PRINCIPLES AND PRACTICE OF BIG DATA

PREPARING, SHARING, AND ANALYZING COMPLEX INFORMATION

SECOND EDITION

JULES J. BERMAN

Principles and Practice of Big Data

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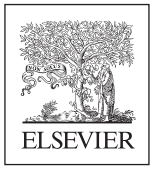
Second Edition

Jules J. Berman



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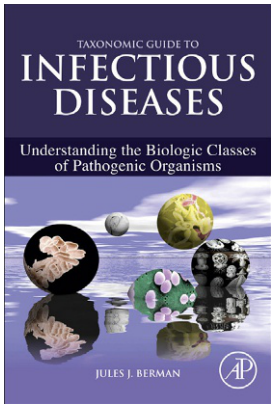

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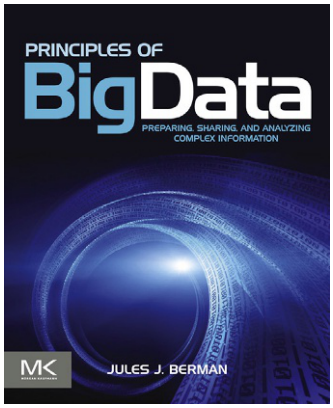

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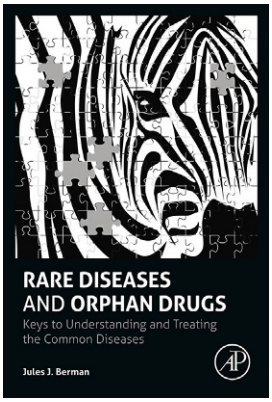

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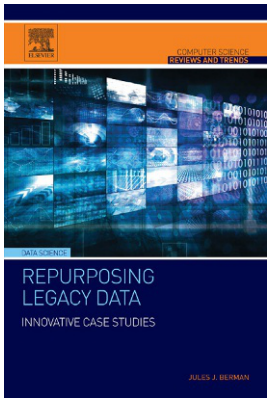

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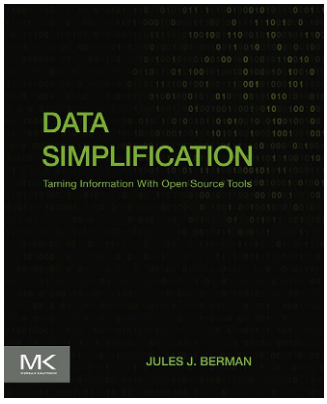

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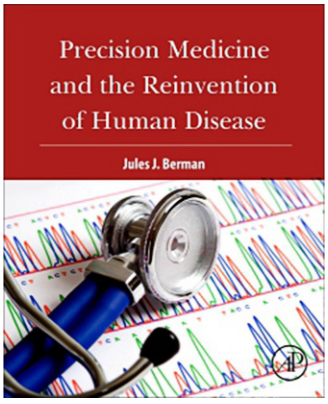

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Dedication

To my wife, Irene, who reads every day, and who understands why books are important.

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About the Author

Jules J. Berman received two baccalaureate degrees from MIT; in Mathematics, and in Earth and Planetary Sciences. He holds a PhD from Temple University, and an MD, from the University of Miami. He was a graduate student researcher in the Fels Cancer Research Institute, at Temple University, and at the American Health Foundation in Valhalla, New York. His postdoctoral studies were completed at the US National Institutes of Health, and his residency was completed at the George Washington University Medical Center in Washington, DC. Dr. Berman served as Chief of Anatomic Pathology, Surgical Pathology, and Cytopathology at the Veterans Administration Medical Center in Baltimore, Maryland, where he held joint appointments at the University of Maryland Medical Center and at the Johns Hopkins Medical Institutions. In 1998, he transferred to the US National Institutes of Health, as a Medical Officer, and as the Program Director for Pathology Informatics in the Cancer Diagnosis Program at the National Cancer Institute. Dr. Berman is a past president of the Association for Pathology Informatics, and the 2011 recipient of the Association's Lifetime Achievement Award. He has first-authored over 100 scientific publications and has written more than a dozen books in the areas of data science and disease biology. Several of his most recent titles, published by Elsevier, include:

Taxonomic Guide to Infectious Diseases: Understanding the Biologic Classes of Pathogenic Organisms (2012)
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Author's Preface to Second Edition

Everything has been said before, but since nobody listens we have to keep going back and beginning all over again.
Andre Gide

Good science writers will always jump at the chance to write a second edition of an earlier work. No matter how hard they try, that first edition will contain inaccuracies and misleading remarks. Sentences that seemed brilliant when first conceived will, with the passage of time, transform into examples of intellectual overreaching. Points too trivial to include in the original manuscript may now seem like profundities that demand a full explanation. A second edition provides rueful authors with an opportunity to correct the record.

When the first edition of Principles of Big Data was published in 2013 the field was very young and there were few scientists who knew what to do with Big Data. The data that kept pouring in was stored, like wheat in silos, throughout the planet. It was obvious to data managers that none of that stored data would have any scientific value unless it was properly annotated with metadata, identifiers, timestamps, and a set of basic descriptors. Under these conditions, the first edition of the Principles of Big Data stressed the proper and necessary methods for collecting, annotating, organizing, and curating Big Data. The process of preparing Big Data comes with its own unique set of challenges, and the First Edition was peppered with warnings and exhortations intended to steer readers clear of disaster.

It is now five years since the first edition was published and there have since been hundreds of books written on the subject of Big Data. As a scientist, it is disappointing to me that the bulk of Big Data, today, is focused on issues of marketing and predictive analytics (e.g., "Who is likely to buy product x, given that they bought product y two weeks previously?"); and machine learning (e.g., driverless cars, computer vision, speech recognition). Machine learning relies heavily on hyped up techniques such as neural networks and deep learning; neither of which are leading to fundamental laws and principles that simplify and broaden our understanding of the natural world and the physical universe. For the most part, these techniques use data that is relatively new (i.e., freshly collected), poorly annotated (i.e., provided with only the minimal information required for one particular analytic process), and not deposited for public evaluation or for re-use. In short, Big Data has followed the path of least resistance, avoiding most of the tough issues raised in the first edition of this book; such as the importance of sharing data with the public, the value of finding relationships (not similarities) among data objects, and the heavy, but inescapable, burden of creating robust, immortal, and well-annotated data.

It was certainly my hope that the greatest advances from Big Data would come as fundamental breakthroughs in the realms of medicine, biology, physics, engineering, and chemistry. Why has the focus of Big Data shifted from basic science over to machine learning? It may have something to do with the fact that no book, including the first edition of this book, has provided readers with the methods required to put the principles of Big Data into practice. In retrospect, it was not sufficient to describe a set of principles and then expect readers to invent their own methodologies.

Consequently, in this second edition, the publisher has changed the title of the book from "The Principles of Big Data," to "The Principles AND PRACTICE of Big Data." Henceforth and herein, recommendations are accompanied by the methods by which those recommendations can be implemented. The reader will find that all of the methods for implementing Big Data preparation and analysis are really quite simple. For the most part, computer methods require some basic familiarity with a programming language, and, despite misgivings, Python was chosen as the language of choice. The advantages of Python are:

- Python is a no-cost, open source, high-level programming language that is easy to acquire, install, learn, and use, and is available for every popular computer operating system.
- Python is extremely popular, at the present time, and its popularity seems to be increasing.
- Python distributions (such as Anaconda) come bundled with hundreds of highly useful modules (such as numpy, matplot, and scipy).
- Python has a large and active user group that has provided an extraordinary amount of documentation for Python methods and modules.
- Python supports some object-oriented techniques that will be discussed in this new edition

As everything in life, Python has its drawbacks:

- The most current versions of Python are not backwardly compatible with earlier versions. The scripts and code snippets included in this book should work for most versions of Python 3.x, but may not work with Python versions 2.x and earlier, unless the reader is prepared to devote some time to tweaking the code. Of course, these short scripts and snippets are intended as simplified demonstrations of concepts, and must not be construed as application-ready code.
- The built-in Python methods are sometimes maximized for speed by utilizing Random Access Memory (RAM) to hold data structures, including data structures built through iterative loops. Iterations through Big Data may exhaust available RAM, leading to the failure of Python scripts that functioned well with small data sets.
- Python's implementation of object orientation allows multiclass inheritance (i.e., a class can be the subclass of more than one parent class). We will describe why this is problematic, and the compensatory measures that we must take, whenever we use our Python programming skills to understand large and complex sets of data objects.

The core of every algorithm described in the book can be implemented in a few lines of code, using just about any popular programming language, under any operating system,

on any modern computer. Numerous Python snippets are provided, along with descriptions of free utilities that are widely available on every popular operating system. This book stresses the point that most data analyses conducted on large, complex data sets can be achieved with simple methods, bypassing specialized software systems (e.g., parallelization of computational processes) or hardware (e.g., supercomputers). Readers who are completely unacquainted with Python may find that they can read and understand Python code, if the snippets of code are brief, and accompanied by some explanation in the text. In any case, readers who are primarily concerned with mastering the principles of Big Data can skip the code snippets without losing the narrative thread of the book.

This second edition has been expanded to stress methodologies that have been overlooked by the authors of other books in the field of Big Data analysis. These would include:

– **Data preparation.**

How to annotate data with metadata and how to create data objects composed of triples. The concept of the triple, as the fundamental conveyor of meaning in the computational sciences, is fully explained.

– **Data structures of particular relevance to Big Data**

Concepts such as triplestores, distributed ledgers, unique identifiers, timestamps, concordances, indexes, dictionary objects, data persistence, and the roles of one-way hashes and encryption protocols for data storage and distribution are covered.

– **Classification of data objects**

How to assign data objects to classes based on their shared relationships, and the computational roles filled by classifications in the analysis of Big Data will be discussed at length.

– **Introspection**

How to create data objects that are self-describing, permitting the data analyst to group objects belonging to the same class and to apply methods to class objects that have been inherited from their ancestral classes.

– **Algorithms that have special utility in Big Data preparation and analysis**

How to use one-way hashes, unique identifier generators, cryptographic techniques, timing methods, and time stamping protocols to create unique data objects that are immutable (never changing), immortal, and private; and to create data structures that facilitate a host of useful functions that will be described (e.g., blockchains and distributed ledgers, protocols for safely sharing confidential information, and methods for reconciling identifiers across data collections without violating privacy).

– **Tips for Big Data analysis**

How to overcome many of the analytic limitations imposed by scale and dimensionality, using a range of simple techniques (e.g., approximations, so-called back-of-the-envelope

tricks, repeated sampling using a random number generator, Monte Carlo simulations, and data reduction methods).

– **Data reanalysis, data repurposing, and data sharing**

Why the first analysis of Big Data is almost always incorrect, misleading, or woefully incomplete, and why data reanalysis has become a crucial skill that every serious Big Data analyst must acquire. The process of data reanalysis often inspires repurposing of Big Data resources. Neither data reanalysis nor data repurposing can be achieved unless and until the obstacles to data sharing are overcome. The topics of data reanalysis, data repurposing, and data sharing are explored at length.

Comprehensive texts, such as the second edition of the Principles and Practice of Big Data, are never quite as comprehensive as they might strive to be; there simply is no way to fully describe every concept and method that is relevant to a multi-disciplinary field, such as Big Data. To compensate for such deficiencies, there is an extensive Glossary section for every chapter, that defines the terms introduced in the text, providing some explanation of the relevance of the terms for Big Data scientists. In addition, when techniques and methods are discussed, a list of references that the reader may find useful, for further reading on the subject, is provided. Altogether, the second edition contains about 600 citations to outside references, most of which are available as free downloads. There are over 300 glossary items, many of which contain short Python snippets that readers may find useful.

As a final note, this second edition uses case studies to show readers how the principles of Big Data are put into practice. Although case studies are drawn from many fields of science, including physics, economics, and astronomy, readers will notice an overabundance of examples drawn from the biological sciences (particularly medicine and zoology). The reason for this is that the taxonomy of all living terrestrial organisms is the oldest and best Big Data classification in existence. All of the classic errors in data organization, and in data analysis, have been committed in the field of biology. More importantly, these errors have been documented in excruciating detail and most of the documented errors have been corrected and published for public consumption. If you want to understand how Big Data can be used as a tool for scientific advancement, then you must look at case examples taken from the world of biology, a well-documented field where everything that can happen has happened, is happening, and will happen. Every effort has been made to limit Case Studies to the simplest examples of their type, and to provide as much background explanation as non-biologists may require.

Principles and Practice of Big Data, Second Edition, is devoted to the intellectual conviction that the primary purpose of Big Data analysis is to permit us to ask and answer a wide range of questions that could not have been credibly approached with small sets of data. There is every reason to hope that the readers of this book will soon achieve scientific breakthroughs that were beyond the reach of prior generations of scientists. Good luck!

Author's Preface to First Edition

We can't solve problems by using the same kind of thinking we used when we created them.
Albert Einstein

Data pours into millions of computers every moment of every day. It is estimated that the total accumulated data stored on computers worldwide is about 300 exabytes (that's 300 billion gigabytes). Data storage increases at about 28% per year. The data stored is peanuts compared to data that is transmitted without storage. The annual transmission of data is estimated at about 1.9 zettabytes or 1,900 billion gigabytes [1]. From this growing tangle of digital information, the next generation of data resources will emerge.

As we broaden our data reach (i.e., the different kinds of data objects included in the resource), and our data timeline (i.e., accruing data from the future and the deep past), we need to find ways to fully describe each piece of data, so that we do not confuse one data item with another, and so that we can search and retrieve data items when we need them. Astute informaticians understand that if we fully describe everything in our universe, we would need to have an ancillary universe to hold all the information, and the ancillary universe would need to be much larger than our physical universe.

In the rush to acquire and analyze data, it is easy to overlook the topic of data preparation. If the data in our Big Data resources are not well organized, comprehensive, and fully described, then the resources will have no value. The primary purpose of this book is to explain the principles upon which serious Big Data resources are built. All of the data held in Big Data resources must have a form that supports search, retrieval, and analysis. The analytic methods must be available for review, and the analytic results must be available for validation.

Perhaps the greatest potential benefit of Big Data is its ability to link seemingly disparate disciplines, to develop and test hypothesis that cannot be approached within a single knowledge domain. Methods by which analysts can navigate through different Big Data resources to create new, merged data sets, will be reviewed.

What exactly, is Big Data? Big Data is characterized by the three V's: volume (large amounts of data), variety (includes different types of data), and velocity (constantly accumulating new data) [2]. Those of us who have worked on Big Data projects might suggest throwing a few more v's into the mix: vision (having a purpose and a plan), verification (ensuring that the data conforms to a set of specifications), and validation (checking that its purpose is fulfilled).

Many of the fundamental principles of Big Data organization have been described in the "metadata" literature. This literature deals with the formalisms of data description (i.e., how to describe data); the syntax of data description (e.g., markup languages such as eXtensible Markup Language, XML); semantics (i.e., how to make computer-parsable statements that convey meaning); the syntax of semantics (e.g., framework specifications such as Resource Description Framework, RDF, and Web Ontology Language, OWL); the creation of data objects that hold data values and self-descriptive information; and the deployment of ontologies, hierarchical class systems whose members are data objects.

The field of metadata may seem like a complete waste of time to professionals who have succeeded very well, in data-intensive fields, without resorting to metadata formalisms. Many computer scientists, statisticians, database managers, and network specialists have no trouble handling large amounts of data, and they may not see the need to create a strange new data model for Big Data resources. They might feel that all they really need is greater storage capacity, distributed over more powerful computers that work in parallel with one another. With this kind of computational power, they can store, retrieve, and analyze larger and larger quantities of data. These fantasies only apply to systems that use relatively simple data or data that can be represented in a uniform and standard format. When data is highly complex and diverse, as found in Big Data resources, the importance of metadata looms large. Metadata will be discussed, with a focus on those concepts that must be incorporated into the organization of Big Data resources. The emphasis will be on explaining the relevance and necessity of these concepts, without going into gritty details that are well covered in the metadata literature.

When data originates from many different sources, arrives in many different forms, grows in size, changes its values, and extends into the past and the future, the game shifts from data computation to data management. I hope that this book will persuade readers that faster, more powerful computers are nice to have, but these devices cannot compensate for deficiencies in data preparation. For the foreseeable future, universities, federal agencies, and corporations will pour money, time, and manpower into Big Data efforts. If they ignore the fundamentals, their projects are likely to fail. On the other hand, if they pay attention to Big Data fundamentals, they will discover that Big Data analyses can be performed on standard computers. The simple lesson, that data trumps computation, will be repeated throughout this book in examples drawn from well-documented events.

There are three crucial topics related to data preparation that are omitted from virtually every other Big Data book: identifiers, immutability, and introspection.

A thoughtful identifier system ensures that all of the data related to a particular data object will be attached to the correct object, through its identifier, and to no other object. It seems simple, and it is, but many Big Data resources assign identifiers promiscuously, with the end result that information related to a unique object is scattered throughout the resource, attached to other objects, and cannot be sensibly retrieved when needed. The concept of object identification is of such overriding importance that a Big Data resource can be usefully envisioned as a collection of unique identifiers to which complex data is attached.

Immutability is the principle that data collected in a Big Data resource is permanent, and can never be modified. At first thought, it would seem that immutability is a ridiculous and impossible constraint. In the real world, mistakes are made, information changes, and the methods for describing information changes. This is all true, but the astute Big Data manager knows how to accrue information into data objects without changing the pre-existing data. Methods for achieving this seemingly impossible trick will be described in detail.

Introspection is a term borrowed from object-oriented programming, not often found in the Big Data literature. It refers to the ability of data objects to describe themselves when interrogated. With introspection, users of a Big Data resource can quickly determine the content of data objects and the hierarchical organization of data objects within the Big Data resource. Introspection allows users to see the types of data relationships that can be analyzed within the resource and clarifies how disparate resources can interact with one another.

Another subject covered in this book, and often omitted from the literature on Big Data, is data indexing. Though there are many books written on the art of the science of so-called back-of-the-book indexes, scant attention has been paid to the process of preparing indexes for large and complex data resources. Consequently, most Big Data resources have nothing that could be called a serious index. They might have a Web page with a few links to explanatory documents, or they might have a short and crude "help" index, but it would be rare to find a Big Data resource with a comprehensive index containing a thoughtful and updated list of terms and links. Without a proper index, most Big Data resources have limited utility for any but a few cognoscenti. It seems odd to me that organizations willing to spend hundreds of millions of dollars on a Big Data resource will balk at investing a few thousand dollars more for a proper index.

Aside from these four topics, which readers would be hard-pressed to find in the existing Big Data literature, this book covers the usual topics relevant to Big Data design, construction, operation, and analysis. Some of these topics include data quality, providing structure to unstructured data, data deidentification, data standards and interoperability issues, legacy data, data reduction and transformation, data analysis, and software issues. For these topics, discussions focus on the underlying principles; programming code and mathematical equations are conspicuously inconspicuous. An extensive Glossary covers the technical or specialized terms and topics that appear throughout the text. As each Glossary term is "optional" reading, I took the liberty of expanding on technical or mathematical concepts that appeared in abbreviated form in the main text. The Glossary provides an explanation of the practical relevance of each term to Big Data, and some readers may enjoy browsing the Glossary as a stand-alone text.

The final four chapters are non-technical; all dealing in one way or another with the consequences of our exploitation of Big Data resources. These chapters will cover legal, social, and ethical issues. The book ends with my personal predictions for the future of Big Data, and its impending impact on our futures. When preparing this book, I debated whether these four chapters might best appear in the front of the book, to whet the reader's

appetite for the more technical chapters. I eventually decided that some readers would be unfamiliar with some of the technical language and concepts included in the final chapters, necessitating their placement near the end.

Readers may notice that many of the case examples described in this book come from the field of medical informatics. The healthcare informatics field is particularly ripe for discussion because every reader is affected, on economic and personal levels, by the Big Data policies and actions emanating from the field of medicine. Aside from that, there is a rich literature on Big Data projects related to healthcare. As much of this literature is controversial, I thought it important to select examples that I could document from reliable sources. Consequently, the reference section is large, with over 200 articles from journals, newspaper articles, and books. Most of these cited articles are available for free Web download.

Who should read this book? This book is written for professionals who manage Big Data resources and for students in the fields of computer science and informatics. Data management professionals would include the leadership within corporations and funding agencies who must commit resources to the project, the project directors who must determine a feasible set of goals and who must assemble a team of individuals who, in aggregate, hold the requisite skills for the task: network managers, data domain specialists, metadata specialists, software programmers, standards experts, interoperability experts, statisticians, data analysts, and representatives from the intended user community. Students of informatics, the computer sciences, and statistics will discover that the special challenges attached to Big Data, seldom discussed in university classes, are often surprising; sometimes shocking.

By mastering the fundamentals of Big Data design, maintenance, growth, and validation, readers will learn how to simplify the endless tasks engendered by Big Data resources. Adept analysts can find relationships among data objects held in disparate Big Data resources if the data is prepared properly. Readers will discover how integrating Big Data resources can deliver benefits far beyond anything attained from stand-alone databases.

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1 Introduction

OUTLINE

Section 1.1. Definition of Big Data

It's the data, stupid.

Jim Gray

Back in the mid 1960s, my high school held pep rallies before big games. At one of these rallies, the head coach of the football team walked to the center of the stage carrying a large box of printed computer paper; each large sheet was folded flip-flop style against the next sheet and they were all held together by perforations. The coach announced that the athletic abilities of every member of our team had been entered into the school's computer (we were lucky enough to have our own IBM-360 mainframe). Likewise, data on our rival team had also been entered. The computer was instructed to digest all of this information and to produce the name of the team that would win the annual Thanksgiving Day showdown. The computer spewed forth the aforementioned box of computer paper; the very last output sheet revealed that we were the pre-ordained winners. The next day, we sallied forth to yet another ignominious defeat at the hands of our long-time rivals.

Fast-forward about 50 years to a conference room at the National Institutes of Health (NIH), in Bethesda, Maryland. A top-level science administrator is briefing me. She explains that disease research has grown in scale over the past decade. The very best research initiatives are now multi-institutional and data-intensive. Funded investigators are using high-throughput molecular methods that produce mountains of data for every tissue sample in a matter of minutes. There is only one solution; we must acquire supercomputers and a staff of talented programmers who can analyze all our data and tell us what it all means!

The NIH leadership believed, much as my high school coach believed, that if you have a really big computer and you feed it a huge amount of information, then you can answer almost any question.

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That day, in the conference room at the NIH, circa 2003, I voiced my concerns, indicating that you cannot just throw data into a computer and expect answers to pop out. I pointed out that, historically, science has been a reductive process, moving from complex, descriptive data sets to simplified generalizations. The idea of developing an expensive supercomputer facility to work with increasing quantities of biological data, at higher and higher levels of complexity, seemed impractical and unnecessary. On that day, my concerns were not well received. High performance supercomputing was a very popular topic, and still is. [Glossary Science, Supercomputer]

Fifteen years have passed since the day that supercomputer-based cancer diagnosis was envisioned. The diagnostic supercomputer facility was never built. The primary diagnostic tool used in hospital laboratories is still the microscope, a tool invented circa 1590. Today, we augment microscopic findings with genetic tests for specific, key mutations; but we do not try to understand all of the complexities of human genetic variations. We know that it is hopeless to try. You can find a lot of computers in hospitals and medical offices, but the computers do not calculate your diagnosis. Computers in the medical workplace are relegated to the prosaic tasks of collecting, storing, retrieving, and delivering medical records. When those tasks are finished, the computer sends you the bill for services rendered.

Before we can take advantage of large and complex data sources, we need to think deeply about the meaning and destiny of Big Data.

Big Data is defined by the three V's:

1. Volume—large amounts of data;.
2. Variety—the data comes in different forms, including traditional databases, images, documents, and complex records;.
3. Velocity—the content of the data is constantly changing through the absorption of complementary data collections, the introduction of previously archived data or legacy collections, and from streamed data arriving from multiple sources.

It is important to distinguish Big Data from "lotsa data" or "massive data." In a Big Data Resource, all three V's must apply. It is the size, complexity, and restlessness of Big Data resources that account for the methods by which these resources are designed, operated, and analyzed. [Glossary Big Data resource, Data resource]

The term "lotsa data" is often applied to enormous collections of simple-format records. For example: every observed star, its magnitude and its location; the name and cell phone number of every person living in the United States; and the contents of the Web. These very large data sets are sometimes just glorified lists. Some "lotsa data" collections are spreadsheets (2-dimensional tables of columns and rows), so large that we may never see where they end.

Big Data resources are not equivalent to large spreadsheets, and a Big Data resource is never analyzed in its totality. Big Data analysis is a multi-step process whereby data is extracted, filtered, and transformed, with analysis often proceeding in a piecemeal, sometimes recursive, fashion. As you read this book, you will find that the gulf between "lotsa data" and Big Data is profound; the two subjects can seldom be discussed productively within the same venue.

Section 1.2. Big Data Versus Small Data

> *Actually, the main function of Big Science is to generate massive amounts of reliable and easily accessible data.... Insight, understanding, and scientific progress are generally achieved by 'small science.'*
>
> *Dan Graur, Yichen Zheng, Nicholas Price, Ricardo Azevedo, Rebecca Zufall, and Eran Elhaik [1].*

Big Data is not small data that has become bloated to the point that it can no longer fit on a spreadsheet, nor is it a database that happens to be very large. Nonetheless, some professionals who customarily work with relatively small data sets, harbor the false impression that they can apply their spreadsheet and database know-how directly to Big Data resources without attaining new skills or adjusting to new analytic paradigms. As they see things, when the data gets bigger, only the computer must adjust (by getting faster, acquiring more volatile memory, and increasing its storage capabilities); Big Data poses no special problems that a supercomputer could not solve. [Glossary Database]

This attitude, which seems to be prevalent among database managers, programmers, and statisticians, is highly counterproductive. It will lead to slow and ineffective software, huge investment losses, bad analyses, and the production of useless and irreversibly defective Big Data resources.

Let us look at a few of the general differences that can help distinguish Big Data and small data.

– **Goals**

small data—Usually designed to answer a specific question or serve a particular goal.

Big Data—Usually designed with a goal in mind, but the goal is flexible and the questions posed are protean. Here is a short, imaginary funding announcement for Big Data grants designed "to combine high quality data from fisheries, coast guard, commercial shipping, and coastal management agencies for a growing data collection that can be used to support a variety of governmental and commercial management studies in the Lower Peninsula." In this fictitious case, there is a vague goal, but it is obvious that there really is no way to completely specify what the Big Data resource will contain, how the various types of data held in the resource will be organized, connected to other data resources, or usefully analyzed. Nobody can specify, with any degree of confidence, the ultimate destiny of any Big Data project; it usually comes as a surprise.

– **Location**

small data—Typically, contained within one institution, often on one computer, sometimes in one file.

Big Data—Spread throughout electronic space and typically parceled onto multiple Internet servers, located anywhere on earth.

– **Data structure and content**

small data—Ordinarily contains highly structured data. The data domain is restricted to a single discipline or sub-discipline. The data often comes in the form of uniform records in an ordered spreadsheet.

Big Data—Must be capable of absorbing unstructured data (e.g., such as free-text documents, images, motion pictures, sound recordings, physical objects). The subject matter of the resource may cross multiple disciplines, and the individual data objects in the resource may link to data contained in other, seemingly unrelated, Big Data resources. [Glossary Data object]

– **Data preparation**

small data—In many cases, the data user prepares her own data, for her own purposes.

Big Data—The data comes from many diverse sources, and it is prepared by many people. The people who use the data are seldom the people who have prepared the data.

– **Longevity**

small data—When the data project ends, the data is kept for a limited time (seldom longer than 7 years, the traditional academic life-span for research data); and then discarded.

Big Data—Big Data projects typically contain data that must be stored in perpetuity. Ideally, the data stored in a Big Data resource will be absorbed into other data resources. Many Big Data projects extend into the future and the past (e.g., legacy data), accruing data prospectively and retrospectively. [Glossary Legacy data]

– **Measurements**

small data—Typically, the data is measured using one experimental protocol, and the data can be represented using one set of standard units. [Glossary Protocol]

Big Data—Many different types of data are delivered in many different electronic formats. Measurements, when present, may be obtained by many different protocols. Verifying the quality of Big Data is one of the most difficult tasks for data managers. [Glossary Data Quality Act]

– **Reproducibility**

small data—Projects are typically reproducible. If there is some question about the quality of the data, the reproducibility of the data, or the validity of the conclusions drawn from the data, the entire project can be repeated, yielding a new data set. [Glossary Conclusions]

Big Data—Replication of a Big Data project is seldom feasible. In general, the most that anyone can hope for is that bad data in a Big Data resource will be found and flagged as such.

– **Stakes**

small data—Project costs are limited. Laboratories and institutions can usually recover from the occasional small data failure.

Big Data—Big Data projects can be obscenely expensive [2,3]. A failed Big Data effort can lead to bankruptcy, institutional collapse, mass firings, and the sudden disintegration

of all the data held in the resource. As an example, a United States National Institutes of Health Big Data project known as the "NCI cancer biomedical informatics grid" cost at least $350 million for fiscal years 2004–10. An ad hoc committee reviewing the resource found that despite the intense efforts of hundreds of cancer researchers and information specialists, it had accomplished so little and at so great an expense that a project moratorium was called [4]. Soon thereafter, the resource was terminated [5]. Though the costs of failure can be high, in terms of money, time, and labor, Big Data failures may have some redeeming value. Each failed effort lives on as intellectual remnants consumed by the next Big Data effort. [Glossary Grid]

– **Introspection**

small data—Individual data points are identified by their row and column location within a spreadsheet or database table. If you know the row and column headers, you can find and specify all of the data points contained within. [Glossary Data point]

Big Data—Unless the Big Data resource is exceptionally well designed, the contents and organization of the resource can be inscrutable, even to the data managers. Complete access to data, information about the data values, and information about the organization of the data is achieved through a technique herein referred to as introspection. Introspection will be discussed at length in Chapter 6. [Glossary Data manager, Introspection]

– **Analysis**

small data—In most instances, all of the data contained in the data project can be analyzed together, and all at once.

Big Data—With few exceptions, such as those conducted on supercomputers or in parallel on multiple computers, Big Data is ordinarily analyzed in incremental steps. The data are extracted, reviewed, reduced, normalized, transformed, visualized, interpreted, and re-analyzed using a collection of specialized methods. [Glossary Parallel computing, MapReduce]

Section 1.3. Whence Comest Big Data?

All I ever wanted to do was to paint sunlight on the side of a house.

Edward Hopper

Often, the impetus for Big Data is entirely ad hoc. Companies and agencies are forced to store and retrieve huge amounts of collected data (whether they want to or not). Generally, Big Data come into existence through any of several different mechanisms:

– An entity has collected a lot of data in the course of its normal activities and seeks to organize the data so that materials can be retrieved, as needed.

The Big Data effort is intended to streamline the regular activities of the entity. In this case, the data is just waiting to be used. The entity is not looking to discover anything or to do anything new. It simply wants to use the data to accomplish what it has always been doing;

only better. The typical medical center is a good example of an "accidental" Big Data resource. The day-to-day activities of caring for patients and recording data into hospital information systems results in terabytes of collected data, in forms such as laboratory reports, pharmacy orders, clinical encounters, and billing data. Most of this information is generated for a one-time specific use (e.g., supporting a clinical decision, collecting payment for a procedure). It occurs to the administrative staff that the collected data can be used, in its totality, to achieve mandated goals: improving quality of service, increasing staff efficiency, and reducing operational costs. [Glossary Binary units for Big Data, Binary atom count of universe]

– An entity has collected a lot of data in the course of its normal activities and decides that there are many new activities that could be supported by their data.

Consider modern corporations; these entities do not restrict themselves to one manufacturing process or one target audience. They are constantly looking for new opportunities. Their collected data may enable them to develop new products based on the preferences of their loyal customers, to reach new markets, or to market and distribute items via the Web. These entities will become hybrid Big Data/manufacturing enterprises.

– An entity plans a business model based on a Big Data resource.

Unlike the previous examples, this entity starts with Big Data and adds a physical component secondarily. Amazon and FedEx may fall into this category, as they began with a plan for providing a data-intense service (e.g., the Amazon Web catalog and the FedEx package tracking system). The traditional tasks of warehousing, inventory, pick-up, and delivery, had been available all along, but lacked the novelty and efficiency afforded by Big Data.

– An entity is part of a group of entities that have large data resources, all of whom understand that it would be to their mutual advantage to federate their data resources [6].

An example of a federated Big Data resource would be hospital databases that share electronic medical health records [7].

– An entity with skills and vision develops a project wherein large amounts of data are collected and organized, to the benefit of themselves and their user-clients.

An example would be a massive online library service, such as the U.S. National Library of Medicine's PubMed catalog, or the Google Books collection.

– An entity has no data and has no particular expertise in Big Data technologies, but it has money and vision.

The entity seeks to fund and coordinate a group of data creators and data holders, who will build a Big Data resource that can be used by others. Government agencies have been the major benefactors. These Big Data projects are justified if they lead to important discoveries that could not be attained at a lesser cost with smaller data resources.

Section 1.4. The Most Common Purpose of Big Data Is to Produce Small Data

> *If I had known what it would be like to have it all, I might have been willing to settle for less.*
>
> *Lily Tomlin*

Imagine using a restaurant locater on your smartphone. With a few taps, it lists the Italian restaurants located within a 10-block radius of your current location. The database being queried is big and complex (a map database, a collection of all the restaurants in the world, their longitudes and latitudes, their street addresses, and a set of ratings provided by patrons, updated continuously), but the data that it yields is small (e.g., five restaurants, marked on a street map, with pop-ups indicating their exact address, telephone number, and ratings). Your task comes down to selecting one restaurant from among the five, and dining thereat.

In this example, your data selection was drawn from a large data set, but your ultimate analysis was confined to a small data set (i.e., five restaurants meeting your search criteria). The purpose of the Big Data resource was to proffer the small data set. No analytic work was performed on the Big Data resource; just search and retrieval. The real labor of the Big Data resource involved collecting and organizing complex data, so that the resource would be ready for your query. Along the way, the data creators had many decisions to make (e.g., Should bars be counted as restaurants? What about take-away only shops? What data should be collected? How should missing data be handled? How will data be kept current? [Glossary Query, Missing data]

Big Data is seldom, if ever, analyzed *in toto*. There is almost always a drastic filtering process that reduces Big Data into smaller data. This rule applies to scientific analyses. The Australian Square Kilometre Array of radio telescopes [8], WorldWide Telescope, CERN's Large Hadron Collider and the Pan-STARRS (Panoramic Survey Telescope and Rapid Response System) array of telescopes produce petabytes of data every day. Researchers use these raw data sources to produce much smaller data sets for analysis [9]. [Glossary Raw data, Square Kilometer Array, Large Hadron Collider, WorldWide Telescope]

Here is an example showing how workable subsets of data are prepared from Big Data resources. Blazars are rare super-massive black holes that release jets of energy that move at near-light speeds. Cosmologists want to know as much as they can about these strange objects. A first step to studying blazars is to locate as many of these objects as possible. Afterwards, various measurements on all of the collected blazars can be compared, and their general characteristics can be determined. Blazars seem to have a gamma ray signature that is not present in other celestial objects. The WISE survey collected infrared data on the entire observable universe. Researchers extracted from the Wise data every celestial body associated with an infrared signature in the gamma ray range that was suggestive of blazars; about 300 objects. Further research on these 300 objects led the researchers to

believe that about half were blazars [10]. This is how Big Data research often works; by constructing small data sets that can be productively analyzed.

Because a common role of Big Data is to produce small data, a question that data managers must ask themselves is: "Have I prepared my Big Data resource in a manner that helps it become a useful source of small data?"

Section 1.5. Big Data Sits at the Center of the Research Universe

Physics is the universe's operating system.

Steven R Garman

In the past, scientists followed a well-trodden path toward truth: hypothesis, then experiment, then data, then analysis, then publication. The manner in which a scientist analyzed his or her data was crucial because other scientists would not have access to the same data and could not re-analyze the data for themselves. Basically, the results and conclusions described in the manuscript was the scientific product. The primary data upon which the results and conclusion were based (other than one or two summarizing tables) were not made available for review. Scientific knowledge was built on trust. Customarily, the data would be held for 7 years, and then discarded. [Glossary Results]

In the Big data paradigm the concept of a final manuscript has little meaning. Big Data resources are permanent, and the data within the resource is immutable (See Chapter 6). Any scientist's analysis of the data does not need to be the final word; another scientist can access and re-analyze the same data over and over again. Original conclusions can be validated or discredited. New conclusions can be developed. The centerpiece of science has moved from the manuscript, whose conclusions are tentative until validated, to the Big Data resource, whose data will be tapped repeatedly to validate old manuscripts and spawn new manuscripts. [Glossary Immutability, Mutability]

Today, hundreds or thousands of individuals might contribute to a Big Data resource. The data in the resource might inspire dozens of major scientific projects, hundreds of manuscripts, thousands of analytic efforts, and millions or billions of search and retrieval operations. The Big Data resource has become the central, massive object around which universities, research laboratories, corporations, and federal agencies orbit. These orbiting objects draw information from the Big Data resource, and they use the information to support analytic studies and to publish manuscripts. Because Big Data resources are permanent, any analysis can be critically examined using the same set of data, or re-analyzed anytime in the future. Because Big Data resources are constantly growing forward in time (i.e., accruing new information) and backward in time (i.e., absorbing legacy data sets), the value of the data is constantly increasing.

Big Data resources are the stars of the modern information universe. All matter in the physical universe comes from heavy elements created inside stars, from lighter elements. All data in the informational universe is complex data built from simple data. Just as stars

can exhaust themselves, explode, or even collapse under their own weight to become black holes; Big Data resources can lose funding and die, release their contents and burst into nothingness, or collapse under their own weight, sucking everything around them into a dark void. It is an interesting metaphor. In the following chapters, we will see how a Big Data resource can be designed and operated to ensure stability, utility, growth, and permanence; features you might expect to find in a massive object located in the center of the information universe.

Glossary

Big Data resource A Big Data collection that is accessible for analysis. Readers should understand that there are collections of Big Data (i.e., data sources that are large, complex, and actively growing) that are not designed to support analysis; hence, not Big Data resources. Such Big Data collections might include some of the older hospital information systems, which were designed to deliver individual patient records upon request; but could not support projects wherein all of the data contained in all of the records were opened for selection and analysis. Aside from privacy and security issues, opening a hospital information system to these kinds of analyses would place enormous computational stress on the systems (i.e., produce system crashes). In the late 1990s and the early 2000s data warehousing was popular. Large organizations would collect all of the digital information created within their institutions, and these data were stored as Big Data collections, called data warehouses. If an authorized person within the institution needed some specific set of information (e.g., emails sent or received in February, 2003; all of the bills paid in November, 1999), it could be found somewhere within the warehouse. For the most part, these data warehouses were not true Big Data resources because they were not organized to support a full analysis of all of the contained data. Another type of Big Data collection that may or may not be considered a Big Data resource are compilations of scientific data that are accessible for analysis by private concerns, but closed for analysis by the public. In this case a scientist may make a discovery based on her analysis of a private Big Data collection, but the research data is not open for critical review. In the opinion of some scientists, including myself, if the results of a data analysis are not available for review, then the analysis is illegitimate. Of course, this opinion is not universally shared, and Big Data professionals hold various definitions for a Big Data resource.

Binary atom count of universe There are estimated to be about 10^80 atoms in the universe. Log2(10) is 3.32192809, so the number of atoms in the universe is 2^80*3.32192809 or 2^266 atoms.

Binary units for Big Data Binary sizes are named in 1000-fold intervals: 1 bit = binary digit (0 or 1); 1 byte = 8 bits (the number of bits required to express an ascii character); 1000 bytes = 1 kilobyte; 1000 kilobytes = 1 megabyte; 1000 megabytes = 1 gigabyte; 1000 gigabytes = 1 terabyte; 1000 terabytes = 1 petabyte; 1000 petabytes = 1 exabyte; 1000 exabytes = 1 zettabyte; 1000 zettabytes = 1 yottabyte.

Conclusions Conclusions are the interpretations made by studying the results of an experiment or a set of observations. The term "results" should never be used interchangeably with the term "conclusions." **Remember, results are verified. Conclusions are validated** [11].

Data Quality Act In the United States the data upon which public policy is based must have quality and must be available for review by the public. Simply put, public policy must be based on verifiable data. The Data Quality Act of 2002 requires the Office of Management and Budget to develop government-wide standards for data quality [12].

Data manager This book uses "data manager" as a catchall term, without attaching any specific meaning to the name. Depending on the institutional and cultural milieu, synonyms and plesionyms (i.e., near-synonyms) for data manager would include: technical lead, team liaison, data quality manager, chief curator, chief of operations, project manager, group supervisor, and so on.

Data object As used in this book, a data object consists of a unique object identifier along with all of the data/metadata pairs that rightly belong to the object identifier, and that includes one data/metadata pair that tells us the object's class.

```
75898039563441
  name                G. Willikers
  gender              male
  age                 35
  is_a_class_member   cowboy
```

In this example, the object identifier, 75898039563441, is followed by its data/metadata pairs, including the one pair that tells us that the object (a 35-year-old man named G. Willikers) belongs to the class of individuals known as "cowboy."

The utility of data objects, in the field of Big Data, is discussed in Section 6.2.

Data point The singular form of data is datum. Strictly speaking, the term should be datum point or datumpoint. Most information scientists, myself included, have abandoned consistent usage rules for the word "data." In this book, the term "data" always refers collectively to information, numeric or textual, structured or unstructured, in any quantity.

Data resource A collection of data made available for data retrieval. The data can be distributed over servers located anywhere on earth or in space. The resource can be static (i.e., having a fixed set of data), or in flux. Plesionyms for data resource are: data warehouse, data repository, data archive, and data store.

Database A software application designed specifically to create and retrieve large numbers of data records (e.g., millions or billions). The data records of a database are persistent, meaning that the application can be turned off, then on, and all the collected data will be available to the user.

Grid A collection of computers and computer resources (typically networked servers) that is coordinated to provide a desired functionality. In the most advanced Grid computing architecture, requests can be broken into computational tasks that are processed in parallel on multiple computers and transparently (from the client's perspective) assembled and returned. The Grid is the intellectual predecessor of Cloud computing. Cloud computing is less physically and administratively restricted than Grid computing.

Immutability Immutability is the principle that data collected in a Big Data resource is permanent and can never be modified. At first thought, it would seem that immutability is a ridiculous and impossible constraint. In the real world, mistakes are made, information changes, and the methods for describing information changes. This is all true, but the astute Big Data manager knows how to accrue information into data objects without changing the pre-existing data. Methods for achieving this seemingly impossible trick are described in Chapter 8.

Introspection Well-designed Big Data resources support introspection, a method whereby data objects within the resource can be interrogated to yield their properties, values, and class membership. Through introspection the relationships among the data objects in the Big Data resource can be examined and the structure of the resource can be determined. Introspection is the method by which a data user can find everything there is to know about a Big Data resource without downloading the complete resource.

Large Hadron Collider The Large Hadron Collider is the world's largest and most powerful particle accelerator and is expected to produce about 15 petabytes (15 million gigabytes) of data annually [13].

Legacy data Data collected by an information system that has been replaced by a newer system, and which cannot be immediately integrated into the newer system's database. For example, hospitals regularly replace their hospital information systems with new systems that promise greater efficiencies, expanded services, or improved interoperability with other information systems. In many cases, the new system cannot readily integrate the data collected from the older system. The previously collected

data becomes a legacy to the new system. In such cases, legacy data is simply "stored" for some arbitrary period of time in case someone actually needs to retrieve any of the legacy data. After a decade or so the hospital may find itself without any staff members who are capable of locating the storage site of the legacy data, or moving the data into a modern operating system, or interpreting the stored data, or retrieving appropriate data records, or producing a usable query output.

MapReduce A method by which computationally intensive problems can be processed on multiple computers, in parallel. The method can be divided into a mapping step and a reducing step. In the mapping step a master computer divides a problem into smaller problems that are distributed to other computers. In the reducing step the master computer collects the output from the other computers. Although MapReduce is intended for Big Data resources, and can hold petabytes of data, most Big Data problems do not require MapReduce.

Missing data Most complex data sets have missing data values. Somewhere along the line data elements were not entered, records were lost, or some systemic error produced empty data fields. Big Data, being large, complex, and composed of data objects collected from diverse sources, is almost certain to have missing data. Various mathematical approaches to missing data have been developed; commonly involving assigning values on a statistical basis; so-called imputation methods. The underlying assumption for such methods is that missing data arises at random. When missing data arises nonrandomly, there is no satisfactory statistical fix. The Big Data curator must track down the source of the errors and somehow rectify the situation. In either case the issue of missing data introduces a potential bias and it is crucial to fully document the method by which missing data is handled. In the realm of clinical trials, only a minority of data analyses bothers to describe their chosen method for handling missing data [14].

Mutability Mutability refers to the ability to alter the data held in a data object or to change the identity of a data object. Serious Big Data is not mutable. Data can be added, but data cannot be erased or altered. Big Data resources that are mutable cannot establish a sensible data identification system, and cannot support verification and validation activities. The legitimate ways in which we can record the changes that occur in unique data objects (e.g., humans) over time, without ever changing the key/value data attached to the unique object, is discussed in Section 8.2.

For programmers, it is important to distinguish data mutability from object mutability, as it applies in Python and other object-oriented programming languages. Python has two immutable objects: strings and tuples. Intuitively, we would probably guess that the contents of a string object cannot be changed, and the contents of a tuple object cannot be changed. This is not the case. Immutability, for programmers, means that there are no methods available to the object by which the contents of the object can be altered. Specifically, a Python tuple object would have no methods it could call to change its own contents. However, a tuple may contain a list, and lists are mutable. For example, a list may have an append method that will add an item to the list object. You can change the contents of a list contained in a tuple object without violating the tuple's immutability.

Parallel computing Some computational tasks can be broken down and distributed to other computers, to be calculated "in parallel." The method of parallel programming allows a collection of desktop computers to complete intensive calculations of the sort that would ordinarily require the aid of a supercomputer. Parallel programming has been studied as a practical way to deal with the higher computational demands brought by Big Data. Although there are many important problems that require parallel computing, the vast majority of Big Data analyses can be easily accomplished with a single, off-the-shelf personal computer.

Protocol A set of instructions, policies, or fully described procedures for accomplishing a service, operation, or task. Protocols are fundamental to Big Data. Data is generated and collected according to protocols. There are protocols for conducting experiments, and there are protocols for measuring the results. There are protocols for choosing the human subjects included in a clinical trial, and there are protocols for interacting with the human subjects during the course of the trial. All network

communications are conducted via protocols; the Internet operates under a protocol (TCP-IP, Transmission Control Protocol-Internet Protocol).

Query The term "query" usually refers to a request, sent to a database, for information (e.g., Web pages, documents, lines of text, images) that matches a provided word or phrase (i.e., the query term). More generally a query is a parameter or set of parameters that are submitted as input to a computer program that searches a data collection for items that match or bear some relationship to the query parameters. In the context of Big Data the user may need to find classes of objects that have properties relevant to a particular area of interest. In this case, the query is basically introspective, and the output may yield metadata describing individual objects, classes of objects, or the relationships among objects that share particular properties. For example, "weight" may be a property, and this property may fall into the domain of several different classes of data objects. The user might want to know the names of the classes of objects that have the "weight" property and the numbers of object instances in each class. Eventually the user might want to select several of these classes (e.g., including dogs and cats, but excluding microwave ovens) along with the data object instances whose weights fall within a specified range (e.g., 20–30 pound). This approach to querying could work with any data set that has been well specified with metadata, but it is particularly important when using Big Data resources.

Raw data Raw data is the unprocessed, original data measurement, coming straight from the instrument to the database with no intervening interference or modification. In reality, scientists seldom, if ever, work with raw data. When an instrument registers the amount of fluorescence emitted by a hybridization spot on a gene array, or the concentration of sodium in the blood, or virtually any of the measurements that we receive as numeric quantities, the output is produced by an algorithm executed by the measurement instrument. Pre-processing of data is commonplace in the universe of Big Data, and data managers should not labor under the false impression that the data received is "raw," simply because the data has not been modified by the person who submits the data.

Results The term "results" is often confused with the term "conclusions." Interchanging the two concepts is a source of confusion among data scientists. In the strictest sense, "results" consist of the full set of experimental data collected by measurements. In practice, "results" are provided as a small subset of data distilled from the raw, original data. In a typical journal article, selected data subsets are packaged as a chart or graph that emphasizes some point of interest. Hence, the term "results" may refer, erroneously, to subsets of the original data, or to visual graphics intended to summarize the original data. Conclusions are the inferences drawn from the results. Results are verified; conclusions are validated.

Science Of course, there are many different definitions of science, and inquisitive students should be encouraged to find a conceptualization of science that suits their own intellectual development. For me, science is all about finding general relationships among objects. In the so-called physical sciences the most important relationships are expressed as mathematical equations (e.g., the relationship between force, mass and acceleration; the relationship between voltage, current and resistance). In the so-called natural sciences, relationships are often expressed through classifications (e.g., the classification of living organisms). Scientific advancement is the discovery of new relationships or the discovery of a generalization that applies to objects hitherto confined within disparate scientific realms (e.g., evolutionary theory arising from observations of organisms and geologic strata). Engineering would be the area of science wherein scientific relationships are exploited to build new technology.

Square Kilometer Array The Square Kilometer Array is designed to collect data from millions of connected radio telescopes and is expected to produce more than one exabyte (1 billion gigabytes) every day [8].

Supercomputer Computers that can perform many times faster than a desktop personal computer. In 2015 the top supercomputers operate at about 30 petaflops. A petaflop is 10 to the 15 power floating point operations per second. By my calculations a 1 petaflop computer performs about 250,000 operations in the time required for my laptop to finish one operation.

WorldWide Telescope A Big Data effort from the Microsoft Corporation bringing astronomical maps, imagery, data, analytic methods, and visualization technology to standard Web browsers. More information is available at: http://www.worldwidetelescope.org/Home.aspx

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2

Providing Structure to Unstructured Data

OUTLINE

Section 2.1. Nearly All Data Is Unstructured and Unusable in Its Raw Form

> *I was working on the proof of one of my poems all the morning, and took out a comma. In the afternoon I put it back again.*
>
> *Oscar Wilde*

In the early days of computing, data was always highly structured. All data was divided into fields, the fields had a fixed length, and the data entered into each field was constrained to a pre-determined set of allowed values. Data was entered into punch cards with pre-configured rows and columns. Depending on the intended use of the cards, various entry and read-out methods were chosen to express binary data, numeric data, fixed-size text, or programming instructions. Key-punch operators produced mountains of punch cards. For many analytic purposes, card-encoded data sets were analyzed without the assistance of a computer; all that was needed was a punch card sorter. If you wanted the data card on all males, over the age of 18, who had graduated high school, and had passed their physical exam, then the sorter would need to make 4 passes. The sorter would pull every card listing a male, then from the male cards it would pull all the cards of people over the age of 18, and from this double-sorted sub-stack, it would pull cards that met the next criterion, and so on.

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As a high school student in the 1960s, I loved playing with the card sorters. Back then, all data was structured data, and it seemed to me, at the time, that a punch-card sorter was all that anyone would ever need to analyze large sets of data. [Glossary Binary data]

How wrong I was! Today, most data entered by humans is unstructured in the form of free-text. The free-text comes in email messages, tweets, and documents. Structured data has not disappeared, but it sits in the shadows cast by mountains of unstructured text. Free-text may be more interesting to read than punch cards, but the venerable punch card, in its heyday, was much easier to analyze than its free-text descendant. To get much informational value from free-text, it is necessary to impose some structure. This may involve translating the text to a preferred language; parsing the text into sentences; extracting and normalizing the conceptual terms contained in the sentences; mapping terms to a standard nomenclature; annotating the terms with codes from one or more standard nomenclatures; extracting and standardizing data values from the text; assigning data values to specific classes of data belonging to a classification system; assigning the classified data to a storage and retrieval system (e.g., a database); and indexing the data in the system. All of these activities are difficult to do on a small scale and virtually impossible to do on a large scale. Nonetheless, every Big Data project that uses unstructured data must deal with these tasks to yield the best possible results with the resources available. [Glossary Parsing, Nomenclature, Nomenclature mapping, Thesaurus, Indexes, Plain-text]

Section 2.2. Concordances

> *The limits of my language are the limits of my mind. All I know is what I have words for. (Die Grenzen meiner Sprache bedeuten die Grenzen meiner Welt.)*
>
> *Ludwig Wittgenstein*

A concordance is a list of all the different words contained in a text with the locations in the text where each word appears. Concordances have been around for a very long time, painstakingly constructed from holy scriptures thought to be of such immense value that every word deserved special attention. Creating a concordance has always been a straightforward operation. You take the first word in the text and you note its location (i.e., word 1, page 1); then onto the second word (word 2 page 1), and so on. When you come to a word that has been included in the nascent concordance, you add its location to the existing entry for the word. Continuing thusly, for a few months or so, you end up with a concordance that you can be proud of. Today a concordance for the Bible can be constructed in a small fraction of a second. [Glossary Concordance]

Without the benefit of any special analyses, skimming through a book's concordance provides a fairly good idea of the following:

– The topic of the text based on the words appearing in the concordance. For example, a concordance listing multiple locations for "begat" and "anointed" and "thy" is most likely to be the Old Testament.

- The complexity of the language. A complex or scholarly text will have a larger vocabulary than a romance novel.
- A precise idea of the length of the text, achieved by adding all of the occurrences of each of the words in the concordance. Knowing the number of items in the concordance, multiplied by the average number of locations of concordance items, provides a rough estimate of the total number of words in the text.
- The care with which the text was prepared, achieved by counting the misspelled words.

Here, in a short Python script, concord_gettysbu.py, that builds a concordance for the Gettysburg address, located in the external file "gettysbu.txt": [Glossary Script]

```
import re, string
word_list=[];word_dict={};key_list=[]
count=0; word=""
in_text_string = open('gettysbu.txt', "r").read().lower()
word_list = re.split(r'[^a-zA-z\_\-]+',in_text_string)
for word in word_list:
   count = count + 1
   if word in word_dict:
     word_dict[word] = word_dict[word] + ',' + str(count)
   else:
     word_dict[word] = str(count)
key_list = list(word_dict)
key_list.sort()
for key in key_list:
   print(key + " " + word_dict[key])
```

The first few lines of output are shown:

```
a 14,36,59,70,76,104,243
above 131
add 136
advanced 185
ago 6
all 26
altogether 93
and 3,20,49,95,122,248
any 45
are 28,33,56
as 75
battlefield 61
be 168,192
before 200
birth 245
```

```
brave 119
brought 9
but 102,151
by 254
can 52,153
cannot 108,111,114
```

The numbers that follow each item in the concordance correspond to the locations (expressed as the nth words of the Gettysburg address) of each word in the text.

At this point, building a concordance may appear to an easy, but somewhat pointless exercise. Does the concordance provide any functionality beyond that provided by the ubiquitous "search" box. There are five very useful properties of concordances that you might not have anticipated.

- You can use a concordance to rapidly search and retrieve the locations where single-word terms appear.
- You can always reconstruct the original text from the concordance. Hence, after you've built your concordance, you can discard the original text.
- You can merge concordances without forfeiting your ability to reconstruct the original texts, provided that you tag locations with some character sequence that identifies the text of origin.
- With a little effort a dictionary can be transformed into a universal concordance (i.e., a merged dictionary/concordance of every book in existence) by attaching the book identifier and its concordance entries to the corresponding dictionary terms.
- You can easily find the co-locations among words (i.e., which words often precede or follow one another).
- You can use the concordance to retrieve the sentences and paragraphs in which a search word or a search term appears, without having access to the original text. The concordance alone can reconstruct and retrieve the appropriate segments of text, on-the-fly, thus bypassing the need to search the original text.
- A concordance provides a profile of the book and can be used to compute a similarity score among different books.

There is insufficient room to explore all of the useful properties of concordances, but let us examine a script, concord_reverse.py, that reconstructs the original text, in lowercase, from the concordance. In this case, we have pasted the output from the concord_gettysbu.py script (vida supra) into the external file, "concordance.txt".

```
import re, string
concordance_hash = {} ; location_array = []
in_text = open('concordance.txt', "r")
for line in in_text:
   line = line.replace("\n","")
   location_word, separator, location_positions = line.partition(" ")
   location_array = location_positions.split(",")
```

```
    location_array = [int(x) for x in location_array]
    for location in location_array:
      concordance_hash[location] = location_word
for n in range(300):
    if n in concordance_hash:
      print((concordance_hash[n]), end = " ")
```

Here is the familiar output:

> *four score and seven years ago our fathers brought forth on this continent a new nation conceived in liberty and dedicated to the proposition that all men are created equal now we are engaged in a great civil war testing whether that nation or any nation so conceived and so dedicated can long endure we are met on a great battlefield of that war we have come to dedicate a portion of that field as a final resting-place for those who here gave their lives that that nation might live it is altogether fitting and proper that we should do this but in a larger sense we cannot dedicate we cannot consecrate we cannot hallow this ground the brave men living and dead who struggled here have consecrated it far above our poor power to add or detract the world will little note nor long remember what we say here but it can never forget what they did here it is for us the living rather to be dedicated here to the unfinished work which they who fought here have thus far so nobly advanced it is rather for us to be here dedicated to the great task remaining before us–that from these honored dead we take increased devotion to that cause for which they gave the last full measure of devotion–that we here highly resolve that these dead shall not have died in vain that this nation under god shall have a new birth of freedom and that government of the people by the people for the people shall not perish from the earth*

Had we wanted to write a script that produces a merged concordance, for multiple documents, we could have simply written a loop that repeated the concordance-building process for each text. Within the loop, we would have tagged each word location with a short notation indicating the particular source book. For example, locations from the Gettysburg address could have been prepended with "G:" and locations from the Bible might have been prepended with a "B:".

We have not finished with the topic of concordances. Later in this chapter (Section 2.8), we will show how concordances can be transformed to speed-up search and retrieval operations on large bodies of text.

Section 2.3. Term Extraction

> *There's a big difference between knowing the name of something and knowing something.*
>
> *Richard Feynman*

One of my favorite movies is the parody version of "Hound of the Baskervilles," starring Peter Cooke as Sherlock Holmes and Dudley Moore as his faithful hagiographer, Dr. Watson. Sherlock, preoccupied with his own ridiculous pursuits, dispatches Watson to the Baskerville family manse, in Dartmoor, to undertake urgent sleuth-related activities. The hapless Watson, standing in the great Baskerville Hall, has no idea how to proceed with the investigation. After a moment of hesitation, he turns to the incurious maid and commands, "Take me to the clues!"

Building an index is a lot like solving a fiendish crime; you need to know how to find the clues. For informaticians, the terms in the text are the clues upon which the index is built. Terms in a text file do not jump into your index file; you need to find them. There are several available methods for finding and extracting index terms from a corpus of text [1], but no method is as simple, fast, and scalable as the "stop word" method [2]. [Glossary Term extraction algorithm, Scalable]

The "stop word" method presumes that text is composed of terms that are somehow connected into sequences known as sentences. [Glossary Sentence]

Consider the following:

The diagnosis is chronic viral hepatitis.

This sentence contains two very specific medical concepts: "diagnosis" and "chronic viral hepatitis." These two concepts are connected to form a sentence, using grammatical bric-a-brac such as "the" and "is", and the sentence delimiter, ".". These grammatical bric-a-brac are found liberally sprinkled in every paragraph you are likely to read.

A term can be defined as a sequence of one or more uncommon words that are demarcated (i.e., bounded on one side or another) by the occurrence of one or more very common words (e.g., "and", "the", "a", "of") and phrase delimiters (e.g., ".", ",", and ";")

Consider the following:

An epidural hemorrhage can occur after a lucid interval.

The medical concepts "epidural hemorrhage" and "lucid interval" are composed of uncommon words. These uncommon word sequences are bounded by common words (i.e., "the", "an", "can", "a") or a sentence delimiter (i.e., ".").

If we had a list of all the words that were considered common, we could write a program that extracts the all the concepts found in any text of any length. The concept terms would consist of all sequences of uncommon words that are uninterrupted by common words. Here is an algorithm for extracting terms from a sentence:

1. Read the first word of the sentence. If it is a common word, delete it. If it is an uncommon word, save it.
2. Read the next word. If it is a common word, delete it, and place the saved word (from the prior step, if the prior step saved a word) into our list of terms found in the text. If it

is an uncommon word, concatenate it with the word we saved in step one, and save the 2-word term. If it is a sentence delimiter, place any saved term into our list of terms, and stop the program.

3. Repeat step two.

This simple algorithm, or something much like it, is a fast and efficient method to build a collection of index terms. The following list of common words might be useful: "about, again, all, almost, also, although, always, among, an, and, another, any, are, as, at, be, because, been, before, being, between, both, but, by, can, could, did, do, does, done, due, during, each, either, enough, especially, etc, for, found, from, further, had, has, have, having, here, how, however, i, if, in, into, is, it, its, itself, just, kg, km, made, mainly, make, may, mg, might, ml, mm, most, mostly, must, nearly, neither, no, nor, obtained, of, often, on, our, overall, perhaps, pmid, quite, rather, really, regarding, seem, seen, several, should, show, showed, shown, shows, significantly, since, so, some, such, than, that, the, their, theirs, them, then, there, therefore, these, they, this, those, through, thus, to, upon, use, used, using, various, very, was, we, were, what, when, which, while, with, within, without, would."

Such lists of common words are sometimes referred to as "stop word" lists or "barrier word" lists, as they demarcate the beginnings and endings of extraction terms. Let us look at a short Python script (terms.py) that uses our list of stop words (contained in the file stop.txt) and extracts the terms from the sentence: "Once you have a method for extracting terms from sentences the task of creating an index associating a list of locations with each term is child's play for programmers"

```
import re, string
stopfile = open("stop.txt",'r')
stop_list = stopfile.readlines()
stopfile.close()
item_list = []
line = "Once you have a method for extracting terms from \
sentences the task of creating an index associating a list \
of locations with each term is child's play for programmers"
for stopword in stop_list:
   stopword = re.sub(r'\n', '', stopword)
   line = re.sub(r' *\b' + stopword + r'\b *', '\n', line)
item_list.extend(line.split("\n"))
item_list = sorted(set(item_list))
for item in item_list:
   print(item)
```

Here is the output:

```
Once
child's play
creating
```

```
extracting terms
index associating
list
locations
method
programmers
sentences
task
term
```

Extracting terms is the first step in building a very crude index. Indexes built directly from term extraction algorithms always contain lots of unnecessary terms having little or no informational value. For serious indexers, the collection of terms extracted from a corpus, along with their locations in the text, is just the beginning of an intellectual process that will eventually lead to a valuable index.

Section 2.4. Indexing

> *Knowledge can be public, yet undiscovered, if independently created fragments are logically related but never retrieved, brought together, and interpreted.*
>
> *Donald R. Swanson [3]*

Individuals accustomed to electronic media tend to think of the Index as an inefficient or obsolete method for finding and retrieving information. Most currently available e-books have no index. It is far easier to pull up the "Find" dialog box and enter a word or phrase. The e-reader can find all matches quickly, providing the total number of matches, and bringing the reader to any or all of the pages containing the selection. As more and more books are published electronically, the book Index, as we have come to know it, may cease to be.

It would be a pity if indexes were to be abandoned by computer scientists. A well-designed book index is a creative, literary work that captures the content and intent of the book and transforms it into a listing wherein related concepts are collected under common terms, and keyed to their locations. It saddens me that many people ignore the book index until they want something from it. Open a favorite book and read the index, from A to Z, as if you were reading the body of the text. You will find that the index refreshes your understanding of the concepts discussed in the book. The range of page numbers after each term indicates that a concept has extended its relevance across many different chapters. When you browse the different entries related to a single term, you learn how the concept represented by the term applies itself to many different topics. You begin to understand, in ways that were not apparent when you read the book as a linear text, the versatility of the ideas contained in the book. When you have finished reading the index, you will notice that the indexer exercised great restraint when selecting terms.

Most indexes are under 20 pages. The goal of the indexer is not to create a concordance (i.e., a listing of every word in a book, with its locations), but to create a keyed encapsulation of concepts, sub-concepts and term relationships.

The indexes we find in today's books are generally alphabetized terms. In prior decades and prior centuries, authors and editors put enormous effort into building indexes, sometimes producing multiple indexes for a single book. For example, a biography might contain a traditional alphabetized term index, followed by an alphabetized index of the names of the people included in the text. A zoology book might include an index specifically for animal names, with animals categorized according to their taxonomic order. A geography index might list the names of localities sub-indexed by country, with countries sub-indexed by continent. A single book might have 5 or more indexes. In nineteenth century books, it was not unusual to publish indexes as stand-alone volumes. [Glossary Taxonomy, Systematics, Taxa, Taxon]

You may be thinking that all this fuss over indexes is quaint, but it cannot apply to Big Data resources. Actually, Big Data resources that lack a proper index cannot be utilized to their full potential. Without an index, you never know what your queries are missing. Remember, in a Big Data resource, it is the relationship among data objects that are the keys to knowledge. Data by itself, even in large quantities, tells only part of a story. The most useful Big Data resources have electronic indexes that map concepts, classes, and terms to specific locations in the resource where data items are stored. An index imposes order and simplicity on the Big Data resource. Without an index, Big Data resources can easily devolve into vast collections of disorganized information. [Glossary Class]

The best indexes comply with international standards (ISO 999) and require creativity and professionalism [4]. Indexes should be accepted as another device for driving down the complexity of Big Data resources. Here are a few of the specific strengths of an index that cannot be duplicated by "find" operations on terms entered into a query box:

- An index can be read, like a book, to acquire a quick understanding of the contents and general organization of the data resource.
- Index lookups (i.e., searches and retrievals) are virtually instantaneous, even for very large indexes (see Section 2.6 of this chapter, for explanation).
- Indexes can be tied to a classification. This permits the analyst to know the relationships among different topics within the index, and within the text. [Glossary Classification]
- Many indexes are cross-indexed, providing relationships among index terms that might be extremely helpful to the data analyst.
- Indexes from multiple Big Data resources can be merged. When the location entries for index terms are annotated with the name of the resource, then merging indexes is trivial, and index searches will yield unambiguously identified locators in any of the Big Data resources included in the merge.
- Indexes can be created to satisfy a particular goal; and the process of creating a made-to-order index can be repeated again and again. For example, if you have a Big Data

resource devoted to ornithology, and you have an interest in the geographic location of species, you might want to create an index specifically keyed to localities, or you might want to add a locality sub-entry for every indexed bird name in your original index. Such indexes can be constructed as add-ons, as needed. [Glossary Ngrams]

- Indexes can be updated. If terminology or classifications change, there is nothing stopping you from re-building the index with an updated specification. In the specific context of Big Data, you can update the index without modifying your data. [Glossary Specification]
- Indexes are created after the database has been created. In some cases, the data manager does not envision the full potential of the Big Data resource until after it is created. The index can be designed to facilitate the use of the resource in line with the observed practices of users.
- Indexes can serve as surrogates for the Big Data resource. In some cases, all the data user really needs is the index. A telephone book is an example of an index that serves its purpose without being attached to a related data source (e.g., caller logs, switching diagrams).

Section 2.5. Autocoding

The beginning of wisdom is to call things by their right names.

Chinese proverb

Coding, as used in the context of unstructured textual data, is the process of tagging terms with an identifier code that corresponds to a synonymous term listed in a standard nomenclature. For example, a medical nomenclature might contain the term renal cell carcinoma, a type of kidney cancer, attaching a unique identifier code for the term, such as "C9385000." There are about 50 recognized synonyms for "renal cell carcinoma." A few of these synonyms and near-synonyms are listed here to show that a single concept can be expressed many different ways, including: adenocarcinoma arising from kidney, adenocarcinoma involving kidney, cancer arising from kidney, carcinoma of kidney, Grawitz tumor, Grawitz tumour, hypernephroid tumor, hypernephroma, kidney adenocarcinoma, renal adenocarcinoma, and renal cell carcinoma. All of these terms could be assigned the same identifier code, "C9385000". [Glossary Coding, Identifier]

The process of coding a text document involves finding all the terms that belong to a specific nomenclature, and tagging each term with the corresponding identifier code.

A nomenclature is a specialized vocabulary, usually containing terms that comprehensively cover a knowledge domain. For example, there may be a nomenclature of diseases, of celestial bodies, or of makes and models of automobiles. Some nomenclatures are ordered alphabetically. Others are ordered by synonymy, wherein all synonyms and plesionyms (near-synonyms) are collected under a canonical (i.e., best or preferred) term. Synonym indexes are always corrupted by the inclusion of polysemous terms (i.e., terms with multiple meanings). In many nomenclatures, grouped synonyms are collected under

a so-called code (i.e., a unique alphanumeric string) assigned to all of the terms in the group.

Nomenclatures have many purposes: to enhance interoperability and integration, to allow synonymous terms to be retrieved regardless of which specific synonym is entered as a query, to support comprehensive analyses of textual data, to express detail, to tag information in textual documents, and to drive down the complexity of documents by uniting synonymous terms under a common code. Sets of documents held in more than one Big Data resource can be harmonized under a nomenclature by substituting or appending a nomenclature code to every nomenclature term that appears in any of the documents. [Glossary Interoperability, Data integration, Plesionymy, Polysemy, Vocabulary, Uniqueness, String]

In the case of "renal cell carcinoma," if all of the 50+ synonymous terms, appearing anywhere in a medical text, were tagged with the code "C938500," then a search engine could retrieve documents containing this code, regardless of which specific synonym was queried (e.g., a query on Grawitz tumor would retrieve documents containing the word "hypernephroid tumor"). To do so the search engine would simply translate the query word, "Grawitz tumor" into its nomenclature code "C938500" and would pull every record that had been tagged by the code.

Traditionally, nomenclature coding, much like language translation, has been considered a specialized and highly detailed task that is best accomplished by human beings. Just as there are highly trained translators who will prepare foreign language versions of popular texts, there are highly trained coders, intimately familiar with specific nomenclatures, who create tagged versions of documents. Tagging documents with nomenclature codes is serious business. If the coding is flawed the consequences can be dire. In 2009 the Department of Veterans Affairs sent out hundreds of letters to veterans with the devastating news that they had contracted Amyotrophic Lateral Sclerosis, also known as Lou Gehrig's disease, a fatal degenerative neurologic condition. About 600 of the recipients did not, in fact, have the disease. The VA retracted these letters, attributing the confusion to a coding error [5]. Coding text is difficult. Human coders are inconsistent, idiosyncratic, and prone to error. Coding accuracy for humans seems to fall in the range of 85%–90% [6]. [Glossary Accuracy versus precision]

When dealing with text in gigabyte and greater quantities, human coding is simply out of the question. There is not enough time or money or talent to manually code the textual data contained in Big Data resources. Computerized coding (i.e., autocoding) is the only practical solution.

Autocoding is a specialized form of machine translation, the field of computer science wherein meaning is drawn from narrative text. Not surprisingly, autocoding algorithms have been adopted directly from the field of machine translation, particularly algorithms for natural language processing. A popular approach to autocoding involves using the natural rules of language to find words or phrases found in text and matching them to nomenclature terms. Ideally the terms found in text are correctly matched to their equivalent nomenclature terms, regardless of the way that the terms were expressed in the text.

For instance, the term "adenocarcinoma of lung" has much in common with alternate terms that have minor variations in word order, plurality, inclusion of articles, terms split by a word inserted for informational enrichment, and so on. Alternate forms would be "adenocarcinoma of the lung," "adenocarcinoma of the lungs," "lung adenocarcinoma," and "adenocarcinoma found in the lung." A natural language algorithm takes into account grammatical variants, allowable alternate term constructions, word roots (i.e., stemming), and syntax variation. Clever improvements on natural language methods might include string similarity scores, intended to find term equivalences in cases where grammatical methods come up short. [Glossary Algorithm, Syntax, Machine translation, Natural language processing]

A limitation of the natural language approach to autocoding is encountered when synonymous terms lack etymologic commonality. Consider the term "renal cell carcinoma." Synonyms include terms that have no grammatical relationship with one another. For example, hypernephroma, and Grawitz tumor are synonyms for renal cell carcinoma. It is impossible to compute the equivalents among these terms through the implementation of natural language rules or word similarity algorithms. The only way of obtaining adequate synonymy is through the use of a comprehensive nomenclature that lists every synonym for every canonical term in the knowledge domain.

Setting aside the inability to construct equivalents for synonymous terms that share no grammatical roots, the best natural language autocoders are pitifully slow. The reason for the slowness relates to their algorithm, which requires the following steps, at a minimum: parsing text into sentences; parsing sentences into grammatical units; re-arranging the units of the sentence into grammatically permissible combinations; expanding the combinations based on stem forms of words; allowing for singularities and pluralities of words, and matching the allowable variations against the terms listed in the nomenclature. A typical natural language autocoder parses text at about 1 kilobyte per second, which is equivalent to a terabyte of text every 30 years. Big Data resources typically contain many terabytes of data; thus, natural language autocoding software is unsuitable for translating Big Data resources. This being the case, what good are they?

Natural language autocoders have value when they are employed at the time of data entry. Humans type sentences at a rate far less than 1 kilobyte per second, and natural language autocoders can keep up with typists, inserting codes for terms, as they are typed. They can operate much the same way as auto-correct, auto-spelling, look-ahead, and other commonly available crutches intended to improve or augment the output of plodding human typists.

– **Recoding and speed**

It would seem that by applying the natural language parser at the moment when the data is being prepared, all of the inherent limitations of the algorithm can be overcome. This belief, popularized by developers of natural language software, and perpetuated by a generation of satisfied customers, ignores two of the most important properties that must be preserved in Big Data resources: longevity, and curation. [Glossary Curator]

Nomenclatures change over time. Synonymous terms and the codes will vary from year to year as new versions of old nomenclature are published and new nomenclatures are developed. In some cases, the textual material within the Big Data resource will need to be annotated using codes from nomenclatures that cover informational domains that were not anticipated when the text was originally composed.

Most of the people who work within an information-intensive society are accustomed to evanescent data; data that is forgotten when its original purpose is served. Do we really want all of our old e-mails to be preserved forever? Do we not regret our earliest blog posts, Facebook entries, and tweets? In the medical world, a code for a clinic visit or a biopsy diagnosis, or a reportable transmissible disease will be used in a matter of minutes or hours; maybe days or months. Few among us place much value on textual information preserved for years and decades. Nonetheless, it is the job of the Big Data manager to preserve resource data over years and decades. When we have data that extends back, over decades, we can find and avoid errors that would otherwise reoccur in the present, and we can analyze trends that lead us into the future.

To preserve its value, data must be constantly curated, adding codes that apply to currently available nomenclatures. There is no avoiding the chore; the entire corpus of textual data held in the Big Data resource needs to be recoded again and again, using modified versions of the original nomenclature, or using one or more new nomenclatures. This time, an autocoding application will be required to code huge quantities of textual data (possibly terabytes), quickly. Natural language algorithms, which depend heavily on regex operations (i.e., finding word patterns in text) are too slow to do the job. [Glossary RegEx]

A faster alternative is so-called lexical parsing. This involves parsing text, word by word, looking for exact matches between runs of words and entries in a nomenclature. When a match occurs, the words in the text that matched the nomenclature term are assigned the nomenclature code that corresponds to the matched term. Here is one possible algorithmic strategy for autocoding the sentence: "Margins positive malignant melanoma." For this example, you would be using a nomenclature that lists all of the tumors that occur in humans. Let us assume that the terms "malignant melanoma," and "melanoma" are included in the nomenclature. They are both assigned the same code, for example "Q5673013," because the people who wrote the nomenclature considered both terms to be biologically equivalent.

Let us autocode the diagnostic sentence, "Margins positive malignant melanoma":

1. Begin parsing the sentence, one word at a time. The first word is "Margins." You check against the nomenclature, and find no match. Save the word "margins." We will use it in step 2.
2. You go to the second word, "positive" and find no matches in the nomenclature. You retrieve the former word "margins" and check to see if there is a 2-word term, "margins positive." There is not. Save "margins" and "positive" and continue.
3. You go to the next word, "malignant." There is no match in the nomenclature. You check to determine whether the 2-word term "positive malignant" and the 3-word term "margins positive malignant" are in the nomenclature. They are not.

4. You go to the next word, "melanoma." You check and find that melanoma is in the nomenclature. You check against the two-word term "malignant melanoma," the three-word term "positive malignant melanoma," and the four-word term "margins positive malignant melanoma." There is a match for "malignant melanoma" but it yields the same code as the code for "melanoma."
5. The autocoder appends the code, "Q5673013" to the sentence, and proceeds to the next sentence, where it repeats the algorithm.

The algorithm seems like a lot of work, requiring many comparisons, but it is actually much more efficient than natural language parsing. A complete nomenclature, with each nomenclature term paired with its code, can be held in a single variable, in volatile memory. Look-ups to determine whether a word or phrase is included in the nomenclature are also fast. As it happens, there are methods that will speed things along. In Section 2.7, we will see a 12-line autocoder algorithm that can parse through terabytes of text at a rate that is much faster than commercial-grade natural language autocoders [7]. [Glossary Variable]

Another approach to the problem of recoding large volumes of textual data involves abandoning the attempt to autocode the entire corpus, in favor of on-the-fly autocoding, when needed. On-the-fly autocoding involves parsing through a text of any size, and searching for all the terms that match one particular concept (i.e., the search term).

Here is a general algorithm on-the-fly coding [8]. This algorithm starts with a query term and seeks to find every synonym for the query term, in any collection of Big Data resources, using any convenient nomenclature.

1. The analyst starts with a query term submitted by a data user. The analyst chooses a nomenclature that contains his query term, as well as the list of synonyms for the term. Any vocabulary is suitable, so long as the vocabulary consists of term/code pairs, where a term and its' synonyms are all paired with the same code.
2. All of the synonyms for the query term are collected together. For instance the 2004 version of a popular medical nomenclature, the Unified Medical Language System, had 38 equivalent entries for the code C0206708, nine of which are listed here:

```
C0206708|Cervical Intraepithelial Neoplasms
C0206708|Cervical Intraepithelial Neoplasm
C0206708|Intraepithelial Neoplasm, Cervical
C0206708|Intraepithelial Neoplasms, Cervical
C0206708|Neoplasm, Cervical Intraepithelial
C0206708|Neoplasms, Cervical Intraepithelial
C0206708|Intraepithelial Neoplasia, Cervical
C0206708|Neoplasia, Cervical Intraepithelial
C0206708|Cervical Intraepithelial Neoplasia
```

If the analyst had chosen to search on "Cervial Intraepithelial Neoplasia," his term will be attached to the 38 synonyms included in the nomenclature.

3. One-by-one, the equivalent terms are matched against every record in every Big Data resource available to the analyst.
4. Records are pulled that contain terms matching any of the synonyms for the term selected by the analyst.

In the case of the example, this would mean that all 38 synonymous terms for "Cervical Intraepithelial Neoplasms" would be matched against the entire set of data records. The benefit of this kind of search is that data records that contain any search term, or its nomenclature equivalent, can be extracted from multiple data sets in multiple Big Data resources, as they are needed, in response to any query. There is no pre-coding, and there is no need to match against nomenclature terms that have no interest to the analyst. The drawback of this method is that it multiplies the computational task by the number of synonymous terms being searched, 38-fold in this example. Luckily, there are published methods for conducting simple and fast synonym searches, using precompiled concordances [8].

Section 2.6. Case Study: Instantly Finding the Precise Location of Any Atom in the Universe (Some Assembly Required)

> *There's as many atoms in a single molecule of your DNA as there are stars in the typical galaxy. We are, each of us, a little universe.*
>
> *Neil deGrasse Tyson, Cosmos*

If you have sat through an introductory course in Computer Science, you are no doubt familiar with three or four sorting algorithms. Indeed, most computer science books devote a substantial portion of their texts to describing sorting algorithms. The reason for this infatuation with sorting is that all sorted lists can be searched nearly instantly, regardless of the size of the list. The so-called binary algorithm for searching a sorted list is incredibly simple. For the sake of discussion, let us consider an alphabetically sorted list of 1024 words. I want to determine if the word "kangaroo" is in the list; and, if so, its exact location in the list. Here is how a binary search would be conducted.

1. Go to the middle entry of the list.
2. Compare the middle entry to the word "kangaroo." If the middle entry comes earlier in the alphabet than "kangaroo," then repeat step 1, this time ignoring the first half of the list and using only the second half of the list (i.e., going to the middle entry of the second half of the file). Otherwise, go to step 1, this time ignoring the second half of the list and using only the first half.

These steps are repeated until you come to the location where kangaroo resides, or until you have exhausted the list without finding your kangaroo.

Each cycle of searching cuts the size of the list in half. Hence, a search through a sorted list of 1024 items would involve, at most, 10 cycles through the two-step algorithm (because $1024 = 2\hat{}10$).

Every computer science student is expected to write her own binary search script. Here is a simple script, binary.py, that does five look-ups through a sorted numeric list, reporting on which items are found, and which items are not.

```
def Search(search_list, search_item):
  first_item = 0
  last_item = len(search_list)-1
  found = False
  while (first_item <= last_item) and not found:
    middle = (first_item + last_item)//2
    if search_list[middle] == search_item:
      found = True
    else:
      if search_item < search_list[middle]:
        last_item = middle - 1
      else:
        first_item = middle + 1
  return found
sorted_list = [4, 5, 8, 15, 28, 29, 30, 45, 67, 82, 99, 101, 1002]
for item in [3, 7, 28, 31, 45, 1002]:
  print(Search(sorted_list, item))

output:
False
False
True
False
True
True
```

Let us say, just for fun, we wanted to search through a sorted list of every atom in the universe. First we would take each atom in the universe and assign it a location. Then we would sort the locations based on their distances from the center of the center of the universe, which is apparently located at the tip of my dog's left ear. We could then substitute the sorted atom list for the sorted_list in the binary.py script, shown above.

How long would it take to search all the atoms of the universe, using the binary.py script. As it happens, we could find the list location for any atom in the universe, almost instantly. The reason is that there are only about 2 ̈260 atoms in the known universe. This means that the algorithm would required, at the very most, 260 2-step cycles. Each cycle is very fast, requiring only that we compare the search atom's distance from my dog's ear, against the middle atom of the list.

Of course, composing the list of atom locations may pose serious difficulties, and we might need another universe, much larger than our own, to hold the sorted list that we

create. Nonetheless, a valid point emerges; that binary searches are fast, and the time to completion of a binary search is not significantly lengthened by any increase in the number of items in the list. Had we chosen, we could have annotated the items of sorted_list with any manner of information (e.g., locations in a file, nomenclature code, links to web addresses, definitions of the items, metadata), so that our binary searches would yield something more useful than the location of the item in the list.

Section 2.7. Case Study (Advanced): A Complete Autocoder (in 12 Lines of Python Code)

Software is a gas; it expands to fill its container.

Nathan Myhrvold

This script requires two external files:

1. The nomenclature file that will be converted into a Python dictionary, wherein each term is a dictionary key, and each nomenclature code is a value assigned to a term. [Glossary Dictionary]

   Here are a few sample lines from the nomenclature file (nomenclature_dict.txt, in this case):

   ```
   oropharyngeal adenoid cystic adenocarcinoma , C6241000
   peritoneal mesothelioma , C7633000
   benign tumour arising from the exocrine pancreas , C4613000
   basaloid penile squamous cell cancer , C6980000
   cns malignant soft tissue tumor , C6758000
   digestive stromal tumour of stomach , C5806000
   bone with malignancy , C4016000
   benign mixed tumor arising from skin , C4474000
   ```

2. The file containing a corpus of sentences that will be autocoded by the script.

   Here are a few sample lines from the corpus file (tumorabs.txt, in this case):

   ```
   local versus diffuse recurrences of meningiomas factors correlated
   to the extent of the recurrence

   the effect of an unplanned excision of a soft tissue sarcoma on
   prognosis

   obstructive jaundice associated burkitt lymphoma mimicking
   pancreatic carcinoma

   efficacy of zoledronate in treating persisting isolated tumor
   cells in bone marrow in patients with breast cancer a phase ii pilot
   study
   ```

```
metastatic lymph node number in epithelial ovarian carcinoma does it
have any clinical significance

extended three dimensional impedance map methods for identifying
ultrasonic scattering sites

aberrant expression of connexin 26 is associated with lung metastasis
of colorectal cancer
```

The 19-line python script, autocode.txt, produces a sentence-by-sentence list of extracted autocoded terms:

```
outfile = open("autocoded.txt", "w")
literalhash = {}
with open("nomenclature_dict.txt") as f:
    for line in f:
       (key, val) = line.split(" , ")
       literalhash[key] = val
corpus_file = open("tumorabs.txt", "r")
for line in corpus_file:
    sentence = line.rstrip()
    outfile.write("\n" + sentence[0].upper() + sentence[1:] + "." +
    "\n")
    sentence_array = sentence.split(" ")
    length = len(sentence_array)
    for i in range(length):
      for place_length in range(len(sentence_array)):
          last_element = place_length + 1
          phrase = ' '.join(sentence_array[0:last_element])
          if phrase in literalhash:
             outfile.write(phrase + " " + literalhash[phrase])
      sentence_array.pop(0)
```

The first seven lines of code are housekeeping chores, in which the external nomenclature is loaded into a Python dictionary (literalhash, in this case), and an external file composed of lines, with one sentence on each line, is opened and prepared for reading, and which another external file, autocoded.txt, is created to accept the script's output. We will not count these first seven lines as belonging to our autocoder because, in all fairness, they are not doing any of the work of autocoding. The meat of the script is the next twelve lines, beginning with "for line in corpus_file."

Here is a sample of the output:

```
Obstructive jaundice associated burkitt lymphoma mimicking pancreatic
carcinoma.
   burkitt lymphoma C7188000
```

```
   lymphoma C7065000
   pancreatic carcinoma C3850000
   carcinoma C2000000

Littoral cell angioma of the spleen.
   littoral cell angioma C8541100
   littoral cell angioma of the spleen C8541100
   angioma C3085000
   angioma of the spleen C8541000

Isolated b cell lymphoproliferative disorder at the dura mater with b
cell chronic lymphocytic leukemia immunophenotype.
   lymphoproliferative disorder C4727100
   b cell chronic lymphocytic leukemia C3163000
   chronic lymphocytic leukemia C3163000
   lymphocytic leukemia C7539000
   leukemia C3161000
```

By observing a few samples of autocoded lines of text, we can see that the autocoder extracts all cancer terms, and supplies its nomenclature code, regardless of whether a term is contained within a longer term.

For example, the autocoder managed to find four terms within the sentence "Littoral cell angioma of the spleen," these being: littoral cell angioma, littoral cell angioma of the spleen, angioma, and angioma of the spleen. The ability to extract every valid term, even when they are subsumed by larger terms, guarantees that a query term and all its synonyms will always be retrieved, if the query term happens to be a valid nomenclature term.

This short autocoding script comes with a few advantages that are of particular interest to Big Data professionals:

– Scalable to any size

All nomenclatures are small. Most of us have a working vocabulary of a few thousand words. Most dictionaries are smaller, containing maybe 60,000 words. The most extreme case of verbiage about verbiage is The 20-volume Oxford English Dictionary, which contains about 170,000 entries. Even in this case, slurping the entire list of Oxford English dictionary items would be a simple matter for any modern computer.

Most importantly, the autocoding algorithm imposes no limits on the size of the Big Data corpus. The software proceeds line-by-line until the task is complete. Memory requirements and other issues of scalability are not a problem.

– Fast

On my modest desktop computer, the 12-line autocoding algorithm processes text at the rate of 1 megabyte every two seconds. A fast and powerful computer, using the same algorithm, would be expected to parse at rates of 1 gigabytes of text per second, or greater.

– Repeatable

Code a gigabyte of data in the morning. Do it all over again in the afternoon. Use another version of the nomenclature, or use a different nomenclature, entirely. Recoding is not a problem.

– Simple and adaptable, with easily maintained code

The larger the program, the more difficult it is to find bugs, or to recover from errors produced when the code is modified. It is nearly impossible to inflict irreversible damage upon a simple, 12-line script. As a general rule, tiny scripts are seldom a problem if you maintain records of where the scripts are located, how the scripts are used, and how the scripts are modified over time.

– Reveals the dirty little secret that every programmer knows, but few are willing to admit.

Virtually all useful algorithms can be implemented in a few lines of code; autocoders are no exception. The thousands, or millions, of lines of code in just about any commercial software application are devoted, in one way or another, to the graphic user interface.

Section 2.8. Case Study: Concordances as Transformations of Text

> *Interviewer: Is there anything from home that you brought over with you to set up for yourself? Creature comforts?*
> *Hawkeye: I brought a book over.*
> *Interviewer: What book?*
> *Hawkeye: The dictionary. I figure it's got all the other books in it.*
> *Interview with the character Hawkeye, played by Alan Alda, from television show M*A*S*H*

A transform is a mathematical operation that takes a function, a signal, or a set of data and changes it into something else, that is easier to work with than the original data. The concept of the transform is a simple but important idea that has revolutionized many scientific fields including electrical engineering, digital signal processing, and data analysis. In the field of digital signal processing, data in the time domain (i.e., wherein the amplitude of a measurement varies over time, as in a signal), is commonly transformed into the frequency domain (i.e., wherein the original data can be assigned to amplitude values for a range of frequencies). There are dozens, possibly hundreds, of mathematical transforms that enable data analysts to move signal data between forward transforms (e.g., time domain to frequency domain), and their inverse counterparts (e.g., frequency domain to time domain). [Glossary Transform, Signal, Digital signal, Digital Signal Processing, DSP, Fourier transform, Burrows-Wheeler transform]

A concordance is transform, for text. A concordance takes a linear text and transforms it a word-frequency distribution list; which can reversed as needed. Like any good transform, we can expect to find circumstances when it is easier to perform certain types of operations on the transformed data than on the original data. [Glossary Concordance]

Here is an example, from the Python script proximate_words.py, where we use a concordance to list the words in close proximity to the concordance entries (i.e., the words contained in the text). In this script, we use the previously constructed (vida supra) concordance of the Gettysburg address.

```
import string
infile = open ("concordance.txt", "r")
places = []
word_array = []
concordance_hash = {}
words_hash = {}
for line in infile:
   line = line.rstrip()
   line_array = line.split(" ")
   word = line_array[0]
   places = line_array[1]
   places_array = places.split(",")
   words_hash[word] = places_array
   for word_position in places_array:
     concordance_hash[word_position] = word
for k, v in words_hash.items():
   print(k, end=" - \n")
   for items in v:
     n=0
     while n < 5:
       nextone = str(int(items) + n)
       if nextone in concordance_hash:
         print(concordance_hash[nextone], end=" ")
       n=n+1
     print()
   print()
```

The script produces a list of the words from the Gettysburg address, along with short sequences of the text that follow each occurrence of the word in the text, as shown in this sampling from the output file:

```
to -
to the proposition that all
to dedicate a portion of
```

```
to add or detract. The
to be dedicated here to
to the unfinished work which
to be here dedicated to
to the great task remaining
to that cause for which

dedicated -
dedicated to the proposition that
dedicated can long endure. We
dedicated here to the unfinished
dedicated to the great task
```

Inspecting some of the output, we see that the word "to" appears 8 times in the Gettysburg address. We used the concordance to reconstruct four words that follow the word "to" wherever it occurs in the text. Likewise we see that the word "dedicated" occurs 4 times in the text, and the concordance tells us the four words that follow at each of the locations where "dedicated" appears. We can construct these proximity phrases very quickly, because the concordance tells us the exact location of the words in the text. If we were working from the original text, instead of its transform (i.e., the concordance), then our algorithm would run much more slowly, because each word would need to be individually found and retrieved, by parsing every word in the text, sequentially.

Section 2.9. Case Study (Advanced): Burrows Wheeler Transform (BWT)

> *All parts should go together without forcing. You must remember that the parts you are reassembling were disassembled by you. Therefore, if you can't get them together again, there must be a reason. By all means, do not use a hammer.*
>
> *IBM Manual, 1925*

One of the most ingenious transforms in the field of data science is the Burrows Wheeler transform. Imagine an algorithm that takes a corpus of text and creates an output string consisting of a transformed text combined with its own word index, in a format that can be compressed to a smaller size than the compressed original file. The Burrows Wheeler Transform does all this, and more [9,10]. A clever informatician may find many ways to use the BWT transform in search and retrieval algorithms and in data merging projects [11]. Using the BWT file, you can re-compose the original file, or you can find any portion of a file preceding or following any word from the file [12]. [Glossary Data merging, Data fusion]

Excellent discussions of the algorithm are available, along with implementations in several languages [9,10,13]. The Python script, bwt.py, shown here, is a modification of a script available on Wikipedia [13]. The script executes the BWT algorithm in just three

lines of code. In this example, the input string is a excerpt from Lincoln's Gettysburg address [12].

```
input = "four score and seven years ago our fathers brought forth upon"
input = input + " this continent a new nation conceived in liberty and"
input = input + "\0"
table = sorted(input[i:] + input[:i] for i in range(len(input)))
last_column = [row[-1:] for row in table]
print("".join(last_column))
```

Here is the transformed output:

```
dtsyesnsrtdnwaordnhn  efni n snenryvcvnhbsn  uatttgl tthe oioe oaai
eogipccc
fr fuuuobaeoerri  nhra naro ooieet
```

Admittedly, the output does not look like much. Let us juxtapose our input string and our BWT's transform string:

```
four score and seven years ago our fathers brought forth upon this
continent a new nation conceived in liberty and
dtsyesnsrtdnwaordnhn  efni n snenryvcvnhbsn  uatttgl tthe oioe oaai
eogipcccfr fuuuobaeoerri  nhra naro ooieet
```

We see that the input string and the transformed output string both have the same length, so there doesn't seem to be any obvious advantage to the transform. If we look a bit closer, though, we see that the output string consists largely of runs of repeated individual characters, repeated substrings, and repeated spaces (e.g., "ttt" "uuu"). These frequent repeats in the transform facilitate compression algorithms that hunt for repeat patterns. BWT's facility for creating runs of repeated characters accounts for its popularity in compression software (e.g., the Bunzip compression utility).

The Python script, bwt_inverse.py, computes the inverse BWT to re-construct the original input string. Notice that the inverse algorithm is implemented in just the last four lines of the python code (the first five lines re-created the forward BWT transform) [12]

```
input = "four score and seven years ago our fathers brought forth upon"
input = input + " this continent a new nation conceived in liberty and"
input = input + "\0"
table = sorted(input[i:] + input[:i] for i in range(len(input)))
last_column = [row[-1:] for row in table]
#The first lines re-created the bwt transform

#The next four lines compute the inverse transform
table = [""] * len(last_column)
for i in range(len(last_column)):
   table = sorted(last_column[i] + table[i] for i in range(len(input)))
print([row for row in table if row.endswith("\0")][0])
```

As we would expect, the output of the bwt_inverse.py script, is our original input string:

```
four score and seven years ago our fathers brought forth upon this
continent a new nation conceived in liberty and
```

The charm of the BWT transform is demonstrated when we create an implementation that parses the input string word-by-word; not character-by-character.

Here is the Python script, bwt_trans_inv.py, that transforms an input string, word-by-word, producing its transform; then reverses the process to yield the original string, as an array of words. As an extra feature, the script produces the first column, as an array, of the transform table [12]. [Glossary Numpy]

```
import numpy as np
input = "\0 four score and seven years ago our fathers brought forth upon"
input = input + " this continent a new nation conceived in liberty and"
word_list = input.rsplit()
table = sorted(word_list[i:] + word_list[:i] for i in range(len
(word_list)))
last_column = [row[-1:] for row in table]
first_column = [row[:1] for row in table]
print("First column of the transform table:\n" + str(first_column) +
"\n")
table = [""] * len(last_column)
for i in range(len(last_column)):
   table = sorted(str(last_column[i]) + " " + str(table[i]) for i in
range(len(word_list)))
original = [row for row in table][0]
print("Inverse transform, as a word array:\n" + str(original))
```

Here is the output of the bwt_trans_inv.py script. Notice once more that the word-by-word transform was implemented in 3 lines of code, and the inverse transform was implemented in four lines of code.

```
First column of the transform table:
[['\x00'], ['a'], ['ago'], ['and'], ['and'], ['brought'],
['conceived'], ['continent'], ['fathers'], ['forth'], ['four'],
['in'], ['liberty'], ['nation'], ['new'], ['our'], ['score'],
['seven'], ['this'], ['upon'], ['years']]
```

```
Inverse transform, as a word array:
['\x00'] ['four'] ['score'] ['and'] ['seven'] ['years'] ['ago']
['our'] ['fathers'] ['brought'] ['forth'] ['upon'] ['this']
['continent'] ['a'] ['new'] ['nation'] ['conceived'] ['in']
['liberty'] ['and']
```

The first column of the transform, created in the forward BWT, is a list of the words in the input string, in alphabetic order. Notice that words that occurred more than one time in the input text were repeated in the first column of the transform table (i.e., [and], [and] in the example sentence). Hence, the transform yields all the words from the original input, along with their frequency of occurrence in the text. As expected, the inverse of the transform yields our original input string.

Glossary

Accuracy versus precision Accuracy measures how close your data comes to being correct. Precision provides a measurement of reproducibility (i.e., whether repeated measurements of the same quantity produce the same result). Data can be accurate but imprecise. If you have a 10 pound object, and you report its weight as 7.2376 pounds, on every occasion when the object is weighed, then your precision is remarkable, but your accuracy is dismal.

Algorithm An algorithm is a logical sequence of steps that lead to a desired computational result. Algorithms serve the same function in the computer world as production processes serve in the manufacturing world and as pathways serve in the world of biology. Fundamental algorithms can be linked to one another, to create new algorithms (just as biological pathways can be linked). Algorithms are the most important intellectual capital in computer science. In the past half century, many brilliant algorithms have been developed for the kinds of computation-intensive work required for Big Data analysis [14,15].

Binary data Computer scientists say that there are 10 types of people. Those who think in terms of binary numbers, and those who do not. Pause for laughter and continue. All digital information is coded as binary data. Strings of 0s and 1s are the fundamental units of electronic information. Nonetheless, some data is more binary than other data. In text files, 8-bite sequences are converted into decimals in the range of 0–256, and these decimal numbers are converted into characters, as determined by the ASCII standard. In several raster image formats (i.e., formats consisting of rows and columns of pixel data), 24-bit pixel values are chopped into red, green and blue values of 8-bits each. Files containing various types of data (e.g., sound, movies, telemetry, formatted text documents), all have some kind of low-level software that takes strings of 0s and 1s and converts them into data that has some particular meaning for a particular use. So-called plain-text files, including HTML files and XML files are distinguished from binary data files and referred to as plain-text or ASCII files. Most computer languages have an option wherein files can be opened as "binary," meaning that the 0s and 1s are available to the programmer, without the intervening translation into characters or stylized data.

Burrows-Wheeler transform Abbreviated as BWT, the Burrows-Wheeler transform produces a compressed version of an original file, along with a concordance to the contents of the file. Using a reverse BWT, you can reconstruct the original file, or you can find any portion of a file preceding or succeeding any location in the file. The BWT transformation is an amazing example of simplification, applied to informatics. A detailed discussion of the BWT is found in Section 2.9, "Case Study (Advanced): Burrows Wheeler Transform."

Class A class is a group of objects that share a set of properties that define the class and that distinguish the members of the class from members of other classes. The word "class," lowercase, is used as a general term. The word "Class," uppercase, followed by an uppercase noun (e.g., Class Animalia), represents a specific class within a formal classification.

Classification A system in which every object in a knowledge domain is assigned to a class within a hierarchy of classes. The properties of superclasses are inherited by the subclasses. Every class has one immediate superclass (i.e., parent class), although a parent class may have more than one immediate subclass (i.e., child class). Objects do not change their class assignment in a classification, unless there

was a mistake in the assignment. For example, a rabbit is always a rabbit, and does not change into a tiger. Classifications can be thought of as the simplest and most restrictive type of ontology, and serve to reduce the complexity of a knowledge domain [16].

Classifications can be easily modeled in an object-oriented programming language and are non-chaotic (i.e., calculations performed on the members and classes of a classification should yield the same output, each time the calculation is performed). A classification should be distinguished from an ontology. In an ontology a class may have more than one parent class and an object may be a member of more than one class. A classification can be considered a special type of ontology wherein each class is limited to a single parent class and each object has membership in one and only one class.

Coding The term "coding" has three very different meanings depending on which branch of science influences your thinking. For programmers, coding means writing the code that constitutes a computer programmer. For cryptographers, coding is synonymous with encrypting (i.e., using a cipher to encode a message). For medics, coding is calling an emergency team to handle a patient in extremis. For informaticians and library scientists, coding involves assigning a alphanumeric identifier, representing a concept listed in a nomenclature, to a term. For example, a surgical pathology report may includes the diagnosis, "Adenocarcinoma of prostate." A nomenclature may assign a code C4863000 that uniquely identifies the concept "Adenocarcinoma." Coding the report may involve annotating every occurrence of the work "Adenocarcinoma" with the "C4863000" identifier. For a detailed explanation of coding, and its importance for searching and retrieving data, see the full discussion in Section 3.4, "Autoencoding and Indexing with Nomenclatures."

Concordance A concordance is an index consisting of every word in the text, along with every location wherein each word can be found. It is computationally trivial to reconstruct the original text from the concordance. Before the advent of computers, concordances fell into the provenance of religious scholars, who painstakingly recorded the locations of the all words appearing in the Bible, ancient scrolls, and any texts whose words were considered to be divinely inspired. Today, a concordance for a Bible-length book can be constructed in about a second. Furthermore, the original text can be reconstructed from the concordance, in about the same time.

Curator The word "curator" derives from the latin, "curatus," the same root for "curative," indicating that curators "take care of" things. A data curator collects, annotates, indexes, updates, archives, searches, retrieves, and distributes data. Curator is another of those somewhat arcane terms (e.g., indexer, data archivist, lexicographer) that are being rejuvenated in the new millennium. It seems that if we want to enjoy the benefits of a data-centric world, we will need the assistance of curators, trained in data organization.

DSP Abbreviation for Digital Signal Processing.

Data fusion Data fusion is very closely related to data integration. The subtle difference between the two concepts lies in the end result. Data fusion creates a new and accurate set of data representing the combined data sources. Data integration is an on-the-fly usage of data pulled from different domains and, as such, does not yield a residual fused set of data.

Data integration The process of drawing data from different sources and knowledge domains in a manner that uses and preserves the identities of data objects and the relationships among the different data objects. The term "integration" should not be confused with a closely related term, "interoperability." An easy way to remember the difference is to note that **integration applies to data; interoperability applies to software.**

Data merging A nonspecific term that includes data fusion, data integration, and any methods that facilitate the accrual of data derived from multiple sources.

Dictionary In general usage a dictionary is a word list accompanied by a definition for each item. In Python a dictionary is a data structure that holds an unordered list of key/value pairs. A dictionary, as used in Python, is equivalent to an associative array, as used in Perl.

Digital Signal Processing Digital Signal Processing (DSP) is the field that deals with creating, transforming, sending, receiving, and analyzing digital signals. Digital signal processing began as a specialized

subdiscipline of signal processing, another specialized subdiscipline. For most of the twentieth century, many technologic advances came from converting non-electrical signals (temperature, pressure, sound, and other physical signals) into electric signals that could be carried via electromagnetic waves, and later transformed back into physical actions. Because electromagnetic waves sit at the center of so many transform process, even in instances when the input and outputs are non-electrical in nature, the field of electrical engineering and signal processing have paramount importance in every field of engineering. In the past several decades the intermediate signals have been moved from the analog domain (i.e., waves) into the digital realm (i.e., digital signals expressed as streams of 0s and 1s). Over the years, as techniques have developed by which any kind of signal can be transformed into a digital signal, the subdiscipline of digital signal processing has subsumed virtually all of the algorithms once consigned to its parent discipline. In fact, as more and more processes have been digitized (e.g., telemetry, images, audio, sensor data, communications theory), the field of digital signal processing has come to play a central role in data science.

Digital signal A signal is a description of how one parameter varies with some other parameter. The most familiar signals involve some parameter varying over time (e.g., sound is air pressure varying over time). When the amplitude of a parameter is sampled at intervals, producing successive pairs of values, the signal is said to be digitized.

Fourier transform A transform is a mathematical operation that takes a function or a time series (e.g., values obtained at intervals of time) and transforms it into something else. An inverse transform takes the transform function and produces the original function (Fig. 2.1). Transforms are useful when there are operations that can be more easily performed on the transformed function than on the original function. Possibly the most useful transform is the Fourier transform, which can be computed with great speed on modern computers, using a modified form known as the fast Fourier Transform. Periodic functions and waveforms (periodic time series) can be transformed using this method. Operations on the transformed function can sometimes eliminate repeating artifacts or frequencies that occur below a selected threshold (e.g., noise). The transform can be used to find similarities between two signals. When the operations on the transform function are complete, the inverse of the transform can be calculated and substituted for the original set of data (Fig. 2.2).

Identifier A string that is associated with a particular thing (e.g., person, document, transaction, data object), and not associated with any other thing [17]. In the context of Big Data, identification usually involves permanently assigning a seemingly random sequence of numeric digits (0–9) and alphabet characters (a-z and A-Z) to a data object. The data object can be a class of objects.

Indexes Every writer must search deeply into his or her soul to find the correct plural form of "index". Is it "indexes" or is it "indices"? Latinists insist that "indices" is the proper and exclusive plural form. Grammarians agree, reserving "indexes" for the third person singular verb form; "The student indexes his thesis." Nonetheless, popular usage of the plural of "index," referring to the section at the end of a book, is almost always "indexes," the form used herein.

$$\hat{f}(\xi) = \int_{-\infty}^{\infty} f(x)\, e^{-2\pi i x \xi}\, dx$$

$$f(x) = \int_{-\infty}^{\infty} \hat{f}(\xi)\, e^{2\pi i x \xi}\, d\xi$$

FIG. 2.1 The Fourier transform and its inverse. In this representation of the transform, *x* represents time in seconds and the transform variable zeta represents frequency in hertz.

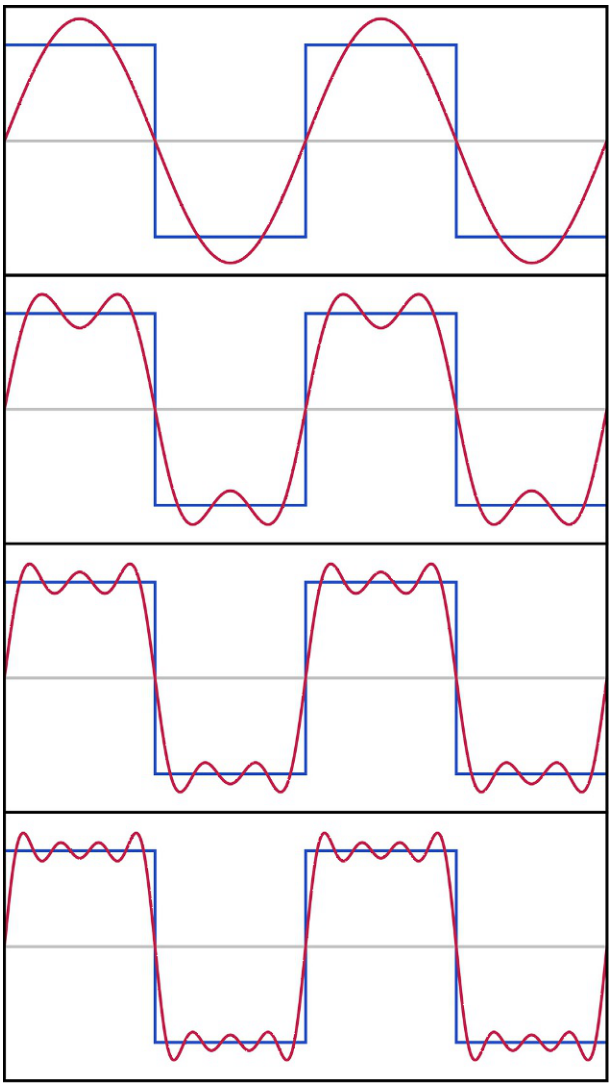

FIG. 2.2 A square wave is approximated by a single sine wave, the sum of two sine waves, three sine waves, and so on. As more components are added, the representation of the original signal or periodic set of data, is more closely approximated. *From Wikimedia Commons.*

Interoperability It is desirable and often necessary to create software that operates with other software, regardless of differences in hardware, operating systems and programming language. Interoperability, though vital to Big Data science, remains an elusive goal.

Machine translation Ultimately, the job of machine translation is to translate text from one language into another language. The process of machine translation begins with extracting sentences from text, parsing the words of the sentence into grammatical parts, and arranging the grammatical parts into an order that imposes logical sense on the sentence. Once this is done, each of the parts can be translated by a dictionary that finds equivalent terms in a foreign language, then re-assembled as a foreign

language sentence by applying grammatical positioning rules appropriate for the target language. Because these steps apply the natural rules for sentence constructions in a foreign language, the process is often referred to as natural language machine translation. It is important to note that nowhere in the process of machine translation is it necessary to find meaning in the source text, or to produce meaning in the output. Good machine translation algorithms preserve ambiguities, without attempting to impose a meaningful result.

Natural language processing A field broadly concerned with how computers interpret human language (i.e., machine translation). At its simplest level this may involve parsing through text and organizing the grammatical units of individual sentences (i.e., tokenization). For example, we might assign the following tokens to the grammatical parts of a sentence: A = adjective, D = determiner, N = noun, P = preposition, V = main verb. A determiner is a word such as "a" or "the", which specifies the noun [18]. Consider the sentence, "The quick brown fox jumped over lazy dogs." This sentence can be grammatically tokenized as:

the::D
quick::A
brown::A
fox::N
jumped::V
over::P
the::D
lazy::A
dog::N

We can express the sentence as the sequence of its tokens listed in the order of occurrence in the sentence: DAANVPDAN. This does not seem like much of a breakthrough, but imagine having a large collection of such token sequences representing every sentence from a large text corpus. With such a data set, we could begin to understand the rules of sentence structure. Commonly recurring sequences, like DAANVPDAN, might be assumed to be proper sentences. Sequences that occur uniquely in a large text corpus are probably poorly constructed sentences. Before long, we might find ourselves constructing logic rules for reducing the complexity of sentences by dropping subsequences which, when removed, yield a sequence that occurs more commonly than the original sequence. For example, our table of sequences might indicate that we can convert DAANVPDAN into NVPAN (i.e., "Fox jumped over lazy dog"), without sacrificing too much of the meaning from the original sentence and preserving a grammatical sequence that occurs commonly in the text corpus.

This short example serves as an overly simplistic introduction to natural language processing. We can begin to imagine that the grammatical rules of a language can be represented by sequences of tokens that can be translated into words or phrases from a second language, and re-ordered according to grammatical rules appropriate to the target language. Many natural language processing projects involve transforming text into a new form, with desirable properties (e.g., other languages, an index, a collection of names, a new text with words and phrases replaced with canonical forms extracted from a nomenclature) [18]. When we use natural language rules to autocode text, the grammatical units are trimmed, reorganized, and matched against concept equivalents in a nomenclature.

Ngrams Ngrams are subsequences of text, of length n words. A complete collection of ngrams consists of all of the possible ordered subsequences of words in a text. Because sentences are the basic units of statements and ideas, when we speak of ngrams, we are confining ourselves to ngrams of sentences. Let us examine all the ngrams for the sentence, "Ngrams are ordered word sequences."

```
Ngrams (1-gram)
are (1-gram)
ordered (1-gram)
word (1-gram)
```

```
sequences (1-gram)
Ngrams are (2-gram)
are ordered (2-gram)
ordered word (2-gram)
word sequences (2-gram)
Ngrams are ordered (3-gram)
are ordered word (3-gram)
ordered word sequences (3-gram)
Ngrams are ordered word (4-gram)
are ordered word sequences (4-gram)
Ngrams are ordered word sequences (5-gram)
```

Here is a short Python script, ngram.py, that will take a sentence and produce a list of all the contained ngrams.

```
import string
text = "ngrams are ordered word sequences"
partslist = []
ngramlist = {}
text_list = text.split(" ")
while(len(text_list) > 0):
   partslist.append(" ".join(text_list))
   del text_list[0]
for part in partslist:
   previous = ""
   wordlist = part.split(" ")
   while(len(wordlist) > 0):
      ngramlist[(" ".join(wordlist))] = ""
      firstword = wordlist[0]
      del wordlist[0]
      ngramlist[firstword] = ""
      previous = previous + " " + firstword
      previous = previous.strip()
      ngramlist[previous] = ""
for key in sorted(ngramlist):
      print(key)
exit
```

```
output:
are
are ordered
are ordered word
are ordered word sequences
ngrams
ngrams are
ngrams are ordered
ngrams are ordered word
ngrams are ordered word sequences
ordered
ordered word
ordered word sequences
sequences
```

```
word
word sequences
```

The ngram.py script can be easily modified to parse through all the sentences of any text, regardless of length, building the list of ngrams as it proceeds.

Google has collected ngrams from scanned literature dating back to 1500. The public can enter their own ngrams into Google's ngram viewer, and receive a graph of the published occurrences of the phrase, through time [18]. We can use the Ngram viewer to find trends (e.g., peaks, valleys and periodicities) in data. Consider the Google Ngram Viewer results for the two-word ngram, "yellow fever" (Fig. 2.3).

We see that the term "yellow fever" (a mosquito-transmitted hepatitis) appeared in the literature beginning about 1800, with several subsequent peaks. The dates of the peaks correspond roughly to outbreaks of yellow fever in Philadelphia (epidemic of 1793), New Orleans (epidemic of 1853), with United States construction efforts in the Panama Canal (1904–14), and with well-documented WWII Pacific outbreaks (about 1942). Following the 1942 epidemic an effective vaccine was available, and the incidence of yellow fever, as well as the literature occurrences of the "yellow fever" n-gram, dropped precipitously. In this case, a simple review of n-gram frequencies provides an accurate chart of historic yellow fever outbreaks [19,18].

Nomenclature A nomenclatures is a listing of terms that cover all of the concepts in a knowledge domain. A nomenclature is different from a dictionary for three reasons: 1) the nomenclature terms are not annotated with definitions, 2) nomenclature terms may be multi-word, and 3) the terms in the nomenclature are limited to the scope of the selected knowledge domain. In addition, most nomenclatures group synonyms under a group code. For example, a food nomenclature might collect submarine sandwich, hoagie, po' boy, grinder, hero, and torpedo under an alphanumeric code such as "F63958." Nomenclatures simplify textual documents by uniting synonymous terms under a common code. Documents that have been coded with the same nomenclature can be integrated with other documents that have been similarly coded, and queries conducted over such documents will yield the same results, regardless of which term is entered (i.e., a search for either hoagie, or po' boy will retrieve the same information, if both terms have been annotated with the synonym code, "F63948"). Optimally, the canonical concepts listed in the nomenclature are organized into a hierarchical classification [20,21,12].

Nomenclature mapping Specialized nomenclatures employ specific names for concepts that are included in other nomenclatures, under other names. For example, medical specialists often preserve their favored names for concepts that cross into different fields of medicine. The term that pathologists use for a certain benign fibrous tumor of the skin is "fibrous histiocytoma," a term spurned by

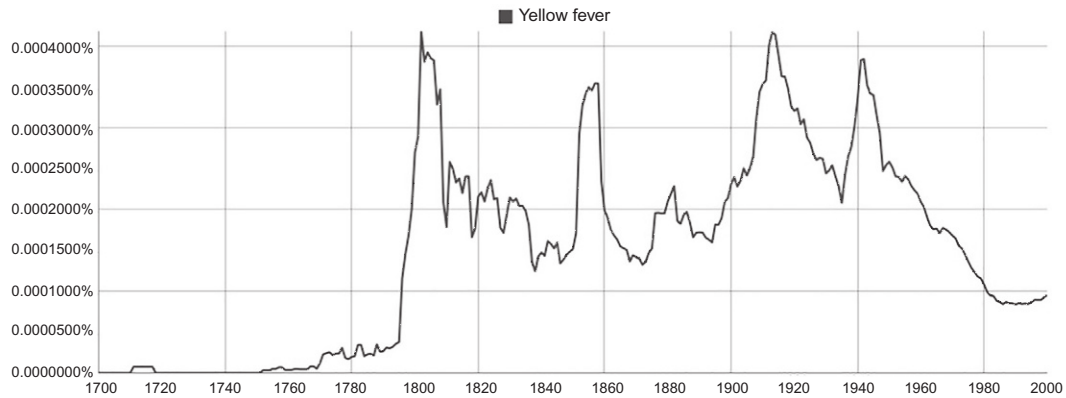

FIG. 2.3 Google Ngram for the phrase "yellow fever," counting occurrences of the term in a large corpus, from the years 1700–2000. Peaks roughly correspond to yellow fever epidemics. *Source: Google Ngram viewer, with permission from Google.*

dermatologists, who prefer to use "dermatofibroma" to describe the same tumor. As another horrifying example, the names for the physiologic responses caused by a reversible cerebral vasoconstricitve event include: thunderclap headache, Call-Fleming syndrome, benign angiopathy of the central nervous system, postpartum angiopathy, migrainous vasospasm, and migraine angiitis. The choice of term will vary depending on the medical specialty of the physician (e.g., neurologist, rheumatologist, obstetrician). To mitigate the discord among specialty nomenclatures, lexicographers may undertake a harmonization project, in which nomenclatures with overlapping concepts are mapped to one another.

Numpy Numpy (Numerical Python) is an open source extension to Python that supports matrix operations, as well as a rich assortment of mathematical functions. Numpy can be easily downloaded from sourceforge.net: http://sourceforge.net/projects/numpy/. Here is a short Python script, numpy_dot.py, that creates a 3x3 matrix, inverts the matrix, and calculates the dot produce of the matrix and its inverted counterpart.

```
import numpy
from numpy.linalg import inv
a = numpy.array([[1,4,6], [9,15,55], [62,-5, 4]])
print(a)
print(inv(a))
c = numpy.dot(a, inv(a))
print(numpy.round_(c))
```

The numpy_dot.py script employs numpy, numpy's linear algebra module, and numpy's matrix inversion method, and the numpy dot product method. Here is the output of the script, displaying the original matrix, its inversion, and the dot product, which happens to be the unity matrix:

```
c:\ftp\py>numpy_dot.py
[[ 1  4  6]
 [ 9 15 55]
 [62 -5  4]]
[[ 4.19746899e-02 -5.76368876e-03 1.62886856e-02]
 [ 4.22754041e-01 -4.61095101e-02 -1.25297582e-04]
 [-1.22165142e-01 3.17002882e-02 -2.63124922e-03]]
[[1. 0. 0.]
 [0. 1. 0.]
 [0. 0. 1.]]
```

Parsing Much of computer programming involves parsing; moving sequentially through a file or some sort of data structure and performing operations on every contained item, one item at a time. For files, this might mean going through a text file line by line, or sentence by sentence. For a data file, this might mean performing an operation on each record in the file. For in-memory data structures, this may mean performing an operation on each item in a list or a tuple or a dictionary.

The parse_directory.py script prints all the file names and subdirectory names in a directory tree.

```
import os
for root, dirs, files in os.walk(".", topdown=False):
  for filename in files:
     print(os.path.join(root, filename))
  for dirname in dirs:
     print(os.path.join(root, dirname))
```

Plain-text Plain-text refers to character strings or files that are composed of the characters accessible to a typewriter keyboard. These files typically have a ".txt" suffix to their names. Plain-text files are sometimes referred to as 7-bit ascii files because all of the familiar keyboard characters have

ASCII vales under 128 (i.e., can be designated in binary with, just seven 0s and 1s. In practice, plain-text files exclude 7-bit ascii symbols that do not code for familiar keyboard characters. To further confuse the issue, plain-text files may contain ascii characters above 7 bits (i.e., characters from 128 to 255) that represent characters that are printable on computer monitors, such as accented letters.

Plesionymy Nearly synonymous words, or pairs of words that are sometimes synonymous; other times not. For example, the noun forms of "smell" and "odor" are synonymous. As verb forms, "smell" applies, but odor does not. You can small a fish, but you cannot odor a fish. Smell and odor are plesionyms. Plesionymy is another challenge for machine translators.

Polysemy Occurs when a word has more than one distinct meaning. The intended meaning of a word can sometimes be determined by the context in which the word is used. For example, "She rose to the occasion," and "Her favorite flower is the rose." Sometimes polysemy cannot be resolved. For example, "Eats shoots and leaves."

RegEx Short for Regular Expressions, RegEx is a syntax for describing patterns in text. For example, if I wanted to pull all lines from a text file that began with an uppercase "B" and contained at least one integer, and ended with the a lowercase x, then I might use the regular expression: "^B.*[0-9].*x$". This syntax for expressing patterns of strings that can be matched by pre-built methods available to a programming language is somewhat standardized. This means that a RegEx expression in Perl will match the same pattern in Python, or Ruby, or any language that employs RegEx. The relevance of RegEx to Big Data is several-fold. RegEx can be used to build or transform data from one format to another; hence creating or merging data records. It can be used to convert sets of data to a desired format; hence transforming data sets. It can be used to extract records that meet a set of characteristics specified by a user; thus filtering subsets of data or executing data queries over text-based files or text-based indexes. The big drawback to using RegEx is speed: operations that call for many RegEx operations, particularly when those operations are repeated for each parsed line or record, will reduce software performance. RegEx-heavy programs that operate just fine on megabyte files may take hours, days or months to parse through terabytes of data.

A 12-line python script, file_search.py, prompts the user for the name of a text file to be searched, and then prompts the user to supply a RegEx pattern. The script will parse the text file, line by line, displaying those lines that contain a match to the RegEx pattern.

```
import sys, string, re
print("What is file would you like to search?")
filename = sys.stdin.readline()
filename = filename.rstrip()
print("Enter a word, phrase or regular expression to search.")
word_to_search = (sys.stdin.readline()).rstrip()
infile = open (filename, "r")
regex_object = re.compile(word_to_search, re.I)
for line in infile:
  m= regex_object.search(line)
  if m:
     print(line)
```

Scalable Software is scalable if it operates smoothly, whether the data is small or large. Software programs that operate by slurping all data into a RAM variable (i.e., a data holder in RAM memory) are not scalable, because such programs will eventually encounter a quantity of data that is too large to store in RAM. As a rule of thumb, programs that process text at speeds less than a megabyte per second are not scalable, as they cannot cope, in a reasonable time frame, with quantities of data in the gigabyte and higher range.

Script A script is a program that is written in plain-text, in a syntax appropriate for a particular programming language, that needs to be parsed through that language's interpreter before it can be compiled

and executed. Scripts tend to run a bit slower than executable files, but they have the advantage that they can be understood by anyone who is familiar with the script's programming language.

Sentence Computers parse files line by line, not sentence by sentence. If you want a computer to perform operations on a sequence of sentences found in a corpus of text, then you need to include a subroutine in your scripts that list the sequential sentences. One of the simplest ways to find the boundaries of sentences is to look for a period followed by one or more spaces, followed by an uppercase letter. Here's a simple Python demonstration of a sentence extractor, using a few famous lines from the Lewis Carroll poem, Jabberwocky.

```
import re
all_text =\
"And, has thou slain the Jabberwock? Come \
to my arms, my beamish boy! O frabjous \
day! Callooh! Callay! He chortled in his \
joy. Lewis Carroll, excerpted from \
Jabberwocky";
sentence_list = re.split(r'[\.\!\?] +(?=[A-Z])', all_text)
print("\n".join(sentence_list))
```

Here is the output:

```
And, has thou slain the Jabberwock
Come to my arms, my beamish boy
O frabjous day
Callooh
Callay
He chortled in his joy
Lewis Carroll, excerpted from Jabberwocky
```

The meat of the script is the following line of code, which splits lines of text at the boundaries of sentences:

```
sentence_list = re.split(r'[\.\!\?] +(?=[A-Z])',in_text_string)
```

This algorithm is hardly foolproof, as periods are used for many purposes other than as sentence terminators. But it may suffice for most purposes.

Signal In a very loose sense a signal is a way of gauging how measured quantities (e.g., force, voltage, or pressure) change in response to, or along with, other measured quantities (e.g., time). A sound signal is caused by the changes in pressure, exerted on our eardrums, over time. A visual signal is the change in the photons impinging on our retinas, over time. An image is the change in pixel values over a two-dimensional grid. Because much of the data stored in computers consists of discrete quantities of describable objects, and because these discrete quantities change their values, with respect to one another, we can appreciate that a great deal of modern data analysis is reducible to digital signal processing.

Specification A specification is a method for describing objects (physical objects such as nuts and bolts or symbolic objects such as numbers). Specifications do not require specific types of information, and do not impose any order of appearance of the data contained in the document. Specifications do not generally require certification by a standards organization. They are generally produced by special interest organizations, and their legitimacy depends on their popularity. Examples of specifications are RDF (Resource Description Framework) produced by the W3C (WorldWide Web Consortium), and TCP/IP (Transfer Control Protocol/Internet Protocol), maintained by the Internet Engineering Task Force.

String A string is a sequence of characters. Words, phrases, numbers, and alphanumeric sequences (e.g., identifiers, one-way hash values, passwords) are strings. A book is a long string. The complete sequence of the human genome (3 billion characters, with each character an A,T,G, or C) is a very long string. Every subsequence of a string is another string.

Syntax Syntax is the standard form or structure of a statement. What we know as English grammar is equivalent to the syntax for the English language. If I write, "Jules hates pizza," the statement would be syntactically valid, but factually incorrect. If I write, "Jules drives to work in his pizza," the statement would be syntactically valid but nonsensical. For programming languages, syntax refers to the enforced structure of command lines. In the context of triplestores, syntax refers to the arrangement and notation requirements for the three elements of a statement (e.g., RDF format or N3 format). Charles Mead distinctly summarized the difference between syntax and semantics: "Syntax is structure; semantics is meaning" [22].

Systematics The term "systematics" is, by tradition, reserved for the field of biology that deals with taxonomy (i.e., the listing of the distinct types of organisms) and with classification (i.e., the classes of organisms and their relationships to one another). There is no reason why biologists should lay exclusive claim to the field of systematics. As used herein, systematics equals taxonomics plus classification, and this term applies just as strongly to stamp collecting, marketing, operations research, and object-oriented programming as it does to the field of biology.

Taxa Plural of taxon.

Taxon A taxon is a class. The common usage of "taxon" is somewhat inconsistent, as it sometimes refers to the class name, and at other times refers to the instances (i.e., members) of the class. In this book, the term "taxon" is abandoned in favor of "class," the plesionym used by computer scientists. Hence, the term "class" is used herein in the same manner that it is used in modern object oriented programming languages.

Taxonomy When we write of "taxonomy" as an area of study, we refer to the methods and concepts related to the science of classification, derived from the ancient Greek taxis, "arrangement," and nomia, "method." When we write of "a taxonomy," as a construction within a classification, we are referring to the collection of named instances (class members) in the classification. To appreciate the difference between a taxonomy and a classification, it helps to think of taxonomy as the scientific field that determines how different members of a classification are named. Classification is the scientific field that determines how related members are assigned to classes, and how the different classes are related to one another. A taxonomy is similar to a nomenclature; the difference is that in a taxonomy, every named instance must have an assigned class.

Term extraction algorithm Terms are phrases, most often noun phrases, and sometimes individual words, that have a precise meaning within a knowledge domain. For example, "software validation," "RDF triple," and "WorldWide Telescope" are examples of terms that might appear in the index or the glossary of this book. The most useful terms might appear up to a dozen times in the text, but when they occur on every page, their value as a searchable item is diminished; there are just too many instances of the term to be of practical value. Hence, terms are sometimes described as noun phrases that have low-frequency and high information content. Various algorithms are available to extract candidate terms from textual documents. The candidate terms can be examined by a curator who determines whether they should be included in the index created for the document from which they were extracted. The curator may also compare the extracted candidate terms against a standard nomenclature, to determine whether the candidate terms should be added to the nomenclature. For additional discussion, see Section 2.3, "Term Extraction."

Thesaurus A vocabulary that groups together synonymous terms. A thesaurus is very similar to a nomenclature. There are two minor differences. Nomenclatures do not always group terms by synonymy; and nomenclatures are often restricted to a well-defined topic or knowledge domain (e.g., names of stars, infectious diseases, etc.).

Transform (noun form) There are three truly great conceptual breakthroughs that have brought with them great advances to science and to civilization. The first two to be mentioned are well known to everyone: equations and algorithms. Equations permit us to relate variable quantities in a highly specific and repeatable way. Algorithms permit us to follow a series of steps that always produce the same

results. The third conceptual breakthrough, less celebrated but just as important, is the transformation; a way of changing things to yield a something new, with properties that provide an advantage over the original item. In the case of reversible transformation, we can return the transformed item to its original form, and often in improved condition, when we have completed our task.

It should be noted that this definition applies only to the noun form of "transform." The meaning of the verb form of transform is to change or modify, and a transformation is the closest noun form equivalent of the verb form, "to transform."

Uniqueness Uniqueness is the quality of being separable from every other thing in the universe. For data scientists, uniqueness is achieved when data is bound to a unique identifier (i.e., a randomly chosen string of alphanumeric characters) that has not, and will never be, assigned to any data. The binding of data to a permanent and inseparable identifier constitutes the minimal set of ingredients for a data object. Uniqueness can apply to two or more indistinguishable objects, if they are assigned unique identifiers (e.g., unique product numbers stamped into identical auto parts).

Variable In algebra, a variable is a quantity, in an equation, that can change; as opposed to a constant quantity, that cannot change. In computer science, a variable can be perceived as a container that can be assigned a value. If you assign the integer 7 to a container named "x," then "x" equals 7, until you re-assign some other value to the container (i.e., variables are mutable). In most computer languages, when you issue a command assigning a value to a new (undeclared) variable, the variable automatically comes into existence to accept the assignment. The process whereby an object comes into existence, because its existence was implied by an action (such as value assignment), is called reification.

Vocabulary A comprehensive collection of the words used in a general area of knowledge. The term "vocabulary" and the term "nomenclature" are nearly synonymous. In common usage, a vocabulary is a list of words and typically includes a wide range of terms and classes of terms. Nomenclatures typically focus on a class of terms within a vocabulary. For example, a physics vocabulary might contain the terms "quark, black hole, Geiger counter, and Albert Einstein"; a nomenclature might be devoted to the names of celestial bodies.

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3

Identification, Deidentification, and Reidentification

OUTLINE

Section 3.1. What Are Identifiers?

> *Where is the 'any' key?*
>
> *Homer Simpson, in response to his computer's instruction to "Press any key"*

Let us begin this chapter with a riddle. "Is the number 5 a data object?" If you are like most people, you will answer "yes" because "5" is an integer and therefore it is represents numeric data, and "5" is an object because it exists and is different from all the other numbers. Therefore "5" is a data object. This line of reasoning happens to be completely erroneous. Five is not a data object. As a pure abstraction with nothing binding it to a physical object (e.g., 5 pairs of shoes, 5 umbrellas), it barely qualifies as data.

When we speak of a data object, in computer science, we refer to something that is identified and described. Consider the following statements:

```
<f183136d-3051-4c95-9e32-66844971afc5><name><Baltimore>
<f183136d-3051-4c95-9e32-66844971afc5><class><city>
<f183136d-3051-4c95-9e32-66844971afc5><population><620,961>
```

Without knowing much about data objects (which we will be discussing in detail in Section 6.2), we can start to see that these three statements are providing information about Baltimore. They tell us that Baltimore is a city of population 620,961, and that

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Baltimore has been assigned an alphanumeric sequence, "f183136d-3051-4c95-9e32-66844971afc5," to which all our available information about Baltimore has been attached. Peeking ahead into Chapter 6, we can now surmise that a data object consists of a unique alphanumeric sequence (the object identifier) plus the descriptive information associated with the identifier (e.g., name, population number, class). We will see that there are compelling reasons for storing all information contained in Big Data resources within uniquely identified data objects. Consequently, one of the most important tasks for data managers is the creation of a dependable identifier system [1]. In this chapter, we will be focusing our attention on the unique identifier and how it is created and utilized in the realm of Big Data.

Identification issues are often ignored by data managers who are accustomed to working on small data projects. It is worthwhile to list, up front, the most important ideas described in this chapter, many of which are counterintuitive and strange to those whose careers are spent outside the confusing realm of Big Data.

- All Big Data resources can be imagined as identifier systems to which we attach our data.
- Without an adequate identification system, a Big Data resource has no value. In this case, the data within the resource cannot be sensibly analyzed.
- Data deidentification is a process whereby links to the public name of the subject of the record are removed.
- Deidentification should not be confused with the act of stripping a record of an identifier. A deidentified record, like any valid data object, must always have an associated identifier.
- Deidentification should not be confused with data scrubbing. Data scrubbers remove unwanted information from a data record, including information of a personal nature, and any information that is not directly related to the purpose of the data record. [Glossary Data cleaning, Data scrubbing]
- Reidentification is a concept that specifically involves personal and private data records. It involves ascertaining the name of the individual who is associated with a deidentified record. Reidentification is sometimes necessary to verify the contents of a record, or to provide information that is necessary for the well-being of the subject of a deidentified data record. Ethical reidentification always requires approval and oversight.
- Where there is no identification, there can be no deidentification and no reidentification.
- When a deidentified data set contains no unique records (i.e., every record has one or more additional records from which it cannot be distinguished, aside from its assigned identifier sequence), then it becomes impossible to maliciously uncover a deidentified record's public name.

Section 3.2. Difference Between an Identifier and an Identifier System

Many errors, of a truth, consist merely in the application the wrong names of things.
Baruch Spinoza

Data identification is among the most underappreciated and least understood Big Data issue. Measurements, annotations, properties, and classes of information have no informational meaning unless they are attached to an identifier that distinguishes one data object from all other data objects, and that links together all of the information that has been or will be associated with the identified data object. The method of identification and the selection of objects and classes to be identified relates fundamentally to the organizational model of the Big Data resource. If data identification is ignored or implemented improperly, the Big Data resource cannot succeed. [Glossary Annotation]

This chapter will describe, in some detail, the available methods for data identification, and the minimal properties of identified information (including uniqueness, exclusivity, completeness, authenticity, and harmonization). The dire consequences of inadequate identification will be discussed, along with real-world examples. Once data objects have been properly identified, they can be deidentified and, under some circumstances, reidentified. The ability to deidentify data objects confers enormous advantages when issues of confidentiality, privacy, and intellectual property emerge. The ability to reidentify deidentified data objects is required for error detection, error correction, and data validation. [Glossary Deidentification, Re-identification, Privacy versus confidentiality, Intellectual property]

Returning to the title of this section, let us ask ourselves, "What is the difference between an identifier and an identifier system?" To answer, by analogy, it is like the difference between having a $100 dollar bill in your pocket and having a savings account with $100 credited to the account. In the case of the $100 bill, anyone in possession of the bill can use it to purchase items. In the case of the $100 credit, there is a system in place for uniquely assigning the $100 to one individual, until such time as that individual conducts an account transaction that increases or decreases the account value. Likewise, an identifier system creates a permanent environment in which the identifiers are safely stored and used.

Every good information system is, at its heart, an identification system: a way of naming data objects so that they can be retrieved by their name, and a way of distinguishing each object from every other object in the system. If data managers properly identified their data, and did absolutely nothing else, they would be producing a collection of data objects with more informational value than many existing Big Data resources.

The properties of a good identifier system are the following:

– **Completeness**

Every unique object in the big data resource must be assigned an identifier.

– **Uniqueness**

Each identifier is a unique sequence.

– **Exclusivity**

Each identifier is assigned to a unique object, and to no other object.

– **Authenticity**

The objects that receive identification must be verified as the objects that they are intended to be. For example, if a young man walks into a bank and claims to be Richie Rich, then the bank must ensure that he is, in fact, who he says he is.

– **Aggregation**

The Big Data resource must have a mechanism to aggregate all of the data that is properly associated with the identifier (i.e., to bundle all of the data that belongs to the uniquely identified objected). In the case of a bank, this might mean collecting all of the transactions associated with an account holder. In a hospital, this might mean collecting all of the data associated with a patient's identifier: clinic visit reports, medication transactions, surgical procedures, and laboratory results. If the identifier system performs properly, aggregation methods will always collect all of the data associated with an object and will never collect any data that is associated with a different object.

– **Permanence**

The identifiers and the associated data must be permanent. In the case of a hospital system, when the patient returns to the hospital after 30 years of absence, the record system must be able to access his identifier and aggregate his data. When a patient dies, the patient's identifier must not perish.

– **Reconciliation**

There should be a mechanism whereby the data associated with a unique, identified object in one Big Data resource can be merged with the data held in another resource, for the same unique object. This process, which requires comparison, authentication, and merging is known as reconciliation. An example of reconciliation is found in health record portability. When a patient visits a hospital, it may be necessary to transfer her electronic medical record from another hospital. Both hospitals need a way of confirming the identity of the patient and combining the records. [Glossary Electronic medical record]

– **Immutability**

In addition to being permanent (i.e., never destroyed or lost), the identifier must never change (see Chapter 6) [2]. In the event that two Big Data resources are merged, or that legacy data is merged into a Big Data resource, or that individual data objects from two different Big Data resources are merged, a single data object will be assigned two

identifiers; one from each of the merging systems. In this case, the identifiers must be preserved as they are, without modification. The merged data object must be provided with annotative information specifying the origin of each identifier (i.e., clarifying which identifier came from which Big Data resource).

– **Security**

The identifier system is vulnerable to malicious attack. A Big Data resource with an identifier system can be irreversibly corrupted if the identifiers are modified. In the case of human-based identifier systems, stolen identifiers can be used for a variety of malicious activities directed against the individuals whose records are included in the resource.

– **Documentation and Quality Assurance**

A system should be in place to find and correct errors in the identifier system. Protocols must be written for establishing the identifier system, for assigning identifiers, for protecting the system, and for monitoring the system. Every problem and every corrective action taken must be documented and reviewed. Review procedures should determine whether the errors were corrected effectively; and measures should be taken to continually improve the identifier system. All procedures, all actions taken, and all modifications of the system should be thoroughly documented. This is a big job.

– **Centrality**

Whether the information system belongs to a savings bank, an airline, a prison system, or a hospital, identifiers play a central role. You can think of information systems as a scaffold of identifiers to which data is attached. For example, in the case of a hospital information system, the patient identifier is the central key to which every transaction for the patient is attached.

– **Autonomy**

An identifier system has a life of its own, independent of the data contained in the Big Data resource. The identifier system can persist, documenting and organizing existing and future data objects even if all of the data in the Big Data resource were to suddenly vanish (i.e., when all of the data contained in all of the data objects are deleted).

In theory, identifier systems are incredibly easy to implement. Here is exactly how it is done:

1. Generate a unique character sequence, such as UUID, or a long random number. [Glossary UUID, Randomness]
2. Assign the unique character sequence (i.e., identifier) to each new object, at the moment that the object is created. In the case of a hospital a patient chart is created at the moment he or she is registered into the hospital information system. In the case of a bank a customer record is created at the moment that he or she is provided with an

account number. In the case of an object-oriented programming language, such as Ruby, this would be the moment when the "new" method is sent to a class object, instructing the class object to create a class instance. [Glossary Object-oriented programming, Instance]

3. Preserve the identifier number and bind it to the object. In practical terms, this means that whenever the data object accrues new data, the new data is assigned to the identifier number. In the case of a hospital system, this would mean that all of the lab tests, billable clinical transactions, pharmacy orders, and so on, are linked to the patient's unique identifier number, as a service provided by the hospital information system. In the case of a banking system, this would mean that all of the customer's deposits and withdrawals and balances are attached to the customer's unique account number.

Section 3.3. Generating Unique Identifiers

A UUID is 128 bits long, and can guarantee uniqueness across space and time.
P. Leach, M. Mealling and R. Salz [3]

Uniqueness is one of those concepts that everyone intuitively understands; explanations would seem unnecessary. Actually, uniqueness in the computational sciences is a somewhat different concept than uniqueness in the natural world. In computational sciences, uniqueness is achieved when a data object is associated with an unique identifier (i.e., a character string that has not been assigned to any other data object). Most of us, when we think of a data object, are probably thinking of a data record, which may consist of the name of a person followed by a list of feature values (height, weight, and age), or a sample of blood followed by laboratory values (e.g., white blood cell count, red cell count, and hematocrit). For computer scientists a data object is a holder for data values (the so-called encapsulated data), descriptors of the data, and properties of the holder (i.e., the class of objects to which the instance belongs). Uniqueness is achieved when the data object is permanently bound to its own identifier sequence. [Glossary Encapsulation]

Unique objects have three properties:

- A unique object can be distinguished from all other unique objects.
- A unique object cannot be distinguished from itself.
- Uniqueness may apply to collections of objects (i.e., a class of instances can be unique).

UUID (Universally Unique IDentifier) is an example of one type of algorithm that creates unique identifiers, on command, at the moment when new objects are created (i.e., during the run-time of a software application). A UUID is 128 bits long and reserves 60 bits for a string computed directly from a computer time stamp, and is usually represented by a sequence of alphanumeric ASCII characters [3]. UUIDs were originally used in the Apollo

Network Computing System and were later adopted in the Open Software Foundation's Distributed Computing Environment [4]. [Glossary Time stamp, ASCII]

Linux systems have a built-in UUID utility, "uuidgen.exe," that can be called from the system prompt.

Here are a few examples of output values generated by the "uuidgen.exe" utility: [Glossary Command line utility, Utility]

```
$ uuidgen.exe
312e60c9-3d00-4e3f-a013-0d6cb1c9a9fe
$ uuidgen.exe
822df73c-8e54-45b5-9632-e2676d178664
$ uuidgen.exe
8f8633e1-8161-4364-9e98-fdf37205df2f
$ uuidgen.exe
83951b71-1e5e-4c56-bd28-c0c45f52cb8a
$ uuidgen -t
e6325fb6-5c65-11e5-b0e1-0ceee6e0b993
$ uuidgen -r
5d74e36a-4ccb-42f7-9223-84eed03291f9
```

Notice that each of the final two examples has a parameter added to the "uuidgen" command (i.e., "-t" and "-r"). There are several versions of the UUID algorithm that are available. The "-t" parameter instructs the utility to produce a UUID based on the time (measured in seconds elapsed since the first second of October 15, 1582, the start of the Gregorian calendar). The "-r" parameter instructs the utility to produce a UUID based on the generation of a pseudorandom number. In any circumstance, the UUID utility instantly produces a fixed length character string suitable as an object identifier. The UUID utility is trusted and widely used by computer scientists. Independent-minded readers can easily design their own unique object identifiers, using pseudorandom number generators, or with one-way hash generators. [Glossary One-way hash, Pseudorandom number generator]

Python has its own UUID generator. The uuid module is included in the standard python distribution and can be called directly from the script.

```
import uuid
print(uuid.uuid4())
```

When discussing UUIDs the question of duplicates (so-called collisions, in the computer science literature) always arises. How can we be certain that a UUID is unique? Isn't it possible that the algorithm that we use to create a UUID may, at some point, produce the same sequence on more than one occasion? Yes, but the odds are small. It has been estimated that duplicate UUIDs are produced, on average, once every 2.71 quintillion (i.e., 2.71 * 10∧18) executions [5]. It seems that reports of UUID collisions, when investigated, have been attributed to defects in the implementation of the UUID algorithms. The general consensus seems to be that UUID collisions are not worth worrying about, even in the realm of Big Data.

Section 3.4. Really Bad Identifier Methods

I always wanted to be somebody, but now I realize I should have been more specific.
Lily Tomlin

Names are poor identifiers. First off, we can never assume that any name is unique. Surnames such as Smith, Zhang, Garcia, Lo, and given names such as John and Susan are very common. In Korea, five last names account for nearly 50% of the population [6]. Moreover, if we happened to find an individual with a truly unique name (e.g., Mr. Mxyzptlk), there would be no guarantee that some other unique individual might one day have the same name. Compounding the non-uniqueness of names, there is the problem of the many variant forms of a single name. The sources for these variations are many. Here is a partial listing:

1. Modifiers to the surname (du Bois, DuBois, Du Bois, Dubois, Laplace, La Place, van de Wilde, Van DeWilde, etc.).
2. Accents that may or may not be transcribed onto records (e.g., acute accent, cedilla, diacritical comma, palatalized mark, hyphen, diphthong, umlaut, circumflex, and a host of obscure markings).
3. Special typographic characters (the combined "ae").
4. Multiple "middle names" for an individual, that may not be transcribed onto records. Individuals who replace their first name with their middle name for common usage, while retaining the first name for legal documents.
5. Latinized and other versions of a single name (Carl Linnaeus, Carl von Linne, Carolus Linnaeus, Carolus a Linne).
6. Hyphenated names that are confused with first and middle names (e.g., Jean-Jacques Rousseau, or Jean Jacques Rousseau; Louis-Victor-Pierre-Raymond, 7th duc de Broglie, or Louis Victor Pierre Raymond Seventh duc deBroglie).
7. Cultural variations in name order that are mistakenly rearranged when transcribed onto records. Many cultures do not adhere to the Western European name order (e.g., given name, middle name, surname).
8. Name changes; through marriage or other legal actions, aliasing, pseudonymous posing, or insouciant whim.

Aside from the obvious consequences of using names as record identifiers (e.g., corrupt database records, forced merges between incompatible data resources, impossibility of reconciling legacy record), there are non-obvious consequences that are worth considering. Take, for example, accented characters in names. These word decorations wreak havoc on orthography and on alphabetization. Where do you put a name that contains an umlauted character? Do you pretend the umlaut is not there, and alphabetize it according to its plain characters? Do you order based on the ASCII-numeric assignment for the character, in which the umlauted letter may appear nowhere near the plain-lettered words in an alphabetized list. The same problem applies to every special character. [Glossary American Standard Code for Information Interchange, ASCII]

A similar problem exists for surnames with modifiers. Do you alphabetize de Broglie under "D" or under "d" or under "B"? If you choose B, then what do you do with the concatenated form of the name, "deBroglie"? When it comes down to it, it is impossible to satisfactorily alphabetize a list of names. This means that searches based on proximity in the alphabet will always be prone to errors.

I have had numerous conversations with intelligent professionals who are tasked with the responsibility of assigning identifiers to individuals. At some point in every conversation, they will find it necessary to explain that although an individual's name cannot serve as an identifier, the combination of name plus date of birth provides accurate identification in almost every instance. They sometimes get carried away, insisting that the combination of name plus date of birth plus social security number provides perfect identification, as no two people will share all three identifiers: same name, same date of birth, same social security number. This argument rises to the height of folly and completely misses the point of identification. As we will see, it is relatively easy to assign unique identifiers to individuals and to any data object, for that matter. For managers of Big Data resources, the larger problem is ensuring that each unique individual has only one identifier (i.e., denying one object multiple identifiers). [Glossary Social Security Number]

Let us see what happens when we create identifiers from the name plus the birthdate. We will examine name + birthdate + social security number later in this section.

Consider this example. Mary Jessica Meagher, born June 7, 1912 decided to open a separate bank account in each of 10 different banks. Some of the banks had application forms, which she filled out accurately. Other banks registered her account through a teller, who asked her a series of questions and immediately transcribed her answers directly into a computer terminal. Ms. Meagher could not see the computer screen and could not review the entries for accuracy.

Here are the entries for her name plus date of birth:

1. Marie Jessica Meagher, June 7, 1912 (the teller mistook Marie for Mary).
2. Mary J. Meagher, June 7, 1912 (the form requested a middle initial, not name).
3. Mary Jessica Magher, June 7, 1912 (the teller misspelled the surname).
4. Mary Jessica Meagher, Jan 7, 1912 (the birth month was constrained, on the form, to three letters; Jun, entered on the form, was transcribed as Jan).
5. Mary Jessica Meagher, 6/7/12 (the form provided spaces for the final two digits of the birth year. Through a miracle of modern banking, Mary, born in 1912, was re-born a century later).
6. Mary Jessica Meagher, 7/6/2012 (the form asked for day, month, year, in that order, as is common in Europe).
7. Mary Jessica Meagher, June 1, 1912 (on the form, a 7 was mistaken for a 1).
8. Mary Jessie Meagher, June 7, 1912 (Marie, as a child, was called by the informal form of her middle name, which she provided to the teller).
9. Mary Jesse Meagher, June 7, 1912 (Marie, as a child, was called by the informal form of her middle name, which she provided to the teller, and which the teller entered as the male variant of the name).

10. Marie Jesse Mahrer, 1/1/12 (an underzealous clerk combined all of the mistakes on the form and the computer transcript, and added a new orthographic variant of the surname).

For each of these ten examples, a unique individual (Mary Jessica Meagher) would be assigned a different identifier at each of 10 banks. Had Mary re-registered at one bank, ten times, the outcome may have been the same.

If you toss the social security number into the mix (name + birth date + social security number) the problem is compounded. The social security number for an individual is anything but unique. Few of us carry our original social security cards. Our number changes due to false memory ("You mean I've been wrong all these years?"), data entry errors ("Character transpositoins, I mean transpositions, are very common"), intention to deceive ("I don't want to give those people my real number"), or desperation ("I don't have a number, so I'll invent one"), or impersonation ("I don't have health insurance, so I'll use my friend's social security number"). Efforts to reduce errors by requiring patients to produce their social security cards have not been entirely beneficial.

Beginning in the late 1930s, the E. H. Ferree Company, a manufacturer of wallets, promoted their product's card pocket by including a sample social security card with each wallet sold. The display card had the social security number of one of their employees. Many people found it convenient to use the card as their own social security number. Over time, the wallet display number was claimed by over 40,000 people. Today, few institutions require individuals to prove their identity by showing their original social security card. Doing so puts an unreasonable burden on the honest patient (who does not happen to carry his/her card) and provides an advantage to criminals (who can easily forge a card).

Entities that compel individuals to provide a social security number have dubious legal standing. The social security number was originally intended as a device for validating a person's standing in the social security system. More recently, the purpose of the social security number has been expanded to track taxable transactions (i.e., bank accounts, salaries). Other uses of the social security number are not protected by law. The Social Security Act (Section 208 of Title 42 U.S. Code 408) prohibits most entities from compelling anyone to divulge his/her social security number.

Considering the unreliability of social security numbers in most transactional settings, and considering the tenuous legitimacy of requiring individuals to divulge their social security numbers, a prudently designed medical identifier system will limit its reliance on these numbers. The thought of combining the social security number with name and date of birth will virtually guarantee that the identifier system will violate the strict one-to-a-customer rule.

Most identifiers are not purely random numbers; they usually contain some embedded information that can be interpreted by anyone familiar with the identification system. For example, they may embed the first three letters of the individual's family name in the identifier. Likewise, the last two digits of the birth year are commonly embedded in many types of identifiers. Such information is usually included as a crude "honesty" check by people "in the know." For instance, the nine digits of a social security number are divided into an

area code (first three digits), a group number (the next two digits), followed by a serial number (last four digits). People with expertise in the social security numbering system can pry considerable information from a social security number, and can determine whether certain numbers are bogus, based on the presence of excluded sub-sequences.

Seemingly inconsequential information included in an identifier can sometimes be used to discover confidential information about individuals. Here is an example. Suppose every client transaction in a retail store is accessioned under a unique number, consisting of the year of the accession, followed by the consecutive count of accessions, beginning with the first accession of the new year. For example, accession 2010-3518582 might represent the 3,518,582nd purchase transaction in the year 2010. Because each number is unique, and because the number itself says nothing about the purchase, it may be assumed that inspection of the accession number would reveal nothing about the transaction.

Actually, the accession number tells you quite a lot. The prefix (2010) tells you the year of the purchase. If the accession number had been 2010-0000001, then you could safely say that accession represented the first item sold on the first day of business in the year 2010. For any subsequent accession number in 2010, simply divide the suffix number (in this case 3,518,582) by the last accession number of the year, and multiply by 365 (the number of days in a non-leap year), and you have the approximate day of the year that the transaction occurred. This day can easily be converted to a calendar date.

Unimpressed? Consider this scenario. You know that a prominent member of the President's staff had visited a Washington, D.C. Hospital on February 15, 2005, for the purpose of having a liver biopsy. You would like to know the results of that biopsy. You go to a Web site that lists the deidentified pathology records for the hospital, for the years 2000–2010. Though no personal identifiers are included in these public records, the individual records are sorted by accession numbers. Using the aforementioned strategy, you collect all of the surgical biopsies performed on or about February 15, 2010. Of these biopsies, only three are liver biopsies. Of these three biopsies, only one was performed on a person whose gender and age matched the President's staff member. The report provides the diagnosis. You managed to discover some very private information without access to any personal identifiers.

The alphanumeric character string composing the identifier should not expose the patient's identity. For example, a character string consisting of a concatenation of the patient's name, birth date, and social security number might serve to uniquely identify an individual, but it could also be used to steal an individual's identity. The safest identifiers are random character strings containing no information whatsoever.

Section 3.5. Registering Unique Object Identifiers

It isn't that they can't see the solution. It's that they can't see the problem.

G. K. Chesterton

Registries are trusted services that provide unique identifiers to objects. The idea is that everyone using the object will use the identifier provided by the central registry. Unique object registries serve a very important purpose, particularly when the object identifiers

are persistent. It makes sense to have a central authority for Web addresses, library acquisitions, and journal abstracts. Such registries include:

- DOI, Digital object identifier
- PMID, PubMed identification number
- LSID (Life Science Identifier)
- HL7 OID (Health Level 7 Object Identifier)
- DICOM (Digital Imaging and Communications in Medicine) identifiers
- ISSN (International Standard Serial Numbers)
- Social Security Numbers (for United States population)
- NPI, National Provider Identifier, for physicians
- Clinical Trials Protocol Registration System
- Office of Human Research Protections FederalWide Assurance number
- Data Universal Numbering System (DUNS) number
- International Geo Sample Number
- DNS, Domain Name Service
- URL, Unique Resource Locator [Glossary URL]
- URN, Unique Resource Name [Glossary URN]

In some cases the registry does not provide the full identifier for data objects. The registry may provide a general identifier sequence that will apply to every data object in the resource. Individual objects within the resource are provided with a non-unique registry number. A unique suffix sequence is appended locally (i.e., not by a central registrar). Life Science Identifiers (LSIDs) serve as a typical example of a registered identifier. Every LSIDs is composed of the following 5 parts: Network Identifier, root DNS name of the issuing authority, name chosen by the issuing authority, a unique object identifier assigned locally, and an optional revision identifier for versioning information.

In the issued LSID identifier, the parts are separated by a colon, as shown:

urn:lsid:pdb.org:1AFT:1

This identifies the first version of the 1AFT protein in the Protein Data Bank. Here are a few LSIDs:

urn:lsid:ncbi.nlm.nih.gov:pubmed:12571434

This identifies a PubMed citation

urn:lsid:ncbi.nlm.nig.gov:GenBank:T48601:2

This refers to the second version of an entry in GenBank

An OID, short for Object Identifier, is a hierarchy of identifier prefixes. Successive numbers in the prefix identify the descending order of the hierarchy. Here is an example of an OID from HL7, an organization that deals with health data interchanges:

1.3.6.1.4.1.250

Each node is separated from the successor by a dot, Successively finer registration detail leads to the institutional code (the final node). In this case the institution identified by the HL7 OID happens to be the University of Michigan.

The final step in creating an OID for a data object involves placing a unique identifier number at the end of the registered prefix. OID organizations leave the final step to the institutional data managers.

The problem with this approach is that the final within-institution data object identifier is sometimes prepared thoughtlessly, corrupting the OID system [7]. Here is an example. Hospitals use an OID system for identifying images, part of the DICOM (Digital Imaging and Communications in Medicine) image standard. There is a prefix consisting of a permanent, registered code for the institution and the department, and a suffix consisting of a number generated for an image as it is created.

A hospital may assign consecutive numbers to its images, appending these numbers to an OID that is unique for the institution and the department within the institution. For example, the first image created with a CT-scanner might be assigned an identifier consisting of the OID (the assigned code for institution and department) followed by a separator such as a hyphen, followed by "1."

In a worst-case scenario, different instruments may assign consecutive numbers to images, independently of one another. This means that the CT-scanner in room A may be creating the same identifier (OID + image number) as the CT-scanner in Room B; for images on different patients. This problem could be remedied by constraining each CT-scanner to avoid using numbers assigned by any other CT-scanner. This remedy can be defeated if there is a glitch anywhere in the system that accounts for image assignments (e.g., if the counters are re-set, broken, replaced or simply ignored).

When image counting is done properly, and the scanners are constrained to assign unique numbers (not previously assigned by other scanners in the same institution), each image may indeed have a unique identifier (OID prefix + image number suffix). Nonetheless, the use of consecutive numbers for images will create havoc over time. Problems arise when the image service is assigned to another department in the institution, or when departments or institutions merge. Each of these shifts produces a change in the OID (the institutional and departmental prefix) assigned to the identifier. If a consecutive numbering system is used, then you can expect to create duplicate identifiers if institutional prefixes are replaced after the merge. The old records in both of the merging institutions will be assigned the same prefix and will contain replicate (consecutively numbered) suffixes (e.g., image 1, image 2, etc.).

Yet another problem may occur if one unique object is provided with multiple different unique identifiers. A software application may be designed to ignore any previously assigned unique identifier and to generate its own identifier, using its own assignment method. Doing so provides software vendors with a strategy that insulates the vendors from bad identifiers created by their competitor's software, and locks the customer to a vendor's software, and identifiers, forever.

In the end the OID systems provide a good set of identifiers for the institution, but the data objects created within the institution need to have their own identifier systems. Here is the HL7 statement on replicate OIDs:

> *Though HL7 shall exercise diligence before assigning an OID in the HL7 branch to third parties, given the lack of a global OID registry mechanism, one cannot make absolutely certain that there is no preexisting OID assignment for such third-party entity [8].*

It remains to be seen whether any of the registration identifier systems will be used and supported with any serious level of permanence (e.g., over decades and centuries).

Section 3.6. Deidentification and Reidentification

Never answer an anonymous letter.

Yogi Berra

For scientists, deidentification serves two purposes:

- To protect the confidentiality and the privacy of the individual (when the data concerns a particular human subject), and
- To remove information that might bias the experiment (e.g., to blind the experimentalist to patient identities).

Deidentification involves stripping information from a data record that might link the record to the public name of the record's subject. In the case of a patient record, this would involve stripping any information from the record that would enable someone to connect the record to the name of the patient. The most obvious item to be removed in the deidentification process is the patient's name. Other information that should be removed would be the patient's address (which could be linked to the name), the patient's date of birth (which narrows down the set of individuals to whom the data record might pertain), and the patient's social security number. In the United States, patient privacy regulations include a detailed discussion of record deidentification and this discussion recommends 18 patient record items for exclusion from deidentified records [9].

Before going any further, it is important to clarify that deidentification is not achieved by removing an identifier from a data object. In point of fact, nothing good is ever achieved by simply removing an identifier from a data object; doing so simply invalidates the data object (i.e., every data object, identified or deidentified, must have an identifier). Deidentification involves removing information contained in the data object that reveals something about the publicly known name of the data object. This kind of information is often referred to as identifying information, but it would be much less confusing if we used another term for such data, such as "name-linking information." The point here is that we do not want to confuse the identifier of a data object with information contained in a data object that can link the object to its public name.

It may seem counterintuitive, but there is very little difference between an identifier and a deidentifier; under certain conditions the two concepts are equivalent. Here is how a dual identification/deidentification system might work:

1. Collect data on unique object. "Joe Ferguson's bank account contains $100."
2. Assign a unique identifier. "Joe Ferguson's bank account is 7540038947134."
3. Substitute name of object with its assigned unique identifier: "754003894713 contains $100.".

4. Consistently use the identifier with data.
5. Do not let anyone know that Joe Ferguson owns account "754003894713."

The dual use of an identifier/deidentifier is a tried and true technique. Swiss bank accounts are essentially unique numbers (identifiers) assigned to a person. You access the bank account by producing the identifier number. The identifier number does not provide information about the identity of the bank account holder (i.e., it is a deidentifier and an identifier).

The purpose of an identifier is to tell you that whenever the identifier is encountered, it refers to the same unique object, and whenever two different identifiers are encountered, they refer to different objects. The identifier, by itself, should contain no information that links the data object to its public name.

It is important to understand that the process of deidentification can succeed only when each record is properly identified (i.e., there can be no deidentification without identification). Attempts to deidentify a poorly identified data set of clinical information will result in replicative records (multiple records for one patient), mixed-in records (single records composed of information on multiple patients), and missing records (unidentified records lost in the deidentification process).

The process of deidentification is best understood as an algorithm performed on-the-fly, in response to a query from a data analyst. Here is how such an algorithm might proceed.

1. The data analyst submits a query requesting a record from a Big Data resource. The resource contains confidential records that must not be shared, unless the records are deidentified.
2. The Big Data resource receives the query and retrieves the record.
3. A copy of the record is parsed and any of the information within the data record that might link the record to the public name of the subject of the record (usually the name of an individual) is deleted from the copy. This might include the aforementioned name, address, date of birth, and social security number.
4. A pseudo-identifier sequence is prepared for the deidentified record. The pseudo-identifier sequence might be generated by a random number generator, by encrypting the original identifier, through a one-way hash algorithm, or by other methods chosen by the Big Data manager. [Glossary Encryption]
5. A transaction record is attached to the original record that includes the pseudo-identifier, the deidentified record, the time of the transaction, and any information pertaining to the requesting entity (e.g., the data analyst who sent the query) that is deemed fit and necessary by the Big Data resource data manager.
6. A record is sent to the data analyst that consists of the deidentified record (i.e., the record stripped of its true identifier and containing no data that links the record to a named person) and the unique pseudo-identifier created for the record.

Because the deidentified record, and its unique pseudo-identifier are stored with the original record, subsequent requests for the pseudo-identified record can be retrieved and

provided, at the discretion of the Big Data manager. This general approach to data deidentification will apply to requests for a single record or to millions of records.

At this point, you might be asking yourself the following question, "What gives the data manager the right to distribute parts of a confidential record, even if it happens to be deidentified?" You might think that if you tell someone a secret, under the strictest confidence, then you would not want any part of that secret to be shared with anyone else. The whole notion of sharing confidential information that has been deidentified may seem outrageous and unacceptable.

We will discuss the legal and ethical issues of Big Data in Chapters 18 and 19. For now, readers should know that there are several simple and elegant principles that justify sharing deidentified data.

Consider the statement "Jules Berman has a blood glucose level of 85." This would be considered a confidential statement because it tells people something about my medical condition.

Consider the phrase, "Blood glucose 85."

When the name "Jules Berman" is removed, we are left with a disembodied piece of data. "Blood glucose 85" is no different from "Temperature 98.6" or "Apples 2" or "Terminator 3." They are simply raw data belonging to nobody in particular. The act of removing information linking data to a person renders the data harmless. Because the use of properly deidentified data poses no harm to human subjects, United States Regulations allow the unrestricted use of such data for research purposes [9,10]. Other countries have similar provisions.

– **Reidentification**

Because confidentiality and privacy concerns always apply to human subject data, it would seem imperative that deidentification should be an irreversible process (i.e., the names of the subjects and samples should be held a secret, forever).

Scientific integrity does not always accommodate irreversible deidentification. On occasion, experimental samples are mixed-up; samples thought to come from a certain individual, tissue, record, or account, may in fact come from another source. Sometimes major findings in science need to be retracted when a sample mix-up has been shown to occur [11,12,13,14,15]. When samples are submitted, without mix-up, the data is sometimes collected improperly. For example, reversing electrodes on an electrocardiogram may yield spurious and misleading results. Sometimes data is purposefully fabricated and otherwise corrupted, to suit the personal agendas of dishonest scientists. When data errors occur, regardless of reason, it is important to retract the publications [16,17]. To preserve scientific integrity, it is sometimes necessary to discover the identity of deidentified records.

In some cases, deidentification stops the data analyst from helping individuals whose confidentiality is being protected. Imagine you are conducting an analysis on a collection of deidentified data, and you find patients with a genetic marker for a disease that is curable, if treated at an early stage; or you find a new biomarker that determines which

patients would benefit from surgery and which patients would not. You would be compelled to contact the subjects in the database to give them information that could potentially save their lives. Having an irreversibly deidentified data sets precludes any intervention with subjects; nobody knows their identities.

Deidentified records can, under strictly controlled circumstances, be reidentified. Reidentification is typically achieved by entrusting a third party with a confidential list that maps individuals to their deidentified records. Obviously, reidentification can only occur if the Big Data resource keeps a link connecting the identifiers of their data records to the identifiers of the corresponding deidentified record (what we've been calling pseudo-identifiers). The act of assigning a public name to the deidentified record must always involve strict oversight. The data manager must have in place a protocol that describes the process whereby approval for reidentification is obtained. Reidentification provides an opportunity whereby confidentiality can be breached and human subjects can be harmed. Consequently, stewarding the reidentification process is one of the most serious responsibilities of Big Data managers [18].

Section 3.7. Case Study: Data Scrubbing

It is a sin to believe evil of others but it is seldom a mistake.

Garrison Keillor

The term "data scrubbing" is sometimes used, mistakenly, as a synonym for deidentification. It is best to think of data scrubbing as a process that begins where deidentification ends. A data scrubber will remove unwanted information from a data record, including information of a personal nature and any information that is not directly related to the purpose of the data record. For example, in the case of a hospital record a data scrubber might remove the names of physicians who treated the patient; the names of hospitals or medical insurance agencies; addresses; dates; and any textual comments that are inappropriate, incriminating, irrelevant, or potentially damaging. [Glossary Data munging, Data scraping, Data wrangling]

In medical data records, there is a concept known as "minimal necessary" that applies to shared confidential data [9]. It holds that when records are shared, only the minimum necessary information should be released. Any information not directly relevant to the intended purposes of the data analyst should be withheld. The process of data scrubbing gives data managers the opportunity to render a data record that is free of information that would link the record to its subject and free of extraneous information that the data analyst does not actually require. [Glossary Minimal necessary]

There are many methods for data scrubbing. Most of these methods require that data managers develop an exception list of items that should not be included in shared records (e.g., cities, states, zip codes, and names of people). The scrubbing application moves through the records, extracting unnecessary information along the way. The end product is cleaned, but not sterilized. Though many undesired items can be successfully removed,

this approach never produces a perfectly scrubbed set of data. In a Big Data resource, it is simply impossible for the data manager to anticipate every objectionable item and to include it in an exception list. Nobody is that smart.

There is, however, a method whereby data records can be cleaned, without error. This method involves creating a list of data (often in the form of words and phrases) that is acceptable for inclusion in a scrubbed and deidentified data set. Any data that is not in the list of acceptable information is automatically deleted. Whatever is left is the scrubbed data. This method can be described as a reverse scrubbing method. Everything is in the data set is automatically deleted, unless it is an approved "exception."

This method of scrubbing is very fast and can produce an error-free deidentified and scrubbed output [4,19,20]. An example of the kind of output produced by such a scrubber is shown:

*Since the time when * * * * * * * * his own * and the * * * *, the anomalous * * have been * and persistent * * *; and especially * true of the construction and functions of the human *, indeed, it was the anomalous that was * * * in the * the attention, * * that were * to develop into the body * * which we now * *. As by the aid * * * * * * * * * our vision into the * * * has emerged *, we find * * and even evidence of *. To the highest type of * * it is the * the ordinary * * * * *. * to such, no less than to the most *, * * * is of absorbing interest, and it is often * * that the * * the most * into the heart of the mystery of the ordinary. * * been said, * * * * *. * * dermoid cysts, for example, we seem to * * * the secret * of Nature, and * out into the * * of her clumsiness, and * of her * * * *, *, * tell us much of * * * used by the vital * * * * even the silent * * * upon the * * *.*

The reverse-scrubber requires the preexistence of a set of approved terms. One of the simplest methods for generating acceptable terms involves extracting them from a nomenclature that comprehensively covers the terms used in a knowledge domain. For example, a comprehensive listing of living species will not contain dates or zip codes or any of the objectionable language or data that should be excluded from a scrubbed data set. In a method that I have published a list of approved doublets (approximately 200,000 two-word phrases collected from standard nomenclatures) are automatically collected for the scrubbing application [4]. The script is fast, and its speed is not significantly reduced by the size of the list of approved terms.

Here is a short python script. scrub.py, that will take any line of text and produce a scrubbed output. It requires an external file, doublets.txt, containing an approved list of doublet terms.

```
import sys, re, string
doub_file = open("doublets.txt", "r")
doub_hash = {}
for line in doub_file:
  line = line.rstrip()
  doub_hash[line] = " "
```

```
doub_file.close()
print("What would you like to scrub?")
line = sys.stdin.readline()
line = line.lower()
line = line.rstrip()
linearray = re.split(r' +', line)
lastword = "*"
for i in range(0, len(linearray)):
  doublet = " ".join(linearray[i:i+2])
  if doublet in doub_hash:
    print(" " + linearray[i], end="")
    lastword = " " + linearray[i+1]
  else:
    print(lastword, end="")
    lastword = " *"
  if (i == len(linearray) + 1):
    print(lastword, end="")
```

Section 3.8. Case Study (Advanced): Identifiers in Image Headers

Plus ca change, plus c'est la meme chose.

Old French saying ("The more things change, the more things stay the same.")

As it happens, nothing is ever as simple as it ought to be. In the case of an implementation of systems that employ long sequence generators to produce unique identifiers, the most common problem involves indiscriminate reassignment of additional unique identifiers to the same data object, thus nullifying the potential benefits of the unique identifier systems.

Let us look at an example wherein multiple identifiers are redundantly assigned to the same image, corrupting the identifier system. In Section 4.3, we discuss image headers, and we provide examples wherein the ImageMagick "identify" utility could extract the textual information included in the image header. One of the header properties created, inserted, and extracted by ImageMagick's "identify" is an image-specific unique string. [Glossary ImageMagick]

When ImageMagick is installed in our computer, we can extract any image's unique string, using the "identify" utility and the "-format" attribute, on the following system command line: [Glossary Command line]

```
c:\>identify -verbose -format "%#" eqn.jpg
```

Here, the image file we are examining is "eqn.jpg". The "%#" character string is ImageMagick's special syntax indicating that we would like to extract the image identifier from the image header. The output is shown.

```
219e41b4c761e4bb04fbd67f71cc84cd6ae53a26639d4bf33155a5f62ee36e33
```

We can repeat the command line whenever we like, for this image; and the same image-specific unique sequence of characters will be produced.

Using ImageMagick, we can insert text into the "comment" section of the header, using the "-set" attribute. Let us add the text, "I'm modifying myself":

```
c:\ftp>convert eqn.jpg -set comment "I'm modifying myself" eqn.jpg
```

Now, let us extract the comment that we just added, to satisfy ourselves that the "-set" attribute operated as we had hoped. We do this using the "-format" attribute and the "%c" character string, which is ImageMagick's syntax for extracting the comment section of the header.

```
c:\ftp>identify -verbose -format "%c" eqn.jpg
```

The output of the command line is:

```
I'm modifying myself
```

Now, let us run, one more time, the command line that produces the unique character string that is unique for the eqn.jpg image file

```
c:\ftp>identify -verbose -format "%#" eqn.jpg
```

The output is:

```
cb448260d6eeeb2e9f2dcb929fa421b474021584e266d486a6190067a278639f
```

What just happened? Why has the unique character string specific for the eqn.jpg image changed? Has our small modification of the file, which consisted of adding a text comment to the image header, resulted in the production of a new image object, worthy of a new unique identifier?

Before answering these very important questions, let us pose the following gedanken question. Imagine you have a tree. This tree, like every living organism, is unique. It has a unique history, a unique location, and a unique genome (i.e., a unique sequence of nucleotides composing its genetic material). In ten years, its leaves drop off and are replaced ten times. Its trunk expands in size and its height increases. In the ten years of its existence, has the identify of the tree changed? [Glossary Gedanken]

You would probably agree that the tree has changed, but that it has maintained its identity (i.e., it is still the same tree, containing the descendants of the same cells that grew within the younger version of itself).

In informatics, a newly created object is given an identifier, and this identifier is immutable (i.e., cannot be changed), regardless of how the object is modified. In the case of the unique string assigned to an image by ImageMagick, the string serves as an authenticator, not as an identifier. When the image is modified a new unique string is created. By comparing the so-called identifier string in copies of the image file, we can determine whether any modifications have been made. That is to say, we can authenticate the file.

Getting back to the image file in our example, when we modified the image by inserting a text comment, ImageMagick produced a new unique string for the image. The identity of the image had not changed, but the image was different from the original image (i.e., no longer authentic). It seems that the string that we thought to be an identifier string was actually an authenticator string. [Glossary Authentication]

If we want an image to have a unique identifier that does not change when the image is modified, we must create our own identifier that persists when the image is modified.

Here is a short Python script, image_id.py, that uses Python's standard UUID method to create an identifier, which is inserted into the comment section of the image's header, and flanking the identifier with XML tags. [Glossary XML, HTML]

```
import sys, os, uuid
my_id = "<image_id>" + str(uuid.uuid4()) + "</image_id>"
in_command = "convert leaf.jpg -set comment \"" + my_id + "\" leaf.jpg"
os.system(in_command)
out_command = "identify -verbose -format \"%c\" leaf.jpg"
print ("\nHere's the unique identifier:")
os.system(out_command)
print ("\nHere's the unique authenticator:")
os.system("identify -verbose -format \"%#\" leaf.jpg")
os.system("convert leaf.jpg -resize 325x500! leaf.jpg")
print ("\nHere's the new authenticator:")
os.system("identify -verbose -format \"%#\" leaf.jpg")
print ("\nHere's the unique identifier:")
os.system(out_command)
```

Here is the output of the image_id.py script:

```
Here's the unique identifier:
<image_id>b0836a26-8f0e-4a6b-842d-9b0dde2b3f59</image_id>

Here's the unique authenticator:
98c9fe07e90ce43f49961ab6226cd1ccffee648edd1a456a9d06a53ad6d3215a

Here's the new authenticator:
017e401d80a41aafa289ae9c2a1adb7c00477f7a943143141912189499d69ad2

Here's the unique identifier:
<image_id>b0836a26-8f0e-4a6b-842d-9b0dde2b3f59</image_id>
```

What did the script do and what does it teach us? It employed the UUID utility to create a unique and permanent identifier for the image (leaf.jpg, in this case), and inserted the unique identifier into the image header. This identifier, "b0836a26-8f0e-4a6b-842d-9b0dde2b3f59," did not change when the image was subsequently modified. A new authenticator string was automatically inserted into the image header, by ImageMagick, when the image was modified. Hence, we achieved what we needed to achieve: a unique

identifier that never changes, and a unique authenticator that changes when the image is modified in any way.

If you have followed the logic of this section, then you are prepared for the following question posed as an exercise for Zen Buddhists. Imagine you have a hammer. Over the years, you have replaced its head, twice, and its handle, thrice. In this case, with nothing remaining of the original hammer, has it maintained its identity (i.e., is it still the same hammer?). The informatician would answer "Yes," the hammer has maintained its unique identity, but it is no longer authentic (i.e., it is what it must always be, though it has become something different).

Section 3.9. Case Study: One-Way Hashes

I live on a one-way street that's also a dead end. I'm not sure how I got there.
Steven Wright

A one-way hash is an algorithm that transforms a string into another string is such a way that the original string cannot be calculated by operations on the hash value (hence the term "one-way" hash). Popular one-way hash algorithms are MD5 and Standard Hash Algorithm (SHA). A one-way hash value can be calculated for any character string, including a person's name, or a document, or even another one-way hash. For a given input string, the resultant one-way hash will always be the same.

Here are a few examples of one-way hash outputs performed on a sequential list of input strings, followed by their one-way hash (md5 algorithm) output.

```
Jules Berman => Ri0oaVTIAilwnS8+nvKhfA
"Whatever" => n2YtKKG6E4MyEZvUKyGWrw
Whatever => OkXaDVQFYjwkQ+MOC8dpOQ
jules berman => SlnuYpmyn8VXLsxBWwO57Q
Jules J. Berman => i74wZ/CsIbxt3goH2aCS+A
Jules J Berman => yZQfJmAf4dIYO6Bd0qGZ7g
Jules Berman => Ri0oaVTIAilwnS8+nvKhfA
```

The one-way hash values are a seemingly random sequence of ASCII characters (the characters available on a standard keyboard). Notice that a small variation among input strings (e.g., exchanging an uppercase for a lowercase character, adding a period or quotation mark) produces a completely different one-way hash output. The first and the last entry (Jules Berman) yield the same one-way hash output (Ri0oaVTIAilwnS8+nvKhfA) because the two input strings are identical. A given string will always yield the same hash value, so long as the hashing algorithm is not altered. Each one-way hash has the same length (22 characters for this particular md5 algorithm) regardless of the length of the input term. A one-way hash output of the same length (22 characters) could have been produced for a string or file or document of any length. Once produced, there is no feasible mathematical algorithm that can reconstruct the input string from its one-way hash output. In our example, there is no way of examining the string "Ri0oaVTIAilwnS8+nvKhfA" and computing the name Jules Berman.

We see that the key functional difference between a one-way hash and a UUID sequence is that the one-way hash algorithm, performed on a unique string, will always yield the same random-appearing alphanumeric sequence. A UUID algorithm has no input string; it simply produces unique alphanumeric output, and never (almost never) produces the same alphanumeric output twice.

One-way hashes values can serve as ersatz ide ntifiers, permitting Big Data resources to accrue data, over time, to a specific record, even when the record is deidentified (e.g., even when its UUID identifier has been stripped from the record). Here is how it works [18]:

1. A data record is chosen, before it is deidentified, and a one-way hash is performed on its unique identifier string.
2. The record is deidentified by removing the original unique identifier. The output of the one-way hash (from step 1) is substituted for the original unique identifier.
3. The record is deidentified because nobody can reconstruct the original identifier from the one-way hash that has replaced it.
4. The same process is done for every record in the database.
5. All of the data records that were associated with the original identifier will now have the same one-way hash identifier and can be collected under this substitute identifier, which cannot be computationally linked to the original identifier.

Implementation of one-way hashes carry certain practical problems. If anyone happens to have a complete listing of all of the original identifiers, then it would be a simple matter to perform one-way hashes on every listed identifier. This would produce a look-up table that can match deidentified records back to the original identifier, a strategy known as a dictionary attack. For deidentification to work, the original identifier sequences must be kept secret.

One-way hash protocols have many practical uses in the field of information science [21,18,4]. It is very easy to implement one-way hashes, and most programming languages and operating systems come bundled with one or more implementations of one-way hash algorithms. The two most popular one-way hash algorithms are md5 (message digest version 5) and SHA (Secure Hash Algorithm). [Glossary HMAC, Digest, Message digest, Check digit]

Here we use Cygwin's own md5sum.exe utility on the command line to produce a one-way hash for an image file, named dash.png:

```
c:\ftp>c:\cygwin64\bin\md5sum.exe dash.png
```

Here is the output:

```
db50dc33800904ab5f4ac90597d7b4ea *dash.png
```

We could call the same command line from a Python script:

```
import sys, os
os.system("c:/cygwin64/bin/md5sum.exe dash.png")
```

The output will always be the same, as long as the input file, dash.png, does not change:

```
db50dc33800904ab5f4ac90597d7b4ea *dash.png
```

OpenSSL contains several one-way hash implementations, including both md5 and several variants of SHA.

One-way hashes on files are commonly used as a quick and convenient authentication tool. When you download a file from a Web site, you are likely to see that the file distributor has posted the file's one-way hash value. When you receive the file, it is a good idea to calculate the one-way hash on the file that you have received. If the one-way hash value is equal to the posted one-way hash value, then you can be certain that the file received is an exact copy of the file that was intentionally sent. Of course, this does not ensure that the file that was intentionally sent was a legitimate file or that the website was an honest file broker. We will be using our knowledge of one-way hashes when we discuss trusted time stamps (Section 8.5), blockchains (Section 8.6) and data security protocols (Section 18.3).

Glossary

ASCII ASCII is the American Standard Code for Information Interchange, ISO-14962-1997. The ASCII standard is a way of assigning specific 8-bit strings (a string of 0s and 1s of length 8) to the alphanumeric characters and punctuation. Uppercase letters are assigned a different string of 0s and 1s than their matching lowercase letters. There are 256 ways of combining 0s and 1s in strings of length 8. This means that that there are 256 different ASCII characters, and every ASCII character can be assigned a number-equivalent, in the range of 0–255. The familiar keyboard keys produce ASCII characters that happen to occupy ASCII values under 128. Hence, alphanumerics and common punctuation are represented as 8-bits, with the first bit, "0", serving as padding. Hence, keyboard characters are commonly referred to as 7-bit ASCII, and files composed exclusively of common keyboard characters are referred to as plain-text files or as 7-bit ASCII files.
These are the classic ASCII characters:

```
!"#$%&'()*+,-./0123456789:;<=>
?@ABCDEFGHIJKLMNOPQRSTUVWXYZ
[\]^_`abcdefghijklmnopqrstuvwxyz{|}~
```

Python has several methods for removing non-printable characters from text, including the "printable" method, as shown in this short script, printable.py.

```
# -*- coding: iso-8859-15 -*-

import string
in_string = "prinüéâäàtable"
out_string = "".join(s for s in in_string if s in string.printable)
print(out_strung)
output:
printable
```

It is notable that the first line of code violates a fundamental law of Python programming; that the pound sign signifies that a comment follows, and that the Python interpreter will ignore the pound

sign and any characters that follow the pound sign on the line in which they appear. For obscure reasons, the top line of the snippet is a permitted exception to the rule. In nonpythonic language, the top line conveys to the Python compiler that it may expect to find non-ASCII characters encoded in the iso-8859-15 standard.

The end result of this strange snippet is that non-ASCII characters are stripped from input strings; a handy script worth saving.

American Standard Code for Information Interchange Long form of the familiar acronym, ASCII.

Annotation Annotation involves describing data elements with metadata or attaching supplemental information to data objects.

Authentication A process for determining if the data object that is received (e.g., document, file, image) is the data object that was intended to be received. The simplest authentication protocol involves one-way hash operations on the data that needs to be authenticated. Suppose you happen to know that a certain file, named temp.txt will be arriving via email and that this file has an MD5 hash of "a0869a42609af6c712caeba454f47429". You receive the temp.txt file, and you perform an MD5 one-way hash operation on the file.

In this example, we will use the md5 hash utility bundled into the CygWin distribution (i.e., the Linux emulator for Windows systems). Any md5 implementation would have sufficed.

```
c:\cygwin64\bin>openssl md5 temp.txt
MD5(temp.txt)= a0869a42609af6c712caeba454f47429
```

We see that the md5 hash value generated for the received file is identical to the md5 hash value produced on the file, by the file's creator, before the file was emailed. This tells us that the received, temp.txt, is authentic (i.e., it is the file that you were intended to receive) because no other file has the same MD5 hash. Additional implementations of one-way hashes are described in **Section 3.9.**

The authentication process, in this example, does not tell you who sent the file, the time that the file was created, or anything about the validity of the contents of the file. These would require a protocol that included signature, time stamp, and data validation, in addition to authentication. In common usage, authentication protocols often include entity authentication (i.e., some method by which the entity sending the file is verified). Consequently, authentication protocols are often confused with signature verification protocols. An ancient historical example serves to distinguish the concepts of authentication protocols and signature protocols. Since earliest of recorded history, fingerprints were used as a method of authentication. When a scholar or artisan produced a product, he would press his thumb into the clay tablet, or the pot, or the wax seal closing a document. Anyone doubting the authenticity of the pot could ask the artisan for a thumbprint. If the new thumbprint matched the thumbprint on the tablet, pot, or document, then all knew that the person creating the new thumbprint and the person who had put his thumbprint into the object were the same individual. Hence, ancient pots were authenticated. Of course, this was not proof that the object was the creation of the person with the matching thumbprint. For all anyone knew, there may have been a hundred different pottery artisans, with one person pressing his thumb into every pot produced. You might argue that the thumbprint served as the signature of the artisan. In practical terms, no. The thumbprint, by itself, does not tell you whose print was used. Thumbprints could not be read, at least not in the same way as a written signature. The ancients needed to compare the pot's thumbprint against the thumbprint of the living person who made the print. When the person died, civilization was left with a bunch of pots with the same thumbprint, but without any certain way of knowing whose thumb produced them. In essence, because there was no ancient database that permanently associated thumbprints with individuals, the process of establishing the identity of the pot-maker became very difficult once the artisan died. A good signature protocol permanently binds an authentication code to a unique entity (e.g., a person). Today, we can find a fingerprint at the scene of a crime; we can find a matching signature in a database; and we can link the fingerprint to one individual. Hence, in modern times,

fingerprints are true "digital" signatures, no pun intended. Modern uses of fingerprints include keying (e.g., opening locked devices based on an authenticated fingerprint), tracking (e.g., establishing the path and whereabouts of an individual by following a trail of fingerprints or other identifiers), and body part identification (i.e., identifying the remains of individuals recovered from mass graves or from the sites of catastrophic events based on fingerprint matches). Over the past decade, flaws in the vaunted process of fingerprint identification have been documented, and the improvement of the science of identification is an active area of investigation [22].

Check digit A checksum that produces a single digit as output is referred to as a check digit. Some of the common identification codes in use today, such as ISBN numbers for books, come with a built-in check digit. Of course, when using a single digit as a check value, you can expect that some transmitted errors will escape the check, but the check digit is useful in systems wherein occasional mistakes are tolerated; or wherein the purpose of the check digit is to find a specific type of error (e.g., an error produced by a substitution in a single character or digit), and wherein the check digit itself is rarely transmitted in error.

Command line Instructions to the operating system, that can be directly entered as a line of text from the a system prompt (e.g., the so-called C prompt, "c:\>", in Windows and DOS operating systems; the so-called shell prompt, "$", in Linux-like systems).

Command line utility Programs lacking graphic user interfaces that are executed via command line instructions. The instructions for a utility are typically couched as a series of arguments, on the command line, following the name of the executable file that contains the utility.

Data cleaning More correctly, data cleansing, and synonymous with data fixing or data correcting. Data cleaning is the process by which errors, spurious anomalies, and missing values are somehow handled. The options for data cleaning are: correcting the error, deleting the error, leaving the error unchanged, or imputing a different value [23]. Data cleaning should not be confused with data scrubbing.

Data munging Refers to a multitude of tasks involved in preparing data for some intended purpose (e.g., data cleaning, data scrubbing, and data transformation). Synonymous with data wrangling.

Data scraping Pulling together desired sections of a data set or text by using software.

Data scrubbing A term that is very similar to data deidentification and is sometimes used improperly as a synonym for data deidentification. Data scrubbing refers to the removal of unwanted information from data records. This may include identifiers, private information, or any incriminating or otherwise objectionable language contained in data records, as well as any information deemed irrelevant to the purpose served by the record.

Data wrangling Jargon referring to a multitude of tasks involved in preparing data for eventual analysis. Synonymous with data munging [24].

Deidentification The process of removing all of the links in a data record that can connect the information in the record to an individual. This usually includes the record identifier, demographic information (e.g., place of birth), personal information (e.g., birthdate), and biometrics (e.g., fingerprints). The deidentification strategy will vary based on the type of records examined. Deidentifying protocols exist wherein deidentificated records can be reidentified, when necessary.

Digest As used herein, "digest" is equivalent to a one-way hash algorithm. The word "digest" also refers to the output string produced by a one-way hash algorithm.

Electronic medical record Abbreviated as EMR, or as EHR (Electronic Health Record). The EMR is the digital equivalent of a patient's medical chart. Central to the idea of the EMR is the notion that all of the documents, transactions, and all packets of information containing test results and other information on a patient are linked to the patient's unique identifier. By retrieving all data linked to the patient's identifier, the EMR (i.e., the entire patient's chart) can be assembled instantly.

Encapsulation The concept, from object oriented programming, that a data object contains its associated data. Encapsulation is tightly linked to the concept of introspection, the process of accessing the data

encapsulated within a data object. Encapsulation, Inheritance, and Polymorphism are available features of all object-oriented languages.

Encryption A common definition of encryption involves an algorithm that takes some text or data and transforms it, bit-by-bit, into an output that cannot be interpreted (i.e., from which the contents of the source file cannot be determined). Encryption comes with the implied understanding that there exists some reverse transform that can be applied to the encrypted data, to reconstitute the original source. As used herein, the definition of encryption is expanded to include any protocols by which files can be shared, in such a way that only the intended recipients can make sense of the received documents. This would include protocols that divide files into pieces that can only be reassembled into the original file using a password. Encryption would also include protocols that alter parts of a file while retaining the original text in other parts of the file. As described in Chapter 5, there are instances when some data in a file should be shared, while only specific parts need to be encrypted. The protocols that accomplish these kinds of file transformations need not always employ classic encryption algorithms (e.g., Winnowing and Chaffing [25], threshold protocols [21]).

Gedanken Gedanken is the German word for "thought." A gedanken experiment is one in which the scientist imagines a situation and its outcome, without resorting to any physical construction of a scientific trial. Albert Einstein, a consummate theoretician, was fond of inventing imaginary scenarios, and his use of the term "gedanken trials" has done much to popularize the concept. The scientific literature contains multiple descriptions of gedanken trials that have led to fundamental breakthroughs in our understanding of the natural world and of the universe [26].

HMAC Hashed Message Authentication Code. When a one-way hash is employed in an authentication protocol, it is often referred to as an HMAC.

HTML HyperText Markup Language is an ASCII-based set of formatting instructions for web pages. HTML formatting instructions, known as tags, are embedded in the document, and double-bracketed, indicating the start point and end points for instruction. Here is an example of an HTML tag instructing the web browser to display the word "Hello" in italics: Hello. All web browsers conforming to the HTML specification must contain software routines that recognize and implement the HTML instructions embedded within in web documents. In addition to formatting instructions, HTML also includes linkage instructions, in which the web browsers must retrieve and display a listed web page, or a web resource, such as an image. The protocol whereby web browsers, following HTML instructions, retrieve web pages from other Internet sites, is known as HTTP (HyperText Transfer Protocol).

ImageMagick An open source utility that supports a huge selection of robust and sophisticated image editing methods. ImageMagick is available for download at: https://www.imagemagick.org/script/download.php

Instance An instance is a specific example of an object that is not itself a class or group of objects. For example, Tony the Tiger is an instance of the tiger species. Tony the Tiger is a unique animal and is not itself a group of animals or a class of animals. The terms instance, instance object, and object are sometimes used interchangeably, but the special value of the "instance" concept, in a system wherein everything is an object, is that it distinguishes members of classes (i.e., the instances) from the classes to which they belong.

Intellectual property Data, software, algorithms, and applications that are created by an entity capable of ownership (e.g., humans, corporations, and universities). The entity holds rights over the manner in which the intellectual property can be used and distributed. Protections for intellectual property may come in the form of copyrights and patent. Copyright applies to published information. Patents apply to novel processes and inventions. Certain types of intellectual property can only be protected by being secretive. For example, magic tricks cannot be copyrighted or patented; this is why magicians guard their intellectual property so closely. Intellectual property can be sold outright, essentially transferring ownership to another entity; but this would be a rare event. In other cases, intellectual property is

retained by the creator who permits its limited use to others via a legal contrivance (e.g., license, contract, transfer agreement, royalty, and usage fee). In some cases, ownership of the intellectual property is retained, but the property is freely shared with the world (e.g., open source license, GNU license, FOSS license, and Creative Commons license).

Message digest Within the context of this book, "message digest", "digest", "HMAC", and "one-way hash" are equivalent terms.

Minimal necessary In the field of medical informatics, there is a concept known as "minimal necessary" that applies to shared confidential data [9]. It holds that when records are shared, only the minimum necessary information should be released. Information not directly relevant to the intended purposes of the study should be withheld.

Object-oriented programming In object-oriented programming, all data objects must belong to one of the classes built into the language or to a class created by the programmer. Class methods are subroutines that belong to a class. The members of a class have access to the methods for the class. There is a hierarchy of classes (with superclasses and subclasses). A data object can access any method from any superclass of its class. All object-oriented programming languages operate under this general strategy. The two most important differences among the object oriented programming languages relate to syntax (i.e., the required style in which data objects call their available methods) and content (the built-in classes and methods available to objects). Various esoteric issues, such as types of polymorphism offered by the language, multi-parental inheritance, and non-Boolean logic operations may play a role in how expert programmer's choose a specific object-oriented language for the job at-hand.

One-way hash A one-way hash is an algorithm that transforms one string into another string (a fixed-length sequence of seemingly random characters) in such a way that the original string cannot be calculated by operations on the one-way hash value (i.e., the calculation is one-way only). One-way hash values can be calculated for any string, including a person's name, a document, or an image. For any given input string, the resultant one-way hash will always be the same. If a single byte of the input string is modified, the resulting one-way hash will be changed, and will have a totally different sequence than the one-way hash sequence calculated for the unmodified string.

Most modern programming languages have several methods for generating one-way hash values. Regardless of the language we choose to implement a one-way hash algorithm (e.g., md5, SHA), the output value will be identical. One-way hash values are designed to produce long fixed-length output strings (e.g., 256 bits in length). When the output of a one-way hash algorithm is very long, the chance of a hash string collision (i.e., the occurrence of two different input strings generating the same one-way hash output value) is negligible. Clever variations on one-way hash algorithms have been repurposed as identifier systems [27,28,29,30]. A detailed discussion of one-way hash algorithms can be found in Section 3.9, "Case Study: One-Way Hashes."

Privacy versus confidentiality The concepts of confidentiality and of privacy are often confused, and it is useful to clarify their separate meanings. Confidentiality is the process of keeping a secret with which you have been entrusted. You break confidentiality if you reveal the secret to another person. You violate privacy when you use the secret to annoy the person whose confidential information was acquired. If you give a friend your unlisted telephone number in confidence, then your fried is expected to protect this confidentiality by never revealing the number to other persons. In addition, your friend may be expected to protect your privacy by resisting the temptation to call you in the middle of the night, complain about a mutual acquaintance. In this case, the same information object (unlisted telephone number) is encumbered by separable confidentiality and privacy obligations.

Pseudorandom number generator It is impossible for computers to produce an endless collection of truly random numbers. Eventually, algorithms will cycle through their available variations and begins to repeat themselves, producing the same set of "random" numbers, in the same order; a phenomenon referred to as the generator's period. Because algorithms that produce seemingly random numbers are imperfect, they are known as pseudorandom number generators. The Mersenne Twister algorithm,

which has an extremely long period, is used as the default random number generator in Python. This algorithm performs well on most of the tests that mathematicians have devised to test randomness.

Randomness Various tests of randomness are available [31]. One of the easiest to implement takes advantage of the property that random strings are uncompressible. If you can show that if a character string, a series of numbers, or a column of data cannot be compressed by gzip, then it is pretty safe to conclude that the data is randomly distributed, and without any informational value.

Reidentification A term casually applied to any instance whereby information can be linked to a specific person after the links between the information and the person associated with the information were removed. Used this way, the term reidentification connotes an insufficient deidentification process. In the healthcare industry, the term "reidentification" means something else entirely. In the United States, regulations define "reidentification" under the "Standards for Privacy of Individually Identifiable Health Information". Reidentification is defined therein as a legally valid process whereby deidentified records can be linked back to the respective human subjects, under circumstances deemed compelling by a privacy board. Reidentification is typically accomplished via a confidential list of links between human subject names and deidentified records, held by a trusted party. As used by the healthcare industry, reidentification only applies to the approved process of re-establishing the identity of a deidentified record. When a human subject is identified through fraud, trickery, or through the deliberate use of computational methods to break the confidentiality of insufficiently deidentified records, the term "reidentification" would not apply.

Social Security Number The common strategy, in the United States, of employing social security numbers as identifiers is often counterproductive, owing to entry error, mistaken memory, or the intention to deceive. Efforts to reduce errors by requiring individuals to produce their original social security cards puts an unreasonable burden on honest individuals, who rarely carry their cards, and provides an advantage to dishonest individuals, who can easily forge social security cards. Institutions that compel patients to provide a social security number have dubious legal standing. The social security number was originally intended as a device for validating a person's standing in the social security system. More recently, the purpose of the social security number has been expanded to track taxable transactions (i.e., bank accounts, salaries). Other uses of the social security number are not protected by law. The Social Security Act (Section 208 of Title 42 U.S. Code 408) prohibits most entities from compelling anyone to divulge his/her social security number. Legislation or judicial action may one day stop healthcare institutions from compelling patients to divulge their social security numbers as a condition for providing medical care. Prudent and forward-thinking institutions will limit their reliance on social security numbers as personal identifiers.

Time stamp Many data objects are temporal events and all temporal events must be given a time stamp indicating the time that the event occurred, using a standard measurement for time. The time stamp must be accurate, persistent, and immutable. The Unix epoch time (equivalent to the Posix epoch time) is available for most operating systems and consists of the number of seconds that have elapsed since January 1, 1970, midnight, Greenwhich mean time. The Unix epoch time can easily be converted into any other standard representation of time. The duration of any event can be easily calculated by subtracting the beginning time from the ending time. Because the timing of events can be maliciously altered, scrupulous data managers employ a trusted time stamp protocol by which a time stamp can be verified. A trusted time stamp must be accurate, persistent, and immutable. Trusted time stamp protocols are discussed in Section 8.5, "Case Study: The Trusted Time stamp."

URL Unique Resource Locator. The Web is a collection of resources, each having a unique address, the URL. When you click on a link that specifies a URL, your browser fetches the page located at the unique location specified in the URL name. If the Web were designed otherwise (i.e., if several different web pages had the same web address, or if one web address were located at several different locations), then the web could not function with any reliability.

URN Unique Resource Name. Whereas the URL identifies objects based on the object's unique location in the Web, the URN is a system of object identifiers that are location-independent. In the URN system, data objects are provided with identifiers, and the identifiers are registered with, and subsumed by, the URN.

For example:

```
urn:isbn-13:9780128028827
```

Refers to the unique book, "Repurposing Legacy Data: Innovative Case Studies," by Jules Berman

```
urn:uuid:e29d0078-f7f6-11e4-8ef1-e808e19e18e5
```

Refers to a data object tied to the UUID identifier e29d0078-f7f6-11e4-8ef1-e808e19e18e5.

In theory, if every data object were assigned a registered URN, and if the system were implemented as intended, the entire universe of information could be tracked and searched.

UUID UUID, the abbreviation for Universally Unique IDentifiers, is a protocol for assigning identifiers to data objects, without using a central registry. UUIDs were originally used in the Apollo Network Computing System [3].

Utility In the context of software, a utility is an application that is dedicated to performing one specific task, very well, and very fast. In most instances, utilities are short programs, often running from the command line, and thus lacking any graphic user interface. Many utilities are available at no cost, with open source code. In general, simple utilities are preferable to multi-purpose software applications [32]. Remember, an application that claims to do everything for the user is, most often, an application that requires the user to do everything for the application.

XML Abbreviation for eXtensible Markup Language. A syntax for marking data values with descriptors (metadata). The descriptors are commonly known as tags. In XML, every data value is enclosed by a start-tag, indicating that a value will follow, and an end-tag, indicating that the value had preceded the tag. For example: <name>Tara Raboomdeay</name>. The enclosing angle brackets, "<>", and the end-tag marker, "/", are hallmarks of XML markup. This simple but powerful relationship between metadata and data allows us to employ each metadata/data pair as though it were a small database that can be combined with related metadata/data pairs from any other XML document. The full value of metadata/data pairs comes when we can associate the pair with a unique object, forming a so-called triple.

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4

Metadata, Semantics, and Triples

OUTLINE

Section 4.1. Metadata

Life is a concept.

Patrick Forterre [1]

When you think about it, numbers are meaningless. The number "8" has no connection to anything in the physical realm until we attach some information to the number (e.g., 8 candles, 8 minutes). Some numbers, like "0" or "−5" have no physical meaning under any set of circumstances. There really is no such thing as "0 dollars"; it is an abstraction indicating the absence of a positive number of dollars. Likewise, there is no such thing as "−5 walnuts"; it is an abstraction that we use to make sense of subtractions ($5-10=-5$).

When we write "8 walnuts," "walnuts" is the metadata that tells us what is being referred to by the data, in this case the number "8."

When we write "8 o'clock", "8" is the data and "o'clock" is the metadata.

Section 4.2. eXtensible Markup Language

The purpose of narrative is to present us with complexity and ambiguity.

Scott Turow

XML (eXtensible Markup Language) is a syntax for attaching descriptors (so-called metadata) to data values. [Glossary Metadata]

In XML, descriptors are commonly known as tags.

Principles and Practice of Big Data. https://doi.org/10.1016/B978-0-12-815609-4.00004-2

XML has its own syntax; a set of rules for expressing data/metadata pairs. Every data value is flanked by a start-tag and an end-tag. Enclosing angle brackets, "<>", and the end-tag marker, "/", are hallmarks of XML markup. For example:

```
<name>Tara Raboomdeay</name>
```

This simple but powerful relationship between metadata and data allows us to employ every metadata/data pair as a miniscule database that can be combined with related metadata/data pairs from the same XML document or from different XML documents.

It is impossible to overstate the importance of XML (eXtensible Markup Language) as a data organization tool. With XML, every piece of data tells us something about itself. When a data value has been annotated with metadata, it can be associated with other, related data, even when the other data is located in a seemingly unrelated database. [Glossary Integration].

When all data is flanked by metadata, it is relatively easy to port the data into spreadsheets, where the column headings correspond to the metadata tags, and the data values correspond to the value found in the cells of the spreadsheet. The rows correspond to the record number.

A file that contains XML markup is considered a proper XML document only if it is well formed. Here are the properties of a well-formed XML document.

- The document must have a proper XML header. The header can vary somewhat, but it usually looks something like:
  ```
  <?xml version="1.0" ?>
  ```
- XML files are ASCII files consisting of characters available to a standard keyboard.
- Tags in XML files must conform to composition rules (e.g., spaces are not permitted within a tag, and tags are case-sensitive).
- Tags must be properly nested (i.e., no overlapping). For example, the following is properly nested XML.

```
<chapter><chapter_title>Introspection</chapter_title></chapter>
```

Compare the previous example, with the following, improperly nested XML.

```
<chapter><chapter_title>Introspection</chapter></chapter_title>
```

Web browsers will not display XML files that are not well formed.

The actual structure of an XML file is determined by another XML file known as an XML Schema. The XML Schema file lists the tags and determines the structure for those XML files that are intended to comply with a specific Schema document. A valid XML file conforms to the rules of structure and content defined in its assigned XML Schema.

Every XML file that is valid under a particular Schema will contain data that is described using the same tags that are listed in that same XML schema, permitting data integration among those files. This is one of the strengths of XML.

The greatest drawback of XML is that data/metadata pairs are not assigned to a unique object. XML describes its data, but it does not tell us the object of the data. This gaping hole in XML was filled by RDF (Resource Description Framework), a modified XML syntax

designed to associate every data/metadata pair with a unique data object. Before we can begin to understand RDF, we need to understand the concept of "meaning," in the context of information science.

Section 4.3. Semantics and Triples

> *Supplementary bulletin from the Office of Fluctuation Control, Bureau of Edible Condiments, Soluble and Indigestible Fats and Glutinous Derivatives, Washington, D.C. Correction of Directive #943456201, . . . the quotation on ground-hog meat should read 'ground hog meat.'*
>
> *Bob Elliot and Ray Goulding, comedy routine*

Metadata gives structure to data values, but it does not tell us anything about how the data value relates to anything else. For example,

```
<height_in_feet_inches>5'11"</height_in_feet_inches>
```

What does it mean to know that 5′11″ is a height attribute, expressed in feet and inches? Nothing really. The metadata/data pair has no meaning, as it stands, because it does not describe anything in particular. If we were to assert that John Harrington has a height of 5′11″, then we would be making a meaningful statement. This brings us to ask ourselves: What is the meaning of meaning? This question sounds like another one of those Zen mysteries that has no answer. In informatics, "meaningfulness" is achieved when described data (i.e., a metadata/data pair) is bound to the unique identifier of a data object.

Let us look once more at our example:

```
"John Harrington's height is five feet eleven inches."
```

This sentence has meaning because there is data (five feet eleven inches), and it is described (person's height), and it is bound to a unique individual (John Harrington). Let us generate a unique identifier for John Harrington using our UUID generator (discussed in Section 3.3) and rewrite our assertion in a format in which metadata/data pairs are associated with a unique identifier:

```
9c7bfe97-e637-461f-a30b-d931b97907fe    name     John Harrington
9c7bfe97-e637-461f-a30b-d931b97907fe    height   5'11"
```

We now have two meaningful assertions: one that associates the name "John Harrington" with a unique identifier (9c7bfe97-e637-461f-a30b-d931b97907fe); and one that tells us that the object associated with the unique identifier (i.e., John Harrington) is 5′11″ tall. We could insert these two assertions into a Big Data resource, knowing that both assertions fulfill our definition of meaning. Of course, we would need to have some process in place to ensure that any future information collected on our unique John Harrington (i.e., the John Harrington assigned the identifier 9c7bfe97-e637-461f-a30b-d931b97907fe) will be assigned the same identifier.

A statement with meaning does not need to be a true statement (e.g., The height of John Harrington was not 5 feet 11 inches when John Harrington was an infant). That is to say, an assertion can be meaningful but false.

Semantics is the study of meaning. In the context of Big Data, semantics is the technique of creating meaningful assertions about data objects. All meaningful assertions, without exception, can be structured as a 3-item list consisting of an identified data object, a data value, and a descriptor for the data value. These 3-item assertions are referred to as "triples." Just as sentences are the fundamental informational unit of spoken languages, the triple is the fundamental unit of computer information systems.

In practical terms, semantics involves making assertions about data objects (i.e., making triples), combining assertions about data objects (i.e., aggregating triples), and assigning data objects to classes; hence relating triples to other triples. As a word of warning, few informaticians would define semantics in these terms, but I would suggest that all legitimate definitions for the term "semantics" are functionally equivalent to the definition offered here. For example every cell in a spreadsheet is a data value that has a descriptor (the column header), and a subject (the row identifier). A spreadsheet can be pulled apart and re-assembled as a set of triples (known as a triplestore) equal in number to the number of cells contained in the original spreadsheet. Each triple would be an assertion consisting of the following:

```
<row identifier> <column header> <content of cell>
```

Likewise, any relational database, no matter how many relational table are included, can be decomposed into a triplestore. The primary keys of the relational tables would correspond to the identifier of the RDF triple. Column header and cell contents complete the triple.

If spreadsheets and relational databases are equivalent to triplestores, then is there any special advantage to creating triplestores? Yes. A triple is a stand-alone unit of meaning. It does not rely on the software environment (e.g., excel spreadsheet or SQL database engine) to convey its meani ng. Hence, triples can be merged without providing any additional structure. Every triple on the planet could be concatenated to create the ultimate superduper triplestore, from which all of the individual triples pertaining to any particular unique identifier, could be collected. This is something that could not be done with spreadsheets and d atabase engines. Enormous triplestores can serve as native databases or as a large relational table, or as pre-indexed tables. Regardless, the final products have all the functionality of any popular database engine [2].

Section 4.4. Namespaces

It is once again the vexing problem of identity within variety; without a solution to this disturbing problem there can be no system, no classification.

Roman Jakobson

A namespace is the metadata realm in which a metadata tag applies. The purpose of a namespace is to distinguish metadata tags that have the same name, but different meaning. For example, within a single XML file, the metadata term "date" may be used to signify a calendar date, or the fruit, or the social engagement. To avoid confusion, the metadata term is given a prefix that is associated with a Web document that defines the term within an assigned Web location. [Glossary Namespace]

For example, an XML page might contain three date-related values, and their metadata descriptors:

```
<calendar:date>June 16, 1904</caldendar:date>
<agriculture:date>Thoory</agriculture:date>
<social:date>Pyramus and Thisbe<social:date>
```

At the top of the XML document you would expect to find declarations for the namespaces used in the XML page. Formal XML namespace declarations have the syntax:

```
xmlns:prefix="URI"
```

In the fictitious example used in this section, the namespace declarations might appear in the "root" tag at the top of the XML page, as shown here (with fake web addresses):

```
<root xmlns:calendar="http://www.calendercollectors.org/"
xmlns:agriculture="http://www.farmersplace.org/"
xmlns:social="http://hearts_throbbing.com/">
```

The namespace URIs are the web locations that define the meanings of the tags that reside within their namespace.

The relevance of namespaces to Big Data resources relates to the heterogeneity of information contained in or linked to a resource. Every description of a value must be provided a unique namespace. With namespaces, a single data object residing in a Big Data resource can be associated with assertions (i.e., object-metadata-data triples) that include descriptors of the same name, without losing the intended sense of the assertions. Furthermore, triples held in different Big Data resources can be merged, with their proper meanings preserved.

Here is an example wherein two resources are merged, with their data arranged as assertion triples.

```
Big Data resource 1

29847575938125      calendar:date      February 4, 1986
83654560466294      calendar:date      June 16, 1904

Big Data resource 2

57839109275632      social:date        Jack and Jill
83654560466294      social:date        Pyramus and Thisbe
```

```
Merged Big Data Resource 1 + 2

29847575938125      calendar:date      February 4, 1986
57839109275632      social:date        Jack and Jill
83654560466294      social:date        Pyramus and Thisbe
83654560466294      calendar:date      June 16, 1904
```

There you have it. The object identified as 83654560466294 is associated with a "date" metadata tag in both resources. When the resources are merged, the unambiguous meaning of the metadata tag is conveyed through the appended namespaces (i.e., social: and calendar:)

Section 4.5. Case Study: A Syntax for Triples

> *I really do not know that anything has ever been more exciting than diagramming sentences.*
>
> *Gertrude Stein*

If you want to represent data as triples, you will need to use a standard grammar and syntax. RDF (Resource Description Framework) is a dialect of XML designed to convey triples. Providing detailed instruction in RDF syntax, or its dialects, lies far outside the scope of this book. However, every Big Data manager must be aware of those features of RDF that enhance the value of Big Data resources. These would include:

1. The ability to express any triple in RDF (i.e., the ability to make RDF statements).
2. The ability to assign the subject of an RDF statement to a unique, identified, and defined class of objects (i.e., that ability to assign the object of a triple to a class).

RDF is a formal syntax for triples. The subjects of triples can be assigned to classes of objects defined in RDF Schemas and linked from documents composed of RDF triples. RDF Schemas will be described in detail in Section 5.9.

When data objects are assigned to classes, the data analysts can discover new relationships among the objects that fall into a class, and can also determine relationships among different related classes (i.e., ancestor classes and descendant classes, also known as superclasses and subclasses). RDF triples plus RDF Schemas provide a semantic structure that supports introspection and reflection. [Glossary Child class, Subclass, RDF Schema, RDFS, Introspection, Reflection]

3. The ability for all data developers to use the same publicly available RDF Schemas and namespace documents with which to describe their data, thus supporting data integration over multiple Big Data resources.

This last feature allows us to turn the Web into a worldwide Big Data resource composed of RDF documents.

We will briefly examine each of these three features in RDF. First, consider the following triple:

```
pubmed:8718907    creator    Bill Moore
```

Every triple consists of an identifier (the subject of the triple), followed by metadata, followed by a value. In RDF syntax the triple is flanked by metadata indicating the beginning and end of the triple. This is the <rdf:description> tag and its end-tag </rdf:description). The identifier is listed as an attribute within the <rdf:description> tag, and is described with the rdf:about tag, indicating the subject of the triple. There follows a metadata descriptor, in this case <author>, enclosing the value, "Bill Moore."

```
<rdf:description rdf:about="urn:pubmed:8718907">
  <creator>Bill Moore</creator>
</rdf:description>
```

The RDF triple tells us that Bill Moore wrote the manuscript identified with the PubMed number 8718907. The PubMed number is the National library of Medicine's unique identifier assigned to a specific journal article. We could express the title of the article in another triple.

```
pubmed:8718907, title, "A prototype Internet autopsy database. 1625
consecutive fetal and neonatal autopsy facesheets spanning 20 years."
```

In RDF, the same triple is expressed as:

```
<rdf:description rdf:about="urn:pubmed:8718907">
  <title>A prototype Internet autopsy database. 1625 consecutive
fetal and neonatal autopsy facesheets spanning 20 years</title>
</rdf:description>
```

RDF permits us to nest triples if they apply to the same unique object.

```
<rdf:description rdf:about="urn:pubmed:8718907">
  <author>Bill Moore</author>
  <title>A prototype Internet autopsy database. 1625 consecutive
fetal and neonatal autopsy facesheets spanning 20 years</title>
</rdf:description>
```

Here we see that the PubMed manuscript identified as 8718907 was written by Bill Moore (the first triple) and is titled "A prototype Internet autopsy database. 1625 consecutive fetal and neonatal autopsy facesheets spanning 20 years" (a second triple).

What do we mean by the metadata tag "title"? How can we be sure that the metadata term "title" refers to the name of a document and does not refer to an honorific (e.g., The Count of Monte Cristo or the Duke of Earl). We append a namespace to the metadata. Namespaces were described in Section 4.4.

```
<rdf:description rdf:about="urn:pubmed:8718907">
  <dc:creator>Bill Moore</dc:creator>
  <dc:title>A prototype Internet autopsy database. 1625 consecutive
fetal and neonatal autopsy facesheets spanning 20 years</dc:title>
</rdf:description>
```

In this case, we appended "dc:" to our metadata. By convention, "dc:" refers to the Dublin Core metadata set at: http://dublincore.org/documents/2012/06/14/dces/.

We will be describing the Dublin Core in more detail, in Section 4.6. [Glossary Dublin Core metadata].

RDF was developed as a semantic framework for the Web. The object identifier system for RDF was created to describe Web addresses or unique resources that are available through the Internet. The identification of unique addresses is done through the use of a Uniform Resource Name (URN) [3]. In many cases the object of a triple designed for the Web will be a Web address. In other cases the URN will be an identifier, such as the PubMed reference number in the example above. In this case, we appended the "urn:" prefix to the PubMed reference in the "about" declaration for the object of the triple.

```
<rdf:description rdf:about="urn:pubmed:8718907">
```

Let us create an RDF triple whose subject is an actual Web address.

```
<rdf:Description rdf:about="http://www.usa.gov/">
  <dc:title>USA.gov: The U.S. Government's Official Web Portal</dc:
title>
</rdf:Description>
```

Here we created a triple wherein the object is uniquely identified by the unique Web address http://www.usa.gov/, and the title of the Web page is "USA.gov: The U.S. Government's Official Web Portal." The RDF syntax for triples was created for the purpose of identifying information with its URI (Unique Resource Identifier). The URI is a string of characters that uniquely identifies a Web resource (such as a unique Web address, or some unique location at a Web address, or some unique piece of information that can be ultimately reached through the Worldwide Web). In theory, using URIs as identifiers for triples will guarantee that all triples will be accessible through the so-called "Semantic Web" (i.e., the Web of meaningful assertions) [3]. Using RDF, Big Data resources can design a scaffold for their information that can be understood by humans, parsed by computers, and shared by other Big Data resources. This solution transforms every RDF-compliant Web page into a an accessible database whose contents can be searched, extracted, aggregated, and integrated along with all the data contained in every existing Big Data resource.

In practice, the RDF syntax is just one of many available formats for packaging triples, and can be used with identifiers that have invalid URIs (i.e., that do not relate in any way to Web addresses or Web resources). The point to remember is that Big Data resources that employ triples can port their data into RDF syntax, or into any other syntax for triples, as needed. [Glossary Notation 3, Turtle]

Section 4.6. Case Study: Dublin Core

> *For myself, I always write about Dublin, because if I can get to the heart of Dublin I can get to the heart of all the cities of the world. In the particular is contained the universal.*
>
> *James Joyce*

James Joyce believed that Dublin held the m eaning of every city in the world. In a similar vein, the Dublin Core metadata descriptors hold the meaning of every document in the world. The principle difference between the two Dublin-centric philosophies is that James Joyce hailed from Dublin, Ireland, while the Dublin Core metadata descriptors hailed from Dublin, Ohio, United States. For it was in Dublin, Ohio, in 1995, that a coterie of interested Interne t technologists and librarians met for the purpose of identifying a core set of descriptive data elements that every electronic document should contain.

The specification resulting from this early workshop came to be known as the Dublin Core [4]. The Dublin Core elements include such information as the date that the file was created, the name of the entity that created the file, and a general comment on the contents of the file. The Dublin Core elements aid in indexing and retrieving electronic files, and should be included in every electronic document, including every image file. The Dublin Core metadata specification is found at:

http://dublincore.org/documents/dces/

Some of the most useful Dublin Core elements are [5]:

- Contributor—the entity that contributes to the document
- Coverage—the general area of information covered in the document
- Creator—the entity primarily responsible for creating the document
- Date—a time associated with an event relevant to the document
- Description—description of the document
- Format—file format
- Identifier—a character string that uniquely and unambiguously identifies the document
- Language—the language of the document
- Publisher—the entity that makes the resource available
- Relation—a pointer to another, related document, typically the identifier of the related document
- Rights—the property rights that apply to the document
- Source—an identifier linking to another document from which the current document was derived
- Subject—the topic of the document
- Title—title of the document
- Type—genre of the document

An XML syntax for expressing the Dublin Core elements is available [6,7].

Glossary

Child class The direct or first generation subclass of a class. Sometimes referred to as the daughter class or, less precisely, as the subclass.

Dublin Core metadata The Dublin Core is a set of metadata elements developed by a group of librarians who met in Dublin, Ohio. It would be very useful if every electronic document were annotated with the Dublin Core elements. The Dublin Core Metadata is discussed in detail in Chapter 4. The syntax for including the elements is found at: http://dublincore.org/documents/dces/

Integration Occurs when information is gathered from multiple data sets, relating diverse data extracted from different data sources. Integration can broadly be categorized as pre-computed or computed on-the fly. Pre-computed integration includes such efforts as absorbing new databases into a Big Data resource or merging legacy data from with current data. On-the-fly integration involves merging data objects at the moment when the individual objects are parsed. This might be done during a query that traverses multiple databases or multiple networks. On-the-fly data integration can only work with data objects that support introspection. The two closely related topics of integration and interoperability are often confused with one another. An easy way to remember the difference is to note that integration refers to data; interoperability refers to software.

Introspection Well-designed Big Data resources support introspection, a method whereby data objects within the resource can be interrogated to yield their properties, values, and class membership. Through introspection the relationships among the data objects in the Big Data resource can be examined and the structure of the resource can be determined. Introspection is the method by which a data user can find everything there is to know about a Big Data resource without downloading the complete resource.

Metadata Data that describes data. For example in XML, a data quantity may be flanked by a beginning and an ending metadata tag describing the included data quantity. <age>48 years</age>. In the example, <age> is the metadata and 48 years is the data.

Namespace A namespace is the metadata realm in which a metadata tag applies. The purpose of a namespace is to distinguish metadata tags that have the same name, but a different meaning. For example, within a single XML file, the metadata term "date" may be used to signify a calendar date, or the fruit, or the social engagement. To avoid confusion the metadata term is given a prefix that is associated with a Web document that defines the term within the document's namespace.

Notation 3 Also called n3. A syntax for expressing assertions as triples (unique subject + metadata + data). Notation 3 expresses the same information as the more formal RDF syntax, but n3 is compact and easy for humans to read. Both n3 and RDF can be parsed and equivalently tokenized (i.e., broken into elements that can be re-organized in a different format, such as a database record).

RDF Schema Resource Description Framework Schema (RDFS). A document containing a list of classes, their definitions, and the names of the parent class(es) for each class (e.g., Class Marsupiala is a subclass of Class Metatheria). In an RDF Schema, the list of classes is typically followed by a list of properties that apply to one or more classes in the Schema. To be useful, RDF Schemas are posted on the Internet, as a Web page, with a unique Web address. Anyone can incorporate the classes and properties of a public RDF Schema into their own RDF documents (public or private) by linking named classes and properties, in their RDF document, to the web address of the RDF Schema where the classes and properties are defined.

RDFS Same as RDF Schema.

Reflection A programming technique wherein a computer program will modify itself, at run-time, based on information it acquires through introspection. For example, a computer program may iterate over a collection of data objects, examining the self-descriptive information for each object in the collection (i.e., object introspection). If the information indicates that the data object belongs to a particular class of objects, the program might call a method appropriate for the class. The program executes in a

manner determined by descriptive information obtained during run-time; metaphorically reflecting upon the purpose of its computational task. Because introspection is a property of well-constructed Big Data resources, reflection is an available technique to programmers who deal with Big Data.

Subclass A class in which every member descends from some higher class (i.e., a superclass) within the class hierarchy. Members of a subclass have properties specific to the subclass. As every member of a subclass is also a member of the superclass, the members of a subclass inherit the properties and methods of the ancestral classes. For example, all mammals have mammary glands because mammary glands are a defining property of the mammal class. In addition, all mammals have vertebrae because the class of mammals is a subclass of the class of vertebrates. A subclass is the immediate child class of its parent class.

Turtle Another syntax for expressing triples. From RDF came a simplified syntax for triples, known as Notation 3 or N3 [8]. From N3 came Turtle, thought to fit more closely to RDF. From Turtle came an even more simplified form, known as N-Triples.

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[5] Berman JJ. Principles of big data: preparing, sharing, and analyzing complex information. Waltham, MA: Morgan Kaufmann; 2013.

[6] Dublin Core Metadata Initiative. Available from: http://dublincore.org/ The Dublin Core is a set of basic metadata that describe XML documents. The Dublin Core were developed by a forward-seeing group library scientists who understood that every XML document needs to include self-describing metadata that will allow the document to be indexed and appropriately retrieved.

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5 Classifications and Ontologies

OUTLINE

Section 5.1. It's All About Object Relationships

Order and simplification are the first steps toward the mastery of a subject.
Thomas Mann

Information has limited value unless it can take its place within our general understanding of the world. When a financial analyst learns that the price of a stock has suddenly dropped, he cannot help but wonder if the drop of a single stock reflects conditions in other stocks in the same industry. If so, the analyst may check to ensure that other industries are following a downward trend. He may wonder whether the downward trend represents a shift in the national or global economies. There is a commonality to all of the questions posed by the financial analyst. In every case, the analyst is asking a variation on a single question: "How does this thing relate to that thing?"

Big Data resources are complex. When data is simply stored in a database, without any general principles of organization, it becomes impossible to find the relationships among the data objects. To be useful the information in a Big Data resource must be divided into classes of data. Each data object within a class shares a set of properties chosen to enhance our ability to relate one piece of data with another.

Relationships are the fundamental properties of an object that determine the class in which it is placed. Every member of a class shares these same fundamental properties. A core set of relational properties is found in all the ancestral classes of an object and in all the descendant classes of an object. Similarities are just features that one or more

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objects have in common, but they are not fundamental relationships upon which classes can be organized. Related objects tend to be similar to one another, but these similarities occur as the consequence of their relationships; not vice versa. For example, you may have many similarities to your father. If so, you are similar to your father because you are related to him; you are not related to him because you are similar to him.

The distinction between grouping data objects by similarity and grouping data objects by relationship is sometimes lost on computer scientists. I have had numerous conversations with intelligent scientists who refuse to accept that grouping by similarity (e.g., clustering) is fundamentally different from grouping by relationship (i.e., building a classification). [Glossary Cluster analysis]

Consider a collection of 300 objects. Each object belongs to one of two classes, marked by an asterisk or by an empty box. The three hundred objects naturally cluster into three groups. It is tempting to conclude that the graph shows three classes of objects that can be defined by their similarities, but we know from the outset that the objects fall into two classes, and we see from the graph that objects from both classes are distributed in all three clusters (Fig. 5.1).

Is this graph far-fetched? Not really. Suppose you have a collection of felines and canines. The collection of dogs might include Chihuahuas, St. Bernards, and other breeds. The collection of cats might include housecats, lions, and other species, and the data collected on each animal might include weight, age, and hair length. We do not know what to expect when we cluster the animals by similarities (i.e., weight, age, and hair length) but we can be sure that short-haired cats and short-haired Chihuahuas of the same age will probably fall into one cluster. Cheetahs and greyhounds, having similar size and build,

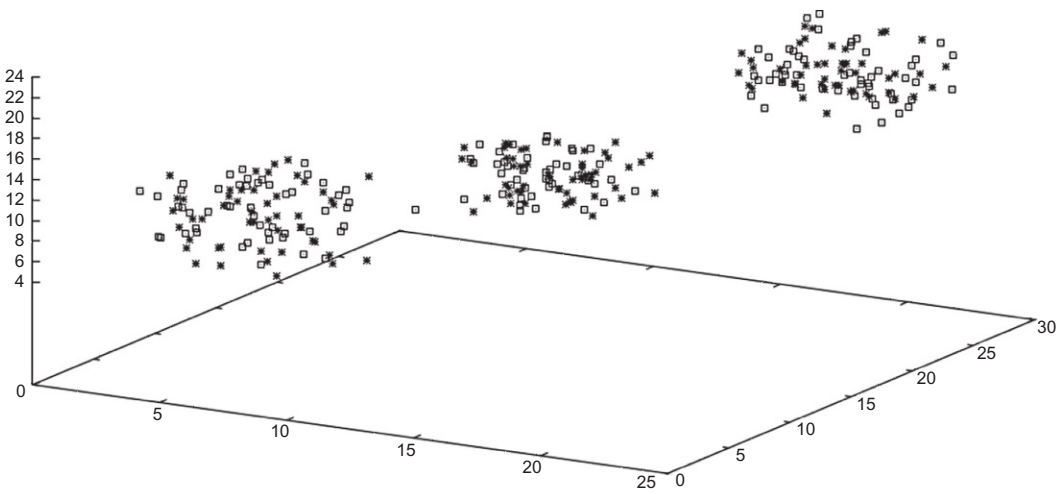

FIG. 5.1 The spatial distribution of 300 objects represented by data points in three dimensions. Each data object falls into one of two classes, represented by an asterisk or an empty box. The data naturally segregates into three clusters. Objects of type asterisk and type box are distributed throughout each cluster.

might fall into another cluster. The similarity clusters will mix together unrelated animals and will separate related animals.

OK, similarities are different from relationships; but how do we know when we are dealing with a similarity and when we are dealing with a true relationship? Here are two stories that may clarify the functional differences between the two concepts:

1. You look up at the clouds, and you begin to see the shape of a lion. The cloud has a tail, like a lion's tail, and a fluffy head, like a lion's mane. With a little imagination, the mouth of the lion seems to roar down from the sky. You have succeeded in finding similarities between the cloud and a lion. If you look at a cloud and you imagine a teakettle producing a head of steam, then you are establishing a relationship between the physical forces that create a cloud and the physical forces that produce steam from a heated kettle, and you understand that clouds are composed of water vapor.
2. You look up at the stars and you see the outline of a flying horse, Pegasus, or the soup ladle, the Big Dipper. You have found similarities upon which to base the names of celestial landmarks, the constellations. The constellations help you orient yourself to the night sky, but they do not tell you much about the physical nature of the twinkling objects. If you look at the stars and you see the relationship between the twinkling stars in the night sky, and the round sun in the daylight sky, then you can begin to understand how the universe operates.

For taxonomists, the importance of grouping by relationship, not by similarity, is a lesson learned the hard way. Literally two thousand years of mis-classifications, erroneous biological theorizations, impediments to progress in medicine and agriculture, have occurred whenever similarities were confused with relationships. Early classifications of animals were based on similarities (e.g., beak shape, color of coat, or number of toes). These kinds of classifications led to the erroneous conclusion that the various juvenile forms of holometabolous insects (i.e., insects that undergo metamorphosis) were distinct organisms, unrelated to the adult form into which they would mature. The vast field of animal taxonomy was a useless mess until taxonomists began to think very deeply about classes of organisms and the fundamental properties that accounted for the relationships among the classes. [Glossary Classification system versus identification system, Classification versus index, Phenetics]

Geneticists have learned that sequence similarities among genes may bear no relationship to their functionalities, their inheritance from higher organisms, their physical locations, or to any biological process whatsoever. Geneticists use the term homology to describe the relationship among sequences that can be credited to descent from a common ancestral sequence. Similarity among different sequences can be non-homologous, developing randomly in non-related organisms, or developing by convergence, through selection for genes that have common functionality. Sequence similarity that is not acquired from a common ancestral sequence seldom relates to the shared fundamental cellular properties that characterize inherited relationships. Biological inferences drawn from gene analyses are more useful when they are built upon

phylogenetic relationships, rather than on superficial genetic or physiologic similarities [1]. [Glossary Nonphylogenetic property]

The distinction between classification by similarity and classification by relationship is vitally important to the field of computer science and to the future of Big Data analysis. I have discussed this point with many of my colleagues, who hold the opposite view: that the distinction between similarity classification and relationship classification is purely semantic. There is no practical difference between the two methods. Regardless of which side you may choose, the issue is worth pondering for a few moments.

Two arguments support the opinion that classification should be based on similarity measures. The first argument is that classification by similarity is the standard method by which relational classifications are built. The second argument is that relational properties are always unknown at the time that the classification is built. The foundation of every classification must be built on measurable features and the only comparison we have for measurable features is similarity. This argument has no scientific merit insofar as comparisons by relationship are always feasible, though not always readily computable.

The second argument, that classification by relationship requires access to unobtainable knowledge is a clever observation that hits on a weakness in the relational theory of classification. To build a classification, you must first know the relational properties that define classes, superclasses, and subclasses; but if you want to know the relationships among the classes, you must refer to the classification. It is another bootstrapping problem. [Glossary Bootstrapping]

Building a classification is an iterative process wherein you hope that your tentative selection of relational properties and your class assignments will be validated by the test of time. You build a classification by guessing which properties are fundamental and relational and by guessing which system of classes will make sense when all of the instances of the classes are assigned. A classification is often likened to a hypothesis that must be tested again and again as the classification grows.

Is it ever possible to build a classification using a hierarchical clustering algorithm based on measuring similarities among objects? The answer is a qualified yes, assuming that the object features that you have measured happen to be the relational properties that define the classes. A good example of this process is demonstrated by the work of Carl Woese and his coworkers in the field of the classification of terrestrial organisms [2]. Woese compared ribosomal RNA sequences among organisms. Ribosomal RNA is involved in the precise synthesis of proteins according to instructions coded in genes. According to Woese, the genes coding for ribosomal RNA mutate more slowly than other genes, because ribosomal RNA has scarcely any leeway in its functionality. Changes in the sequence of ribosomal RNA act like a chronometer for evolution. Using sequence similarities Woese developed a brilliant classification of living organisms that has revolutionized evolutionary genetics. Woese's analysis is not perfect and where there are apparent mistakes in his classification, disputations focus on the limitations of using similarity as a substitute for fundamental relational properties [3,4]. [Glossary Non-living organism]

The field of medical genetics has been embroiled in a debate, lasting well over a decade, on the place of race in science. Some would argue that when the genomes of humans from different races are compared, there is no sensible way to tell one genome from another, on the basis of assigned race. The genes of a tall man and the short man are more different than the genes of an African-American man and a white man. Judged by genetic similarity, race has no scientific meaning [5]. On the other hand, every clinician understands that various diseases, congenital and acquired, occur at different rates in the African-American population than in the white population. Furthermore, the clinical symptoms, clinical outcome, and even the treatment of these diseases in African-American and white individuals will sometimes differ among ethnic or racial groups. Hence, many medical epidemiologists and physicians perceive race as a clinical reality [6]. The discord stems from a misunderstanding of the meanings of similarity and of relationship. It is quite possible to have a situation wherein similarities are absent, while relationships pertain. The lack of informative genetic similarities that distinguish one race from another does not imply that race does not exist. The basis for race is the relationship created by shared ancestry. The morphologic and clinical by-product of the ancestry relationship may occur as various physical features and epidemiologic patterns found by clinicians. [Glossary Cladistics]

Fundamentally, all analysis is devoted to finding relationships among objects or classes of objects. All we ever know about the universe, and the processes that play out in our universe, can be reduced to simple relationships. In many cases the process of finding and establishing relationships often begins with finding similarities; but it must never end there.

Section 5.2. Classifications, the Simplest of Ontologies

Consciousness is our awareness of our own awareness.

Descartes

The human brain is constantly processing visual and other sensory information collected from the environment. When we walk down the street, we see images of concrete and asphalt and millions of blades of grass, birds, dogs, and other persons. Every step we take conveys a new world of sensory input. How can we process it all? The mathematician and philosopher Karl Pearson (1857–1936) has likened the human mind to a "sorting machine" [7]. We take a stream of sensory information and sort it into objects; we then collect the individual objects into general classes. The green stuff on the ground is classified as "grass," and the grass is subclassified under some larger grouping, such as "plants." A flat stretch of asphalt and concrete may be classified as a "road" and the road might be subclassified under "man-made constructions." If we lacked a culturally determined classification of objects for our world, we would be overwhelmed by sensory input, and we would have no way to remember what we see, and no way to draw general inferences about anything. Simply put, without our ability to classify, we would not be human [8].

Every culture has some particular way to impose a uniform way of perceiving the environment. In English-speaking cultures, the term "hat" denotes a universally recognized object. Hats may be composed of many different types of materials, and they may vary greatly in size, weight, and shape. Nonetheless, we can almost always identify a hat when we see one, and we can distinguish a hat from all other types of objects. An object is not classified as a hat simply because it shares a few structural similarities with other hats. A hat is classified as a hat because it has a class relationship; all hats are items of clothing that fit over the head. Likewise, all biological classifications are built by relationships, not by similarities[9,8].

Aristotle was one of the first experts in classification. His greatest insight came when he correctly identified a dolphin as a mammal. Through observation, he knew that a large group of animals was distinguished by a gestational period in which a developing embryo is nourished by a placenta, and the offspring are delivered into the world as formed, but small versions of the adult animals (i.e., not as eggs or larvae), and the newborn animals feed from milk excreted from nipples, overlying specialized glandular organs (mammae). Aristotle knew that these features, characteristic of mammals, were absent in all other types of animals. He also knew that dolphins had all these features; fish did not. He correctly reasoned that dolphins were a type of mammal, not a type of fish. Aristotle was ridiculed by his contemporaries for whom it was obvious that dolphins were a type of fish. Unlike Aristotle, they based their classification on similarities, not on relationships. They saw that dolphins looked like fish and dolphins swam in the ocean like fish, and this was all the proof they needed to conclude that dolphins were indeed fish. For about two thousand years following the death of Aristotle, biologists persisted in their belief that dolphins were a type of fish. For the past several hundred years, biologists have acknowledged that Aristotle was correct after all; dolphins are mammals. Aristotle discovered and taught the most important principle of classification; that classes are built on relationships among class members; not by counting similarities [8].

Today, the formal systems that assign data objects to classes, and that relate classes to other classes, are known as ontologies. When the data within a Big Data resource is classified within an ontology, data analysts can determine whether observations on a single object will apply to other objects in the same class.

A classification is a very simple form of ontology, in which each class is allowed to have only one parent class. To build a classification, the ontologist must do the following: (1) define classes (i.e., find the properties that define a class and extend to the subclasses of the class); (2) assign instances to classes; (3) position classes within the hierarchy; and (4) test and validate all the above. [Glossary Parent class]

The constructed classification becomes a hierarchy of data objects conforming to a set of principles:

1. The classes (groups with members) of the hierarchy have a set of properties or rules that extend to every member of the class and to all of the subclasses of the class, to the exclusion of unrelated classes. A subclass is itself a type of class wherein the members have the defining class properties of the parent class plus some additional property(ies) specific for the subclass.

2. In a hierarchical classification, each subclass may have no more than one parent class. The root (top) class has no parent class. The biological classification of living organisms is a hierarchical classification.
3. At the bottom of the hierarchy is the class instance. For example, your copy of this book is an instance of the class of objects known as "books."
4. Every instance belongs to exactly one class.
5. Instances and classes do not change their positions in the classification. As examples, a horse never transforms into a sheep, and a book never transforms into a harpsichord. [Glossary Intransitive property]
6. The members of classes may be highly similar to one another, but their similarities result from their membership in the same class (i.e., conforming to class properties), and not the other way around (i.e., similarity alone cannot define class inclusion).

Classifications are always simple; the parental classes of any instance of the classification can be traced as a simple, non-branched list, ascending through the class hierarchy. As an example, here is the lineage for the domestic horse (Equus caballus), from the classification of living organisms:

Equus caballus
Equus subg. Equus
Equus
Equidae
Perissodactyla
Laurasiatheria
Eutheria
Theria
Mammalia
Amniota
Tetrapoda
Sarcopterygii
Euteleostomi
Teleostomi
Gnathostomata
Vertebrata
Craniata
Chordata
Deuterostomia
Coelomata
Bilateria
Eumetazoa
Metazoa
Fungi/Metazoa group
Eukaryota
cellular organisms

The words in this zoological lineage may seem strange to laypersons, but taxonomists who view this lineage instantly grasp the place of domestic horses in the classification of all living organisms.

A classification is a list of every member class along with their relationships to other classes. Because each class can have only one parent class, a complete classification can be provided when we list all the classes, adding the name of the parent class for each class on the list. For example, a few lines of the classification of living organisms might be:

```
Craniata, subclass of Chordata
Chordata, subclass of Duterostomia
Deuterostomia, subclass of Coelomata
Coelomata, subclass of Bilateria
Bilateria, subclass of Eumetazoa
```

Given the name of any class a programmer can compute (with a few lines of code), the complete ancestral lineage for the class, by iteratively finding the parent class assigned to each ascending class [10]. [Glossary Iterator]

A taxonomy is a classification with the instances "filled in." This means that for each class in a taxonomy, all the known instances (i.e., member objects) are explicitly listed. For the taxonomy of living organisms the instances are named species. Currently, there are several million named species of living organisms, and each of these several million species is listed under the name of some class included in the full classification.

Classifications drive down the complexity of their data domain because every instance in the domain is assigned to a single class and every class is related to the other classes through a simple hierarchy.

It is important to distinguish a classification system from an identification system. An identification system puts a data object into its correct slot within the classification. For example, a fingerprint matching system may look for a set of features that puts a fingerprint into a special subclass of all fingerprint, but the primary goal of fingerprint matching is to establish the identity of an instance (i.e., to determine whether two sets of fingerprints belong to the same person). In the realm of medicine, when a doctor renders a diagnosis on a patient's diseases, she is not classifying the disease; she is finding the correct slot, within the preexisting classification of diseases, that holds her patient's diagnosis.

Section 5.3. Ontologies, Classes With Multiple Parents

...science is in reality a classification and analysis of the contents of the mind...
Karl Pearson [7]

Ontologies are constructions that permit an object to be a direct subclass of more than one classes. In an ontology, the class "horse" might be a subclass of Equu, a zoological term; as well as a subclass of "racing animals" and "farm animals," and "four-legged animals." The class "book" might be a subclass of "works of literature," as well as a subclass of

"wood-pulp materials," and "inked products." Ontologies are unrestrained classifications. Hence, all classifications are ontologies, but not all ontologies are classifications. Ontologies are predicated on the belief that a single object or class of objects might have multiple different fundamental identities, and that these different identities will often place one class of objects directly under more than one superclass. [Glossary Multiclass classification, Multiclass inheritance]

Data analysts sometimes prefer ontologies to classifications because they permit the analyst to find relationships among classes of objects that would have been impossible to find under a classification. For example, a data analyst might be interested in determining the relationships among groups of flying animals, such as butterflies, birds, and bats. In the classification of living organisms, these animals occupy classes that are not closely related to one another; no two of the different types of flying animals share a single parent class. Because classifications follow relationships through a lineage, they cannot connect instances of classes that fall outside the line of descent.

Ontologies are not subject to the analytic limitations imposed by classifications. In an ontology, a data object can be an instance of many different kinds of classes; thus, the class does not define the essence of the object, as it does in a classification. In an ontology the assignment of an object to a class and the behavior of the members of the objects of a class, are determined by rules. An object belongs to a class when it behaves like the other members of the class, according to a rule created by the ontologist. Every class, subclass, and superclass is defined by rules; and rules can be programmed into software.

Classifications were created and implemented at a time when scientists did not have powerful computers that were capable of handling the complexities of ontologies. For example, the classification of all living organisms on earth was created over a period of two millennia. Several million species have been assigned to date to the classification. It is currently estimated that we will need to add another 10–50 million species before we come close to completing the taxonomy of living organisms. Prior generations of scientists could cope with a simple classification, wherein each class of organisms falls under a single superclass; they could not hope to cope with a complex ontology of organisms.

The advent of powerful and accessible computers has spawned a new generation of computer scientists who have developed powerful methods for building complex ontologies. It is the goal of these computer scientists to analyze data in a manner that allows us to find and understand ontologic relationships among data objects.

In simple data collections, such as spreadsheets, data is organized in a very specific manner that preserves the relationships among specific types of data. The rows of the spreadsheet are the individual data objects (i.e., people, experimental samples, and class of information). The left-hand field of the row is typically the name assigned to the data object and the cells of the row are the attributes of the data object (e.g., quantitative measurements, categorical data, and other information). Each cell of each row occurs in a specific order and the order determines the kind of information contained in the cell. Hence, every column of the spreadsheet has a particular type of information in each spreadsheet cell. [Glossary Categorical data, Observational data]

Big Data resources are much more complex than spreadsheets. The set of features belonging to an object (i.e., the values, sometimes called variables, belonging to the object, and corresponding to the cells in a spreadsheet row) will be different for different classes of objects. For example, a member of Class Automobile may have a feature such as "average miles per gallon in city driving," while a member of Class Mammal would not. Every data object must be assigned membership in a class (e.g., Class Persons, Class Tissue Samples, and Class Bank Accounts), and every class must be assigned a set of class properties. In Big Data resources that are based on class models, the data objects are not defined by their location in a rectangular spreadsheet; they are defined by their class membership. Classes, in turn, are defined by their properties and by their relations to other classes. [Glossary Properties versus classes]

The question that should confront every Big Data manager is, "Should I model my data as a classification, wherein every class has one direct parent class; or should I model the resource as an ontology, wherein classes may have multiparental inheritance?"

Section 5.4. Choosing a Class Model

Taxonomy is the oldest profession practiced by people with their clothes on.
Quentin Wheeler, referring to the belief that Adam was assigned the task of naming all the creatures.

The simple, and fundamental question, "Can a class of objects have more than one parent class?" lies at the heart of several related fields: database management, computational informatics, object oriented programming, semantics, and artificial intelligence. Computer scientists are choosing sides, often without acknowledging the problem or fully understanding the stakes. For example, when a programmer builds object libraries in the Python or the Perl programming languages, he is choosing to program in a permissive environment that supports multiclass object inheritance. In Python and Perl, any object can have as many parent classes as the programmer prefers. When a programmer chooses to program in the Ruby programming language, he shuts the door on multiclass inheritance. A Ruby object can have only one direct parent class. Many programmers are totally unaware of the liberties and restrictions imposed by their choice of programming language, until they start to construct their own object libraries, or until they begin to use class libraries prepared by another programmer. [Glossary Artificial intelligence]

In object oriented programming the programming language provides a syntax whereby a named method is "sent" to data objects and a result is calculated. The named methods are functions and short programs contained in a library of methods created for a class. For example, a "close" method, written for file objects, typically shuts a file so that it cannot be accessed for read or write operations. In object-oriented languages a "close" method is sent to an instance of class "File" when the programmer wants to prohibit access to the file. The programming language, upon receiving the "close" method, will look for a method named "close" somewhere in the library of methods prepared for the "File" class.

If it finds the "close" method in the "File" class library, it will apply the method to the object to which the method was sent. In simplest terms the specified file would be closed.

If the "close" method were not found among the available methods for the "File" class library, the programming language would automatically look for the "close" method in the parent class of the "File" class. In some languages the parent class of the "File" class is the "Input/Output" class. If there were a "close" method in the "Input/Output" class, the method would be sent to the "File" Object. If not, the process of looking for a "close" method would be repeated for the parent class of the "Input/Output" class. You get the idea. Object oriented languages search for methods by moving up the lineage of ancestral classes for the object instance that receives the method.

In object oriented programming, every data object is assigned membership to a class of related objects. Once a data object has been assigned to a class, the object has access to all of the methods available to the class in which it holds membership, and to all of the methods in all the ancestral classes. This is the beauty of object oriented programming. If the object oriented programming language is constrained to single parental inheritance, as happens in the Ruby programming language, then the methods available to the programmer are restricted to a tight lineage. When the object oriented language permits multiparental inheritance, as happens in the Perl and Python programming languages, a data object can have many different ancestral classes spread horizontally and vertically through the class libraries. [Glossary Beauty]

Freedom always has its price. Imagine what happens in a multiparental object oriented programming language when a method is sent to a data object, and the data object's class library does not contain the method. The programming language will look for the named method in the library belonging to a parent class. Which parent class library should be searched? Suppose the object has two parent classes, and each of those two parent classes has a method of the same name in their respective class libraries? The functionality of the method will change depending on its class membership (i.e., a "close" method may have a different function within class File than it may have within class Transactions or class Boxes). There is no way to determine how a search for a named method will traverse its ancestral class libraries; hence, the output of a software program written in an object oriented language that permits multiclass inheritance is unpredictable.

The rules by which ontologies assign class relationships can become computationally difficult. When there are no restraining inheritance rules, a class within the ontology might be an ancestor of a child class that is an ancestor of its parent class (e.g., a single class might be a grandfather and a grandson to the same class). An instance of a class might be an instance of two classes, at once. The combinatorics and the recursive options can become impossible to compute. [Glossary Combinatorics]

Those who use ontologies that allow multiclass inheritance will readily acknowledge that they have created a system that is complex and unpredictable. The ontology expert justifies his complex and unpredictable model on the observation that reality itself is complex and unpredictable. A faithful model of reality cannot be created with a simple-minded classification. With time and effort, modern approaches to complex systems will

isolate and eliminate computational impedimenta; these are the kinds of problems that computer scientists are trained to solve. For example, recursion within an ontology can be avoided if the ontology is acyclic (i.e., class relationships are not permitted to cycle back onto themselves). For every problem created by an ontology an adept computer scientist will find a solution. Basically, many modern ontologists believe that the task of organizing and understanding information cannot reside within the ancient realm of classification.

For those non-programmers who believe in the supremacy of classifications, over ontologies, their faith may have nothing to do with the computational dilemmas incurred with multiclass parental inheritance. They base their faith on epistemological grounds; on the nature of objects. They hold that an object can only be one thing. You cannot pretend that one thing is really two or more things simply because you insist that it is so. One thing can only belong to one class. Once class can only have one ancestor class; otherwise, it would have a dual nature. For classical taxonomists, assigning more than one parental class to an object indicates that you have failed to grasp the essential nature of the object. The classification expert believes that ontologies (i.e., classifications that permit one class to have more than one parent classes and that permit one object to hold membership in more than one class), do not accurately represent reality.

At the heart of traditional classifications is the notion that everything in the universe has an essence that makes it one particular thing and nothing else. This belief is justified for many different kinds of systems. When an engineer builds a radio, he knows that he can assign names to components, and these components can be relied upon to behave in a manner that is characteristic of its type. A capacitor will behave like a capacitor, and a resistor will behave like a resistor. The engineer need not worry that the capacitor will behave like a semiconductor or an integrated circuit.

What is true for the radio engineer may not hold true for the Big Data analyst. In many complex systems the object changes its function depending on circumstances. For example, cancer researchers discovered an important protein that plays a very important role in the development of cancer. This protein, p53, was, at one time, considered to be the primary cellular driver for human malignancy. When p53 mutated, cellular regulation was disrupted and cells proceeded down a slippery path leading to cancer. In the past few decades, as more information was obtained, cancer researchers have learned that p53 is just one of many proteins that play some role in carcinogenesis, but the role changes depending on the species, tissue type, cellular microenvironment, genetic background of the cell, and many other factors. Under one set of circumstances, p53 may play a role in DNA repair; under another set of circumstances, p53 may cause cells to arrest the growth cycle [11,12]. It is difficult to classify a protein that changes its primary function based on its biological context.

As someone steeped in the ancient art of classification, and as someone who has written extensively on object oriented programming, I am impressed, but not convinced, by arguments on both sides of the ontology/classification debate. As a matter of practicality, complex ontologies are nearly impossible to implement in Big Data projects. The job of building and operating a Big Data resource is always difficult. Imposing a complex

ontology framework onto a Big Data resource tends to transform a tough job into an impossible job. Ontologists believe that the Big Data resources must match the complexity of their data domain. They would argue that the dictum "Keep it simple, stupid!" only applies to systems that are simple at the outset. I would comment here that one of the problems with ontology builders is that they tend to build ontologies that are much more complex than our reality. They do so because it is actually quite easy to add layers of abstraction to an ontology without incurring any immediate penalty. [Glossary KISS]

Without stating a preference for single-class inheritance (classifications) or multi-class inheritance (ontologies), I would suggest that when modeling a complex system, you should always strive to design a model that is as simple as possible. The wise ontologist will settle for a simplified approximation of the truth. Regardless of your personal preference, you should learn to recognize when an ontology has become too complex for its own good.

Here are the danger signs of an overly-complex ontology:

- You realize that the ontology makes no sense. The solutions obtained by data analysts contradict direct observations. The ontologists perpetually tinker with the model in an effort to achieve a semblance of reality and rationality. Meanwhile, the data analysts tolerate the flawed model because they have no choice in the matter.
- For a given problem, no two data analysts seem able to formulate the query the same way and no two query results are ever equivalent.
- The time spent on ontology design and improvement exceeds the time spent on collecting the data that populates the ontology.
- The ontology lacks modularity. It is impossible to remove a set of classes within the ontology without reconstructing the entire ontology. When anything goes wrong the entire ontology must be fixed or redesigned.
- The ontology cannot be fitted into a higher level ontology or a lower-level ontology.
- The ontology cannot be debugged when errors are detected.
- Errors occur without anyone knowing where the error has occurred.
- Nobody, even the designers, fully understands the ontology model.

Simple classifications are not flawless. Here are a few danger signs of an overly-simple classifications.

1. The classification is too granular.

You find it difficult to associate observations with particular instances within a class or to particular classes within the classification.

2. The classification excludes important relationships among data objects.

For example, dolphins and fish both live in water. As a consequence, dolphins and fish will both be subject to some of the same influences (e.g., ocean pollutants and water-borne infectious agents). In this case, relationships that are not based on species ancestry are simply excluded from the classification of living organisms and cannot be usefully examined.

3. The classes in the classification lack inferential competence.

Competence in the ontology field is the ability to infer answers based on the rules for class membership. For example, in an ontology you can subclass wines into white wines and red wines and you can create a rule that specifies that the two subclasses are exclusive. If you know that a wine is white, then you can infer that the wine does not belong to the subclass of red wines. Classifications are built by understanding the essential features of an object that make it what it is; they are not generally built on rules that might serve the interests of the data analyst or the computer programmer. Unless a determined effort has been made to build a rule-based classification, the ability to draw logical inferences from observations on data objects will be sharply limited.

4. The classification contains a "miscellaneous" class.

A formal classification requires that every instance belongs to a class with well-defined properties. A good classification does not contain a "miscellaneous" class that includes objects that are difficult to assign. Nevertheless, desperate taxonomists will occasionally assign objects of indeterminate nature to a temporary class, waiting for further information to clarify the object's correct placement. In the field of biological taxonomy, the task of creating and assigning the correct classes for the members of these unnatural and temporary groupings, has frustrated biologists over many decades, and is still a source of some confusion [13]. [Glossary Unclassifiable objects]

5. The classification is unstable.

Simplistic approaches may yield a classification that serves well for a limited number of tasks, but fails to be extensible to a wider range of activities or fails to integrate well with classifications created for other knowledge domains. All classifications require review and revision, but some classifications are just awful and are constantly subjected to major overhauls.

It seems obvious that in the case of Big Data, a computational approach to data classification is imperative, but a computational approach that consistently leads to failure is not beneficial. Many of the ontologies that have been created for data collected in many of the fields of science have been ignored or abandoned by their intended beneficiaries. Ontologies, due to their multi-lineage ancestries, are simply too difficult to understand and too difficult to implement.

Section 5.5. Class Blending

> *It ain't what you don't know that gets you into trouble. It's what you know for sure that just ain't so.*
>
> *Mark Twain*

A blended class, also known as a noisy class, results when the taxonomist assigns unrelated objects to the same class. This almost always leads to errors in data analysis

whose cause is nearly impossible to find. As an example of class blending, suppose you were testing the effectiveness of an antibiotic on a group of subjects all having a specific type of bacterial pneumonia. In this case, the accuracy of your results will be forfeit when your study population includes subjects with viral pneumonia, smoking-related lung damage, or a pneumonia produced by some bacteria other than the bacteria that is known to be sensitive to the antibiotic under study. Basically, a classification has no value if its classes contain unrelated members.

Errors induced by blending classes are often overlooked by data analysts who incorrectly assume that the experiment was designed to ensure that each data group is composed of a uniform and representative population. Sometimes class blending occurs when an incompetent curator misplaces data objects into the wrong class. For example, you would not want to hire an astronomer who cannot distinguish a moon from a planet. More commonly, however, the problem lies within the classification itself. It is not uncommon for the formal class definition (which includes objective criteria for including or excluding objects from the class) to be ill-conceived.

One caveat. Efforts to eliminate class blending can be counterproductive if undertaken with excessive zeal. For example, in an effort to reduce class blending, a researcher may choose groups of subjects who are uniform with respect to every known observable property. For example, suppose you want to actually compare apples with oranges. To avoid class blending, you might want to make very sure that your apples do not include any cumquats or persimmons. You should be certain that your oranges do not include any limes or grapefruits. Imagine that you go even further, choosing only apples and oranges of one variety (e.g., Macintosh apples and Navel oranges), size (e.g., 10 cm), and origin (e.g., California). How will your comparisons apply to the varieties of apples and oranges that you have excluded from your study? You may actually reach conclusions that are invalid and irreproducible for more generalized populations within each class. In this case, you have succeeded in eliminated class blending at the expense of losing representative subpopulations of the classes. Some days, the more you try, the more you lose. [Glossary Representation bias, Confounder]

Section 5.6. Common Pitfalls in Ontology Development

> *The hallmark of good science is that it uses models and theory but never believes them.*
>
> *Martin Wilk*

Do ontologies serve a necessary role in the design and development of Big Data resources? Yes. Because every Big Data resource is composed of many different types of information, it becomes important to assign types of data into groups that have similar properties: images, music, movies, documents, and so forth. The data manager needs to distinguish one type of data object from another, and must have a way of knowing the set of properties that apply to the members of each class. When a query comes in asking for a list of songs

written by a certain composer, or performed by a particular musician, the data manager will need to have a software implementation wherein the features of the query are matched to the data objects for which those features apply. The ontology that organizes the Big Data resource may be called by many other names (class systems, tables, data typing, database relationships, object model), but it will always come down to some way of organizing information into groups that share a set of properties.

Despite the importance of ontologies to Big Data resources the process of building an ontology is seldom undertaken wisely. There is a rich and animated literature devoted to the limitations and dangers of ontology-building [14,15]. Here are just a few pitfalls that you should try to avoid:

– **Do not build transitive classes.**

Class assignment is permanent. If you assign your pet beagle to the "dog" class, you cannot pluck him from this class and reassign him to the "feline" class. Once a dog, always a dog. This may seem like an obvious condition for an ontology, but it can be very tempting to make a class known as "puppy." This practice is forbidden because a dog assigned to class "puppy" will grow out of his class when he becomes an adult. It is better to assign "puppy" as a property of Class Dog, with a property definition of "age less than one year."

– **Do not build miscellaneous classes.**

As previously mentioned, even experienced ontologists will stoop to creating a "miscellaneous" class, as an act of desperation. The temptation to build a "miscellaneous" class arises when you have an instance (of a data object) that does not seem to fall into any of the well-defined classes. You need to assign the instance to a class, but you do not know enough about the instance to define a new class for the instance. To keep the project moving forward, you invent a "miscellaneous" class to hold the object until a better class can be created. When you encounter another object that does not fit into any of the defined classes, you simply assign it to the "miscellaneous" class. Now you have two objects in the "miscellaneous" class. Their only shared property is that neither object can be readily assigned to any of the defined classes. In the classification of living organisms, Class Protoctista was invented in the mid-nineteenth century to hold, temporarily, some of the organisms that could not be classified as animal, plant, or fungus. It has taken a century for taxonomists to rectify the oversight, and it may take another century for the larger scientific community to fully adjust to the revisions. Likewise, mycologists (fungus experts) have accumulated a large group of unclassifiable fungi. A pseudoclass of fungi, deuteromycetes (spelled with a lowercase "d", signifying its questionable validity as a true biologic class) was created to hold these indeterminate organisms until definitive classes can be assigned. At present, there are several thousand such fungi, sitting in taxonomic limbo, until they can be placed into a definitive taxonomic class [16]. [Glossary Negative classifier]

Sometimes, everyone just drops the ball and miscellaneous classes become permanent [17]. Successive analysts, unaware that the class is illegitimate, assumed that the "miscellaneous" objects were related to one another (i.e., related through their

"miscellaneousness"). Doing so led to misleading interpretations (e.g., finding similarities among unrelated data objects, and failing to see relationships that would have been obvious had the objects been assigned to their correct classes). The creation of an undefined "miscellaneous" class is an example of a general design flaw known as "ontological promiscuity" [14]. When an ontology is promiscuous the members of one class cannot always be distinguished from members of other classes.

– **Do not confuse properties with classes.**

Whenever I lecture on the topic of classifications and ontologies, I always throw out the following question: "Is a leg a subclass of the human body?" Most people answer yes. They reason that the normal human body contains a leg; hence leg is a subclass of the human body. They forget that a leg is not a type of human body, and is therefore not a subclass of the human body. As a part of the human body, "leg" is a property of a class. Furthermore, lots of different classes of things have legs (e.g., dogs, cows, tables). The "leg" property can be applied to many different classes and is usually asserted with a "has_a" descriptor (e.g., "Fred has_a leg"). The fundamental difference between classes and properties is one of the more difficult concepts in the field of ontology.

– **Do not invent classes and properties that have already been invented** [18].

Time-pressured ontologists may not wish to search, find, and study the classes and properties created by other ontologists. It is often easier to invent classes and properties as you need them, defining them in your own Schema document. If your ambitions are limited to using your own data for your own purposes, there really is no compelling reason to hunt for external ontologies. Problems will surface only if you need to integrate your data objects with the data objects held in other Big Data resources. If every resource invented its own set of classes and properties, then there could be no sensible comparisons among classes, and the relationships among the data objects from the different resources could not be explored.

Most data records, even those that are held in seemingly unrelated databases, contain information that applies to more than one type of class of data. A medical record, a financial record and a music video may seem to be heterogeneous types of data, but each is associated with the name of a person, and each named person might have an address. The classes of information that deal with names and addresses can be integrated across resources is they all fit into the same ontology, and if they all have the same intended meanings in each resource. [Glossary Heterogeneous data]

– **Do not use a complex data description language.**

If you decide to represent your data objects as triples, you will have a choice of languages, each with their own syntax, with which to describe your data objects. Examples of "triple" languages, roughly listed in order of increasing complexity, are: Notation 3, Turtle, RDF, DAML/OIL, and OWL. Experience suggests that syntax languages start out simple; complexity is added as users demand additional functionalities. The task of expressing triples

in DAML/OIL or OWL has gradually become a job for highly trained specialists who work in the obscure field of descriptive logic. As the complexity of the descriptive language increases the number of people who can understand and operate the resource tends to diminish. In general, complex descriptive languages should only be used by well-staffed and well-funded Big Data resources capable of benefiting from the added bells and whistles. [Glossary RDF, Triple]

Section 5.7. Case Study: An Upper Level Ontology

An idea can be as flawless as can be, but its execution will always be full of mistakes.
Brent Scowcroft

Knowing that ontologies reach into higher ontologies, ontologists have endeavored to create upper level ontologies to accommodate general classes of objects, under which the lower ontologies may take their place. Once such ontology is SUMO, the Suggested Upper Merged Ontology, created by a group of talented ontologists [19]. SUMO is owned by IEEE (Institute of Electrical and Electronics Engineers), and is freely available, subject to a usage license [14]. [Glossary RDF Ontology]

As an upper level ontology, SUMO contains classes of objects that other ontologies can refer to as their superclasses. SUMO permits multiple class inheritance. For example, in SUMO, the class of humans is assigned to two different parent classes: Class Hominid and Class CognitiveAgent. "HumanCorpse," another SUMO class, is defined in SUMO as "A dead thing that was formerly a Human." Human corpse is a subclass of Class OrganicObject; not of Class Human. This means that a human, once it ceases to live, transits to a class that is not directly related to the class of humans. Consequently, members of Class Human, in the SUMO ontology, will change their class and their ancestral lineage, at different moments in time, thus violating the non-transitive rule of classification. [Glossary Superclass]

What went wrong?

– Class HumanCorpse was not created as a subclass of Class Human. This was a mistake, as all humans will eventually die. If we were to create two classes, one called Class Living Human and one called Class Deceased Human, we would certainly cover all possible human states of being, but we would be creating a situation where members of a class are forced to transition out of their class and into another (violating the intransitive rule of classification). The solution, in this case, is simple. Life and death are properties of organisms, and all organisms can and will have both properties, but never at the same time. Assign organisms the properties of life and of death, and stop there.

One last quibble. Consider these two classes from the SUMO ontology, both of which happen to be subclasses of Class Substance.

```
Subclass NaturalSubstance
Subclass SyntheticSubstance
```

It would seem that these two subclasses are mutually exclusive. However, diamonds occur naturally, and diamonds can be synthesized. Hence, diamond belongs to Subclass NaturalSubstance and to Subclass SyntheticSubstance. The ontology creates two mutually exclusive classes that contain members of the same objects. This is problematic, because it violates the uniqueness rule of classifications. We cannot create sensible inference rules for objects that occupy mutually exclusive classes.

What went wrong?

– At first glance, the concepts "NaturalSubstance" and "SyntheticSubstance" would appear to be subclasses of "Substance." Are they really? Would it not be better to think that being "natural" or being "synthetic" are just properties of substances; not types of substances. If we agree that diamonds are a member of class substance, we can say that any specific diamond may have occurred naturally or through synthesis. We can eliminate two subclasses (i.e., "NaturalSubstance" and "SyntheticSubstance") and replace them with two properties of class "Substance": synthetic and natural. By assigning properties to a class of objects, we simplify the ontology (by reducing the number of subclasses), and we eliminate problems created when a class member belongs to two mutually exclusive subclasses. We will discuss the role of properties in classifications in Section 5.9.

As ontologies go, SUMO is one of the best, serving a useful purpose as an upper level repository of classes that can be used freely by Big Data scientists who are trying to simplify how they classify their data objects. Nonetheless, SUMO is not perfect and we are reminded that all ontologies are works-in-progress that must be critically examined, tested, and improved, in perpetuity. [Glossary Data scientist]

Section 5.8. Case Study (Advanced): Paradoxes

> *Owners of dogs will have noticed that, if you provide them with food, water, shelter, and affection, they will think you are god. Whereas owners of cats are compelled to realize that, if you provide them with food, water, shelter, and affection, they draw the conclusion that they are gods.*
>
> *Christopher Hitchens*

The rules for constructing classifications seem obvious and simplistic. Surprisingly, the task of building a logical, self-consistent classification is extremely difficult. Most classifications are rife with logical inconsistencies and paradoxes. Let us look at a few examples.

In 1975, while touring the Bethesda, Maryland, campus of the National Institutes of Health, I was informed that their Building 10 was the largest all-brick building in the world, providing a home to over 7 million bricks. Soon thereafter, an ambitious construction project was undertaken to greatly expand the size of Building 10. When the work was finished, building 10 was no longer the largest all-brick building in the world. What

happened? The builders used material other than brick, and Building 10 lost its classification as an all-brick building, violating the immutability rule of class assignments.

Apparent paradoxes that plague any formal conceptualization of classifications are not difficult to find. Let us look at a few more examples.

Consider the geometric class of ellipses; planar objects in which the sum of the distances to two focal points is constant. Class Circle is a child of Class Ellipse, for which the two focal points of instance members occupy the same position, in the center, producing a radius of constant size. Imagine that Class Ellipse is provided with a class method called "stretch," in which the foci are moved further apart, thus producing flatter objects. When the parent class "stretch" method is applied to members of the Class Circle the circle stops being a circle and becomes an ordinary ellipse. Hence the inherited "stretch" method forces members of Class Circle to transition out of their assigned class, violating the intransitive rule of classifications. [Glossary Method]

Let us look at the "Bag" class of objects. A "Bag" is a collection of objects and the Class Bag is included in most object oriented programming languages. A "Set" is also a collection of objects (i.e., a subclass of Bag), with the special feature that duplicate instances are not permitted. For example, if Kansas is a member of the set of United States states, then you cannot add a second state named "Kansas" to the set. If Class Bag were to have an "increment" method, that added "1" to the total count of objects in the bag, whenever an object is added to Class Bag, then the "increment" method would be inherited by all of the subclasses of Class Bag, including Class Set. But Class Set cannot increase in size when duplicate items are added. Hence, inheritance creates a paradox in the Class Set. [Glossary Inheritance]

How does a data scientist deal with class objects that disappear from their assigned class and reappear elsewhere? In the examples discussed here, we saw the following:

1. Building 10 at NIH was defined as the largest all-brick building in the world. Strictly speaking, Building 10 was a structure; it had a certain weight and dimensions, and it was constructed of brick. "Brick" is an attribute or property of buildings and properties cannot form the basis of a class of building, if they are not a constant feature shared by all members of the class (i.e., some buildings have bricks; others do not). Had we not conceptualized an "all-brick" class of building, we would have avoided any confusion.
2. Class Circle qualified as a member of Class Ellipse, because a circle can be imagined as an ellipse whose two focal points happen to occupy the same location. Had we defined Class Ellipse to specify that class members must have two separate focal points, we could have excluded circles from class Ellipse. Hence, we could have safely included the stretch method in Class Ellipse without creating a paradox.
3. Class Set was made a subset of Class Bag, but the increment method of class Bag could not apply to Class Set. We created Class Set without taking into account the basic properties of Class Bag, which must apply to all its subclasses. Perhaps it would have been better if Class Set and Class Bag were created as children of Class Collection; each with its own set of properties.

Section 5.9. Case Study (Advanced): RDF Schemas and Class Properties

> *It's OK to figure out murder mysteries, but you shouldn't need to figure out code. You should be able to read it.*
>
> *Steve McConnell*

In Section 4.5, "Case Study: A Syntax for Triples," we introduced the topic of RDF Schemas, and defined them as web-accessible documents that contain the definitions of classes. How does the RDF schema know how to describe the classes in such a way that computers can understand the class definitions and determine the properties that convey to all the members of a class, and to every member of every subclass of a class? Without moving too far beyond the scope of this book, we can discuss here the marvelous "trick" that RDF Schema employs that solves many of the complexity problems of ontologies and many of the over-simplification issues associated with classifications. It does so by introducing the new concept of class property. The class property permits the developer to assign features that can be associated with a class and its members. A property can apply to more than one class, and may apply to classes that are not directly related (i.e., neither an a ncestor class nor a descendant class). The concept of the assigned class property permits developers to create simple ontologies, by reducing the need to create classes to account for every feature of interest to the developer. Moreover, the concept of the assigned property gives classification developers the ability to relate instances belonging to unrelated classes through their shared property features. The RDF Schema permits developers to build class structures that preserve the best qualities of both complex ontologies and simple classifications.

How do the Class and Property definitions of RDF Schema work? The RDF Schema is a file that defines Classes and Properties. When an RDF Schema is prepared, it is simply posted onto the Internet, as a pub lic Web page, with a unique Web address.

An RDF Schema contains a list of classes, their definition, and the names of the parent class(es). This is followed by a list of properties that apply to one or more classes in the Schema. The following is an example of an RDF Schema written in plain English, without formal RDF syntax.

```
Class: Fungi
Definition: Contains all fungi
Subclass of: Class Opisthokonta (described in another RDF Schema)

Class Plantae
Definition: Includes multicellular organisms such as flowering plants,
conifers, ferns and mosses.
Subclass of: Class Archaeplastida (described in another RDF Schema)
```

```
Property: Stationary existence
Definition: Adult organism does not ambulate under its own power.
Range of classes: Class Fungi, Class Plantae

Property: Soil-habitation
Definition: Lives in soil.
Range of classes: Class Fungi, Class Plantae

Property: Chitinous cell wall
Definition: Chitin is an extracellular material often forming part of
the matrix surrounding cells.
Range of classes: Class Opisthokonta

Property: Cellulosic cell wall
Definition: Cellulose is an extracellular material often forming part
of the matric surrounding cells.
Range of classes: Class Archaeplastida
```

This Schema defines two classes: Class Fungi, containing all fungal species, and Class Plantae containing the flowering plants, conifers and mosses. The Schema defines four properties. Two of the properties (Property Stationary existence and Property Soil-habitation apply to two different classes. Two of the properties (Property Chitinous cell wall and Property Cellulosic cell wall) apply to only one class.

By assigning properties that apply to several unrelated classes, we keep the class system small, but we permit property comparisons among unrelated classes. In this case, we defined Property Stationary growth and we indicated that the property applied to instances of Class Fungi and Class Plantae. This schema permits databases that contain data objects assigned to Class Fungi or data objects assigned to Class Plantae to include data object values related to Property Stationary Growth. Data analysts can collect data from any plant or fungus data object and examine these objects for data values related to Stationary Growth.

Property Soil-habitation applies to Class Fungi and to Class Plantae. Objects of either class may include soil-habitation data values. Data objects from two unrelated classes (Class Fungi and Class Plantae) can be analyzed by a shared property.

The schema lists two other properties, Property Chitinous cell wall and Property Cellulosic cell wall. In this case each property is assigned to one class only. Property Chitinous cell wall applies to Class Opisthokonta. Property Cellulosic cell wall applies to Class Archaeplastidae. These two properties are exclusive to their class. If a data object is described as having a cellulosic cell wall, it cannot be a member of Class Opisthokonta. If a data object is described as having a chitinous cell wall, then it cannot be a member of Class Archaeplastidae.

A property assigned to a class will extend to every member of every descendant class. Class Opisthokonta includes Class Fungi and it also includes Class Animalia, the class of

all animals. This means that all animals may have the property of chitinous cell wall. In point of fact, chitin is distributed widely through the animal kingdom, but is not found in mammals.

As the name implies, RDF Schema are written in RDF syntax. In practice, many of the so-called RDF Schema documents found on the web are prepared in alternate formats. They are nominally RDF syntax because they create a namespace for classes and properties referred by triples listed in RDF documents.

Here is a short schema, written as Turtle triples, and held in a fictitious web site, "http://www.fictitious_site.org/schemas/life#" [Glossary Turtle]

```
@prefix rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#>
@prefix rdfs: <http://www.w3.org/2000/01/rdf-schema#>
@base <http://www.fictitious_site.org/schemas/life#>
:Homo instance_of rdfs:Class.
:HomoSapiens instance_of rdfs:Class;
   rdfs:subClassOf :Homo.
```

Turtle triples have a somewhat different syntax than N-triples or N3 triples. As you can see, the turtle triple resembles RDF syntax in form, allowing for nested metadata/data pairs assigned to the same object. Nonetheless, turtle triples use less verbiage than RDF, but convey equivalent information. In this minimalist RDF Schema, we specify two classes that would normally be included in the much larger classification of living organisms: Homo and HomoSapiens.

A triple that refers to our "http://www.fictitious_site.org/schemas/life#" Schema might look something like this:

```
:Batman instance_of <http://www.fictitious_site.org/schemas/
life#>:HomoSapiens.
```

The triple asserts that Batman is an instance of Homo Sapiens. The data "HomoSapiens" links us to the RDF Schema, which in turn tells us that HomoSapiens is a class and is the subclass of Class Homo.

One of the many advantages of triples is their fungibility. Once you have created your triple list, you can port them into spreadsheets, or databases, or morph them into alternate triple dialects, such as RDF or N3. Triples in any dialect can be transformed into any other dialect with simple scripts using your preferred programming language.

RDF documents can be a pain to create, but they are very easy to parse. Even in instances when an RDF file is composed of an off-kilter variant of RDF, it is usually quite easy to write a short script that will parse through the file, extracting triples, and using the components of the triples to serve the programmer's goals. Such goals may include: counting occurrences of items in a class, finding properties that apply to specific subsets of items in specific classes, or merging triples extracted from various triplestore databases. [GlossaryTriplestore]

RDF seems like a panacea for ontologists, but it is seldom used in Big Data resources. The reasons for its poor acceptance are largely due to its strangeness. Savvy data

mangers who have led successful careers using standard database technologies are understandably reluctant to switch over to an entirely new paradigm of information management. Realistically, a novel and untested approach to data description, such as RDF, will take decades to catch on. Whether RDF emerges as the data description standard for Big Data resources is immaterial. The fundamental principles upon which RDF is built are certain to dominate the world of Big Data.

Section 5.10. Case Study (Advanced): Visualizing Class Relationships

The ignoramus is a leaf who doesn't know he is part of a tree

Attributed to Michael Crichton

When working with classifications or ontologies, it is useful to have an image that represents the relationships among the classes. GraphViz is an open source software utility that produces graphic representations of object relationships.

The GraphViz can be downloaded from:
http://www.graphviz.org/

GraphViz comes with a set of applications that generate graphs of various styles. Here is an example of a GraphViz dot file, number.dot, constructed in GraphViz syntax [20]. Aside from a few lines that provide instructions for line length and graph size the dot file is a list of classes and their child classes.

```
digraph G {
  size="7,7";
  Object -> Numeric;
  Numeric -> Integer;
  Numeric -> Float;
  Integer -> Fixnum
  Integer -> Bignum
}
```

After the GraphViz exe file (version graphviz-2.14.1.exe, on my computer) is installed, you can launch the various GraphViz methods as command lines from its working directory, or through a system call from within a script. [Glossary Exe file, System call]

```
c:\ftp\dot>dot -Tpng number.dot -o number.png
```

The command line tells GraphViz to use the dot method to produce a rendering of the number.dot text file, saved as an image file, with filename number.png. The output file contains a class hierarchy, beginning with the highest class and branching until it reaches the lowest descendant class.

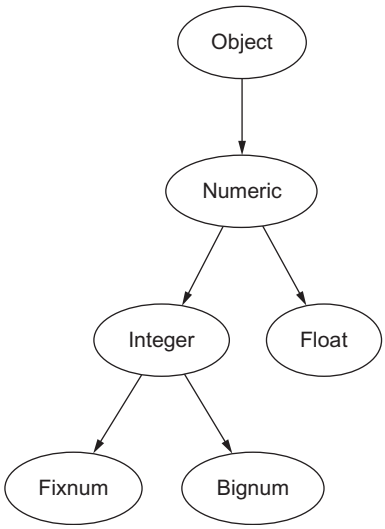

FIG. 5.2 A class hierarchy, described by the number.dot file and converted to a visual file, using GraphViz.

With a glance, we see that the highest class is Class Object (Fig. 5.2). Class Object has one child class, Class Numeric. Numeric has two child classes, Class Integer and Class Float. Class Integer has two child classes, Class Fixnum and Class Bignum. You might argue that a graphic representation of classes was unnecessary; the textual listing of class relationships was all that you needed. Maybe so, but when the class structure becomes complex, visualization can greatly simplify your understanding of the relationships among classes.

Here is a visualization of a classification of human neoplasms (Fig. 5.3). It was produced by GraphViz, from a .dot file containing a ranking of classes and their subclasses, and rendered with the "twopi" method, shown: [Glossary Object rank]

```
c:\ftp>twopi -Tpng neoplasms.dot -o neoplasms_classes.png
```

We can look at the graphic version of the classification and quickly make the following observations:

1. The root class (i.e., the ancestor to every class) is Class Neoplasm. The GraphViz utility helped us find the root class, by placing it in the center of the visualization.
2. Every class is connected to other classes. There are no classes sitting out in space, unrelated to other classes.
3. Every class that has a parent class has exactly one parent class.
4. There are no recursive branches to the graph (e.g., the ancestor of a class cannot also be a descendant of the class).

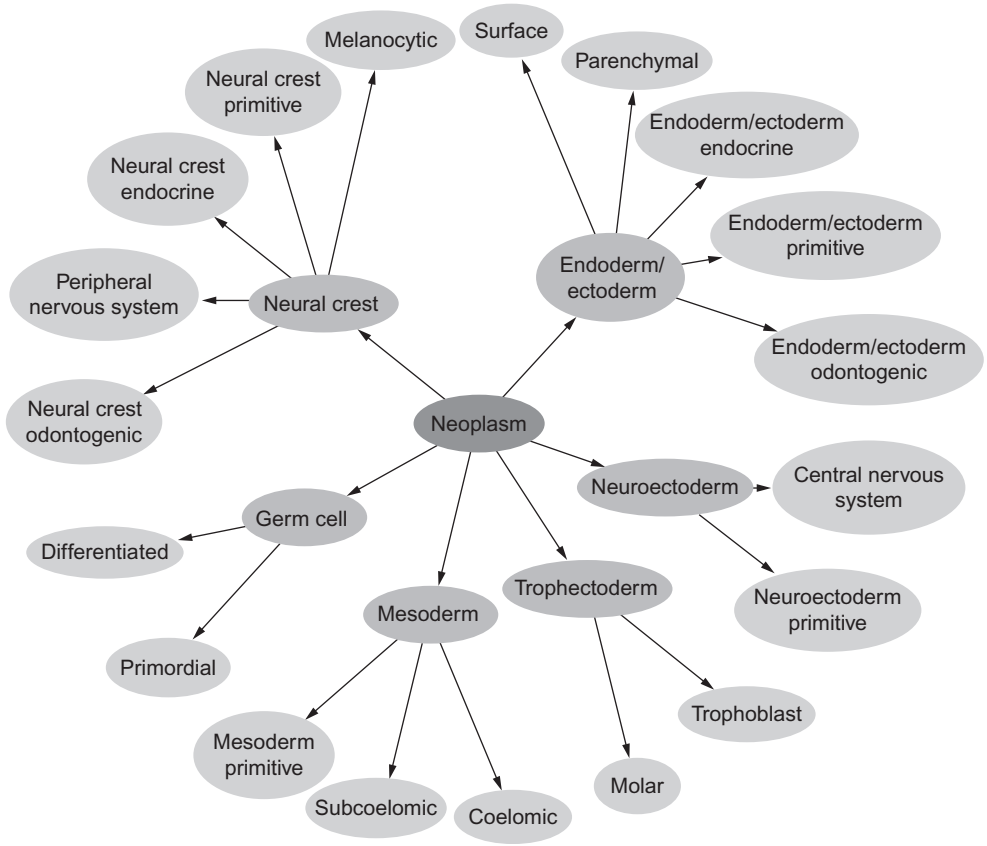

FIG. 5.3 A visualization of relationships in a classification of tumors. The image was rendered with the GraphViz utility, using the twopi method, which produced a radial classification, with the root class in the center.

If we had only the textual listing of class relationships, without benefit of a graphic visualization, it would be very difficult for a human to verify, at a glance, the internal logic of the classification.

With a few tweaks to the neo.dot GraphViz file, we can create a nonsensical graphic visualization:

Notice that one cluster of classes is unconnected to the other, indicating that class Endoderm/Ectoderm has no parent classes (Fig. 5.4). Elsewhere, Class Mesoderm is both child and parent to Class Neoplasm. Class Melanocytic and Class Molar are each the child class to two different parent classes. At a glance, we have determined that the classification is highly flawed. The visualization simplified the relationships among classes, and allowed us to see where the classification went wrong. Had we only looked at the textual listing of classes and subclasses, we may have missed some or all of the logical flaws in our classification.

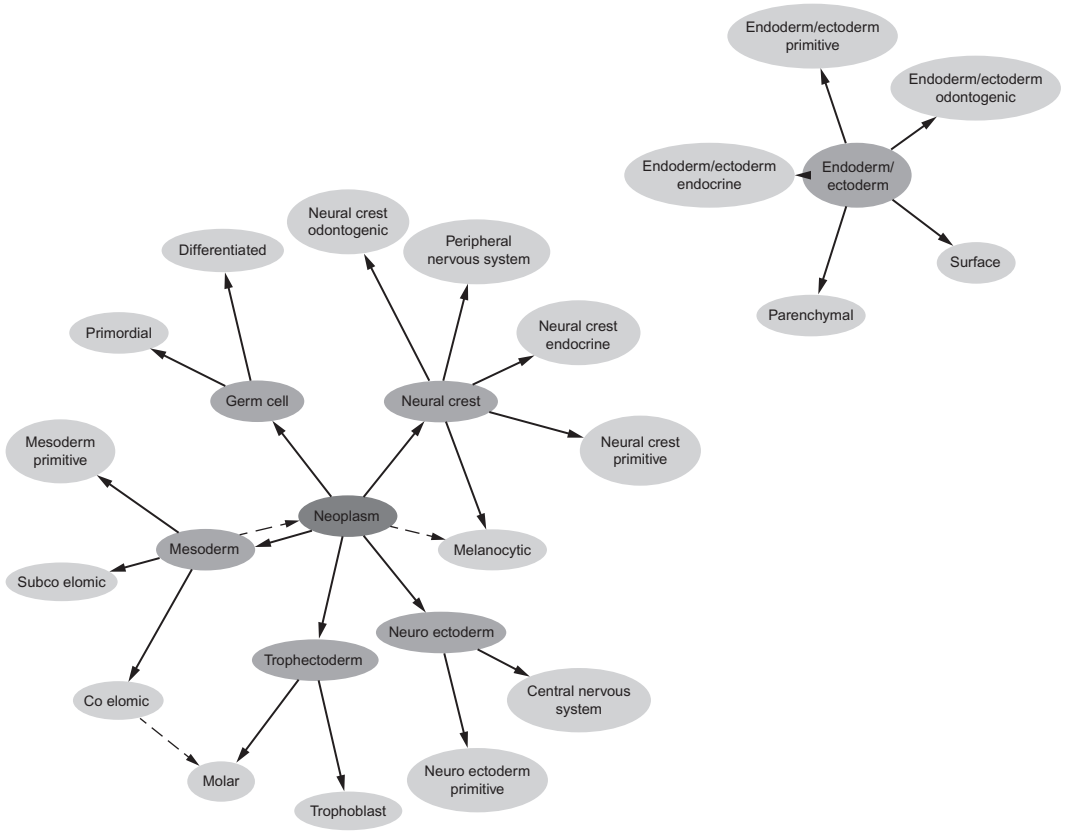

FIG. 5.4 A corrupted classification that might qualify as a valid ontology.

At this point, you may be thinking that visualizations of class relationships are nice, but who has the time and energy to create the long list of classes and subclasses, in GraphViz syntax, that are the input files for the GraphViz methods? Now comes one of the great payoffs of data specifications. You must remember that good data specifications are fungible. A modestly adept programmer can transform a specification into whatever format is necessary to do a particular job. In this case, the classification of neoplasms had been specified as an RDF Schema (vida supra). An RDF Schema includes the definitions of classes and properties, with each class provided with the name of its parent class and each property provided with its range (i.e., the classes to which the property applies). Because class relationships in an RDF Schema are specified, it is easy to transform an RDF Schema into a .dot file suitable for Graphviz.

Here is a short RDF python script, dot.py that parses an RDF Schema (contained in the plain-text file, schema.txt) and produces a GraphViz .dot file, named schema.dot. [Glossary Metaprogramming]

```
import re, string
infile = open('schema.txt', "r")
outfile = open("schema.dot", "w")
outfile.write("digraph G {\n")
outfile.write("size=\"15,15\";\n")
outfile.write("ranksep=\"3.00\";\n")
clump = ""
for line in infile:
  namematch = re.match(r'\<\/rdfs\:Class>', line)
  if (namematch):
    father = ""
    child = ""
    clump = re.sub(r'\n', ' ', clump)
    fathermatch = re.search(r'\:resource\=\"[a-zA-Z0-9\:\/\_\.\-]*
\#([a-zA-Z\_]+)\"', clump)
    if fathermatch:
      father = fathermatch.group(1)
    childmatch = re.search(r'rdf\:ID\=\"([a-zA-Z\_]+)\"', clump)
    if childmatch:
      child = childmatch.group(1)
    outfile.write(father + " -> " + child + ";\n")
    clump = ""
  else:
    clump = clump + line
outfile.write("}\n")
```

The first 15 lines of output of the dot.pl script:

```
digraph G {
size="15,15";
ranksep="2.00";
Class -> Tumor_classification;
Tumor_classification -> Neoplasm;
Tumor_classification -> Unclassified;
Neural_tube -> Neural_tube_parenchyma;
Mesoderm -> Sub_coelomic;
Neoplasm -> Endoderm_or_ectoderm;
Unclassified -> Syndrome;
Neoplasm -> Neural_crest;
Neoplasm -> Germ_cell;
Neoplasm -> Pluripotent_non_germ_cell;
Sub_coelomic -> Sub_coelomic_gonadal;
Trophectoderm -> Molar;
```

The full schema.dot file, not shown, is suitable for use as an input file for the GraphViz utility.

Glossary

Artificial intelligence Artificial intelligence is the field of computer science that seeks to create machines and computer programs that seem to have human intelligence. The field of artificial intelligence sometimes includes the related fields of machine learning and computational intelligence. Over the past few decades the term "artificial intelligence" has taken a battering from professionals inside and outside the field, for good reasons. First and foremost is that computers do not think in the way that humans think. Though powerful computers can now beat chess masters at their own game, the algorithms for doing so do not simulate human thought processes. Furthermore, most of the predicted benefits from artificial intelligence have not come to pass, despite decades of generous funding. The areas of neural networks, expert systems, and language translation have not met expectations. Detractors have suggested that artificial intelligence is not a well-defined subdiscipline within computer science as it has encroached into areas unrelated to machine intelligence, and has appropriated techniques from other fields, including statistics and numerical analysis. Some of the goals of artificial intelligence have been achieved (e.g., speech-to-text translation), and the analytic methods employed in Big Data analysis should be counted among the enduring successes of the field.

Beauty To mathematicians, beauty and simplicity are virtually synonymous, both conveying the idea that someone has managed to produce something of great meaning or value from a minimum of material. Euler's identity, relating e, i, pi, 0, and 1 in a simple equation, is held as an example of beauty in mathematics. When writing this book, I was tempted to give it the title, "The Beauty of Data," but I feared that a reductionist flourish, equating data simplification with beauty, was just too obscure.

Bootstrapping The act of self-creation, from nothing. The term derives from the ludicrous stunt of pulling oneself up by one's own bootstraps. Its shortened form, "booting" refers to the startup process in computers in which the operating system is somehow activated via its operating system, which has not been activated. The absurd and somewhat surrealistic quality of bootstrapping protocols serves as one of the most mysterious and fascinating areas of science. As it happens, bootstrapping processes lie at the heart of some of the most powerful techniques in data simplification (e.g., classification, object oriented programming, resampling statistics, and Monte Carlo simulations).

It is worth taking a moment to explore the philosophical and the pragmatic aspects of bootstrapping. Starting from the beginning, how was the universe created? For believers, the universe was created by an all-powerful deity. If this were so, then how was the all-powerful deity created? Was the deity self-created, or did the deity simply bypass the act of creation altogether? The answers to these questions are left as an exercise for the reader, but we can all agree that there had to be some kind of bootstrapping process, if something was created from nothing. Otherwise, there would be no universe, and this book would be much shorter than it is. Getting back to our computers, how is it possible for any computer to boot its operating system, when we know that the process of managing the startup process is one of the most important functions of the fully operational operating system? Basically, at startup, the operating system is non-functional. A few primitive instructions hardwired into the computer's processors are sufficient to call forth a somewhat more complex process from memory, and this newly activated process calls forth other processes, until the operating system is eventually up and running. The cascading rebirth of active processes takes time and explains why booting your computer may seem to be a ridiculously slow process.

What is the relationship between bootstrapping and classification? The ontologist creates a classification based on a worldview in which objects hold specific relationships with other objects. Hence, the ontologist's perception of the world is based on preexisting knowledge of the classification of

things; which presupposes that the classification already exists. Essentially, you cannot build a classification without first having the classification. How does an ontologist bootstrap a classification into existence? She may begin with a small assumption that seems, to the best of her knowledge, unassailable. In the case of the classification of living organisms, she may assume that the first organisms were primitive, consisting of a few self-replicating molecules and some physiologic actions, confined to a small space, capable of a self-sustaining system. Primitive viruses and prokaryotes (i.e., bacteria) may have started the ball rolling. This first assumption might lead to observations and deductions, which eventually yield the classification of living organisms that we know today. Every thoughtful ontologist will admit that a classification is, at its best, a hypothesis-generating machine; not a factual representation of reality. We use the classification to create new hypotheses about the world and about the classification itself. The process of testing hypotheses may reveal that the classification is flawed; that our early assumptions were incorrect. More often, testing hypotheses will reassure us that our assumptions were consistent with new observations, adding to our understanding of the relations between the classes and instances within the classification.

Categorical data Non-numeric data in which objects are assigned categories, with categories having no numeric order. Yes or no, male or female, heads or tails, snake-eyes or boxcars, are types of unordered categorical data. Traditional courses in mathematics and statistics stress the analysis of numeric data, but data scientists soon learn that much of their work involves the collection and analysis of non-numeric data.

Cladistics The technique of producing a hierarchy of clades, wherein each branch includes a parent species and all its descendant species, while excluding species that did not descend from the parent (Fig. 5.5). If a subclass of a parent class omits any of the descendants of the parent class, then the parent class is said to be paraphyletic. If a subclass of a parent class includes organisms that did not descend from the parent, then the parent class is polyphyletic. A class can be paraphyletic and polyphyletic, if it excludes organisms that were descendants of the parent and if it includes organisms that did not descend from the parent. The goal of cladistics is to create a hierarchical classification that consists exclusively of monophyletic classes (i.e., no paraphyly, no polyphyly). Classifications of the kinds described in this chapter, are monophyletic.

Classification system versus identification system It is important to distinguish a classification system from an identification system. An identification system matches an individual organism with its assigned object name (or species name, in the case of the classification of living organisms). Identification is based on finding several features that, taken together, can help determine the name of an organism. For example, if you have a list of characteristic features: large, hairy, strong, African, jungle-dwelling, knuckle-walking; you might correctly identify the organisms as a gorilla. These identifiers are different from the phylogenetic features that were used to classify gorillas within the hierarchy of

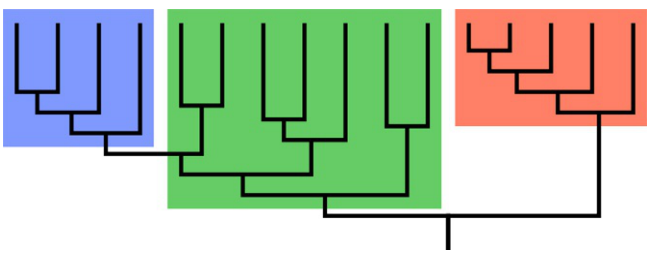

FIG. 5.5 Schematic (cladogram) of all the descendant branches of a common ancestor (stem at bottom of image). The left and the right groups represent clades insofar as they contain all their descendants and exclude classes that are not descendants of the group root. The middle group is not a valid clade because it does not contain all of the descendants of its group root (i.e., it is paraphyletic). Specifically, it excludes the left-most group in the diagram. *From Wikimedia Commons, author "Life of Riley".*

organisms (Animalia: Chordata: Mammalia: Primates: Hominidae: Homininae: Gorillini: Gorilla). Specifically, you can identify an animal as a gorilla without knowing that a gorilla is a type of mammal. You can classify a gorilla as a member of Class Gorillini without knowing that a gorilla happens to be large. One of the most common mistakes in science is to confuse an identification system with a classification system. The former simply provides a handy way to associate an object with a name; the latter is a system of relationships among objects.

Classification versus index In practice, an index is an alphabetized listing of the important terms in a work (e.g., book), with the locations of each term within the work. Ideally, though, an index should be much more than that. An idealized index is a conceptualization of a corpus of work that enables users to locate the concepts that are discussed and created within the work. How does an idealized index differ from a classification? A classification is a way of organizing concepts in classes, wherein the relationships of the concepts are revealed. The classification can incorporate all of the information held in an index by encapsulating the concept locations together with the names of the concepts. Because the relationships among the objects in a classification can be used to draw inferences about the objects, we can think of a classification as an index that can help us think.

Cluster analysis Clustering algorithms provide a way of taking a large set of data objects that seem to have no relationship to one another, and to produce a visually simple collection of clusters wherein each cluster member is similar to every other member of the same cluster. The algorithmic methods for clustering are simple. One of the most popular clustering algorithms is the k-means algorithm, which assigns any number of data objects to one of k clusters [21]. The number k of clusters is provided by the user. The algorithm is easy to describe and to understand, but the computational task of completing the algorithm can be difficult when the number of dimensions in the object (i.e., the number of attributes associated with the object), is large. There are some serious drawbacks to the algorithm: (1) The final set of clusters will sometimes depend on the initial, random choice of k data objects. This means that multiple runs of the algorithm may produce different outcomes; (2) The algorithms are not guaranteed to succeed. Sometimes, the algorithm does not converge to a final, stable set of clusters; (3) When the dimensionality is very high, the distances between data objects (i.e., the square root of the sum of squares of the measured differences between corresponding attributes of two objects) can be ridiculously large and of no practical meaning. Computations may bog down, cease altogether, or produce meaningless results. In this case, the only recourse may require eliminating some of the attributes (i.e., reducing dimensionality of the data objects); (4) The clustering algorithm may succeed, producing a set of clusters of similar objects, but the clusters may have no practical value. They may miss important relationships among the objects, or they might group together objects whose similarities are totally non-informative. The biggest drawback associated with cluster analyses is that researchers may mistakenly believe that that the groupings produced by the method constitute a valid biological classification. This is not the case because biological entities (genes, proteins, cells, organs, organisms) may share many properties and still be fundamentally different. For example, two genes may have the same length and share some sub-sequences, but both genes may have no homology with one another (i.e., no shared ancestry) and may have no common or similar expressed products. Another set of genes may be structurally dissimilar but may belong to the same family. The groupings produced by cluster analysis should never be equated with a classification. At best, cluster analysis produces groups that can be used to start piecing together a biological classification.

Combinatorics The analysis of complex data often involves combinatorics; the evaluation, on some numeric level, of combinations of things. Often, combinatorics involves pairwise comparisons of all possible combinations of items. When the number of comparisons becomes large, as is the case with virtually all combinatoric problems involving large data sets, the computational effort becomes massive. For this reason, combinatorics research has become a subspecialty in applied mathematics and data science. There are four "hot" areas in combinatorics. The first involves building increasingly powerful computers capable of solving complex combinatoric problems. The second involves

developing methods whereby combinatoric problems can be broken into smaller problems that can be distributed to many computers, to provide relatively fast solutions to problems that could not otherwise be solved in any reasonable length of time The third area of research involves developing new algorithms for solving combinatoric problems quickly and efficiently. The fourth area, perhaps the most promising area, involves developing innovative non-combinatoric solutions for traditionally combinatoric problems, a golden opportunity for experts in the field of data simplification.

Confounder Unanticipated or ignored factor that alters the outcome of a data analysis. Confounders are particularly important in Big Data analytics, because most analyses are observational; based on collected parameters from large numbers of data records, and there is very little control over confounders. Confounders are less of a problem in controlled prospective experiments, in which a control group and a treated group are alike, to every extent feasible; only differing in their treatment. Differences between the control group and the treated group are presumed to be caused by the treatment, as all of the confounders have been eliminated. One of the greatest challenges of Big Data analytics involves developing new analytic protocols that reduce the effect of confounders in observational studies.

Data scientist Anyone who practices data science and who has some expertise in a field subsumed by data science (i.e., informatics, statistics, data analysis, programming, and computer science).

Exe file Short for executable file and also known as application file. A file containing a program, in binary code, that can be executed when the name of the file is invoked on the command line.

Heterogeneous data Sets of data that are dissimilar with regard to content, purpose, format, organization, and annotations. One of the purposes of Big Data is to discover relationships among heterogeneous data sources. For example, epidemiologic data sets may be of service to molecular biologists who have gene sequence data on diverse human populations. The epidemiologic data is likely to contain different types of data values, annotated and formatted in a manner that is completely different from the data and annotations in a gene sequence database. The two types of related data, epidemiologic and genetic, have dissimilar content; hence they are heterogeneous to one another.

Inheritance The method by which a child is endowed with features of the parent. In object oriented programming, inheritance is passed from parent class to child class, meaning that the child class has access to all of the methods and properties that are held in the parent class.

Intransitive property One of the criteria for a classification is that every object (sometimes referred to as member or as instance) belongs to exactly one class. From this criteria comes the intransitive property of classifications; namely, an object cannot change its class. Otherwise an object would belong to more than one class at different times. It is easy to apply the intransitive rule under most circumstances. A cat cannot become a dog and a horse cannot become a sheep. What do we do when a caterpillar becomes a butterfly? In this case, we must recognize that caterpillar and butterfly represent phases in the development of one particular instance of a species, and do not belong to separate classes.

Iterator Iterators are simple programming shortcuts that call functions that operate on consecutive members of a data structure, such as a list, or a block of code. Typically, complex iterators can be expressed in a single line of code. Perl, Python and Ruby all have iterator methods. In Ruby, the iterator methods are each, find, collect, and inject. In Python, there are types of objects that are iterable (not to be confused with "irritable"), and these objects accept implicit or scripted iteration methods.

KISS Acronym for Keep It Simple Stupid. With respect to Big Data, there are basically two schools of thought. This first is that reality is quite complex, and the advent of powerful computers and enormous data collections allows us to tackle important problems, despite their inherent size and complexity. KISS represents a second school of thought; that Big Problems are just small problems that are waiting to be simplified.

Metaprogramming A metaprogram is a program that creates or modifies other programs. Metaprogramming is a particularly powerful feature of languages that are modifiable at runtime. Perl, Python, and Ruby are all metaprogramming languages. There are several techniques that facilitate metaprogramming features, including introspection and reflection.

Method Roughly equivalent to functions, subroutines, or code blocks. In object-oriented languages, a method is a subroutine available to an object (class or instance). In Ruby and Python, instance methods are declared with a "def" declaration followed by the name of the method, in lowercase. Here is an example, in Ruby, for the "hello" method, is written for the Salutations class.

```
class Salutations
  def hello
     puts "hello there"
  end
end
```

Multiclass classification A misnomer imported from the field of machine translation, and indicating the assignment of an instance to more than one class. Classifications, as defined in this book, impose one-class classification (i.e., an instance can be assigned to one and only one class). It is tempting to think that a ball should be included in class "toy" and in class "spheroids," but multiclass assignments create unnecessary classes of inscrutable provenance, and taxonomies of enormous size, consisting largely of replicate items.

Multiclass inheritance In ontologies, multiclass inheritance occurs when a child class has more than one parent class. For example, a member of Class House may have two different parent classes: Class Shelter, and Class Property. Multiclass inheritance is generally permitted in ontologies but is forbidden in classifications that restrict inheritance to a single parent class (i.e., each class can have at most one parent class, though it may have multiple child classes). When an object-oriented program language permits multiparental inheritance (e.g., Perl and Python programming languages), data objects may have many different ancestral classes spread horizontally and vertically through the class libraries. There are many drawbacks to multi-class inheritance in object oriented programming languages and these have been discussed at some length in the computer science literature [22]. Medical taxonomists should understand that when multi-class inheritance is permitted, a class may be an ancestor of a child class that is an ancestor of its parent class (e.g., a single class might be a grandfather and a grandson to the same class). An instance of a class might be an instance of two classes, at once. The combinatorics and the recursive options can become computationally difficult or impossible. Those who use taxonomies that permit multiclass inheritance will readily acknowledge that they have created a system that is complex. Ontology experts justify the use of multiclass inheritance on the observation that such ontologies provide accurate models of nature and that faithful models of reality cannot be created with simple, uniparental classification. Taxonomists who rely on simple, uniparental classifications base their model on epistemological grounds; on the nature of objects. They hold that an object can have only one nature and can belong to only one defining class, and can be derived from exactly one parent class. Taxonomists who insist upon uniparental class inheritance believe that assigning more than one parental class to an object indicates that you have failed to grasp the essential nature of the object [22–24].

Negative classifier One of the most common mistakes committed by ontologists involves classification by negative attribute. A negative classifier is a feature whose absence is used to define a class. An example is found in the Collembola, popularly known as springtails, a ubiquitous member of Class Hexapoda, and readily found under just about any rock. These organisms look like fleas (same size, same shape) and were formerly misclassified among the class of true fleas (Class Siphonaptera). Like fleas, springtails are wingless, and it was assumed that springtails, like fleas, lost their wings somewhere in evolution's murky past. However, true fleas lost their wings when they became parasitic. Springtails never had wings, an important taxonomic distinction separating springtails from fleas. Today, springtails (Collembola) are assigned to Class Entognatha, a separate subclass of Class Hexapoda. Alternately, taxonomists may be deceived by a feature whose absence is falsely conceived to be a

fundamental property of a class of organisms. For example, all species of Class Fungi were believed to have a characteristic absence of a flagellum. Based on the absence of a flagellum, the fungi were excluded from Class Opisthokonta and were put in Class Plantae, which they superficially resembled. However, the chytrids, which have a flagellum, were have been shown to be a primitive member of Class Fungi. This finding places fungi among the true descendants of Class Opisthokonta (from which Class Animalia descended). This means that fungi are much more closely related to people than to plants, a shocking revelation [13]!

Non-living organism Herein, viruses and prions are referred to as non-living organisms. Viruses lack key features that distinguish life from non-life. They depend entirely on host cells for replication; they do not partake in metabolism, and do not yield energy; they cannot adjust to changes in their environment (i.e., no homeostasis), nor can they respond to stimuli. Most scientists consider viruses to be mobile genetic elements that can travel between cells (much as transposons are considered mobile genetic elements that travel within a cell). All viruses have a mechanism that permits them to infect cells and to use the host cell machinery to replicate. At minimum, viruses consist of a small RNA or DNA genome, encased by a protective protein coat, called a capsid. Class Mimiviridae, discovered in 1992, occupies a niche that seems to span the biological gulf separating living organisms from viruses. Members of Class Mimiviridae are complex, larger than some bacteria, with enormous genomes (by viral standards), exceeding a million base pairs and encoding upwards of 1000 proteins. The large size and complexity of Class Mimiviridae exemplifies the advantage of a double-stranded DNA genome. Class Megaviridae is a newly reported (October, 2011) class of viruses, related to Class Mimiviridae, but even larger [25]. Biologically, the life of a mimivirus is not very different from that of obligate intracellular bacteria (e.g., Rickettsia). The discovery of Class Mimiviridae inspires biologists to reconsider the "non-living" status relegated to viruses and compels taxonomists to examine the placement of viruses within the phylogenetic development of prokaryotic and eukaryotic organisms [13].

Nonphylogenetic property Properties that do not hold true for a class; hence, cannot be used by ontologists to create a classification. For example, we do not classify animals by height, or weight because animals of greatly different heights and weights may occupy the same biological class. Similarly, animals within a class may have widely ranging geographic habitats; hence, we cannot classify animals by locality. Case in point: penguins can be found virtually anywhere in the southern hemisphere, including hot and cold climates. Hence, we cannot classify penguins as animals that live in Antarctica or that prefer a cold climate. Scientists commonly encounter properties, once thought to be class-specific that prove to be uninformative, for classification purposes. For many decades, all bacteria were assumed to be small; much smaller than animal cells. However, the bacterium *Epulopiscium fishelsoni* grows to about 600 microns by 80 microns, much larger than the typical animal epithelial cell (about 35 microns in diameter) [26]. *Thiomargarita namibiensis*, an ocean-dwelling bacterium, can reach a size of 0.75 mm, visible to the unaided eye. What do these admittedly obscure facts teach us about the art of classification? Superficial properties, such as size, seldom inform us how to classify objects. The ontologist must think very deeply to find the essential defining features of classes.

Object rank A generalization of Page rank, the indexing method employed by Google. Object ranking involves providing objects with a quantitative score that provides some clue to the relevance or the popularity of an object. For the typical object ranking project, objects take the form of a key word phrase.

Observational data Data obtained by measuring existing things or things that occurred without the help of the scientist. Observational data needs to be distinguished from experimental data. In general, experimental data can be described with a Gaussian curve, because the experimenter is trying to measure what happens when a controlled process is performed on every member of a uniform population. Such experiments typically produce Gaussian (i.e., bell-shaped or normal) curves for the control population and the test population. The statistical analysis of experiments reduces to the chore

of deciding whether the resulting Gaussian curves are different from one another. In observational studies, data is collected on categories of things, and the resulting data sets often follow a Zipf distribution, wherein a few types of data objects account for the majority of observations For this reason, many of the assumptions that apply to experimental data (i.e., the utility of parametric statistical descriptors including average, standard deviation and p-values), will not necessarily apply to observational data sets [24].

Parent class The immediate ancestor, or the next-higher class (i.e., the direct superclass) of a class. For example, in the classification of living organisms, Class Vertebrata is the parent class of Class Gnathostomata. Class Gnathostomata is the parent class of Class Teleostomi. In a classification, which imposes single class inheritance, each child class has exactly one parent class; whereas one parent class may have several different child classes. Furthermore, some classes, in particular the bottom class in the lineage, have no child classes (i.e., a class need not always be a superclass of other classes). A class can be defined by its properties, its membership (i.e., the instances that belong to the class), and by the name of its parent class. When we list all of the classes in a classification, in any order, we can always reconstruct the complete class lineage, in their correct lineage and branchings, if we know the name of each class's parent class [13].

Phenetics The classification of organisms by feature similarity, rather than through relationships. Starting with a set of feature data on a collection of organisms, you can write a computer program that will cluster the organisms into classes, according to their similarities. In theory, one computer program, executing over a large dataset containing measurements for every earthly organism, could create a complete biological classification. The status of a species is thereby reduced from a fundamental biological entity, to a mathematical construction.

There are a host of problems consequent to computational methods for classification. First, there are many different mathematical algorithms that cluster objects by similarity. Depending on the chosen algorithm, the assignment of organisms to one species or another would change. Secondly, mathematical algorithms do not cope well with species convergence. Convergence occurs when two species independently acquire identical or similar traits through adaptation; not through inheritance from a shared ancestor. Examples are: the wing of a bat and the wing of a bird; the opposable thumb of opossums and of primates; the beak of a platypus and the beak of a bird. Unrelated species frequently converge upon similar morphologic adaptations to common environmental conditions or shared physiological imperatives. Algorithms that cluster organisms based on similarity are likely to group divergent organisms under the same species.

It is often assumed that computational classification, based on morphologic feature similarities, will improve when we acquire whole-genome sequence data for many different species. Imagine an experiment wherein you take DNA samples from every organism you encounter: bacterial colonies cultured from a river, unicellular non-bacterial organisms found in a pond, small multicellular organisms found in soil, crawling creatures dwelling under rocks, and so on. You own a powerful sequencing machine, that produces the full-length sequence for each sampled organism, and you have a powerful computer that sorts and clusters every sequence. At the end, the computer prints out a huge graph, wherein all the samples are ordered and groups with the greatest sequence similarities are clustered together. You may think you have created a useful classification, but you have not really, because you do not know anything about the organisms that are clustered together. You do not know whether each cluster represents a species, or a class (a collection of related species), or whether a cluster may be contaminated by organisms that share some of the same gene sequences, but are phylogenetically unrelated (i.e., the sequence similarities result from chance or from convergence, but not by descent from a common ancestor). The sequences do not tell you very much about the biological properties of specific organisms, and you cannot infer which biological properties characterize the classes of clustered organisms. You have no certain knowledge whether the members of any given cluster of organisms can be characterized by any particular gene sequence (i.e., you do not know the characterizing

gene sequences for classes of organisms). You do not know the genus or species names of the organisms included in the clusters, because you began your experiment without a presumptive taxonomy. Basically, you simply know what you knew before you started; that individual organisms have unique gene sequences that can be grouped by sequence similarity.

Taxonomists, who have long held that a species is a natural unit of biological life, and that the nature of a species is revealed through the intellectual process of building a consistent taxonomy [27], are opposed to the process of phenetics-based classification [27,13]. In the realm of big data, computational phenetics may create a complex web of self-perpetuating nonsense that cannot be sensibly analyzed. Over the next decade or two, the brilliance or the folly of computational phenetics will most likely be revealed.

Properties versus classes When creating classifications, the most common mistake is to assign class status to a property. When a property is inappropriately assigned as a class, then the entire classification is ruined. Hence, it is important to be very clear on the difference between these two concepts, and to understand why it is human nature to confuse one with the other. A class is a holder of related objects (e.g., items, records, categorized things). A property is a feature or trait that can be assigned to an item. When inclusion in a class requires items to have a specific property, we often name the class by its defining property. For example Class Rodentia, which includes rats, mice, squirrels, and gophers, are all gnawing mammals. The word rodent derives from the Latin roots rodentem, rodens, from rodere, "to gnaw." Although all rodents gnaw, we know that gnawing is not unique to rodents. Rabbits (Class Lagormorpha) also gnaw.

Objects from many different classes may have some of the same properties. Here's another example. Normal human anatomy includes two legs. This being the case, is "leg" a subclass of "human." The answer is no. A leg is not a type of human. Having a leg is just one of many properties associated with normal human anatomy. You would be surprised how many people can be tricked into thinking that a leg, which is itself an object, should be assigned as a subclass of the organisms to which it is attached. Some of this confusion comes from the way that we think about relationships between objects and properties. We say "He is hungry," using a term of equality, "is" to describe the relationship between "He" and "hungry." Technically, the sentence, "He is hungry" asserts that "He" and "hungry" are equivalent objects. We never bother to say "He has hunger," but other languages are more fastidious. A German might say "Ich habe Hunger," indicating that he has hunger, and avoiding any inference that he and hunger are equivalent terms (i.e., never "Ich bin Hunger"). It may seem like a trivial point, but mistaking classes for properties is a common error that nearly always leads to disaster.

RDF Resource Description Framework (RDF) is a syntax in XML notation that formally expresses assertions as triples. The RDF triple consists of a uniquely identified subject plus a metadata descriptor for the data plus a data element. Triples are necessary and sufficient to create statements that convey meaning. Triples can be aggregated with other triples from the same data set or from other data sets, so long as each triple pertains to a unique subject that is identified equivalently through the data sets. Enormous data sets of RDF triples can be merged or functionally integrated with other massive or complex data resources.

RDF Ontology A term that, in common usage, refers to the class definitions and relationships included in an RDF Schema document. The classes in an RDF Schema need not comprise a complete ontology. In fact, a complete ontology could be distributed over multiple RDF Schema documents.

Representation bias Occurs when the population sampled does not represent the population intended for study. For example, the population for which the normal range of prostate specific antigen (PSA) was based, was selected from a county in the state of Minnesota. The male population under study consisted almost exclusively of white men (i.e., virtually no African-Americans, Asians, Hispanics, etc.). It may have been assumed that PSA levels would not vary with race. It was eventually determined that the normal PSA ranges varied greatly by race [28]. The Minnesota data, though plentiful, did not represent racial subpopulations. A sharp distinction must drawn between Big-ness and Whole-ness [29].

Superclass Any of the ancestral classes of a subclass. For example, in the classification of living organisms, the class of vertebrates is a superclass of the class of mammals. The immediate superclass of a class is its parent class. In common parlance, when we speak of the superclass of a class, we are usually referring to its parent class.

System call Refers to a command, within a running script, that calls the operating system into action, momentarily bypassing the programming interpreter for the script. A system call can do essentially anything the operating system can do via a command line.

Triple In computer semantics, a triple is an identified data object associated with a data element and the description of the data element. In theory, all Big Data resources can be composed as collections of triples. When the data and metadata held in sets of triples are organized into ontologies consisting of classes of objects and associated properties (metadata), the resource can potentially provide introspection (the ability of a data object to be self-descriptive). An in-depth discussion of triples is found in Chapter 4, "Metadata, Semantics, and Triples."

Triplestore A list or database composed entirely of triples (statements consisting of an item identifier plus the metadata describing the item plus an item of data. The triples in a triplestore need not be saved in any particular order, and any triplestore can be merged with any other triplestore; the basic semantic meaning of the contained triples is unaffected. Additional discussion of triplestores can be found in Section 6.5, "Case Study: A Visit to the TripleStore."

Turtle Another syntax for expressing triples. From RDF came a simplified syntax for triples, known as Notation 3 or N3 [30]. From N3 came Turtle, thought to fit more closely to RDF. From Turtle came an even more simplified form, known as N-Triples.

Unclassifiable objects Classifications create a class for every object and taxonomies assign each and every object to its correct class. This means that a classification is not permitted to contain unclassified objects; a condition that puts fussy taxonomists in an untenable position. Suppose you have an object, and you simply do not know enough about the object to confidently assign it to a class. Or, suppose you have an object that seems to fit more than one class, and you can't decide which class is the correct class. What do you do?

Historically, scientists have resorted to creating a "miscellaneous" class into which otherwise unclassifiable objects are given a temporary home, until more suitable accommodations can be provided. I have spoken with numerous data managers, and everyone seems to be of a mind that "miscellaneous" classes, created as a stopgap measure, serve a useful purpose. Not so. Historically, the promiscuous application of "miscellaneous" classes has proven to be a huge impediment to the advancement of science. In the case of the classification of living organisms, the class of protozoans stands as a case in point. Ernst Haeckel, a leading biological taxonomist in his time, created the Kingdom Protista (i.e., protozoans), in 1866, to accommodate a wide variety of simple organisms with superficial commonalities. Haeckel himself understood that the protists were a blended class that included unrelated organisms, but he believed that further study would resolve the confusion. In a sense, he was right, but the process took much longer than he had anticipated; occupying generations of taxonomists over the following 150 years.

Today, Kingdom Protista no longer exists. Its members have been reassigned to positions among the animals, plants, and fungi. Nonetheless, textbooks of microbiology still describe the protozoans, just as though this name continued to occupy a legitimate place among terrestrial organisms. In the meantime, therapeutic opportunities for eradicating so-called protozoal infections, using class-targeted agents, have no doubt been missed [13].

You might think that the creation of a class of living organisms, with no established scientific relation to the real world, was a rare and ancient event in the annals of biology, having little or no chance of being repeated. Not so. A special pseudoclass of fungi, deuteromyctetes (spelled with a lowercase "d," signifying its questionable validity as a true biologic class) has been created to hold fungi of

indeterminate speciation. At present, there are several thousand such fungi, sitting in a taxonomic limbo, waiting to be placed into a definitive taxonomic class [16,13].

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6

Introspection

OUTLINE

Section 6.1. Knowledge of Self

All science is description and not explanation.

Karl Pearson [1]

Not very long ago a cancer researcher sent me one of his published papers. For his study, he used a publicly available collection of gene micro-array data collected on tumors. He knew that I was a long-time proponent of open access scientific data sets and that I had been encouraging my colleagues to use these available data sources for various analytic projects. I read the paper with admiration, but the "methods" section of the paper did not provide much description of the human lung cancer tissues that were used to generate the micro-array data. [Glossary Open access]

I called the researcher and asked, perhaps a bit undiplomatically, the following question: "The methods section indicates that data on 12 lung cancer tissues, provided by the repository, were studied. How do you distinguish whether these were 12 lung cancer samples from 12 different patients, or 12 samples of tissue all taken from one lung cancer, in one patient?" If it were the former (12 lung cancers from each of 12 patients), his study conclusions would have applied to a sampling of different tumors and might reasonably apply to lung cancers in general. If it were the latter (12 samples of one tumor), then his generalized conclusion was unjustified.

There was a pause on the line, and I was told that he had neglected to include that information in the manuscript, but the paper included a link to the repository Web site, where the detailed sample information was stored.

After our conversation, I visited the Web site, and found that there was very little information describing the samples included in the database. There was a sample number, followed by the name of a type of cancer (lung cancer, in this case), and then there was

Principles and Practice of Big Data. https://doi.org/10.1016/B978-0-12-815609-4.00006-6

the raw gene-array data. Were the multiple samples taken from multiple patients, or were all those samples taken from one tumor, in one patient? We could not say, because the data would not tell us.

I contacted the researcher again and reiterated the problem. He agreed that the people at the repository should have been more attentive to data annotation. It has been my experience that some data analysts believe that their professional responsibility begins with the received data. In their opinion, pre-analytic issues, such as those described above, do not fall under their professional jurisdiction. This approach to Big Data analysis is an invitation for disaster. Studies emanating from Big Data resources have no scientific value and the Big Data resources are all a waste of time and money, if data analysts cannot uncover all the information that fully describes their data.

The aforementioned story serves as an introduction to the concept of introspection, a term that is not commonly applied to Big Data resources; but should be. Introspection is a term taken from the field of object oriented programming, and it refers to the ability of data objects to describe themselves, when called upon. In object oriented programming languages, everything is objectified. Variables are objects, parameters are objects, methods are objects, and so on. Every object carries around its own data values, as well as an identifier, and self-descriptive information, including its class assignment (i.e., the name of the class of objects to which it belongs). An object can have its own methods (similar to subroutines), and it has access to a library of methods built for its class (i.e., class methods) and from the ancestor classes in its lineage (i.e., superclass methods).

Most object oriented programming languages have methods that can call an object to describe itself. To illustrate, let us see how Ruby, a popular object oriented programming language, implements introspection.

First, let us create a new object, "x"; we will assign "hello world" to the object.

```
x = "hello world"    yields "hello world"
```

Ruby knows that "hello world" is a string and automatically assigns "x" to Class String. We can check any object to see determine its class by sending the "class" method to the object, as shown.

```
x.class        yields String
```

When we send the "class" method to x, Ruby outputs its class assignment, "String." Every class (except the top level class in the hierarchy) has a single parent class, also known as a superclass. We can learn the name of the superclass of Class String, by sending the superclass method, as shown.

```
x.class.superclass    yields Object
```

Ruby tells us that the superclass of Class String is Class Object.

Ruby assigns a unique identifier to every created object. We can find the object identifier by sending "x" the object_id method.

```
x.object_id      yields 22502910
```

The unique object identifier for "x" is 22502910.

If we ever need to learn the contents of "x," we can send the inspect method to the object.

```
x.inspect        yields "hello world"
```

Ruby reminds us that "x" contains the string, "hello world."

Every data object in Ruby inherits dozens of class methods. We can generate a list of methods available to "x" by sending it the "methods" method.

```
x.methods
```

Ruby yields a list of dozens of methods, including a few that we can try out here: "length", "is_a?", "upcase", "downcase", "capitalize", and "reverse."

```
x.length        yields 11
```

The length method, sent to "x" yields the number of characters in "hello world."

```
x.is_a?(String)     yields true
```

When Ruby uses the is_a? method to determine if x is a member of Class String, it yields "true."

```
x.is_a?(Integer)     yields false
```

When Ruby uses the is_a? method to determine if x is a member of Class Integer, it yields "false."

```
x.upcase          yields "HELLO WORLD"
x.downcase        yields "hello world"
x.capitalize      yields "Hello world"
x.reverse         yields "dlrow olleh"
```

String methods sent to the "x" object return appropriate values, as shown above.

What happens when we send "x" a method from a library of methods built for some other class?

The "nonzero?" method tests to see whether an object of Class Integer is zero. This method is useful to avoid division by zero.

Let us see what happens when we send "x" the "nonzero?" method.

```
x.nonzero?       Yields NoMethodError: undefined method `nonzero?'
                 for "hello world":String
```

Ruby sends us an error message, indicating that "nonzero?" is an undefined method for an object of Class String.

How does introspection, a feature of object oriented programming languages, apply to Big Data? In principle, Big Data resources must have the same features of introspection that are automatically provided by object oriented programming languages. Specifically, all data pertaining to the object must be encapsulated within data objects to include the raw data, a description for the raw data (the so-called metadata), the name of the class to

which the data object belongs, and a unique identifier that distinguishes the data object from all other data objects.

I must admit that most Big Data resources lack introspection. Indeed, most Big Data managers are unfamiliar with the concept of introspection as it applies to Big Data. When you speak to the people who manage and use these resources, you may be surprised to learn that they are happy, even ecstatic, about their introspection-free resource. As far as they are concerned, their resource functions just fine, without introspection. When pressed on the subject of data introspection, data managers may confess that their Big Data resources may fall short of perfection, but their users have accommodated themselves to minor deficiencies.

There is always a price to pay when Big Data resources lack introspection. Symptoms of an introspection-free Big Data resource include:

- The resource is used for a narrow range of activities, somewhat less than was originally proposed when the resource was initiated.
- The resource is used by a small number of domain experts; to all others, the resource is inscrutable.
- The data records for the resource cannot be verified. It is impossible to eliminate the possibility that records may have been duplicated or that data may have been mistakenly inserted into the wrong records (i.e., the data records may have been corrupted).
- The resource cannot merge its data with data contained in other Big Data resources.
- The resource cannot match its record identifiers with record identifiers from other resources. For example, if each of two Big Data resources has a record on the same individual, the resources cannot sensibly combine the two records into a single record.
- The resource cannot add legacy data, collected by their own institution on older software system, into the current Big Data resource.
- Despite employing a crew of professionals for the resource, only one individual seems to be privy to the properties of data objects in the largely undocumented system. When he is absent, the system tends to crash.

Introspection is not a feature that you can attach to a Big Data resource, as an afterthought. Introspection is a foundational component of any well-designed data resource. Most Big Data resources will never attain the level of introspection available in object oriented programming languages, but some introspective features would seem essential.

Section 6.2. Data Objects: The Essential Ingredient of Every Big Data Collection

Computer Science is no more about computers than astronomy is about telescopes.
Edsger W. Dijkstra

If you have been following the computer science literature, you may have noticed that the term "data object" has been slowly replacing the shorter, simpler, and more understandable term "data." Do we really need to clutter our minds with yet another example of dispensable technojargon?

Yes, we must. Despite every intention to minimize the use of jargon in this book, the term "data object" has already insinuated itself into this book dozens of times. Back in Section 3.1, we offered a loose definition of data object as "a collection of data that contains self-describing information, and one or more data values." In this section, we will expand the definition to indicate the role of data objects in Big Data construction and analyses.

Like everything else in this fledgling field of Big Data, there is no canonical definition for "data object." As you might expect, practitioners of subdisciplines of computer science provide definitions of data object that coincide with the way they happen to employ data objects in their work. For example, someone who works exclusively with relational databases will refer to data tables, indexes, and views as data objects. A programmer who uses assembly language might refer to a data object as any data that can be referenced from a particular address in memory. A programmer who works with a typed language, such as Ada, might think of a data object as being data that has been assigned a particular type (e.g., string, integer, float).

We can try to find a reasonable definition for data object that serves the imperatives of Big Data, but before we do, let us look at a few triples.

```
75898039563441  name              G. Willikers
75898039563441  gender            male
75898039563441  age               35
75898039563441  is_a_class_member human
```

These triples tell us a few things about a 35-year-old male named G. Willikers, who is a human. Without losing any information, we can rearrange this collection of triples under its identifier, as shown here:

```
75898039563441
 name              G. Willikers
 gender            male
 age               35
 is_a_class_member human
```

Now, we can begin to see how a collection of triples, all having the same identifier, might compose a single data object. What we have is one identifier followed by all the available meta/data data pairs that bind to the same identifier. Someone who prefers working with spreadsheets might interpret this as a row (with "75898039563441" as its key); having metadata as its column headers, and having the data as the contents of the row's cells. We can guess that the relational database programmer would recognize this as a table.

The assembly language programmer would look at the same collection and surmise that it represents the data culled from a referenced address in memory.

For our purposes, let us try to think of the collection as a data object, defined as an object identifier along with all of the data/metadata pairs that rightly belong to the object identifier, and that includes one data/metadata pair that tells us the object's class (i.e., "human" in this example).

By adding a triple that provides class membership, the data object immediately gains all of the properties associated with its class "Human," and this might include a birth date, a social security number, and an address. If a programmer were to write a set of computational methods for the class "Human," then every member of class "Human," including instance 75898039563441, would be qualified to access those methods. In the next section, we will describe how programmers use the information available within data objects to understand and to utilize the relationships among data objects. Before proceeding, there are a few properties of data objects that we should examine. Notice that there is no special order for the data/metadata pairs encapsulated within the data object. We could shuffle the data/metadata pairs any way we please. Furthermore, if each data/metadata pair was attached to its identifier (75898039563441, in this case), as a triple, then there would be no special reason to store the components of the data object in one particular memory location.

The following triple could be stored in a server in California:

```
75898039563441  name      G. Willikers
```

The next triple could be stored in a server in Iceland:

```
75898039563441  gender     male
```

The triples that compose the data object may exist anywhere and everywhere (i.e., stored as replicates), and we might have no knowledge of the number of object's data/metadata pairs that exist at any moment of time. Wherever the pieces of the data object may reside, they will forever have the same unique identifier, and will always belong to the same data object. It is best to think of a data object as an abstraction that is made practical by software created by programmers. Object oriented programming languages are designed to create data objects assigned to classes, and provide them with useful computational methods.

Section 6.3. How Big Data Uses Introspection

"Si sol deficit, respicit me nemo" ("If the sun's gone, nobody looks at me")

Latin motto

Let us look at how data objects are used to understand and explore Big Data. First, we must understand a few new concepts that have been developed for Object-Oriented programming languages, but which apply to all data that supports introspection: encapsulation, inheritance, polymorphism, and reflection.

Encapsulation refers to general property of a data object to contain the data pertaining to itself (i.e., its identifier and its data/metadata pairs). When we say "contain," we are not referring to a physical container. We are indicating that there is some way by which a programmer can access an object's identifier and its data/metadata pairs, through methods provided by a programming language. The data can be scattered on servers throughout the globe. So long as there are methods for retrieving the data/metadata pairs, and ascertaining that these pairs belong to a unique data object, and to no other data object, then we say that the data object encapsulates its data.

Inheritance refers to the ability of a data object to respond appropriately to methods created for its class, and for all of its ancestral classes. For example, all members of Class Document can respond to methods created for its class, such as a "screen_display" method, or a "printer_print" or a "copy_me" method. Furthermore, since all documents are composed of strings of alphanumeric sequences, we know that Class Document is a descendant of Class String. Hence, members of Class Document will inherit the methods created for Class String, such as a "lowercase" method, a "concatenate" method, or a "find_substring" method.

This object oriented concept of inheritance fits nicely with the concept of inheritance, as known to zoologists: every animal inherits the properties of its ancestors. For example, humans are descendants of the class of animals known as the vertebrates (i.e., Class Vertebrata). This means that every human, like all animal classes that descend from Class Vertebrata, contains a vertebra, and all such animals have shared properties inherited from their common ancestor (e.g., they all have anatomic structures derived from gill arches that appear in embryologic development and they all share genes and proteins that were included in the vertebrates from which they descended).

The key thing to understand, whether you are a computer programmer or a zoologist, is that inheritance only helps us if we have created a sensible classification (see the principles of classification in Section 5.2).

Polymorphism is the ability of an object to respond to a named method in a manner that is appropriate for its own class. For example, if I sent a "double" method to an object belonging to Class Integer, I might expect it to multiply its contained integer by itself (e.g., 5 * 2 = 10). If I sent the "double" method to an object belonging to Class String, I might expect it to simply concatenate the contained string to itself (e.g., "3y228hw" would become "3y228hw3y228hw").

How does a data object know how to respond polymorphically (i.e., in a manner appropriate for its class) to a method? In object oriented programming, classes have methods that apply to every instance (i.e., member) belonging to the class. When you send the "double" method to an integer object the integer object knows the name of its own class and will look inside its class object for a class method named "double." If it finds the method, it will do whatever its class method tells it to do; in this case, it will multiply its integer contents by two. If the double method were sent to a member of Class String, the data object would pull the "double" method written for objects of the String class, and would respond appropriately; by concatenating its contained string to itself.

Polymorphism is achieved by having objects respond to different methods, written for different classes. The different methods may happen to have the same name (i.e., "double" in this example), but each data object only has access to the "double" method that was written for its class.

Now, suppose the data object looks within the collection of methods available to its class, and fails to find what it's looking for. In that case, it will look at the methods contained in the parent class of Class String. Remember, in a good classification, every class contains the name of its parent class; hence the ancestral lineage of any class object can be computationally traced, up to the root class of the classification. This means that a class object can search its entire ancestry, if need be, looking for a "double" method. When it finds the method, it stops and does whatever the method instructs it to perform. This is known as inheritance polymorphism.

Underlying all these methods (encapsulation, inheritance, and polymorphism) is a technique known as abstraction. Abstraction encompasses all techniques wherein data objects are unencumbered by the details of their operational repertoires. For example, the programmer who sends a method to an object does not need to create the program by which the method operates. Object methods can be chosen from class libraries. The object that receives the method does not need to contain the instructions for executing the method. The object simply needs to know the class to which it has been assigned membership. Objects will always pull the methods that are appropriate for their own classes. In object oriented languages, the class libraries subsume the nitty-gritty of programming, and the burden of holding all the information required by data objects is abstracted into the class structure of the data domain. Not surprisingly, programs written in object oriented programming languages are famously short, consisting mostly of one-word methods, sent to one-word names for complex data objects.

There is one more concept that we must discuss: reflection. If you were to take introspective data gleaned on-the-fly during the execution of a program and you used that data to modify the run-time instructions of the same program, then you would be achieving reflection. There are many situations when reflection might come in handy. For example, you might use introspection to determine that a data object was created prior to 2010; and then exclude that data object from subsequent computations intended to show the average value of measurements performed from 2010 to the present.

What are the benefits of these object-oriented concepts. For the purposes of Big Data, object-oriented approaches drive down the complexity of the system. Once the classification has been created, and all of the data objects are assigned to one and only one class within the classification, all of the wonderful concepts of object-oriented programming (encapsulation, inheritance, polymorphism, and reflection) come to us gratis. The methods in the class libraries can be written without knowing anything about the individual class objects. The instances of class objects can exist unencumbered by any information pertaining to the classification, other than the name of the class in which they belong.

Section 6.4. Case Study: Time Stamping Data

People change and forget to tell each other.

Lillian Hellman, playwright (1905–1984)

Consider the following assertions:

```
Alexander Goodboy, 34 inches height
Alexander Goodboy, 42 inches height
Alexander Goodboy, 46 inches height
Alexander Goodboy, 52 inches height
```

At first glance these assertions seem contradictory. How can Alexander Goodboy be 34, 42, 46, and 52 inches tall? The confusion is lifted when we add some timing information to the assertions:

```
Alexander Goodboy, age 3 years, 34 inches height
Alexander Goodboy, age 5 years, 42 inches height
Alexander Goodboy, age 7 years, 46 inches height
Alexander Goodboy, age 9 years, 52 inches height
```

All events, measurements and transactions occur at a particular time, and it is essential to annotate data objects with their moment of creation and with every moment when additional data is added to the data object (i.e., event times) [2]. It is best to think of data objects as chronicles of a temporal sequence of immutable versions of the object. In the case of Alexander Goodboy, the boy changes in height as he grows, but each annotated version of Alexander Goodboy (e.g., Alexander Goodboy, age 3 years, height 34 inches) is eternal and immutable. [Glossary Immutability]

Time stamping is nothing new. Ancient scribes were fastidious time stampers. It would be an unusual Sumerian, Egyptian, or Mayan document that lacked an inscribed date. In contrast, it is easy to find modern, Web-based news reports that lack any clue to the date that the Web page was created. Likewise, it is a shameful fact that most spreadsheet data lacks time stamps for individual data cells. Data sets that lack time stamps, unique identifiers, and metadata have limited value to anyone other than the individual who created the data and who happens to have personal knowledge of how the data was created and what the data means.

Fortunately, all computers have an internal clock. This means that all computer events can be time stamped. Most programming languages have a method for generating the epoch time; the number of seconds that have elapsed since a particular moment in time. On most systems the epoch is the first second of January 1, 1970. Perl, Python, and Ruby have methods for producing epoch time. For trivia-sake, we must observe that the UUID time stamp is generated for an epoch time representing the number of seconds elapsed since the first second of Friday, October 15, 1582 (See Section 5.1, “Unique Identifiers”). This moment marks the beginning of the Gregorian calendar. The end of the Julian

calendar occurred on October 4, 1582. The 11 days intervening, from the end of the Julian calendar to the start of the Gregorian calendar, are lost somewhere in time and space.

From Python's interactive environment:

```
import time
print(time.time())
output:
1442353742.456994
```

if you would like the GMT (Greenwich Mean Time), try this gmtime.py script:

```
import time
print(time.gmtime())
output:
time.struct_time(tm_year=2017, tm_mon=10, tm_mday=12, tm_hour=14,
tm_min=3, tm_sec=0, tm_wday=3, tm_yday=285, tm_isdst=0)
```

It is very important to understand that country-specific styles for representing the date are a nightmare for data scientists. As an example, consider: "2/4/97." This date signifies February 4, 1997 in America; and April 2, 1997 in Great Britain and much of the world. There basically is no way of distinguishing with certainty 2/4/97 and 4/2/97.

It is not surprising that an international standard, the ISO-8601, has been created for representing date and time [3]. The international format for date and time is: YYYY-MM-DD hh:mm:ss.

The value "hh" is the number of complete hours that have passed since midnight. The upper value of hh is 24 (midnight). If hh = 24, then the minute and second values must be zero (think about it). An example of and ISO-8601-compliant data and time is:

```
1995-02-04 22:45:00
```

An alternate form, likewise ISO-8601-compliant, is:

```
1995-02-04T22:45:00Z
```

In the alternate form, a "T" replaces the space left between the date and the time, indicating that time follows date. A "Z" is appended to the string indicating that the time and date are computed for UTC (Coordinated Universal Time, formerly known as Greenwich Mean Time, and popularly known as Zulu time, hence the "Z").

Here is a Python script, format_time.py, that generates the date and time, compliant with ISO-8601.

```
import time, datetime
timenow = time.time()
print(datetime.datetime.fromtimestamp(timenow).strftime('%Y-%m-%d
%H:%M:%S'))
```

Here is the output of the format_time.py script:

```
2015-09-16 07:44:09
```

It is sometimes necessary to establish, beyond doubt, that a time stamp is accurate and has not been modified. Through the centuries, a great many protocols have been devised to prove that a time stamp is trustworthy. One common implementation of a trusted time stamp protocol involves sending a message digest (i.e., a one-way hash) of a confidential document to a time stamp authority. The timestamp authority adds a date to the received message digest and returns a time-annotated message, encrypted with the time stamp authority's private key, containing the original one-way hash plus the trusted date. The received message can be decrypted with the timestamp authority's public key to reveal the date/time and the message digest that is unique for the original document. It might seem as though the trusted time stamp process is a lot of work, but regular users of these services can routinely process hundreds of documents in seconds. We will be revisiting the subject of time stamps in Chapter 8, Immutability and Immortality. [Glossary Message digest, Symmetric key, Trusted time stamp]

Section 6.5. Case Study: A Visit to the TripleStore

Before I speak, I have something important to say.

Groucho Marx

Enormous benefits follow when data objects are expressed as triples and assigned to defined classes. All of the attributes of object oriented programming languages (i.e., inheritance, encapsulation, abstraction, and polymorphism) are available to well-organized collections of triples. Furthermore, desirable features in any set of data, including integration, interoperability, portability, and introspection are available to data scientists who analyze triplestore data. Most importantly, when triples are collected as a triplestore, a simple analysis of the triplestore yields all the relations among data objects, and all the information needed to assemble every data object,

Here is a small example of a triplestore:

```
9f0ebdf2^^object_name^^Class
9f0ebdf2^^property^^subclass_of
9f0ebdf2^^property^^property
9f0ebdf2^^property^^definition
9f0ebdf2^^property^^object_name
9f0ebdf2^^property^^instance_of
9f0ebdf2^^subclass_of^^Class
9f0ebdf2^^instance_of^^Class
701cb7ed^^object_name^^Property
701cb7ed^^subclass_of^^Class
```

```
701cb7ed^^definition^^^the metadata class
77cb79d5^^object_name^^instance_of
77cb79d5^^instance_of^^Property
77cb79d5^^definition^^the name of the class to which the object is an
instance
a03fbc3b^^object_name^^object_name
a03fbc3b^^instance_of^^Property
a03fbc3b^^definition^^word equivalent of its predicate identifying
sequence
de0e5aa1^^object_name^^subclass_of
de0e5aa1^^instance_of^^Property
de0e5aa1^^definition^^the name of the parent class of the referred object
4b675067^^object_name^^property
4b675067^^instance_of^^Property
4b675067^^definition^^an identifier a for class property
c37529c5^^object_name^^definition
c37529c5^^instance_of^^Property
c37529c5^^definition^^the meaning of the referred object
a29c59c0^^object_name^^dob
a29c59c0^^instance_of^^Property
a29c59c0^^definition^^date of birth, as Day, Month, Year
a34a1e35^^object_name^^glucose_at_time
a34a1e35^^instance_of^^Property
a34a1e35^^definition^^glucose level in mg/Dl at time drawn (GMT)
03cc6948^^object_name^^Organism
03cc6948^^subclass_of^^Class
7d7ff42b^^object_name^^Hominidae
7d7ff42b^^subclass_of^^Organism
7d7ff42b^^property^^dob
a0ce8ec6^^object_name^^Homo
a0ce8ec6^^subclass_of^^Hominidae
a0ce8ec6^^property^^glucose_at_time
a1648579^^object_name^^Homo sapiens
a1648579^^subclass_of^^Homo
98495efc^^object_name^^Andy Muzeack
98495efc^^instance_of^^Homo sapiens
98495efc^^dob^^1 January, 2001
98495efc^^glucose_at_time^^87, 02-12-2014 17:33:09
```

Perusal of the triples provides the following observations:

1. Individual triples are easy to understand, consisting only of a unique identifier followed by a metadata/data pair. We could have used any

separator, but in this example, we chose to separate the parts of the triple by a double caret, "^^".

```
7d7ff42b^^subclass_of^^Organism
```

As noted, the individual parts of the triple are:

```
7d7ff42b is the identifier
subclass_of is the metadata
Organism is the data
```

Notice that these triples are expressed in a format different from RDF, Notation3, or Turtle. Do we care? Not at all. We know that with a few lines of code, we could convert our triplestore into any alternate format we might prefer. Furthermore, our triplestore could be converted into a spreadsheet, in which the identifiers are record keys, the metadata are column headings, and the data occupy cells. We could also port our triples into a database, if we so desired.

2. Using triples, we have defined various classes and properties. For example:

```
03cc6948^^object_name^^Organism
03cc6948^^subclass_of^^Class
```

With one triple, we create a new object, with name Organism, and we associate it with a unique identifier (03cc6948). With another triple, we establish that the Organism object is a class that happens to be the child class of the root class, Class. Because Organism is a subclass of Class, it will inherit all of the properties of its parent class.

Let's skip down to the bottom of the file:

```
98495efc^^object_name^^Andy Muzeack
98495efc^^instance_of^^Homo sapiens
98495efc^^dob^^1 January, 2001
98495efc^^glucose_at_time^^87, 02-12-2014 17:33:09
```

Here we create a few triples that provide information about a person named Andy Muzeack. First, we assign a unique identifier to our new object, named Andy Muzeack. We learn, from the next triple that Andy Muzeack is a member of class Homo Sapiens. As such, we infer that Andy Muzeack inherits all the properties contained in class Homo (the parent class of class Homo Sapiens) and all the ancestors of class Homo, leading to the top, or root ancestor, class Class. We learn that Andy Muzeack has a "dob" of January 1, 2001. By ascending the list of triples, we learn that "dob" is a property, with a unique identifier (a29c59c0), and a definition, "date of birth, as Day, Month, Year." Finally, we learn that Andy Muzeack has a glucose_at_time of "87, 02-12-2014 17:33:09." Elsewhere in the triplestore, we find that the "glucose_at_time" metadata is defined as the glucose level in mg/Dl at time drawn, in Greenwich Mean Time.

If we wished, we could simply concatenate our triplestore with other triplestores that contain triples relevant to Andy Muzeack. It would not make any difference how the triples are ordered. If Andy Muzeack's identifier is reconcilable, the metadata is defined, and each

triple is assigned to a class, then we will be able to fully understand and analyze the data held in the triplestore. [Glossary Reconciliation]

Of course, when we have millions and billions of triples, we could not perform our analyses by reading through the file. We would need scripts and/or a database application. Here is a simple Python script, nested.py, that loads a triplestore into a nested dictionary, and reads the dictionary items:

```
import collections, sys, re, string, os
from collections import defaultdict
def make_dictionary():
    return defaultdict(make_dictionary)
tripledictionary=defaultdict(make_dictionary)
triple_file = open("triple_2.txt", "r")
for line in triple_file:
  line = line.rstrip()
  triple_items = line.split("^^")
  tripledictionary[triple_items[0]][triple_items[1]][triple_items
[2]] = ""
triple_file.close()
def iter_all(tripledictionary,depth=0):
    for key,value in tripledictionary.items():
        if (depth == 0):
          print("\nidentifier " + key)
    else:
      print("-"*(depth) + key)
    if type(value) is defaultdict:
        iter_all(value,depth+1)
iter_all(tripledictionary)
```

Here is the partial output of the nested.py script:

```
identifier a34a1e35
-definition
--glucose level in mg/Dl at time drawn (GMT)
-object_name
--glucose_at_time
-instance_of
--Property
identifier a29c59c0
-definition
--date of birth, as Day, Month, Year
-object_name
--dob
```

```
-instance_of
--Property
identifier 7d7ff42b
-object_name
--Hominidae
-subclass_of
--Organism
-property
--dob
identifier a0ce8ec6
-object_name
--Homo
-subclass_of
--Hominidae
-property
--glucose_at_time
identifier 98495efc
-object_name
--Andy Muzeack
-instance_of
--Homo sapiens
-glucose_at_time
--87, 02-12-2014 17:33:09
-dob
--1 January, 2001
```

The first listed data object, followed by its nested metadata/data pairs, is "a34a1e35."

```
identifier a34a1e35
-definition
--glucose level in mg/Dl at time drawn (GMT)
-object_name
--glucose_at_time
-instance_of
--Property
```

The triples belonging to "a34a1e35" tell us that the data object is a Property. The property's name is "glucose_at_time," and the object is defined as the "glucose level in mg/Dl at time drawn (GMT)." Had we examined all of the output of the nested.py script, we would have learned that "glucose_at_time" is a property of Class Homo, the subclass of Class Hominidae.

The last listed data object is "98495efc."

```
identifier 98495efc
-object_name
--Andy Muzeack
-instance_of
--Homo sapiens
-glucose_at_time
--87, 02-12-2014 17:33:09
-dob
--1 January, 2001
```

The triples are telling us what we have previously learned; that "98495efc" is a member of Class Homo sapiens, named Andy Muzeack, and that he has a glucose_at_time of 87 mg/Dl drawn at December 2, 2014, at 5:33 Greenwhich Mean Time. He was born on January 1, 2001.

Triplestores can be difficult to understand, at first, owing to the seemingly convoluted self-definitions of the highest-level classes and properties. For example, must we really know that a property is a member of Class Property and that Class Property is a subclass of Class Class? Yes and no. These preliminary triples must exist somewhere, but they need not appear in every triplestore. Ideally, the high level triples would be stored, for reference, in an upper level ontology. Most triplestores would have the appearance of a list of spreadsheet cells with row and column headers attached. The power of a well-designed triplestore comes from the ease with which they can be merged, integrated, and introspected.

Section 6.6. Case Study (Advanced): Proof That Big Data Must Be Object-Oriented

The worst form of inequality is to try to make unequal things equal.

Aristotle

Everyone knows what the meaning of the following equation (or do we?):

```
x=y
```

Does it mean that x and y are the same thing? Certainly, if x is equal to zero, and x equals y, then y must also equal zero. But what if x is the truck blocking my view in traffic? Must I assume that y is the same truck, also blocking my view in traffic? Or does it mean that y is the same kind of truck as x, but not blocking my view?

Perhaps the equation is an assignment function, indicating that the value of y is being assigned to x. In this case, if y is 5, then x is assigned the value of 5. In that case, what happens when y is incremented by 1, to become y + 1, or 6. Does x, being equal to y, also become equal to 6, or does it keep its assigned value of 5?

Suppose x is a global variable (i.e., a variable that persists for the life of the executing program) and y is a local variable (a variable that persists only for the life of the subroutine in which it is created). Then what happens to x when y's subroutine ends?

Maybe the equivalency between x and y indicates that x and y happen to contain the same types and quantities of data objects. For example x is equivalent to y if x contains an orange and an apple and y contains an orange and an apple. If y gives x its apple and its orange, then does x become 2x? If so, then how do we describe the result of a transaction where y gives x its apple but retains its orange. Do we then have 1.5x and 0.5y. Have we become guilty of falsely comparing apples and oranges?

What is the point of all this annoying sophistry? The "=" sign is an example of a polymorphic method. Equality can indicate the assignment of a variable, the establishment of identity, a property of belonging to sets of objects, or any number of alternate meanings. Each meaning of "=" is determined by the class of objects it operates upon.

You can see that if the simple "=" sign is polymorphic, then other methods that operate on objects of different types can also be polymorphic. For example, a "rounding" method applied to a geometric object would be quite different from a "rounding" method applied to a floating point number.

How does this relate to Big Data? Remember that Big Data is complex, meaning that it contains heterogeneous data types. When Big Data contains may different types of data (i.e., may different classes of data objects), we must be prepared to accommodate polymorphic methods. The only way to accommodate polymorphic methods is with object-oriented rules. Doing so guarantees that an object will respond to a method based on the method's defined functionality within the object's class.

Hence, Big Data must be object oriented.

Glossary

Immutability Immutability is the principle that data collected in a Big Data resource is permanent, and can never be modified. At first thought, it would seem that immutability is a ridiculous and impossible constraint. In the real world, mistakes are made, information changes, and the methods for describing information changes. This is all true, but the astute Big Data manager knows how to accrue information into data objects without changing the pre-existing data. Methods for achieving this seemingly impossible trick are described in Chapter 8.

Message digest Within the context of this book, "message digest", "digest", "HMAC", and "one-way hash" are equivalent terms.

Open access A document is open access if its complete contents are available to the public. Open access applies to documents in the same manner as open source applies to software.

Reconciliation Usually refers to identifiers, and involves verifying an object that is assigned a particular identifier in one information system will be provided the same identifier in some other system. For example, if you were assigned identifier 967bc9e7-fea0-4b09-92e7-d9327c405d78 in a legacy record system, you should like to be assigned the same identifier in the new record system. If that were the case, your records in both systems could be combined. If you were assigned an identifier in one system that is different from your assigned identifier in another system, then the two identifiers must be reconciled to determine that they both refer to the same unique data object (i.e., yourself). This may involve creating a link between the two identifiers. Despite claims to the contrary, there is no possible way by which information systems with poor identifier systems can be sensibly reconciled. Consider this example. A hospital has two separate registry systems: one for dermatology cases and another for psychiatry cases. The hospital would like to merge records from the two services. Because of sloppy identifier and registration protocols, a single patient has been registered 10 times

in the dermatology system, and 6 times in the psychiatry system, each time with different addresses, social security numbers, birthdates and spellings of the name. A reconciliation algorithm is applied, and one of the identifiers from the dermatology service is matched positively against one of the records from the psychiatry service. Performance studies on the algorithm indicate that the merged records have a 99.8% chance of belonging to the same patient. So what? Though the two merged identifiers correctly point to the same patient, there are 14 (9 + 5) residual identifiers for the patient still unmatched. The patient's merged record will not contain his complete clinical history. Furthermore, in this hypothetical instance, analyses of patient population data will mistakenly attribute one patient's clinical findings to as many as 15 different patients, and the set of 15 records in the corrupted deidentified dataset may contain mixed-in information from an indeterminate number of additional patients! If the preceding analysis seems harsh, consider these words, from the Healthcare Information and Management Systems Society, "A local system with a poorly maintained or 'dirty' master person index (MPI) will only proliferate and contaminate all of the other systems to which it links" [4].

Symmetric key A key (i.e., a password) that can be used to encrypt and decrypt the same file. AES is an encryption/decryption algorithm that employs a symmetric key.

For example, you may wish to use the AES protocol to encrypt the file myfile.txt, using the following command line code:

```
openssl.exe aes128 -in myfile.txt -out myfile.aes -pass pass:12345
```

In this example, the encrypted output file is myfile.aes, and the password is "12345".
To decrypt the encrypted file, you would use the same password that you used to encrypt the file, and a decrypt instruction ("-d" in this case):

```
openssl aes128 -d -in myfile.aes -out myfiledecrypted.txt -pass pass:12345
```

Trusted time stamp It is sometimes necessary to establish, beyond doubt, that a time stamp is accurate and has not been modified. Through the centuries, a great many protocols have been devised to prove that a time stamp is trustworthy. One of the simplest methods, employed in the late twentieth century, involved creating a digest of a document (e.g., a concatenated sequence consisting of the first letter of each line in the document) and sending the sequence to a newspaper for publication in the "Classifieds" section. After publication of the newspaper, anyone in possession of the original document could extract the same sequence from the document, thus proving that the document had existed on the date that the sequence appeared in the newspaper's classified advertisements.

Near the end of the twentieth century, one-way hash values become the sequences of choice for trusted time stamp protocols. Today, newspapers are seldom used to establish trust in time stamps. More commonly, a message digest of a confidential document is sent to a time stamp authority that adds a date to the digest and returns a message, encrypted with the time stamp authority's private key, containing the original one-way hash plus the trusted date. The received message can be decrypted with the time stamp authority's public key, to reveal the data/time and the message digest that is unique for the original document. It seems like the modern trusted time stamp protocol is a lot of work, but those who use these services can quickly and automatically process huge batches of documents.

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7

Standards and Data Integration

OUTLINE

Section 7.1. Standards

The nice thing about standards is that you have so many to choose from.
Andrew S. Tanenbaum

Everyone is taught, at an early age, the standard composition of a written letter. You start with the date, then you include the name and address of your correspondent, then you write a salutation (e.g., "Dear Abby,"), then comes the body of the letter, followed by a closing (e.g., "Best wishes,") and your name and signature on the next lines. It is all rather rigid and anyone can recognize a page of correspondence, from across the room, just by the configuration of lines and paragraphs on the page.

Now, consider the reminder notes that you leave for yourself. You might jot a thought down on a Post-it and hang your Post-it notes on your refrigerator, you might use a small paper notepad, or you might write something on your computer or your smartphone. You might carry a little voice recorder for this purpose. The point is that there are an endless variety of methods whereby people leave notes for themselves, yet there is only one format for writing a letter to a friend.

The reason for this disparity in available options relates to the important distinction between self and non-self. When you write a note to yourself, you are free to do as you please. When you write a note to another person, you must conform to a standard.

The entire concept of data integration, and software interoperability draws from the same basic rule. If you intend to create your own data to serve your own purposes, then you need not be concerned with data integration and software interoperability. Everyone else must toe the line.

Until the last decade or two, most data systems were created for use within one organization or corporation. The last thing on anyone's minds was providing access to outsiders. All this has changed. Today, data means very little if it cannot be integrated with

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related data sources. Today's software protocols operate with standard application programming interfaces that mediate the interchange of data over operating systems and networks. [Glossary Data interfaces]

In small data projects, a single standard will often support the successful interchange of data. In a Big Data project, data integration and system interoperability might involve the use of multiple standards with data conforming to multiple versions of each standard. Sharing the data across networks may involve the use of many different interchange protocols. The purpose of this chapter is familiarize data managers with standards issues that are important to Big Data resources.

Standards are sometimes touted as the solution to every data integration issue [1]. When implemented as intended, they can support the exchange of data between heterogeneous systems [2]. Such exchanges may involve non-equivalent databases (i.e., databases with different data models, different software holding different types of data). Exchanges may also involve information transfer between humans and databases, or between software agents and mechanical devices. Any exchanges between one data source and another data source can benefit from standards for describing the data and standards for transferring the data.

Whereas a single, all-purpose, unchanging, and perpetual standard is a blessing for Big Data managers, an assortment of incompatible standards can be a curse. The utility of data standards has been undermined by the proliferation of standards, the frequent versioning of data standards, the intellectual property encumbrances placed upon standards, the tendency for standards to increase in complexity over time, the abandonment of unpopular standards, and the idiosyncratic ways in which standards are implemented by data managers.

Look at the field of information science and the growing role of Big Data in science and society; it is tempting to believe that the profusion of standards that we see today is the result of rapid growth in a new field. As the field matures, there will be a filtering-out process wherein the weaker standards are replaced by the strongest, most useful standards, until we reach a point when a few tested and stable standards dominate. This scenario will probably never happen. To the contrary, there is every indication that the number of standards will increase, that the newly created standards will not serve their intended purposes, and that future revisions of these early and inadequate standards will be more complex and less useful than their inadequate predecessors.

Of course, the future need not be so dreary, but it is worth taking a look at some of the scientific, economic, legal, and social forces that push us to create more and more standards of lower and lower quality.

1. **There is no guiding force that has either the authority or the popular support to limit the flood of new standards. They just keep coming**

Today, there are thousands of organizations that develop standards; these are called Standards Development Organizations (SDOs). The development of standards has become part of the established culture of technology. SDOs may become members of a Standards Activities Organization, such as the American National Standards Institute

(ANSI), which coordinates between Standards Development Organizations and Standards Organizations, providing guidance and procedures to attain certified new standards. Above the Standards Activities Organizations are the standards certifying agencies. The two most important are ISO (International Organization for Standardization) and IEC (International Electrochemical Commission).

Aside from SDOs, there are independent-minded groups that create their own standards without following the aforementioned route. These groups often develop standards for their members of for their own private consumption. They see no reason to make the effort to follow a path to the ISO or the IEC. There is no way to count the number of independent standards that are being created.

In addition to the standards produced by SDOs and independent groups, there are the *de facto* standards that seem to arise out of thin air and rapidly gain in popularity. These represent the "better mousetraps" that somebody builds and to which the world beats a path. In the long run, de facto standards such as TCP/IP, QWERTY keyboards, PDF files, and Microsoft Word DOC documents, will have a much greater influence than any official standards.

2. Standards can be easy to create, especially if they are narrowly focused.

Many standards are created for a niche audience. When the topic is very narrow, a standard can be developed in under a month, through the part-time efforts of a few motivated individuals. The time-consuming component of the standards process is vetting; getting your committee members and your user community to read, understand, approve, support, and use the finished product. For the technically-minded, the vetting process can be an insurmountable obstacle. The creators of the standard may not have the stamina, social skills, money, or influence to produce a popular and widely implemented standard. Nonetheless, it is relatively easy to write a standards document and publish it as a journal article or as a Web posting, vetted or not.

3. Standards are highly profitable, with many potential revenue streams.

When there is no industry standard for data representation, then each vendor may prepare his or her own proprietary data model to establish "vendor lock-in." The customer's data is held in the format provided by the vendor. Because the format is proprietary, competing vendors cannot appropriate the format in their own hardware and software. The customer becomes locked into the vendor's original system, upgrades, and add-ons. Proprietary systems provide vendors with an opportunity to gain customer loyalty, without necessarily producing a superior product.

One of the purposes of industry-wide standards is to abolish proprietary systems. The hope is that if every vendor's software, hardware and data models were equivalent, then buyers could break away from locked-in systems; the free market would prevail.

Who sits on standards development committees? Who has the time to invest in the vetting process? Who has the expertise to write a standard? Who can afford to send representatives across the globe to attend committee meetings? Vendors; vendors write the standards, vendors vet the standards, and vendors implement the standards.

Large corporations can afford to send a delegation of standards experts to a standards committee. Furthermore, the corporation that sends delegates will pay for membership in the committee. Consequently, the standards committee becomes dependent on corporations that finance the standards process, and this dependence strengthens the corporation's influence. The corporation will work to create a standard that can be technically supported by the products in place or under development. The standards-making corporations secure an advantage over competitors who do not participate in the standards committee meetings and who cannot anticipate the outcome of the standards process or who cannot comply with finalized rulings for reasons of system incompatibility or simply because the proposed standard is technically beyond the capacity of their staff.

It is one of the great ironies of informatics that standards are written by the very same people who are the standard's intended targets of restraint. Vendors are clever and have learned to benefit from the standards-making process. In some cases, a member of a standards committee may knowingly insert a fragment of patented property into the standard. After the standard is released and implemented in many different vendor systems, the patent holder rises to assert the hidden patent. In this case, all those who implemented the standard may find themselves required to pay a royalty for the use of some intellectual property sequestered within the standard. The practice of hiding intellectual property within a standard or device is known as patent farming or patent ambushing [3]. The patent farmer plants seeds in the standard and harvests his crop when the standard has grown to maturity; a rustic metaphor for some highly sophisticated and cynical behavior.

Savvy standards committees take measures to reduce patent farming. This often takes the form of an agreement, signed by all members of the standards committee, to refrain from asserting patent claims on the users of the standards. There are several ways to circumvent these agreements. If a corporation holds patents on components of a standard, the corporation can sell their patents to a third party. The third party would be a so-called patent holding company that buys patents in selected technologies with the intention of eventually asserting patents over an array of related activities [4]. If the patent holder asserts the patent, the corporation might profit from patent farming, through their sale of the patent, without actually breaking the agreement. [Glossary Patent farming]

Corporations can profit from standards indirectly by obtaining patents on the uses of the standard; not on the patent itself. For example, an open standard may have been created that can be obtained at no cost, is popular among its intended users, and contains no hidden intellectual property. An interested corporation or individual may discover a use for the standard that is non-obvious, novel, and useful; these are the three criteria for awarding patents. The corporation or individual can patent the use of the standard, without needing to patent the standard itself. The patent holder will have the legal right to assert the patent over anyone who uses the standard for the purpose claimed by the patent. This patent protection will apply even when the standard is free and open.

The world of standards is a very strange place. Big Data managers are particularly vulnerable to the legal trappings associated with standards because Big Data is complex and diverse and requires different standards for different types of data and for different types of software.

4. Standards are popular (everyone wants one of their own).

Having your own standard is somewhat of a status symbol. Whenever a team of scientists develops a new method, a variant of an old method, and an organized way of collecting the data produced by the method, there will be a natural urge to legitimize and aggrandize their efforts with a new standard. The standard will dictate how the method is used, and how the data is collected, labeled, and stored. In the late 1990s the most favored way to represent data was through a new markup language; basically a list of specialized XML tags and a Schema that dictated the nesting hierarchy of the tags. In almost every case, these niche markup languages were self-contained constructs that did not re-use tags from related markup languages. For example, many different markup languages contained an equivalent tag that described the sample name or the sample identifier, but these mark-up languages did not refer to pre-existing equivalent tags in other Schemas (i.e., they did not make use of established namespaces). Consequently, a Babel of markup languages sprang into existence, with no attempt at harmonizing the languages or sharing content among the different languages. Thankfully, the markup language fad has passed, but a basic problem persists. Deep down, scientists believe that their way of organizing their own data should be the standard for the entire world. This irrational belief accounts for much of the unchecked proliferation of personalized standards.

5. Most standards are created for reasons that applied in the past, but which do not apply in the Big Data era.

For the last half century the purpose of a standard was to ensure that everyone who created a particular type of object (e.g., a physical object, or a document, or a collection of a specific type of information) would do so in the same way, so that the objects could be compared and categorized.

For example, imagine an international standard for death certificates. You would naturally want each certificate to contain the same information, including the name of the deceased, identifying information (e.g., date of birth, gender, race), causes of death and contributing factors, all coded in accordance with a standard nomenclature. With the cause of death, you would want to find details of the circumstances of the death (e.g., date and time of death, time at which the certificate was signed). Regarding format, you might want every country to list the contents of the document in the same order, numbered identically, so that item 4 in a Portuguese death certificate would correspond to item 4 in an Australian certificate. You may want the layout of the documents to be identical (e.g., name of deceased in the upper left, date of birth of deceased in the upper right). These restrictions are intended to facilitate comparisons among death certificates worldwide. This detailed approach to layout is terribly outdated and largely irrelevant to the purposes of standards in Big Data resources.

In the Big Data universe the purpose of a standard is not to compare one document with another document of the same kind; the purpose of a standard is to enable data analysts to relate data objects within a document to data objects contained in documents of a different kind.

This last point is the most difficult for people to accept, particularly those people who have been supporters of data standards and who have used them to good effect in their work. It is a near-impossible task to convince someone to abandon a paradigm that has served him or her well. But it is worth a try!

Let us reexamine the role of the standard death certificate in Big Data analysis. The "cause of death" section will contain the primary cause of death plus any diseases that contributed to the primary cause of death. Another database, in a hospital information system, might list various diseases that co-exist in living patients. By comparing data in the database of death certificates with data in a hospital information system, it may be possible to find sets of diseases that co-occur with a high risk of death. By comparing the average age at which a particular disease is associated with death, it may be possible to predict when a disease under treatment is likely to lead to death. The occurrence of diseases in particular racial groups included in death certificate data may lead to disparities found in the occurrence of the same diseases in a living population. These are extremely simple examples wherein data values included in one standard data set (death certificates) are compared with data values in another standard data set (Electronic Health Records). The comparisons are made between selected data values in heterogeneous data sets; the comparisons are not made between two documents that conform to the same standard.

The phenomenon of data integration over heterogeneous sources is repeated in virtually every Big Data effort. A real estate property with a known address is matched against crime statistics collected for its listed zip code. A planting chart based on a list of popular flowers and vegetables within a locality is matched against a climate zone dataset matched to geographic region. A data set of personal buying preferences for a population of individuals is matched against a list of previously sold items, and their features, and a list of items-for-sale and their features. In each case, the comparisons are made for data values held in heterogeneous data sets.

In an earlier era, standards served to create data homogeneity. In the Big Data era, standards should help us find the data relationships in heterogeneous data sources.

Section 7.2. Specifications Versus Standards

> *Good specifications will always improve programmer productivity far better than any programming tool or technique.*
>
> *Milt Bryce*

The two terms, "standards" and "specifications" are used interchangeably in the informatics literature, but they are different from one another in very important ways. A "standard" is a set of construction rules that tells you how to represent a required set of information.

For a given subject (i.e., an image, a movie, a legal certificate, a programming language), the standard tells you exactly how the contents must be organized, from top to bottom, and the contents that must be included, and how those contents are expressed. For a standard to have value, it generally requires approval from a standards-certifying organization (such as the ISO), or from some large and influential industry group.

A specification is a general way of describ ing objects (i.e., physical objects such as nuts and bolts or symbolic objects such as numbers) so that anyone can fully understand your intended meaning. Specifications do not force you to include specific types of information, and do not impose a specific order on the data contained in the document. Specifications are not generally certifie d by a standards organization. Their legitimacy depends on their popularity. Exampl es of specifications are RDF (Resource Description Framework) produced by the W3C (WorldWide Web Consortium), and TCP/IP (Transfer Control Protocol/Internet Protocol), maintained by the Internet Engineering Task Force.

The strength of a standard is that it imposes uniformity; the weakness of a standard is that it has no flexibility and impedes innovation. An engineer might want to manufacture a cup with a very wide bottom rim and a narrow top rim; or with no handle; or with three handles; or with an attached computer chip. If the standard prohibits the bottom rim diameter to exceed the top rim diameter, or requires exactly one handle, or has no method for describing ancillary attachments, then the innovator cannot comply with the standard.

The strength of the specification is that it is highly flexible; the weakness of the specification that its flexibility allows designers to omit some of the information required to fully specify the object. In practice, proper implementation of specifications is ensured by usability tests. If everyone seems to understand your implementation of a specification, and if your implementation functions adequately, and operates with other systems without problems, then the specification has served its intended purpose.

Both standards and specifications suffer from the following:

1. **New versions may appear, without much notice, and the new versions may not be fully compatible with older versions.**

For example, Python 3.x has a somewhat different syntax than Python 2.x. Your Python 2.x programs will not necessarily run in a Python 3.x environment, and your Python 3.x programs may not run in a Python 2.x environment. Incompatible programs may run for a while, and then stop when a conflict arises. Because the glitch is caused by a language incompatibility, not a programming error, you may find the debugging process exasperating.

2. **Both standards and specifications may be overly complex.**

It is easy for a standards committee to create a complex standard or for an organization to develop a specification language that contains thousands of metadata tags. A complex standard or specification can easily exceed human comprehension. Data managers may be hesitant to stake their resource on tools that they cannot understand.

3. There are too many standards and specifications from which to choose.

Big Data managers would like to stay in conformance with industry standards. The problem is that Big Data serves many different purposes and must comply with many different standards, all at the same time.

After a standard has been created, there follows a Darwinian struggle for supremacy. Standards committees sometimes display group behavior that can be described as antisocial or even sociopathic. They want their standard to be the only standard used in a data domain. If there are other standards in the data domain, they sometimes use coercive methods to force everyone to use their standard.

The most common coercive argument involves threatening colleagues with the inflated claim that everyone will be using the standard; failing to switch to the standard will result in loss of business opportunities. The proponents of a standard may suggest that those who fail to adopt the standard will be ostracized and marginalized by their colleagues. I have personally heard coercive arguments from some of my colleagues who, in every other respect, are decent and altruistic individuals. The reason for their nastiness often comes down to economics. Vendors and Big Data managers select a standard in the full knowledge that a poor choice may bring financial ruin. If the vendor builds a data model to fit a standard, and their market does not adapt the standard, then they will not be able to sell their software. If a Big Data manager annotates terabytes of data in conformance with an ontology that is soon-to-be-abandoned by its user community, then the value of the resource will plummet. Nevertheless, there can be no excuses for bad behavior; coercion should not be tolerated.

A few commonsense measures might help the data manager:

- Learn how to decompose the standard document into an organized collection of data objects that can be merged with other data object collections or inserted into a preferred data model.
- If feasible, avoid using any standard as your data object model for the resource. It is often best to model your own data in a simple but flexible format that can be ported into any selected standard, as needed.
- Know the standards you use. Read the license agreements. Keep your legal staff apprised of your pending decisions.
- Try your best to use standards that are open source or that belong to the public domain. [Glossary Public domain]

Section 7.3. Versioning

I visited the Sage of reverend fame
And thoughtful left more burden'd than I came.
I went- - and ere I left his humble door
The busy World had quite forgot his name.

Ecclesiastes

In the year 2000 I attended a workshop in San Diego whose purpose was to introduce pathologists to new, standardized protocols for describing different types of cancer specimens (e.g., cancer of the adrenal gland, cancer of the prostate, cancer of the lung, etc.) This was not the first such standardization effort. Over the past decade, several groups had been pushing for standards that would ensure that pathology reports prepared in any United States hospital would contain the same kind of information for a given type of specimen. Having a reporting standard seemed like a good idea, but as I looked at the protocols I saw lots of problems. Lists of required items seemed incomplete and many of the descriptors were poorly defined. Some of the descriptors were non-qualitative and required subjective data. The final reports would not be highly reproducible between laboratories or within a single laboratory. These deficiencies are par for the course in any standards effort. I asked the chairman how she planned to deal with producing and controlling new versions of the standard. She replied that because the standards had been prepared by experts and thoroughly tested by a panel of implementers, there would be no need to develop new versions of the standard. She was telling me that the new standard had been born perfect! Eighteen years have passed, during which time the standards have been subjected to unceasing modifications. [Glossary Reproducibility]

For most types of standards and specifications, versioning is a requirement. Nomenclatures in every area of science and technology are constantly being updated. Every year, the Medical Subject Headings comes out with an updated version. Some nomenclatures are actually named according to the version (e.g., ICD-10 is the tenth version of the International Classification of Diseases). New versions of nomenclatures are not simple expansions of older versions. Aside from the addition of new terms, old terms must be retired, and new coding sequences are sometimes created. The relationships among terms (i.e., the class or classes to which a term belongs) might change.

Without exception, all large nomenclatures are unstable. Changes in a nomenclature may have a ripple effect, changing the meaning of terms that are not included in the nomenclature. Here is an example from the world of mycology (the study of fungi). When the name of a fungus changes, so must the name of the associated infection. Consider "Allescheria boydii," People infected with this organisms were said to suffer from the disease known as allescheriasis. When the organism's name was changed to *Petriellidium boydii*, the disease name was changed to petriellidosis. When the fungal name was changed, once more, to *Pseudallescheria boydii*, the disease name was changed to pseudallescheriasis [5]. All three names appear in the literature (past and present). In this case, changes in the fungal nomenclature necessitate reciprocal changes in every disease nomenclature. Such changes may require months, years, and even decades to adjudicate and finalize in the newer version of the nomenclature. Within this period, the term may change again and the corrected version of the disease nomenclature may be obsolete on its release date.

We discussed classifications and ontologies in Chapter 5. Classifications have a very strong advantage over ontologies with regard to the ease of versioning. Because each class in a classification is restricted to a single parent, the hierarchical tree of a classification is

simple. When a class needs to be repositioned in the classification tree, it is a simple matter to move the class, with its intact branches, to another node on the tree. We do this from time to time with the classification of living organisms.

Unlike the case with uniparental classifications, it is virtually impossible to make sweeping changes in multiparental ontologies. In every complex ontology, we can expect to encounter class branches insinuated across multiple classes. A class cannot simply be cut and repositioned elsewhere. The more complex the ontology, the more difficult it is to modify its structure.

Section 7.4. Compliance Issues

> *It's not worth doing something unless someone, somewhere, would much rather you weren't doing it.*
>
> *Terry Pratchett.*

When it comes to complex standards, compliance is in the eye of the beholder. One vendor's concept of standard-compliant software might be entirely different from another vendor's concept. Standards organizations seldom have the time, manpower, money, or energy to ensure compliance with their standards; consequently, the implementations of standards are often non-standard and incompatible with one another.

In large part, non-compliance is caused by the instability of modern standards. As we have seen, standards themselves may contain flaws related to the complexity of the technologies they model. When a technology outpaces the standard built for the technology, it may be impossible for businesses to adequately model all of their data and processes within the standard.

Small businesses may not have the manpower to keep abreast of every change in a complex standard. Large businesses may have the staff and the expertise to stay compliant; but they may lack the incentive. If they produce a product that works well, and is believed, wrongly or not, to be compliant with a standard, then it may be in the best interest of the business to purposefully introduce a bit of non-compliance. The expectation being that small deviations from the standard will create incompatibilities between their products and their competitors; thus achieving vendor lock-in. Their customers will be loath to switch to another vendor's products if they fear that their original system will not support software or hardware produced by rival companies.

Compliance with specifications is, in general, much easier than compliance with standards. Data specifications provide a syntax and a general method for describing data objects, without demanding much in the way of structuring the data. In most cases, it is relatively easy to produce a program that determines whether a file conforms to a specification.

When a file conforms to the syntax of a specification, it is said to be well formed. When a file conforms to a document that describes how certain types of objects should be

annotated (e.g., which tags should be used, the relationships among tags, the data value properties that can be assigned to tags, the inclusion of all required tags), then the file is said to be valid. A file that is fully compliant with a specification is said to be well formed and valid.

In the case of RDF (as discussed in Section 4.5), a well-formed document would comply with RDF syntax rules. A valid file would conform to the classes and properties found in the RDF Schemas linked from within the RDF statements contained in the file.

Section 7.5. Case Study: Standardizing the Chocolate Teapot

History doesn't repeat itself, but it rhymes.
Attributed variously to Mark Twain and to Joseph Anthony Wittreich

Malcolm Duncan has posted an insightful and funny essay entitled "The Chocolate Teapot (Version 2.3)" [6]. In this essay, he shows how new versions of nomenclatures may unintentionally alter the meanings of classes of terms contained in earlier versions, making it impossible to compare or sensibly aggregate and interpret terms and concepts contained in any of the versions. The essay is a must-read for anyone seriously interested in terminologies, but we can examine a few of the points raised by Duncan.

Suppose you have a cooking-ware terminology with a single "teapot" item. We will call this Version 1.0. Early teapots were made of porcelain and porcelain came in two colors; white and blue. Version 2 of the terminology might accommodate the two sub-types: blue teapot and white teapot. If a teapot were neither blue nor white, it would presumably be coded under the parent term, "teapot." Suppose version 3 expands to accommodate some new additions to the teapot pantheon: chocolate teapot, ornamental teapot, china teapot, and industrial teapot. Now the teapot world is shaken by a tempest of monumental proportions. The white and the blue teapots, implicitly considered to be made of porcelain, like all china teapots, stand divided across the subtypes. How does one deal with a white porcelain teapot that is not a china teapot? If we had previously assumed that a teapot was an item in which tea is made, how do we adjust, conceptually, to the new term "ornamental teapot?" If the teapot is ornamental, then it has no tea-making functionality, and if it cannot be used to make tea, how can it be a teapot? Must we change our concept of the teapot to include anything that looks like a teapot? If so, how can we deal with the new term "industrial teapot," which is likely to be a big stainless steal vat that has more in common, structurally, with a microbrewery fermenter than with an ornamental teapot? What is the meaning of a chocolate teapot? Is it something made of chocolate, is it chocolate-colored, or does it brew chocolate-flavored tea? Suddenly we have lost the ability to map terms in version 3 to terms in versions 1 and 2. We no longer understand the classes of objects (i.e., teapots) in the various versions of our cookware nomenclature. We cannot unambiguously attach nomenclature terms to objects in our data collection (e.g., blue china teapot). We no longer have a precise definition of a teapot or of the subtypes of teapot.

Glossary

Data interfaces Interfaces to Big Data resources often come in one of several types including:

Direct user interfaces. These interfaces permit individuals to submit simple queries, constructed within a narrow range of options, producing an output that is truncated to produce a manageable visual display. Google is an example. You never know what information is excluded from the indexed resource, or exactly how the search is conducted, and the output may or may not have the results you actually need. Regarding the actual query, it is limited to words and phrases entered into a box, and although it permits some innovative methods to specify the query, it does not permit you to enter hundreds of items at once, or to search based on a user-invented algorithms, or to download the entire search output into a file. Basically, Google gives users the opportunity to enter a query according to a set of Google-specified query rules, and Google provides an output. What happens in the very short moment that begins when the query has been launched, and ends when the reply is displayed, is something that only Google fully understands. For most users, the Google reply may as well be conjured by magic.

Programmer or software interfaces. These are standard commands and instructions that a data service releases to the public, and that individual developers can use to link to and interact with the service. The usual term applied to these interfaces is API (Application Programming Interface), but other related terms, including SaaS (Software as a Service) might also apply. Amazon is an example of a company that provides an API. Web developers can use the Amazon API to link to information related to specific Amazon products. Current information for the product can be displayed on the third party Web site, and a buyer's link can broker a purchase. The API enables transactions to be completed through interactions between the developer's software and the company's software.

Autonomous agent interfaces. These are programs that are launched into a network of communicating computers, carrying a query. The program contains communication and interface protocols that enable it to interrogate various databases. The response from a database is stored and examined. Depending on the information received, the autonomous agent might proceed to another database or may modify its interrogation of the first database. The agent continues to collect and process information, traveling to different networked databases in the process. At some point, the software program returns to the client (the user who initiated the query) with its collected output. Web crawlers, familiar to anyone who reviews Internet server logs, are somewhat primitive examples of partly autonomous software agents. They use an interface (Internet protocols) to visit servers, conducting an inventory of the contents, and visiting other servers based on the addresses of links listed on Web pages. If a Big Data resource opens its data to programs that employ a compatible communications protocol (such as a Web services language), then the problem of constructing a software agent becomes relatively straightforward. Opening a system to autonomous agents comes with risk. The consequences of opening a system to complex interactions with innumerable agents, each operating under its own set of instructions, is difficult, or impossible, to predict and control [7].

Patent farming Also known as patent ambushing [3]. The practice of hiding intellectual property within a standard or device, at the time of its creation, is known as patent farming. After the property is marketed, the patent farmer announces the presence of his or her hidden patented material and presses for royalties; metaphorically harvesting his crop.

Public domain Data that is not owned by an entity. Public domain materials include documents whose copyright terms have expired, materials produced by the federal government, materials that contain no creative content (i.e., materials that cannot be copyrighted), or materials donated to the public domain by the entity that holds copyright. Public domain data can be accessed, copied, and re-distributed without violating piracy laws. It is important to note that plagiarism laws and rules of ethics apply to public domain data. You must properly attribute authorship to public domain documents. If you fail to attribute authorship or if you purposefully and falsely attribute authorship to the wrong person (e.g., yourself), then this would be an unethical act and an act of plagiarism.

Reproducibility Reproducibility is achieved when repeat studies produce the same results, over and over. Reproducibility is closely related to validation, which is achieved when you draw the same conclusions, from the data, over and over again. Implicit in the concept of "reproducibility" is that the original research must somehow convey the means by which the study can be reproduced. This usually requires the careful recording of methods, algorithms, and materials. In some cases, reproducibility requires access to the data produced in the original studies. If there is no feasible way for scientists to undertake a reconstruction of the original study, or if the results obtained in the original study cannot be obtained in subsequent attempts, then the study is irreproducible. If the work is reproduced, but the results and the conclusions cannot be repeated, then the study is considered invalid.

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8

Immutability and Immortality

OUTLINE

Section 8.1. The Importance of Data That Cannot Change

Cheese is milk's leap toward immortality

Clifton Fadiman (editor of Mathematical Magpie)

Immutability is one of those issues, like identifiers and introspection, that seem unimportant, until something goes terribly wrong. Then, in the midst of the problem, you realize that your entire information system was designed incorrectly, and there really is nothing you can do to cope.

Here is an example of a immutability problem. You are a pathologist working in a university hospital that has just installed a new, $600 million information system. On Tuesday, you released a report on a surgical biopsy, indicating that it contained cancer. On Friday morning, you showed the same biopsy to your colleagues, who all agreed that the biopsy was not malignant, and contained a benign condition that simulated malignancy (looked a little like a cancer, but was not). Your original diagnosis was wrong, and now you must rectify the error. You return to the computer, and access the prior report, changing the wording of the diagnosis to indicate that the biopsy is benign. You can do this, because pathologists are granted "edit" access for pathology reports. Now, everything seems to have been set right. The report has been corrected, and the final report in the computer is the official diagnosis.

Unknown to you, the patient's doctor read the incorrect report on Wednesday, the day after the incorrect report was issued, and two days before the correct report replaced the incorrect report. Major surgery was scheduled for the following Wednesday (five days after the corrected report was issued). Most of the patient's liver was removed. No cancer was

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found in the excised liver. Eventually, the surgeon and patient learned that the original report had been altered. The patient sued the surgeon, the pathologist, and the hospital.

You, the pathologist, argued in court that the computer held one report issued by the pathologist (following the deletion of the earlier, incorrect report) and that report was correct and available to the surgeon prior to the surgery date. Therefore, you said, you made no error. The patient's lawyer had access to a medical chart in which paper versions of the diagnosis had been kept. The lawyer produced, for the edification of the jury, two reports from the same pathologist, on the same biopsy: one positive for cancer, the other negative for cancer. The hospital, conceding that they had no credible defense, settled out of court for a very large quantity of money. Meanwhile, back in the hospital, a fastidious intern is deleting an erroneous diagnosis, and substituting her improved rendition.

One of the most important features of serious Big Data resources (such as the data collected in hospital information systems) is immutability. The rule is simple. Data is immortal and cannot change. You can add data to the system, but you can never alter data and you can never erase data. Immutability is counterintuitive to most people, including most data analysts. If a patient has a glucose level of 100 on Monday, and the same patient has a glucose level of 115 on Tuesday, then it would seem obvious that his glucose level changed between Monday and Tuesday. Not so. Monday's glucose level remains at 100. For the end of time, Monday's glucose level will always be 100. On Tuesday, another glucose level was added to the record for the patient. Nothing that existed prior to Tuesday was changed. [Glossary Serious Big Data]

Section 8.2. Immutability and Identifiers

People change and forget to tell each other.

Lillian Hellman

Immutability applies to identifiers. In a serious Big Data resource, data objects never change their identity (i.e., their identifier sequences). Individuals never change their names. A person might add a married name, but the married name does not change the maiden name. The addition of a married name might occur as follows:

```
18843056488  is_a         patient
18843056488  has_a        maiden_name
18843056488  has_a        married_name
9937564783   is_a         maiden_name
4401835284   is_a         married_name
18843056488  maiden_name  Karen Sally Smith
18843056488  married_name Karen Sally Smythe
```

Here, we have a woman named Karen Sally Smith. She has a unique, immutable identifier, "18843056488." Her patient record has various metadata/data pairs associated with her unique identifier. Karen is a patient, Karen has a maiden name, and Karen has a married

name. The metadata tags that describe the data that is associated with Karen include "maiden_name" and "married_name." These metadata tags are themselves data objects. Hence, they must be provided with unique, immutable identifiers. Though metadata tags are themselves unique data objects, each metadata tag can be applied to many other data objects. In the following example, the unique maiden_name and married_name tags are associated with two different patients.

```
9937564783  is_a         maiden_name
4401835284  is_a         married_name
18843056488 is_a         patient
18843056488 has_a        maiden_name
18843056488 has_a        married_name
18843056488 maiden_name  Karen Sally Smith
18843056488 married_name Karen Sally Smythe
73994611839 is_a         patient
73994611839 has_a        maiden_name
73994611839 has_a        married_name
73994611839 maiden_name  Barbara Hay Wire
73994611839 married_name Barbara Haywire
```

The point here is that patients may acquire any number of names over the course of their lives, but the Big Data resource must have a method for storing, and describing each of those names and associating them with the same unique patient identifier. Everyone who uses a Big Data resource must be confident that all the data objects in the resource are unique, identified, and immutable.

By now, you should be comfortable with the problem confronted by the pathologist who changed his mind. Rather than simply replacing one report with another, the pathologist might have issued a modification report, indicating that the new report supercedes the earlier report. In this case, the information system does not destroy or replace the earlier report, but creates a companion report. As a further precaution the information system might flag the early report with a link to the ensuant entry. Alternately, the information system might allow the pathologist to issue an addendum (i.e., add-on text) to the original report. The addendum could have clarified that the original diagnosis is incorrect, stating the final diagnosis is the diagnosis in the addendum. Another addendum might indicate that the staff involved in the patient's care was notified of the updated diagnosis. The parts of the report (including any addenda) could be dated and authenticated with the electronic signature of the pathologist. Not one byte in the original report is ever changed. Had these procedures been implemented, the unnecessary surgery, the harm inflicted on the patient, the lawsuit, and the settlement, might have all been avoided. [Glossary Digital signature]

The problem of updating diagnoses may seem like a problem that is specific for the healthcare industry. It is not. The content of Big Data resources is constantly changing; the trick is to accommodate all changes by the addition of data, not by the deletion or

modification of data. For example, suppose a resource uses an industry standard for catalog order numbers assigned to parts of an automobile. These 7-digit numbers are used whenever a part needs to be purchased. The resource may inventory millions of different parts, each with an order number annotation. What happens when the standard suddenly changes, and 12-digit numbers replace all of the existing 7-digit numbers? A well-managed resource will preserve all of the currently held information, including the metadata tag that describe the 7-digit standard and the 7-digit order number for each part in the resource inventory. The new standard, containing 12-digit numbers, will have a different metadata tag from the prior standard, and the new metadata/data pair will be attached to the internal identifier for the part. This operation will work if the resource maintains its own unique identifiers for every data object held in the resource and if the data objects in the resource are associated with metadata/data pairs. All of these actions involve adding information to data objects, not deleting information.

In the days of small data, this was not much of a problem. The typical small data scenario would involve creating a set of data, all at once, followed soon thereafter by a sweeping analytic procedure applied against the set of data, culminating in a report that summarized the conclusions. If there was some problem with the study, a correction would be made, and everything would be repeated. A second analysis would be performed in the new and improved data set. It was all so simple.

A procedure for replicative annotations to accommodate the introduction of new standards and nomenclatures as well as new versions of old standards and nomenclatures is one of the more onerous jobs of the Big Data curator. Over the years, dozens of new or additional annotations could be required. It should be stressed that replicative annotations for nomenclatures and standards can be avoided if the data objects in the resource are not tied to any specific standard. If the data objects are well specified (i.e., providing adequate and uniform descriptions), queries can be matched against any standard nomenclature on-the-fly (i.e., as needed, in response to queries), as previously discussed in Section 2.5, "Autocoding" [1]. [Glossary Curator]

Why is it always bad to change the data objects held in a Big Data resource? Though there are many possible negative repercussions to deleting and modifying data, most of the problems come down to data verification, and time stamping. All Big Data resources must be able to verify that the data held in the resource conforms to a set of protocols for preparing data objects and measuring data values. When you change pre-existing data, all of your efforts at resource verification are wasted, because the resource that you once verified no longer exists. The resource has become something else. Aside from producing an unverifiable resource, you put the resource user into the untenable position of deciding which data to believe; the old data or the new data. Time stamping is another component of data objects. Events (e.g., a part purchased, a report issued, a file opened) have no meaning unless you know when they occurred. Timestamps applied to data objects must be unique and immutable. A single event cannot occur at two different times. [Glossary Time stamp, Verification and validation]

– Immortal Data Objects

In Section 6.2, we defined the term "data object." To review, a data object is a collection of triples that have the same identifier. A respectable data object should always encapsulate two very specific triples: one that tells us the class to which the data object holds membership, and another that tells us the name of the parent class from which the data object descends. When these two triples are included in the data object, we can apply the logic and the methods of object-oriented programming to Big Data objects.

In addition, we should note that if the identifier and the associated metadata/data pairs held by the data object are immutable (as they must be, vida supra), and if all the data held in the Big Data resource is preserved indefinitely (as it should be), then the data objects achieve immortality. If every data object has metadata/data pairs specifying its class and parent class, then all of the relationships among every data object in the Big Data resource will apply forever. In addition, all the class-specific methods can be applied to objects belonging to its class and its subclass descendants, can always be applied; and all of the encapsulated data can always be reconstructed. This would hold true, even if the data objects were reduced to their individual triples, scattered across the planet, and deposited into countless data clouds. The triples could, in theory, reassemble into data objects under their immortal identifier.

Big Data should be designed to last forever. Hence, Big Data managers must do what seems to be impossible; they must learn how to modify data without altering the original content. The rewards are great.

Section 8.3. Coping With the Data That Data Creates

> *The chief problem in historical honesty isn't outright lying. It is omission or de-emphasis of important data.*
>
> *Howard Zinn*

Imagine this scenario. A data analyst extracts a large set of data from a Big Data resource. After subjecting the data to several cycles of the usual operations (data cleaning, data reduction, data filtering, data transformation, and the creation of customized data metrics), the data analyst is left with a new set of data, derived from the original set. The data analyst has imbued this new set of data with some added value, not apparent in the original set of data.

The question becomes, "How does the data analyst insert her new set of derived data back into the original Big Data resource, without violating immutability?" The answer is simple but disappointing; re-inserting the derived data is impossible, and should not be attempted. The transformed data set is not a collection of original measurements; the data manager of the Big Data Resource can seldom verify it. Data derived from other data (e.g., age-adjustments, normalized data, averaged data values, and filtered data) will not sensibly fit into the data object model upon which

the resource was created. There simply is no substitute for the original and primary data.

The data analyst should make her methods and her transformed data available for review by others. Every step involved in creating the new data set needs to be carefully recorded and explained, but the transformed set of data should not be absorbed back into the resource. The Big Data resource may provide a link to sources that hold the modified data sets. Doing so provides the public with an information trail leading from the original data to the transformed data prepared by the data analyst. [Glossary Raw data]

Section 8.4. Reconciling Identifiers Across Institutions

Mathematics is the art of giving the same name to different things.

Henri Poincare

In math, we are taught that variables are named "x" or "y," or sometimes "n," (if you are sure the variable is an integer). Using other variable names, such as "h" or "s," is just asking for trouble. Computer scientists have enlarged their list of familiar variables to include "foo" and "bar." A long program with hundreds of different local variables, all named "foo" is unreadable, even to the person who wrote the code. The sloppiness with which mathematicians and programmers assign names has carried over into the realm of Big Data. Sometimes, it seems that data professionals just don't care much about how we name our data records, just so long as we have lots of them to play with. Consequently, we must deal with the annoying problem that arises when multiple data records, for one unique object, are assigned different identifiers (e.g., when identifier x and identifier y and identifier foo all refer to the same unique data object). The process of resolving identifier replications is known as reconciliation. [Glossary Metasyntactic variable]

In many cases, the biggest obstacle to achieving Big Data immutability is data record reconciliation [2]. When different institutions merge their data systems, it is crucial that no data is lost, and all identifiers are sensibly preserved. Cross-institutional identifier reconciliation is the process whereby institutions determine which data objects, held in different resources, are identical (i.e., the same data object). The data held in reconciled identical data objects can be combined in search results, and the identical data objects themselves can be merged (i.e., all of the encapsulated data can be combined into one data object), when Big Data resources are integrated, or when legacy data is absorbed into a Big data resource.

In the absence of successful reconciliation, there is no way to determine the unique identity of records (i.e., duplicate data objects may exist across institutions and data users will be unable to rationally analyze data that relates to or is dependent upon the distinctions among objects in a data set). For all practical purposes, without data object reconciliation, there is no way to understand data received from multiple sources.

Reconciliation is particularly important for healthcare agencies. Some countries provide citizens with a personal medical identifier that is used in every medical facility in the nation. Hospital A can send a query to Hospital B for medical records pertaining to a patient sitting Hospital A's emergency room. The national patient identifier insures that the cross-institutional query will yield all of Hospital B's data on the patient, and will not include data on other patients. [Glossary National Patient Identifier]

Consider the common problem of two institutions trying to reconcile personal records (e.g., banking records, medical charts, dating service records, credit card information). When both institutions are using the same identifiers for individuals in their resources, then reconciliation is effortless. Searches on an identifier will retrieve all the information attached to the identifier, if the search query is granted access to the information systems in both institutions. However, universal identifier systems are rare. If any of the institutions lack an adequate identifier system, the data from the systems cannot be sensibly reconciled. Data pertaining to a single individual may be unattached to any identifier, attached to one or more of several different identifiers, or mixed into the records of other individuals. The merging process would fail, at this point.

Assuming both institutions have adequate identifiers, then the two institutions must devise a method whereby a new identifier is created, for each record, that will be identical to the new identifier created for the same individual's record, in the other institution. For example, suppose each institution happens to store biometric data (e.g., retinal scan, DNA sequences, fingerprints), then the institutions might agree on a way to create a new identifier validated against these unique markers. With some testing, they could determine whether the new identifier works as specified (i.e., either institution will always create the same identifier for the same individual, and the identifier will never apply to any other individual). Once testing is finished, the new identifiers can be used for cross-institutional searches.

Lacking a unique biometric for individuals, reconciliation between institutions is feasible, but difficult. Some combination of identifiers (e.g., date of birth, social security number, name) might be developed. Producing an identifier from a combination of imperfect attributes has its limitations (as discussed in detail in Section 3.4, "Really Bad Identifier Methods"), but it has the advantage that if all the pre-conditions of the identifier are met, errors in reconciliation will be uncommon. In this case, both institutions will need to decide how they will handle the set of records for which there is no identifier match in the other institution. They may assume that some individuals will have records in both institutions, but their records were not successfully reconciled by the new identifier. They may also assume that unmatched group contains individuals that actually have no records in the other institution. Dealing with unreconciled records is a nasty problem. In most cases, it requires a curator to slog through individual records, using additional data from records or new data supplied by individuals, to make adjustments, as needed. This issue will be explored further, in Section 18.5, "Case Study: Personal Identifiers."

Section 8.5. Case Study: The Trusted Timestamp

Time is what keeps everything from happening at once.
Ray Cummings in his 1922 novel, "The Girl in the Golden Atom"

Time stamps are not tamper-proof. In many instances, changing a recorded time residing in a file or data set requires nothing more than viewing the data on your computer screen and substituting one date and time for another. Dates that are automatically recorded, by your computer system, can also be altered. Operating systems permit users to reset the system date and time. Because the timing of events can be altered, scrupulous data managers employ a trusted timestamp protocol by which a timestamp can be verified.

Here is a description of how a trusted time stamp protocol might work. You have just created a message, and you need to document that the message existed on the current date. You create a one-way hash on the message (a fixed-length sequence of seemingly random alphanumeric characters). You send the one-way hash sequence to your city's newspaper, with instructions to publish the sequence in the classified section of that day's late edition. You are done. Anyone questioning whether the message really existed on that particular date can perform their own one-way hash on the message and compare the sequence with the sequence that was published in the city newspaper on that date. The sequences will be identical to each other. [Glossary One-way hash]

Today, newspapers are seldom used in trusted time stamp protocols. A time authority typically receives the one-way hash value on the document, appends a time, and encrypts a message containing the one-way hash value and the appended time, using a private key. Anyone receiving this encrypted message can decrypt it using the time authority's public key. The only messages that can be decrypted with the time authority's public key are messages that were encrypted using the time authority's private key; hence establishing that the message had been sent by the time authority. The decrypted message will contain the one-way hash (specific for the document) and the time that the authority received the document. This time stamp protocol does not tell you when the message was created; it tells you when the message was stamped.

Section 8.6. Case Study: Blockchains and Distributed Ledgers

It's worse than tulip bulbs.
JP Morgan CEO Jamie Dimon, referring to Bitcoin, a currency exchange system based on blockchains

Today, no book on the subject of Big Data would be complete without some mention of blockchains, which are likely to play an important role in the documentation and management of data transactions for at least the next decade, or until something better

comes along. Fortunately, blockchains are built with two data structures that we have already introduced: one-way hashes and triples. All else is mere detail, determined by the user's choice of implementation.

At its simplest, a blockchain is a collection of short data records, with each record consisting of some variation on the following:

```
<head>-<message>-<tail>
```

Here are the conditions that the blockchain must accommodate:

1. The head (i.e., first field) in each blockchain record consists of the tail of the preceding data record.
2. The tail of each data record consists of a one-way hash of the head of the record concatenated with the record message.
3. Live copies of the blockchain (i.e., a copy that grows as additional blocks are added) are maintained on multiple servers.
4. A mechanism is put in place to ensure that every copy of the blockchain is equivalent to one another, and that when a blockchain record is added, it is added to every copy of the blockchain, in the same sequential order, and with the same record contents.

We will soon see that conditions 1 through 3 are easy to achieve. Condition 4 can be problematic, and numerous protocols have been devised, with varying degrees of success, to ensure that the blockchain is updated identically, at every site. Most malicious attacks on blockchains are targeted against condition 4, which is considered to be the most vulnerable point in every blockchain enterprise.

By convention, records are real-time transactions, acquired sequentially, so that we can usually assume that the nth record was created at a moment in time prior to the creation of the $n+1$th record.

Let us assume that the string that lies between the head and the tail of each record is a triple. This assumption is justified because all meaningful information can be represented as a triple or as a collection of triples.

Here is our list of triples that we will be blockchaining.

```
a0ce8ec6^^object_name^^Homo
a0ce8ec6^^subclass_of^^Hominidae
a0ce8ec6^^property^^glucose_at_time
a1648579^^object_name^^Homo sapiens
a1648579^^subclass_of^^Homo
98495efc^^object_name^^Andy Muzeack
98495efc^^instance_of^^Homo sapiens
98495efc^^dob^^1 January, 2001
98495efc^^glucose_at_time^^87, 02-12-2014 17:33:09
```

Let us create our own blockchain using these nine triples as our messages.

Each blockchain record will be of the form:

```
<tail of prior blockchain link——the current record's triple——md5 hash
of the current triple concatenated with the header>
```

For example, to compute the tail of the second link, we would perform an md5 hash on:

```
ufxOaEaKfw7QBrgsmDYtIw——a0ce8ec6^^subclass_of^^Hominidae
```

Which yields:

```
=> PhjBvwGf6dk9oUK/+yxrCA
```

The resulting blockchain is shown here.

```
            a0ce8ec6^^object_name^^Homo——ufxOaEaKfw7QBrgsmDYtIw
ufxOaEaKfw7QBrgsmDYtIw——a0ce8ec6^^subclass_of^^Hominidae——
PhjBvwGf6dk9oUK/+yxrCA
PhjBvwGf6dk9oUK/+yxrCA——a0ce8ec6^^property^^glucose_at_time——
P40p5GHp4hE1gsstKbrFPQ
P40p5GHp4hE1gsstKbrFPQ——a1648579^^object_name^^Homo sapiens——
2wAF1kWPFi35f6jnGOecYw
2wAF1kWPFi35f6jnGOecYw——a1648579^^subclass_of^^Homo——
N2y3fZgiOgRcqfx86rcpwg
N2y3fZgiOgRcqfx86rcpwg——98495efc^^object_name^^Andy Muzeack——
UXSrchXFR457g4JreErKiA
UXSrchXFR457g4JreErKiA——98495efc^^instance_of^^Homo sapiens——
5wDuJUTLWBJjQIu0Av1guw
5wDuJUTLWBJjQIu0Av1guw——98495efc^^glucose_at_time^^87, 02-12-2014
17:33:09——Y1jCYB7YyRBVIhm4PUUbaA
```

Whether you begin with a list of triples that you would like to convert into a blockchain data structure, or whether you are creating a blockchain one record at a time, through transactions that occur over time, it is easy to write a short script that will generate the one-way hashes and attach them to the end of the nth triple and the beginning of the $n+1$th triple, as needed.

Looking back at our blockchain, we can instantly spot an anomaly, in the header of the very first record. The header to the record is missing. Whenever we begin to construct a new blockchain, the first record will have no antecedent record from which a header can be extracted. This poses another computational bootstrap paradox. In this instance, we cannot begin until there is a beginning. The bootstrap paradox is typically resolved with the construction of a root record (record 0). The root record is permitted to break the rules.

Now that we have a small blockchain, what have we achieved? Here are the properties of a blockchain

– Every blockchain header is built from the values in the entire succession of preceding blockchain links

- The blockchain is immutable. Changing any of the messages contained in any of the blockchain links, would produce a totally different blockchain. Dropping any of the links of the blockchain or inserting any new links (anywhere other than as an attachment to the last validated link) will produce an invalid blockchain.
- The blockchain is recomputable. Given the same message content, the entire blockchain, with all its headers and tails, can be rebuilt. If it cannot recompute, then the blockchain is invalid.
- The blockchain, in its simplest form, is a trusted "relative time" stamp. Our blockchain does not tell us the exact time that a record was created, but it gives its relative time of creation compared with the preceding and succeeding records.

With a little imagination, we can see that a blockchain can be used as a true time stamp authority, if the exact time were appended to each of the records in the container at the moment when the record was added to the blockchain. The messages contained in blockchain records could be authenticated by including data encrypted with a private key. Tampering of the blockchain data records could be prevented by having multiple copies of the blockchain at multiple sites, and routinely checking for discrepancies among the different copies of the data.

We might also see that the blockchain could be used as a trusted record of documents, legal transactions (e.g., property deals), monetary exchanges (e.g., Bitcoin). Blockchains may also be used for authenticating voters, casting votes, and verifying the count. The potential value of blockchains in the era of Big Data is enormous, but the devil hides in the details. Every implementation of a blockchain comes with its own vulnerabilities and much has been written on this subject [3,4].

Section 8.7. Case Study (Advanced): Zero-Knowledge Reconciliation

Experience is what you have after you've forgotten her name.

Milton Berle

Though record reconciliation across institutions is always difficult, the task becomes truly Herculean when it must be done blindly, without directly comparing records. This awkward situation occurs quite commonly whenever confidential data records from different institutions must be checked to see if they belong to the same person. In this case, neither institution is permitted to learn anything about the contents of records in the other institutions. Reconciliation, if it is to occur, must implement a zero-knowledge protocol; a protocol that does not reveal any information concerning the reconciled records [5].

We will be describing a protocol for reconciling identifiers without exchanging information about the contents of data records. Because the protocol is somewhat abstract and unintuitive, a physical analogy may clarify the methodology. Imagine two people each holding a box containing an item. Neither person knows the contents of the box that they are holding or of the box that the other person is holding. They want to determine whether

they are holding identical items, but they don't want to know anything about the items. They work together to create two identical imprint stamps, each covered by a complex random collection of raised ridges. With eyes closed, each one pushes his imprint stamp against his item. By doing so, the randomly placed ridges in the stamp are compressed in a manner characteristic of the object's surface. The stamps are next examined to determine if the compression marks on the ridges are distributed identically in both stamps. If so, the items in the two boxes, whatever they may be, are considered to be identical. Not all of the random ridges need to be examined-just enough of them to reach a high level of certainty. It is theoretically possible for two different items to produce the same pattern of compression marks, but it is highly unlikely. After the comparison is made, the stamps are discarded.

The physical analogy demonstrates the power of a zero-knowledge protocol. Neither party knows the identity of his own item. Neither party learns anything about his item or the other party's item during the transaction. Yet, somehow, the parties can determine whether the two items are identical.

Here is how the zero-knowledge protocol to reconcile confidential records across institutions [5]:

1. Both institutions generate a random number of a pre-determined length and each institution sends the random number to the other institution.
2. Each institution sums their own random number with the random number provided by the other institution. We will refer to this number as Random_A. In this way, both institutions have the same final random number and neither institution has actually transmitted this final random number. The splitting of the random number was arranged as a security precaution.
3. Both institutions agree to create a composite representation of information contained in the record that could establish the human subject of the record. The composite might be a concatenation of the social security number, the date of birth, the first initial of the surname.
4. Both institutions create a program that automatically creates the composite numeric representation of the record (which we will refer to as the record signature) and immediately sums the signature with Random_A, the random number that was negotiated between the two institutions (steps 1 and 2). The sum of the composite representation of the record plus Random_A is a random number that we will call Random_B.
5. If the two records being compared across institutions belong to the same human subject, then Random_B will the identical in both institutions. At this point, the two institutions must compare their respective versions of Random_B in such a way that they do not actually transmit Random_B to the other institution. If they were to transmit Random_B to the other institution, then the receiving institution could subtract Random_A from Random B and produce the signature string for a confidential record contained in the other institution. This would be a violation of the requirement to share zero knowledge during the transaction.

6. The institutions take turns sending consecutive characters of their versions of Random_B. For example, the first institution sends the first character to the second institution. The second institution sends the second character to the first institution. The first institution sends the third character to the second institution. The exchange of characters proceeds until the first discrepancy occurs, or until the first 8 characters of the string match successfully. If any of the characters do not match, both institutions can assume that the records belong to different human subjects (i.e., reconciliation failed). If the first 8 characters match, then it is assumed that both institutions are holding the same Random_B string, and that the records are reconciled.

At the end, both institutions learn whether their respective records belong to the same individual; but neither institution has learned anything about the records held in the other institution. Anyone eavesdropping on the exchange would be treated to a succession of meaningless random numbers.

Glossary

Curator The word "curator" derives from the Latin, "curatus," and the same root for "curative," indicating that curators "take care of" things. A data curator collects, annotates, indexes, updates, archives, searches, retrieves and distributes data. Curator is another of those somewhat arcane terms (e.g., indexer, data archivist, lexicographer) that are being rejuvenated in the new millennium. It seems that if we want to enjoy the benefits of a data-centric world, we will need the assistance of curators, trained in data organization.

Digital signature As it is used in the field of data privacy a digital signature is an alphanumeric sequence that could only have been produced by a private key owned by one particular person. Operationally, a message digest (e.g., a one-way hash value) is produced from the document that is to be signed. The person "signing" the document encrypts the message digest using her private key, and submits the document and the encrypted message digest to the person who intends to verify that the document has been signed. This person decrypts the encrypted message digest with her public key (i.e., the public key complement to the private key) to produce the original one-way hash value. Next, a one-way hash is performed on the received document. If the resulting one-way hash is the same as the decrypted one-way hash, then several statements hold true: the document received is the same document as the document that had been "signed." The signer of the document had access to the private key that complemented the public key that was used to decrypt the encrypted one-way hash. The assumption here is that the signer was the only individual with access to the private key. Digital signature protocols, in general, have a private method for encrypting a hash, and a public method for verifying the signature. Such protocols operate under the assumption that only one person can encrypt the hash for the message, and that the name of that person is known; hence, the protocol establishes a verified signature. It should be emphasized that a digital signature is quite different from a written signature; the latter usually indicates that the signer wrote the document or somehow attests to agreement with the contents of the document. The digital signature merely indicates that the document was received from a particular person, contingent on the assumption that the private key was available only to that person. To understand how a digital signature protocol may be maliciously deployed, imagine the following scenario: I contact you and tell you that I am Elvis Presley and would like you to have a copy of my public key plus a file that I have encrypted using my private key. You receive the file and the public key; and you use the public key to decrypt the file. You conclude that the file was indeed sent by Elvis Presley. You read the decrypted file and learn that Elvis advises you to invest all your money in a

company that manufactures concrete guitars; which, of course, you do. Elvis knows guitars. The problem here is that the signature was valid, but the valid signature was not authentic.

Metasyntactic variable A variable name that imports no specific meaning. Popular metasyntactic variables are x, y, n, foo, bar, foobar, spam, eggs, norf, wubble, and blah. Dummy variables are often used in iterating loops. For example:

```
for($i=0;$i<1000;$i++)
```

Good form dictates against the liberal use of metasyntactic variables. In most cases, programmers should create variable names that describe the purpose of the variable (e.g., time_of_day, column_sum, current_line_from_file).

National Patient Identifier Many countries employ a National Patient Identifier (NPI) system. In these cases, when a citizen receives treatment at any medical facility in the country, the transaction is recorded under the same permanent and unique identifier. Doing so enables the data collected on individuals, from multiple hospitals, to be merged. Hence, physicians can retrieve patient data that was collected anywhere in the nation. In countries with NPIs, data scientists have access to complete patient records and can perform healthcare studies that would be impossible to perform in countries that lack NPI systems. In the United States, where a system of NPIs has not been adopted, there is a perception that such a system would constitute an invasion of privacy and would harm citizens.

One-way hash A one-way hash is an algorithm that transforms one string into another string (a fixed-length sequence of seemingly random characters) in such a way that the original string cannot be calculated by operations on the one-way hash value (i.e., the calculation is one-way only). One-way hash values can be calculated for any string, including a person's name, a document, or an image. For any given input string, the resultant one-way hash will always be the same. If a single byte of the input string is modified, the resulting one-way hash will be changed, and will have a totally different sequence than the one-way hash sequence calculated for the unmodified string.

Most modern programming languages have several methods for generating one-way hash values. Regardless of the language we choose to implement a one-way hash algorithm (e.g., md5, SHA), the output value will be identical. One-way hash values are designed to produce long fixed-length output strings (e.g., 256 bits in length). When the output of a one-way hash algorithm is very long, the chance of a hash string collision (i.e., the occurrence of two different input strings generating the same one-way hash output value) is negligible. Clever variations on one-way hash algorithms have been repurposed as identifier systems [6–9]. A detailed discussion of one-way hash algorithms can be found in Section 3.9, "Case Study: One-Way Hashes."

Raw data Raw data is the unprocessed, original data measurement, coming straight from the instrument to the database, with no intervening interference or modification. In reality, scientists seldom, if ever, work with raw data. When an instrument registers the amount of fluorescence emitted by a hybridization spot on a gene array, or the concentration of sodium in the blood, or virtually any of the measurements that we receive as numeric quantities, an algorithm executed by the measurement instrument produces the output. Pre-processing of data is commonplace in the universe of Big Data, and data managers should not labor under the false impression that the data received is "raw," simply because the data has not been modified by the person who submits the data.

Serious Big Data 3 V's (data volume, data variety and data velocity) plus "seriousness." Seriousness is a tongue-in-cheek term that the author applies to Big Data resources whose objects are provided with an adequate identifier and a trusted timestamp and provide data users with introspection, including pointers to the protocols that produced the data objects. The metadata in Big Data resources are appended with namespaces. Serious Big Data resources can be merged with other serious Big Data resources. In the opinion of the author, Big Data resources that lack seriousness should not be used in science, legal work, banking, and in the realm of public policy.

Time stamp Many data objects are temporal events and all temporal events must be given a time stamp indicating the time that the event occurred, using a standard measurement for time. The time stamp must be accurate, persistent, and immutable. The Unix epoch time (equivalent to the Posix epoch time) is available for most operating systems and consists of the number of seconds that have elapsed since January 1, 1970, midnight, Greenwhich mean time. The Unix epoch time can easily be converted into any other standard representation of time. The duration of any event can be easily calculated by subtracting the beginning time from the ending time. Because the timing of events can be maliciously altered, scrupulous data managers employ a trusted time stamp protocol by which a time stamp can be verified. A trusted time stamp must be accurate, persistent, and immutable. Trusted time stamp protocols are discussed in Section 8.5, "Case Study: The Trusted Time stamp."

Verification and validation As applied to data resources, verification is the process that ensures that data conforms to a set of specifications. Validation is the process that checks whether the data can be applied in a manner that fulfills its intended purpose. This often involves showing that correct conclusions can be obtained from a competent analysis of the data. For example, a Big Data resource might contain position, velocity, direction, and mass data for the earth and for a meteor that is traveling sunwards. The data may meet all specifications for measurement, error tolerance, data typing, and data completeness. A competent analysis of the data indicates that the meteor will miss the earth by a safe 50,000 miles, plus or minus 10,000 miles. If the asteroid smashes into the earth, destroying all planetary life, then an extraterrestrial observer might conclude that the data was verified, but not validated.

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9

Assessing the Adequacy of a Big Data Resource

OUTLINE

Section 9.1. Looking at the Data

discovery is ".....seeing what others have seen, but thinking what others have not."
Albert Szent-Gyorgyi

Big Data must not be a Big Waste of time. Looking at the data will tell you immediately if you can use the data. Moving forward with calculations before looking at the data is inexcusable. Before you choose and apply analytic methods to data sets, you should spend time studying your raw data. The following steps may be helpful:

1. Find a free ASCII editor.

When I encounter a large data file, in plain ASCII format, the first thing I do is open the file and take a look at its contents. Unless the file is small (i.e., under about 20 megabytes), most commercial word processors will fail at this task. They simply cannot open really large files (in the Gigabyte range). You will want to use an editor designed to work with large ASCII files. Two of the more popular, freely available editors are Emacs and vi (also available under the name vim). Downloadable versions are available for Linux, Windows, and Macintosh systems. On most computers, these editors will open files in the range of a Gigabyte. For even larger files, there are operating system utilities that can do the job. These will be discussed in Section 9.4, "Case Study: Utilities for Viewing and Searching Large Files." [Glossary Text editor]

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2. Download and study the "readme" or index files, or their equivalent.

In prior decades, large collections of data were often assembled as files within subdirectories and these files could be downloaded in part or *in toto*, via ftp (file transfer protocol). Traditionally, a "readme" file would be included with the files, and the "readme" file would explain the purpose, contents, and organization of all the files. In some cases, an index file might be available, providing a list of terms covered in the files and their locations in the various files. When such files are prepared thoughtfully, they are of great value to the data analyst. It is always worth a few minutes time to open and browse the "readme" file. I think of "readme" files as treasure maps. The data files contain great treasure, but you are unlikely to find anything of value unless you study and follow the map.

In the past few years, data resources have grown in size and complexity. Today, Big Data resources are often collections of resources, housed on multiple servers. New and innovative access protocols are continually being developed, tested, released, updated, and replaced. Still, some things remain the same. There will always be documents to explain how the Big Data resource "works" for the user. It behooves the data analyst to take the time to read and understand this prepared material. If there is no prepared material, or if the prepared material is unhelpful, then you may want to reconsider using the resource.

3. Assess the number of records in the Big Data resource.

There is a tendency among some data managers to withhold information related to the number of records held in the resource. In many cases, the number of records says a lot about the inadequacies of the resource. If the total number of records is much smaller than the typical user might have expected or desired, then the user might seek their data elsewhere. Data managers, unlike data users, sometimes dwell in a perpetual future that never merges into the here and now. They think in terms of the number of records they will acquire in the next 24 hours, the next year, or the next decade. To the data manager, limitations in the present are often irrelevant.

Data managers may be reluctant to divulge the number of records held in the Big Data resource when the number is so large as to defy credibility. Consider this example. There are about 5700 hospitals in the United States serving a population of about 313 million people. If each hospital served a specific subset of the population with no overlap in service between neighboring hospitals, then each would provide care for about 54,000 people. In practice, there is always some overlap in catchment population and a popular estimate for the average (overlapping) catchment for United States hospitals is 100,000. The catchment population for any particular hospital can be estimated by factoring in a parameter related to its size. For example, if a hospital hosts twice the number of beds than the average United States hospital, then one would guess that its catchment population would be about 200,000. The catchment population represents the approximate number of electronic medical records for living patients served by the hospital (one living individual, one hospital record). If you are informed that a hospital, of average size,

contains 10 million records (when you are expecting about 100,000), then you can infer that something is very wrong. Most likely, the hospital is creating multiple records for individual patients. In general, institutions do not voluntarily provide users with information that casts doubt on the quality of their information systems. Hence, the data analyst, ignorant of the total number of records in the system, might proceed under the false assumption that each patient is assigned one and only one hospital record. Suffice it to say that the data user must know the number of records available in a resource, and the manner in which records are identified and internally organized.

A related issue of particular importance is the sample number/sample dimension dichotomy. Some resources with enormous amounts of data may have very few data records. This occurs when individual records contain mountains of data (e.g., sequences, molecular species, images), but the number of individual records is woefully low (e.g., hundreds or thousands). This problem, falling under the curse of dimensionality, will be further discussed in Section 14.6, "Case Study (Advanced): Curse of Dimensionality."

4. Determine how data objects are identified and classified.

As discussed in previous chapters, if you know the identifier for a data object, then you can collect all of the information associated with the object, regardless of its location in the resource. If other Big Data resources use the same identifier for the data object, you can integrate all of the data associated with the data object, regardless of its location in external resources. Furthermore, if you know the class that holds a data object, you can combine objects of a class and study all of the members of the class. Consider the following example.

```
Big Data resource 1

75898039563441   name              G. Willikers
75898039563441   gender            male

Big Data resource 2

75898039563441   age               35
75898039563441   is_a_class_member cowboy
94590439540089   name              Hopalong Tagalong
94590439540089   is_a_class_member cowboy

Merged Big Data Resource 1 + 2

75898039563441   name              G. Willikers
75898039563441   gender            male
75898039563441   is_a_class_member cowboy
75898039563441   age               35
94590439540089   name              Hopalong Tagalong
94590439540089   is_a_class_member cowboy
```

The merge of two Big Data resources combines data related to identifier 75898039563441 from both resources. We now know a few things about this data object that we did not know before the merge. The merge also tells us that the two data objects identified as 75898039563441 and 94590439540089 are both members of class cowboy. We now have two instance members from the same class, and this gives us information related to the types of instances contained in the class.

The consistent application of standard methods for object identification and for class assignments, using a standard classification or ontology, greatly enhances the value of a Big Data resource. A savvy data analyst will quickly determine whether the resource provides these important features. [Glossary Identification]

5. Determine whether data objects contain self-descriptive information.

Data objects should be well specified. All values should be described with metadata, all metadata should be defined, and the definitions for the metadata should be found documents whose unique names and locations are provided. The data should be linked to protocols describing how the data was obtained and measured. [Glossary ISO metadata standard]

6. Assess whether the data is complete and representative.

You must be prepared to spend hours reading through the records; otherwise, you will never really understand the data. After you have spent a few weeks of your life browsing through Big Data resources, you will start to appreciate the value of the process. Nothing comes easy. Just as the best musicians spend thousands of hours practicing and rehearsing their music, the best data analysts must devote thousands of hours to studying their data sources. It is always possible to run sets of data through analytic routines that summarize the data, but drawing insightful observations from the data requires thoughtful study.

An immense Big Data resource may contain spotty data. On one occasion, I was given a large hospital-based data set, with assurances that the data was complete (i.e., containing all necessary data relevant to the project). After determining how the records and the fields were structured, I looked at the distribution frequency of diagnostic entities contained in the data set. Within a few minutes I had the frequencies of occurrence of the different diseases, categorized under broad diagnostic categories. I spent another few hours browsing through the list, and before long I noticed that there were very few skin diseases included in the data. I am not a dermatologist, but I knew that skin diseases are among the most common conditions encountered in medical clinics. Where were the missing skin diseases? I asked one of the staff clinicians assigned to the project. He explained that the skin clinic operated somewhat autonomously from the other hospital departments. The dermatologists maintained their own information system, and their cases were not integrated into the general disease data set. I inquired as to why I had been assured that the data set was complete, when everyone other than myself knew full well that the data set lacked skin cases. Apparently, the staff had become so accustomed to ignoring the field of dermatology that it never crossed their minds to mention the matter.

It is a quirk of human nature to ignore anything outside one's own zone of comfort and experience. Otherwise fastidious individuals will blithely omit relevant information from Big Data resources if they consider the information to be inconsequential, irrelevant, or insubstantial. I have had conversations with groups of clinicians who requested that the free-text information in radiology and pathology reports (the part of the report containing descriptions of findings and other comments) be omitted from the compiled electronic records on the grounds that it is all unnecessary junk. Aside from the fact that "junk" text can serve as important analytic clues (e.g., measurements of accuracy, thoroughness, methodological trends), the systematic removal of parts of data records produces a biased and incomplete Big Data resource. In general, data managers should not censor data. It is the job of the data analyst to determine what data should be included or excluded from analysis; and to justify his or her decision. If the data is not available to the data analyst, then there is no opportunity to reach a thoughtful and justifiable determination.

On another occasion, I was given an anonymized set of clinical data from an undisclosed hospital. As I always do, I looked at the frequency distributions of items on the reports. In a few minutes, I noticed that germ cell tumors, rare tumors that arise from a cell lineage that includes oocytes and spermatocytes, were occurring in high numbers. At first, I thought that I might have discovered an epidemic of germ cell tumors in the hospital's catchment population. When I looked more closely at the data, I noticed that the increased incidence occurred in virtually every type of germ cell tumor, and there did not seem to be any particular increase associated with gender, age, or ethnicity. Cancer epidemics raise the incidence of one or maybe two types of cancer and may involve a particular at-risk population. A cancer epidemic would not be expected to raise the incidence of all types of germ cell tumors, across ages and genders. It seemed more likely that the high numbers of germ cell tumors were explained by a physician or specialized care unit that concentrated on treating patients with germ cell tumors, receiving referrals from across the nation. Based on the demographics of the data set (the numbers of patients of different ethnicities), I could guess the geographic region of the hospital. With this information and knowing that the institution probably had a prestigious germ cell clinic, I guessed the name of the "undisclosed" hospital. My suspicions were eventually confirmed. [Glossary Anonymization versus deidentification]

It sometimes helps to compare the distribution of data in a new collection against the distribution in data in a known and trusted population. For example, you may want to stratify data records by the age of individuals and compare it with the distribution of ages in a control or normal population of individuals. You might also create a word list or index of terms extracted from the data to determine if the frequency of occurrences of the included words or terms are similar to what you have come to expect from comparable data sets. If you find that there are too many kinds of data that are missing from your new collection of data, then you may need to abandon the project. You may find that the information contained in the new collection is similar in kind, but dissimilar in frequency to other populations. For example, if you encounter a population of men and women of all ages, but with a woman:male ration of 5:1 and with very few men

over the age of 70 included in the population, then you might want to normalize your population against a control population. [Glossary Age-adjusted incidence]

The point here is that if you take the time to study raw data, you can spot systemic deficiencies or excesses in the data, if they exist, and you may gain deep insights that would not be obtained by mathematical techniques.

7. Plot some of the data.

Plotting data is quick, easy, and surprisingly productive. Within minutes, the data analyst can assess long-term trends, short-term and periodic trends, the general shape of data distribution and general notions of the kinds of functions that might represent the data (e.g., linear, exponential, power series). Simply knowing that the data can be expressed as a graph is immeasurably reassuring to the data analyst.

There are many excellent data visualization tools that are widely available. Without making any recommendation, I mention that graphs produced for this book were made with Matplotlib, a plotting library for the Python programming language; and Gnuplot, a graphing utility available for a variety of operating systems. Both Matplotlib and Gnuplot are open source applications that can be downloaded, at no cost, and are available at sourceforge.net. [Glossary Open source]

Gnuplot is extremely easy to use, either as stand-alone scripts containing gnuplot commands, or from the system command line. Most types of plots can be created with a single gnuplot command line. Gnuplot can fit a mathematically expressed curve to a set of data using the nonlinear least-squares Marquardt-Levenberg algorithm [1,2]. Gnuplot can also provide a set of statistical descriptors (e.g., median, mean, and standard deviation) for plotted sets of data.

Gnuplot operates from data held in tab-delimited ASCII files. Typically, data extracted from a Big Data resource is ported into a separate ASCII file, with column fields separated with a tab character, and rows separated by a newline character. In most cases, you will want to modify your raw data, readying it for plotting. Use your favorite programming language to normalize, shift, transform, covert, filter, translate, or munge your raw data, as you see fit. Export the data as a tab-delimited file, named with a .dat suffix.

It takes about a second to generate a plot for 10,000 data points (Fig. 9.1).

One command line in Gnuplot produced the graph, from the data.

```
splot 'c:\ftp\xyz_rand.dat'
```

It is very easy to plot data, but one of the most common mistakes of the data analyst is to assume that the available data actually represents the full range of data that may occur. If the data under study does not include the full range of the data, the data analyst will often reach a completely erroneous explanation for the observed data distribution.

Data distributions will almost always appear to be linear at various segments of their range. An oscillating curve that reaches equilibrium may look like a sine wave early in its course, and a flat-line later on. In the larger oscillations, it may appear linear along the length of a half-cycle. Any of these segmental interpretations of the data will miss observations that would lead to a full explanation of the data (Fig. 9.2).

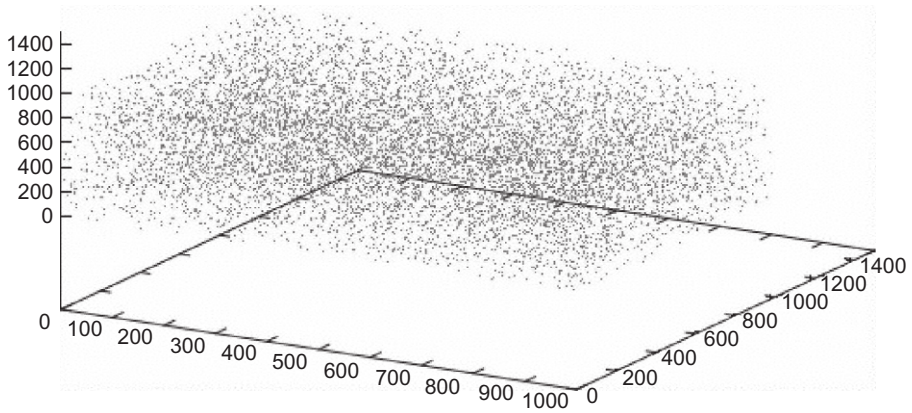

FIG. 9.1 A plot of 10,000 random data points, in three coordinates. The data for this figure was created with a 7 line script using the Perl programming language, but any scripting language would have been sufficient [3]. Ten thousand data points were created, with the *x*, *y*, and *z* coordinates for each point produced by a random number generator. The point coordinates were put into a file named xyz_rand.dat.

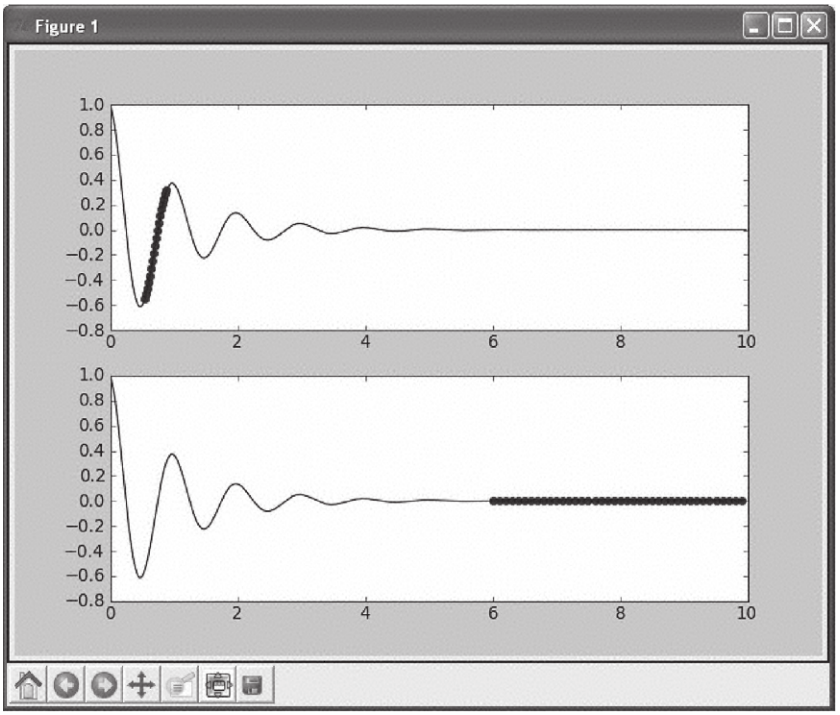

FIG. 9.2 An oscillating wave reaching equilibrium. The top graph uses circle-points to emphasize a linear segment for a half-cycle oscillation. The bottom graph of the same data emphasizes a linear segment occurring at equilibrium.

An adept data analyst can eyeball a data distribution and guess the kind of function that might model the data. For example, a symmetric bell-shaped curve is probably a normal or Gaussian distribution. A curve with an early peak and a long, flat tail is often a power law distribution. Curves that are simple exponential or linear can also be assayed

by visual inspection. Distributions that may be described by a Fourier series or a power series, or that can be segmented into several different distributions, can also be assessed. [Glossary Power law, Power series, Fourier series]

8. Estimate the solution to your multi-million dollar data project, on day 1.

This may seem difficult to accept, and there will certainly be exceptions to the rule, but the solution to almost every multi-million dollar analytic problem can usually be estimated in just a few hours, sometimes minutes, at the outset of the project. If an estimate cannot be attained fairly quickly, then there is a good chance that the project will fail. If you do not have the data for a quick and dirty estimate, then you will probably not have the data needed to make a precise determination.

The past several decades have witnessed a profusion of advanced mathematical techniques for analyzing large data sets. It is important that we have these methods, but in most cases, newer methods serve to refine and incrementally improve older methods that do not rely on powerful computational techniques or sophisticated mathematical algorithms. As someone who was raised prior to the age of hand-held calculators and personal computers, I was taught quick-and-dirty estimation methods for adding, subtracting, multiplying, and dividing lists of numbers. The purpose of the estimation was to provide a good idea of the final answer, before much time was spent on a precise solution. If no mistake was introduced in either the estimate or the long calculation, then the two numbers would come close to one another. Conversely, mistakes in the long calculations could be detected if the two calculations yielded different numbers.

If data analysts go straight to the complex calculations before they perform a simple estimation, they will find themselves accepting wildly ridiculous calculations. For comparison purposes, there is nothing quite like a simple, intuitive estimate to pull a overly-eager analyst back to reality. Often, the simple act of looking at a stripped-down version of the problem opens a new approach that can drastically reduce computation time [4]. In some situations, analysts will find that a point is reached when higher refinements in methods yield diminishing returns. When everyone has used their most advanced algorithms to make an accurate prediction, they may sometimes find that their best effort offers little improvement over a simple estimator.

Section 9.2. The Minimal Necessary Properties of Big Data

In God we trust, all others bring data.

William Edwards Deming (1900–1993)

Many of today's statisticians and scientists came of age in the world of small data. When you are working with a few hundred measurements, most of the issues discussed in this book have almost no relevance. Small data does not need to be dressed up with identifiers and metadata. Scientists did not worry very much about creating self-explanatory data; each scientist understood their own data, and that was usually good enough.

Big Data, with its volume, complexity, velocity, and permanence, requires a remarkable amount of annotation and curation. For the most part, the issues raised in this book are unknown to the bulk of individuals who collect Big Data. Hence, most of the Big Data that has been collected and stored has no scientific value; it is simply incomprehensible and unusable [5–8]. This may seem like an outrageous claim, particularly when you consider how much of the world's activities are data-driven. If you speak with scientists who collect and analyze data, and that would include just about every scientist you are likely to encounter, you will hear them tell you that their data is just fine, and perfectly suitable for their own scientific studies. The point that must be made is that the scientists who collected and analyzed the data cannot judge the value of scientific data. The true value of data must be assessed by the scientists who verify, validate, and re-analyze the data that was collected by other scientists. If the original data cannot be obtained and analyzed by the scientific community, now and in the future, then the original assertions cannot be confirmed, and the data cannot be usefully merged with other data sets, extended, and repurposed. [Glossary Abandonware, Dark data, Universal and perpetual, Data versus datum, Identifier, Data repurposing]

For data to be useful to the scientific community, it must have a set of basic properties, and, unfortunately, these properties are seldom taught or utilized. Here are the universal properties of good data that has lasting scientific value.

- Data that has been annotated with metadata
- Data that establishes uniqueness or identity
- Time stamped data that accrues over time [Glossary Time, Time stamp]
- Data that resides within a data object
- Data that has membership in a defined class
- Introspective data—data that explains itself
- Immutable data
- Data that has been simplified

Let us take a moment to examine each of these data features:

- **Data that has been annotated with metadata**

Metadata, the data that explains data, was discussed in Sections 4.1 through 4.3. The modern specification for metadata is the eXtensible Markup Language (XML). The importance of XML to data scientists cannot be overstated. As a data-organizing technology, it is as important as the invention of written language (circa 3000 bc) or the appearance of mass-printed books (circa 1450 ad). Markup allows us to convey any message as XML (a pathology report, a radiology image, a genome database, a workflow process, a software program, or an e-mail). [Glossary Data annotation, Annotation, Data sharing]

- **Data that establishes uniqueness or identity**

The most useful data establishes the identity of objects. In many cases, objects have their own, natural identifiers that come very close to establishing uniqueness.

Examples include fingerprints, iris patterns, and the sequence of nucleotides in an organism's genetic material.

In regard to identifying data objects, we need not depend on each data object having its own naturally occurring identifier. As discussed in Section 3.1, we can simply generate and assign unique identifiers to our data objects [3,8–10]. Identifiers are data simplifiers, when implemented properly. They allow us to collect all of the data associated with a unique object, while ensuring that we exclude that data that should be associated with some other object.

– **Time stamped data that accrues over time**

When a data set contains data records that collect over time, it becomes possible to measure how the attributes of data records may change as the data accumulates. Signals analysts use the term time series to refer to attribute measurements that change over time. The shape of the time series can be periodic (i.e., repeating over specific intervals), linear, non-linear, Gaussian, or multimodal (i.e., having multiple peaks and troughs), or chaotic. A large part of data science is devoted to finding trends in data, determining simple functions that model the variation of data over time, or predicting how data will change in the future. All these analytic activities require data that is annotated with the time that a measurement is made, or the time that a record is prepared, or the time that an event has occurred. [Glossary Data science, Waveform]

You may be shocked to learn that many, if not most, web pages lack a time stamp to signify the date and time when the page's textual content was created. This oversight applies to news reports, announcements from organizations and governments, and even scientific papers; all being instances for which a time stamp would seem to be an absolute necessity. When a scientist publishes an undated manuscript, how would anyone know if the results are novel? If a news article describes an undated event, how would anyone know whether the report is current? For the purposes of data analysis, undated documents and data records are useless [5].

Whereas undated documents have very little value, all transactions, statements, documents and data points that are annotated with reliable time stamps will always have some value, particularly if the information continues to collect over time. Today, anyone with a computer can easily time stamp his or her data, with the date and the time, accurate to within a second. As discussed in Section 6.4, "Case Study: Time stamping Data," every operating system and every programming language has access to the time, and can easily annotate any data point with the time that it was created. Time data can be formatted in any of dozens of ways, all of which can be instantly converted to an international standard [11].

It's human nature to value newly collected data and to dismiss old data as being outdated or irrelevant. Nothing could be further from the truth. New data, in the absence of old data, has little value. All historical events develop through time, and the observations made at any given moment in time are always influenced by events that transpired at earlier times. Whenever we speak of "new" data, alternately known as prospectively acquired data, we must think in terms that relate the new data to the "old" data that

preceded it. Old data can be used to analyze trends over time and to predict the data values into the future. Essentially, old data provides the opportunity to see the past, the present, and the future. The dependence of new data on old data can be approached computationally. The autocorrelation function is a method for producing a type of measurement indicating the dependence of data elements on prior data elements. Long-range dependence occurs when a value is dependent on many prior values. Long-range dependence is determined when the serial correlation (i.e., the autocorrelation over multiple data elements) is high when the number of sequential elements is large [12]. These are nifty tools for data analysis, but they cannot be employed if the data is not time stamped [6]. [Glossary Correlation distance]

– **Data that is held in a data object**

In Section 6.2, "Data Objects: The Essential Ingredient of Every Big Data Collection," we defined a data object as an object identifier plus all of the data/metadata pairs that rightly belong to the object identifier, including a data/metadata pair that tells us the object's class. Lucky for us, some of the most common data creations (e.g., emails and photographic images) are automatically composed as data objects by our software (i.e., email clients and digital cameras).

When you send a message, your email client automatically creates a data object that holds the contents of your message, descriptive information about the message, a message identifier, and a time stamp. Here is a sample email header, obtained by selecting the email client's long or detailed version of the message. The actual message contents would normally follow, but are omitted here for brevity.

```
– MIME-Version: 1.0
– Received: by 10.36.165.75 with HTTP; Tue, 2 May 2017 14:46:47 -0700
  (PDT)
– Date: Tue, 2 May 2017 17:46:47 -0400
– Delivered-To: you@gmail.com
– Message-ID: <CALVNVe-
  kk7fqYJ82MfsV6a4kFKW4v57c4y9BLp0UYf1cBHq9pQ@mail.gmail.com>
– Subject: tiny fasts
– From: Anybody <me@gmail.com>
– To: Anybody Else <you@gmail.com>
– Content-Type: multipart/alternative;
  boundary=94eb2c07ab4c054062054e917a03
```

Notice that each line of the header consists of a colon ":" flanked to the right by metadata (e.g., Subject, From, To) and on the left by the described data. There is a line for a time stamp and a line for an identifier assigned by the email client.

```
– Date: Tue, 2 May 2017 17:46:47 -0400
– Message-ID: <CALVNVe-
  kk7fqYJ82MfsV6a4kFKW4v57c4y9BLp0UYf1cBHq9pQ@mail.gmail.com>
```

Email messages are an example of data objects that are automatically created when you push the "send" button. When we read about the remarkable results achieved by forensic data analysts, who gather time stamped, immutable, and identified evidence from millions of stored messages, we must give credit to the power of data objects.

– **Data that has membership in a defined class**

In Chapter 5, we discussed classifications and ontologies and explained the importance of assigning instances (e.g., diseases, trucks, investments) to classes wherein every instance shares a set of features typical of the class. All good classifications have a feature that is known as competence; the ability to draw inferences about data objects, and their relationships to other data objects, based on class definitions. Data that is unclassified may have some immediate observational or experimental value to scientists, but such data cannot be used to draw inferences from classes of data objects obtained from Big Data resources.

– **Introspective data (data that explains itself)**

Introspection, as previously discussed in Chapter 6, refers to the ability of data (e.g., data records, documents, and all types of data objects) to describe itself when interrogated. Introspection gives data users the opportunity to see relationships among the individual data records that are distributed in different data sets, and is one of the most useful features of data objects, when implemented properly.

Modern programming languages allow us to interrogate data, and learn everything there is to know about the information contained in data objects. Information about data objects, acquired during the execution of a program, can be used to modify a program's instructions, during run-time, a useful feature known as "reflection". Detailed information about every piece of data in a data set (e.g., the identifier associated with the data object, the class of objects to which the data object belongs, the metadata and the data values that are associated with the data object), permit data scientists to integrate data objects collected from multiple Big Data resources.

It should be noted that the ability to perform introspection is not limited to object oriented programming languages. Introspection is provided by the data, and any programming language will suffice, so long as the data itself is organized as data objects assigned to classes within a sensibly structured classification.

– **Immutable data**

When you are permitted to change preexisting data, all of your collected data becomes tainted. None of the analyses performed on the data in the database can be verified, because the data that was originally analyzed no longer exists. It has become something else, which you cannot fully understand. Aside from producing an unverifiable data collection, you put the data analyst in the impossible position of deciding which data to believe; the old data or the new data.

– **Data that has been simplified**

Big Data is complex data, and complex data is difficult to understand and analyze. As it happens, all of the properties that we consider the minimal necessary for Big Data preparation happen to be simplifying. Metadata, identifiers, data objects, and classifications all work to drive down the complexity of data and render the data understandable to man or machine.

It is easy for data managers to shrug off the data requirements described in this section as high-tech nuisances. Big Data requires an enormous amount of fussy work that was simply not necessary when data was small. Nonetheless, it is necessary, if we hope to use more than an insignificant fraction of the data that is being collected every day.

Section 9.3. Data That Comes With Conditions

This site has been moved.
We'd tell you where, but then we'd
have to delete you.

Computer-inspired haiku by Charles Matthews

I was involved in one project where the data holders could not be deterred from instituting a security policy wherein data access would be restricted to pre-approved users. Anyone wishing to query the database would first submit an application, which would include detailed information about themselves and their employer. The application required users to explain how they intended to use the resource, providing a description of their data project. Supplying this information was a warm-up exercise for the next step.

A screening committee composed primarily of members of the Big Data team would review the submitted application. A statistician would be consulted to determine if the applicant's plan was feasible. The committee would present their findings to an executive committee that would compare each application's merits against those of the other applicants. The very best applications would be approved for data access.

The data team could not seem to restrain their enthusiasm for adding layers of complexity to the security system. They decided that access to data would be tiered. Some users would be given less access to data than other users. No users would be given free access to the entire set of data. No user would have access to individual deidentified records; only aggregate views of record data would be released. A system would be designed to identify users and to restrict data access based on the identity and assigned access status.

These security measures were unnecessary. The data in the system had been rendered harmless via deidentification and could be distributed without posing any risk to the data subjects or to the data providers. The team seemed oblivious to the complexities engendered by a tiered access system. Bruce Schneier, a widely cited security expert, wrote an essay entitled, "A plea for simplicity: you can't secure what you don't understand" [13].

In this essay, he explained that as you add complexity to a system, the system becomes increasingly difficult to secure. I doubted that the team had the resources or the expertise to implement a complex, multi-tiered access system for a Big Data resource. I suspected that if the multi-tiered access system were actually put into place, the complexity of the system would render the resource particularly vulnerable to attack. In addition, the difficulty of accessing the system would discourage potential users and diminish the scientific value of the Big Data resource.

Many data holders believe that their job, as responsible stewards of data, is to deny data access to undeserving individuals and to ensure that any incorrect conclusions drawn from their data will never see the light of day. I have seen examples wherein the data holders require data users to sign an agreement indicating that the results of their analyses must be submitted back to the data holders before being released to the public in the form of manuscripts, public announcements, or conference presentations. The data holders typically reserve the right to forbid releasing results with which they disapprove. It is easy to see that a less-than-saintly committee might disapprove results that cast their Big Data resource in a bad light, or results that compete in any way with the products of their own research, or results that they hold in disfavor for any capricious reason whatsoever.

Aside from putting strict restrictions on who gets access to data, and which results are permitted to be published, it is commonplace to impose strict restrictions on how the data can be viewed. Anyone who has visited online databases is familiar with the query box. The idea is that the user enters a query and waits for some output to appear on the screen. The assumption here is that the user knows how the query must be composed to produce the most complete output. Of course, this is never the case. When a user enters a query, she cannot know, in advance, whether some other query term might have yielded a better output. Such query boxes almost never return details about the data set or the algorithm employed in responding to the query. It is difficult, under these circumstances, to imagine any scenario wherein these kinds of queries have any scientific merit.

If Big Data resources are to add significantly to the advancement of science, the kinds of complex and stingy data sharing practices that have evolved over the past few decades must face extinction.

Section 9.4. Case Study: Utilities for Viewing and Searching Large Files

It isn't that they can't see the solution. It's that they can't see the problem.

G. K. Chesterton

In Section 9.1, we discussed the importance of looking at your data. Several free and open source text editors were suggested (Open Office, vi, emacs). These text editors can open immense files (gigabytes in length and longer), but they have their limits. Files much

larger than a gigabyte may be slow to load, or may actually be unloadable on systems with small memory capacity. In such cases, your computer's operating system may offer a convenient alternative to text editors.

In the Windows operating system, then you can read any text file, one screen at a time, with the "more" command.

For example, on Windows systems, at the prompt:

```
c:\>type huge_file.txt |more
```

The first lines from the huge_file.txt file will fill the screen, and you can proceed through the file by pressing and holding the <Enter> key. [Glossary Line]

Using this simple command, you can assess the format and general organization of any file. For the uninitiated, ASCII data files are inscrutable puzzles. For those who take a few moments to learn the layout of the record items, ASCII records can be read and understood, much like any book.

In contrarian Unix and Linux systems the "less" command functions much like the Windows "more" command, but offers many additional options. At the Unix (or Linux) system prompt, type the following command (substituting your preferred file for "huge_file.txt"):

```
$ less huge_file.txt
```

This will load a screen-sized chunk of huge_file.txt onto your monitor. By pressing the "enter" key, or the "arrow down" key, additional lines will scroll onto the monitor, one line at a time. For fast screen scrolls, keep your finger on the "Page Down" key. The "Page Up" key lets you back the screens.

The less command accommodates various options.

```
$ less -S huge_file.txt
```

the use of the -S switch cuts off line wrap so that the lines are truncated at the edge of the screen. In general, this speeds up the display.

When you use the Unix "less" command, you will find that the last line at the bottom of the screen is a ":". The ":" is a prompt for additional instructions. If you were to enter a slash character ("/") followed by a word or phrase or regex pattern, you would immediately see the line in which the first occurrence of your search term appeared. If you typed "&" and the pattern, at the ":" prompt, you would see all the lines from the file, in which your search pattern appears.

The Unix "less" command is a versatile and fast utility for viewing and searching very large files. If you do not use Unix systems, do not despair. Windows users can install Cygwin, a free Unix-like interface. Cygwin, and supporting documentation, can be downloaded from:

http://www.cygwin.com/

Cygwin opens in a window that produces a shell prompt (equivalent to Windows C prompt) from which Unix programs can be launched. For myself, I use Cygwin primarily as a source of Unix and Linux utilities, of which there are hundreds. In addition, Cygwin comes bundled with some extremely useful applications, such as Perl, Python, OpenSSL, and Gnuplot.

Windows users are not restricted to launching Unix and Linux applications from within the Cygwin shell prompt. A command line from the Windows C prompt will launch Cygwin utilities. For example:

```
c:\cygwin64\bin>wc temp.txt
  11587 217902 1422378 temp.txt
```

The command "wc temp.txt," launched the Unix/Linux word counter utility ("wc") from the Windows C prompt, yielding a count of the lines, words, and bytes in the temp.txt file. Likewise, a system call from a Python script can invoke Cygwin utilities and applications.

Big Data scientists eventually learn that there are some tasks that are best left to Unix/Linux. Having Cygwin installed on your Windows system will make life easier for you, and for your collaborators, who may prefer to work in Linux.

Section 9.5. Case Study: Flattened Data

Everything should be made as simple as possible, but not simpler.

Albert Einstein

Data flattening is a term that is used differently by data analysts, database experts, and informaticians. Though the precise meaning changes from subfield to subfield, the term always seems to connote a simplification of the data and the elimination of unnecessary structural restraints.

In the field of informatics, data flattening is a popular but ultimately counterproductive method of data organization and data reduction. Data flattening involves removing data annotations that are not needed for the interpretation of data [5].

Imagine, for the sake of illustration, a drastic option that was seriously considered by a large medical institution. This institution, that shall remain nameless, had established an excellent Electronic Medical Record (EMR) system. The EMR assigns a unique and permanent identifier string to each patient, and attaches the identifier string to every hospital transaction involving the patient (e.g., biopsy reports, pharmacy reports, nursing notes, laboratory reports). All of the data relevant to a patient, produced anywhere within the hospital system is linked by the patient's unique identifier. The patient's EMR can be assembled, instantly, whenever needed, via a database query.

Over time, the patient records in well-designed information systems accrue a huge number of annotations (e.g., time stamped data elements, object identifiers, linking elements, metadata). The database manager is saddled with the responsibility of

maintaining the associations among all of the annotations. For example, an individual with a particular test, conducted at a particular time, on a particular day, will have annotations that link the test to a test procedure protocol, an instrument identifier, a test code, a laboratory name, a test sample, a sample accession time, and so on. If data objects could be stripped of most of their annotations, after some interval of time, then it would reduce the overall data management burden on the hospital information system. This can be achieved by composing simplified reports and deleting the internal annotations. For example, all of the data relevant to a patient's laboratory test could be reduced to the patient's name, the date, the name of the test, and the test result. All of the other annotations can be deleted. This process is called data flattening.

Should a medical center, or any entity that collects data, flatten their data? The positive result would be a streamlining of the system, with a huge reduction in annotation overhead. The negative result would be the loss of the information that connects well-defined data objects (e.g., test result with test protocol, test instrument with test result, name of laboratory technician with test sample, name of clinician with name of patient). Because the fundamental activity of the data scientist is to find relationships among data objects, data flattening will reduce the scope and value of data repurposing projects. Without annotations and metadata, the data from different information systems cannot be sensibly merged. Furthermore, if there is a desire or a need to reanalyze flattened data, then the data scientist will not be able to verify the data and validate the conclusions drawn from the data [5]. [Glossary Verification and validation, Validation]

Glossary

Abandonware Software that that is abandoned (e.g., no longer updated, supported, distributed, or sold) after its economic value is depleted. In academic circles, the term is often applied to software that is developed under a research grant. When the grant expires, so does the software. Most of the software in existence today is abandonware.

Age-adjusted incidence An age-adjusted incidence is the crude incidence of disease occurrence within an age category (e.g., age 0–10 years, age 70–80 years), weighted against the proportion of persons in the age groups of a standard population. When we age-adjust incidence, we cancel out the changes in the incidence of disease occurrence, in different populations, that result from differences in the proportion of people in different age groups. For example, suppose you were comparing the incidence of childhood leukemia in two populations. If the first population has a large proportion of children, then it will likely have a higher number of childhood leukemia in its population, compared with another population with a low proportion of children. To determine whether the first population has a true, increased rate of leukemia, we need to adjust for the differences in the proportion of young people in the two populations [14].

Annotation Annotation involves describing data elements with metadata or attaching supplemental information to data objects.

Anonymization versus deidentification Anonymization is a process whereby all the links between an individual and the individual's data record are irreversibly removed. The difference between anonymization and deidentification is that anonymization is irreversible. There is no method for re-establishing the identity of the patient from anonymized records. Deidentified records can, under

strictly controlled circumstances, be reidentified. Reidentification is typically achieved by entrusting a third party with a confidential list that maps individuals to deidentified records. Obviously, reidentification opens another opportunity of harming individuals, if the confidentiality of the reidentification list is breached. The advantages of reidentification is that suspected errors in a deidentified database can be found, and corrected, if permission is obtained to reidentify individuals. For example, if the results of a study based on blood sample measurements indicate that the original samples were mislabeled, it might be important to reidentify the samples and conduct further tests to resolve the issue. In a fully anonymized data set, the opportunities for verifying the quality of data are highly limited.

Correlation distance Also known as correlation score. The correlation distance provides a measure of similarity between two variables. Two similar variables will rise and fall together [15,16]. The Pearson correlation score is popular, and can be easily implemented [3,17]. It produces a score that varies from -1 to 1. A score of 1 indicates perfect correlation; a score of -1 indicates perfect anti-correlation (i.e., one variable rises while the other falls). A Pearson score of 0 indicates lack of correlation. Other correlation measures can be applied to Big Data sets [15,16].

Dark data Unstructured and ignored legacy data, presumed to account for most of the data in the "infoverse". The term gets its name from "dark matter" which is the invisible stuff that accounts for most of the gravitational attraction in the physical universe.

Data annotation The process of supplementing data objects with additional data, often providing descriptive information about the data (i.e., metadata, identifiers, time information, and other forms of information that enhances the utility of the data object.

Data repurposing Involves using old data in new ways, that were not foreseen by the people who originally collected the data. Data repurposing comes in the following categories: (1) Using the preexisting data to ask and answer questions that were not contemplated by the people who designed and collected the data; (2) Combining preexisting data with additional data, of the same kind, to produce aggregate data that suits a new set of questions that could not have been answered with any one of the component data sources; (3) Reanalyzing data to validate assertions, theories, or conclusions drawn from the original studies; (4) Reanalyzing the original data set using alternate or improved methods to attain outcomes of greater precision or reliability than the outcomes produced in the original analysis; (5) Integrating heterogeneous data sets (i.e., data sets with seemingly unrelated types of information), for the purpose an answering questions or developing concepts that span diverse scientific disciplines; (6) Finding subsets in a population once thought to be homogeneous; (7) Seeking new relationships among data objects; (8) Creating, on-the-fly, novel data sets through data file linkages; (9) Creating new concepts or ways of thinking about old concepts, based on a reexamination of data; (10) Fine-tuning existing data models; and (11) Starting over and remodeling systems [5].

Data science A vague term encompassing all aspects of data collection, organization, archiving, distribution, and analysis. The term has been used to subsume the closely related fields of informatics, statistics, data analysis, programming, and computer science.

Data sharing Providing one's own data to another person or entity. This process may involve free or purchased data, and it may be done willingly, or under coercion, as in compliance with regulations, laws, or court orders.

Data versus datum The singular form of data is datum, but the word "datum" has virtually disappeared from the computer science literature. The word "data" has assumed both a singular and plural form. In its singular form, it is a collective noun that refers to a single aggregation of many data points. Hence, current usage would be "The data is enormous," rather than "These data are enormous."

Fourier series Periodic functions (i.e., functions with repeating trends in the data, including waveforms and periodic time series data) can be represented as the sum of oscillating functions (i.e., functions involving sines, cosines, or complex exponentials). The summation function is the Fourier series.

ISO metadata standard ISO 11179 is the standard produced by the International Standards Organization (ISO) for defining metadata, such as XML tags. The standard requires that the definitions for metadata used in XML (the so-called tags) be accessible and should include the following information for each tag: Name (the label assigned to the tag), Identifier (the unique identifier assigned to the tag), Version (the version of the tag), Registration Authority (the entity authorized to register the tag), Language (the language in which the tag is specified), Definition (a statement that clearly represents the concept and essential nature of the tag), Obligation (indicating whether the tag is required), Datatype (indicating the type of data that can be represented in the value of the tag), Maximum Occurrence (indicating any limit to the repeatability of the tag), and Comment (a remark describing how the tag might be used).

Identification The process of providing a data object with an identifier, or the process of distinguishing one data object from all other data objects on the basis of its associated identifier.

Identifier A string that is associated with a particular thing (e.g., person, document, transaction, data object), and not associated with any other thing [18]. In the context of Big Data, identification usually involves permanently assigning a seemingly random sequence of numeric digits (0–9) and alphabet characters (a–z and A–Z) to a data object. The data object can be a class of objects.

Line A line in a non-binary file is a sequence of characters that terminate with an end-of-line character. The end-of-line character may differ among operating systems. For example, the DOS end of line character is ASCII 13 (i.e., the carriage return character) followed by ASCII 10 (i.e., the line feed character), simulating the new line movement in manual typewriters. The Linux end-of-line character is ASCII 10 (i.e., the line feed character only). When programming in Perl, Python or Ruby, the newline character is represented by "\n" regardless of which operating system or file system is used. For most purposes, use of "\n" seamlessly compensates for discrepancies among operating systems with regard to their preferences for end-of-line characters. Binary files, such as image files or telemetry files, have no designated end-of-line characters. When a file is opened as a binary file, any end-of-line characters that happen to be included in the file are simply ignored as such, by the operating system.

Open source Software is open source if the source code is available to anyone who has access to the software.

Power law A mathematical formula wherein a particular value of some quantity varies as an inverse power of some other quantity [19,20]. The power law applies to many natural phenomena and describes the Zipf distribution or Pareto's principle. The power law is unrelated to the power of a statistical test.

Power series A power series of a single variable is an infinite sum of increasing powers of x, multiplied by constants. Power series are very useful because it is easy to calculate the derivative or the integral of a power series, and because different power series can be added and multiplied together. When the high exponent terms of a power series are small, as happens when x is less than one, or when the constants associated with the higher exponents all equal 0, the series can be approximated by summing only the first few terms. Many different kinds of distributions can be represented as a power series. Distributions that cannot be wholly represented by a power series may sometimes by segmented by ranges of x. Within a segment, the distribution might be representable as a power series. A power series should not be confused with a power law distribution.

Text editor A text editor (also called ASCII editor) is a software application designed to create, modify, and display simple unformatted text files. Text editors are different from word processes that are designed to include style, font, and other formatting symbols. Text editors are much faster than word processors because they display the contents of files without having to interpret and execute formatting instructions. Unlike word processors, text editors can open files of enormous size (e.g., gigabyte range).

Time A large portion of data analysis is concerned, in one way or another, with the times that events occur or the times that observations are made, or the times that signals are sampled. Here are three examples demonstrate why this is so: (1) most scientific and predictive assertions relate how variables change

with respect to one another, over time; and (2) a single data object may have many different data values, over time, and only timing data will tell us how to distinguish one observation from another; (3) computer transactions are tracked in logs, and logs are composed of time-annotated descriptions of the transactions. Data objects often lose their significance if they are not associated with an accurate time measurement. Because modern computers easily capture accurate time data, there is not annotating all data points with the time when they are measured.

Time stamp Many data objects are temporal events and all temporal events must be given a time stamp indicating the time that the event occurred, using a standard measurement for time. The time stamp must be accurate, persistent, and immutable. The Unix epoch time (equivalent to the Posix epoch time) is available for most operating systems and consists of the number of seconds that have elapsed since January 1, 1970, midnight, Greenwhich mean time. The Unix epoch time can easily be converted into any other standard representation of time. The duration of any event can be easily calculated by subtracting the beginning time from the ending time. Because the timing of events can be maliciously altered, scrupulous data managers employ a trusted time stamp protocol by which a time stamp can be verified. A trusted time stamp must be accurate, persistent, and immutable. Trusted time stamp protocols are discussed in Section 8.5, "Case Study: The Trusted Time Stamp."

Universal and perpetual Wherein a set of data or methods can be understood and utilized by anyone, from any discipline, at any time. It is a tall order, but a worthy goal. Much of the data collected over the centuries of recorded history is of little value because it was never adequately described when it was recorded (e.g., unknown time of recording, unknown source, unfamiliar measurements, unwritten protocols). Efforts to resuscitate large collections of painstakingly collected data are often abandoned simply because there is no way of verifying, or even understanding, the original data [5]. Data scientists who want their data to serve for posterity should use simple specifications, and should include general document annotations such as the Dublin Core. The importance of creating permanent data is discussed elsewhere [6].

Validation Involves demonstrating that the conclusions that come from data analyses fulfill their intended purpose and are consistent [21]. You validate a conclusion (which my appear in the form of an hypothesis, or a statement about the value of a new laboratory test, or a therapeutic protocol) by showing that you draw the same conclusion repeatedly whenever you analyze relevant data sets, and that the conclusion satisfies some criteria for correctness or suitability. Validation is somewhat different from reproducibility. Reproducibility involves getting the same measurement over and over when you perform the test. Validation involves drawing the same conclusion over and over.

Verification and validation As applied to data resources, verification is the process that ensures that data conforms to a set of specifications. Validation is the process that checks whether the data can be applied in a manner that fulfills its intended purpose. This often involves showing that correct conclusions can be obtained from a competent analysis of the data. For example, a Big Data resource might contain position, velocity, direction, and mass data for the earth and for a meteor that is traveling sunwards. The data may meet all specifications for measurement, error tolerance, data typing, and data completeness. A competent analysis of the data indicates that the meteor will miss the earth by a safe 50,000 miles, plus or minus 10,000 miles. If the asteroid smashes into the earth, destroying all planetary life, then an extraterrestrial observer might conclude that the data was verified, but not validated.

Waveform A graph showing a signal's amplitude over time. By convention, the amplitude of the signal is shown on the y-axis, while the time is shown on the x-axis. A .wav file can be easily graphed as a waveform, in python.

The waveform.py script graphs a sample .wav vile, alert.wav, but any handy .wav file should suffice (Fig. 9.3).

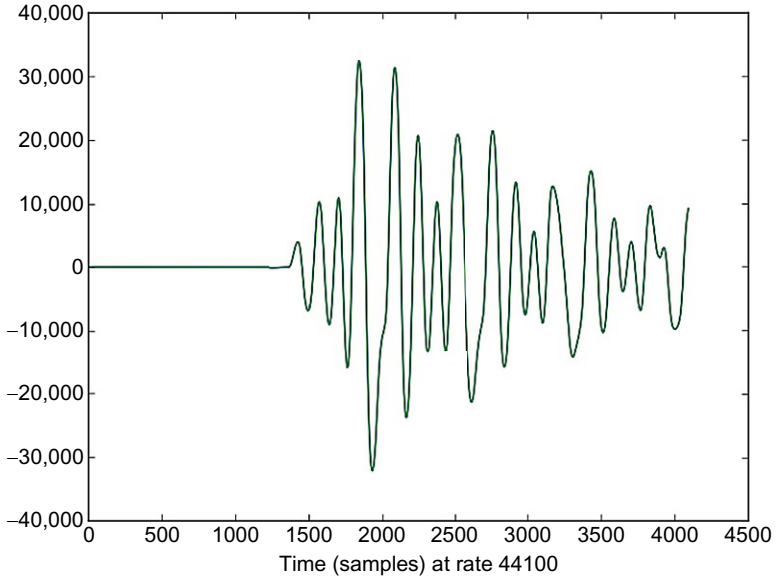

FIG. 9.3 The plotted waveform of a .wav file, alert.wav.

```
from scipy.io.wavfile import read
import matplotlib.pyplot as plt
input_data = read("alert.wav")
# returns a two-item tuple with sampling rate as
#the 0th item and audio samples as the 1st item
audio = input_data[1]
# we'll plot the first 4096 samples
plt.plot(audio[0:4096])
plt.xlabel("time (samples) at rate " + str(input_data[0]))
plt.show()
```

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10

Measurement

OUTLINE

Section 10.1. Accuracy and Precision

Get your facts first, then you can distort them as you please.

Mark Twain

Precision is the degree of exactitude of a measurement and is verified by its reproducibility (i.e., whether repeated measurements of the same quantity produce the same result). Accuracy measures how close your data comes to being correct. Data can be accurate but imprecise or precise but inaccurate. If you have a 10-pound object, and you report its weight as 7.2376 pounds, every time you weigh the object, then your precision is remarkable, but your accuracy is dismal.

What are the practical limits of precision measurements? Let us stretch our imaginations, for a moment, and pretend that we have just found an artifact left by an alien race that excelled in the science of measurement. As a sort of time capsule for the universe, their top scientists decided to collect the history of their civilization, and encoded it in binary. Their story looked something like "001011011101000..." extended to about 5 million places. Rather than print the sequence out on a piece of paper or a computer disc, these aliens simply converted the sequence to a decimal length (i.e., .001011011101000...") and marked the length on a bar composed of a substance that would never change its size. To decode the bar and recover the history of the alien race, one would simply need to have a highly precise measuring instrument that would yield the original binary sequence. Computational linguists could translate the sequence to text, and the recorded history of the alien race would be revealed! Of course, the whole concept is built on an impossible premise. Nothing

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can be measured accurately to 5 million places. We live in a universe with practical limits (i.e., the sizes of atomic particles, the speed of light, the Heisenberg uncertainty principle, the maximum mass of a star, the second law of thermodynamics, the unpredictability of highly complex systems). There are many things that we simply cannot do, no matter how hard we try. The most precise measurement achieved by modern science has been in the realm of atomic clocks, where accuracy of 18 decimal places has been claimed [1]. Nonetheless, many scientific disasters are caused by our ignorance of our own limitations, and our persistent gullibility, leading us to believe that precision claimed is precision obtained.

It is quite common for scientists to pursue precision when they should be seeking accuracy. For an example, we need look no further than the data-intensive field of "Precision Medicine" [2]. One of the goals of precision medicine is to determine the specific genetic alterations that account for human disease. In many cases, this means finding a change in a single nucleotide (from among the 3 billion nucleotides in the DNA sequence that accounts for the human genome) responsible for the development of a disease. Precision Medicine has had tremendous success for a variety of rare diseases and for rare subtypes of common diseases, but has had less luck with common diseases such as type 2 diabetes and adult onset hypertension. Why is this? The diagnosis of diabetes and hypertension are based on a cut-off measurement. Above a certain glucose level in the blood, the patient is said to have diabetes. Above a certain pressure, the patient is said to have hypertension. It is not much different from being overweight (i.e., above a certain weight) or tall (i.e., above a certain height). Theory, strengthened by empiric observations, informs us that quantitative traits have multiple genetic and environmental influences, a phenomenon recognized since the early studies of RA Fisher, in 1919 [3–5]. Hence, we would expect that hypertension and diabetes would not be amenable to precise diagnosis [2].

At this point, we can determine, with credible accuracy, whether a person is diabetic, hypertensive, obese, tall, able to hold his breath for a long time, or able to run 100 m in record time. We cannot determine, with any precision, the precise genes that are necessary for the development of any acquired human traits. Should we be devoting time and money to attain higher and higher precision in the genetic diagnosis of common, polygenic diseases, if increasing precision brings us no closer to a practical cure for these diseases? Put plainly, shouldn't we be opting for "Accurate Medicine" rather than "Precision Medicine"?

The conflict between seeking accuracy and seeking precision is a common dilemma in the universe of Big Data, wherein access to highly precise measurements is ridiculously abundant.

– **Steganography: using imprecision to your advantage**

You look at them every day, the ones that others create, and that you create your own, that you share with your friends or with the world. They are part of your life, and you would feel a deep sense of loss if you lost them. I am referring to high resolution digital images. We love them, but we give them more credit than they deserve. When you download a

16-megapixel image of your sister's lasagna, you can be certain that most of the pixel information is padded with so-called empty resolution; pixel precision that is probably inaccurate and certainly exceeding the eye's ability to meaningfully resolve. Most images in the megabyte size range can safely be reduced to the kilobyte size range, without loss of visual information. Steganography is an encryption technique that takes advantage of the empty precision in pixel data by inserting secret text messages into otherwise useless bits of pseudodata.

Steganography is one of several general techniques in which a message is hidden within an object, such as a book or a painting. The forerunners of modern steganography have been around for centuries and were described as early as AD 1500 by Trithemious [6]. Watermarking is closely related to steganography. Digital watermarking is a way of secretly insinuating the name of the owner or creator of a digital object into the object, as a mechanism of rights management [7]. [Glossary Steghide]

Section 10.2. Data Range

> *Many an object is not seen, though it falls within the range of our visual ray, because it does not come within the range of our intellectual ray, i.e., we are not looking for it. So, in the largest sense, we find only the world we look for.*
>
> *Henry David Thoreau*

Always determine the highest and the lowest observed values in your data collection. These two numbers are often the most important numbers in any set of data; even more important than determining the average or the standard deviation. There is always a compelling reason, relating to the measurement of the data or to the intrinsic properties of the data set, to explain the high and the low of data.

Here is an example. You are looking at human subject data that includes weights. The minimum weight is a pound (the round-off weight of a viable but premature newborn infant). You find that the maximum weight in the data set is 300 pounds, exactly. There are many individuals in the data set who have a weight of 300 pounds, but no individuals with a weight exceeding 300 pounds. You also find that the number of individuals weighing 300 pounds is much greater than the number of individuals weighting 290 pounds or 280 pounds. What does this tell you? Obviously, the people included in the data set have been weighed on a scale that tops off at 300 pounds. Most of the people whose weight was recorded as 300 will have a false weight measurement. Had we not looked for the maximum value in the data set, we would have assumed, incorrectly, that the weights were always accurate.

It would be useful to get some idea of how weights are distributed in the population exceeding 300 pounds. One way of estimating the error is to look at the number of people weighing 295 pounds, 290 pounds, 285 pounds, etc. By observing the trend, and knowing the total number of individuals whose weight is 300 pounds or higher, you can estimate the number of people falling into weight categories exceeding 300 pounds.

Here is another example where knowing the maxima for a data set measurement is useful. You are looking at a collection of data on meteorites. The measurements

include weights. You notice that the largest meteorite in the large collection weighs 66 tons (equivalent to about 60,000 kg), and has a diameter of about 3 m. Small meteorites are more numerous than large meteorites, but one or more meteorites account for almost every weight category up to 66 tons. There are no meteorites weighing more than 66 tons. Why do meteorites have a maximum size of about 66 tons?

A little checking tells you that meteors in space can come in just about any size, from a speck of dust to a moon-sized rock. Collisions with earth have involved meteorites much larger than 3 m. You check the astronomical records and you find that the meteor that may have caused the extinction of large dinosaurs about 65 million years ago was estimated at 6–10 km (at least 2000 times the diameter of the largest meteorite found on earth).

There is a very simple reason why the largest meteorite found on earth weighs about 66 tons, while the largest meteorites to impact the earth are known to be thousands of time heavier. When meteorites exceed 66 tons, the impact energy can exceed the energy produced by an atom bomb blast. Meteorites larger than 66 tons leave an impact crater, but the meteor itself disintegrates on impact.

As it turns out, much is known about meteorite impacts. The kinetic energy of the impact is determined by the mass of the meteor and the square of the velocity. The minimum velocity of a meteor at impact is about 11 km/s (equivalent to the minimum escape velocity for sending an object from earth into space). The fastest impacts occur at about 70 km/s. From this data, the energy released by meteors, on impact with the earth, can be easily calculated.

By observing the maximum weight of meteors found on earth we learn a great deal about meteoric impacts. When we look at the distribution of weights, we can see that small meteorites are more numerous than larger meteorites. If we develop a simple formula that relates the size of a meteorite with its frequency of occurrence, we can predict the likelihood of the arrival of a meteorite on earth, for every weight of meteorite, including those weighing more than 66 tons, and for any interval of time.

Here is another profound example of the value of knowing the maximum value in a data distribution. If you look at the distance from the earth to various cosmic objects (e.g., stars, black holes, nebulae) you will quickly find that there is a limit for the distance of objects from earth. Of the many thousands of cataloged stars and galaxies, none of them have a distance that is greater than 13 billion light years. Why? If astronomers could see a star that is 15 billion light years from earth, the light that is received here on earth must have traveled 15 billion light years to reach us. The time required for light to travel 15 billion light years is 15 billion years; by definition. The universe was born in a big bang about 14 billion years ago. This would imply that the light from the star located 15 billion miles from earth must have begun its journey about a billion years before the universe came into existence. Impossible!

By looking at the distribution of distances of observed stars and noting that the distances never exceed about 13 billion years, we can infer that the universe must be at least 13 billion years old. You can also infer that the universe does not have an infinite age and size; otherwise, we would see stars at a greater distance than 13 billion light years.

If you assume that stars popped into the universe not long after its creation, then you can infer that the universe has an age of about 13 or 14 billion years. All of these deductions, confirmed independently by theoreticians and cosmologists, were made without statistical analysis, simply by noting the maximum number in a distribution of numbers.

Section 10.3. Counting

> *On two occasions I have been asked, 'If you put into the machine wrong figures, will the right answers come out?' I am not able rightly to apprehend the kind of confusion of ideas that could provoke such a question.*
>
> *Charles Babbage*

For the bulk of Big Data projects, analysis begins with counting. If you cannot count the data held in a Big Data resource, then you will derive little benefit from the resource. Systemic counting errors account for irreproducible or misleading results. Surprisingly, there is very little written about this issue in the Big Data literature. Presumably, the subject is considered too trivial for serious study. To rectify this oversight, this section describes, in some depth, the surprising intellectual challenges of Big Data counting.

Most people would agree that the simple act of counting data is something that can be done accurately and reproducibly, from laboratory to laboratory. Actually, this is not the case. Counting is fraught with the kinds of errors previously described in this chapter, plus many other hidden pitfalls. Consider the problem of counting words in a paragraph. It seems straightforward, until you start asking yourself how you might deal with hyphenated words. "Deidentified" is certainly one word. "Under-represented" is probably one word, but sometimes the hyphen is replaced by a space, and then it is certainly two words. How about the term "military-industrial," which seems as though it should be two words? When a hyphen occurs at the end of a line, should we force a concatenation between the syllables at the end of one line and the start of the next?

Slashes are a tougher nut to crack than hyphens. How should we count terms that combine two related words by a slash, such as "medical/pharmaceutical"; one word or two words? If we believe that the slash is a word separator (i.e., slashes mark the end of one word and the beginning of another), then we would need to parse Web addresses into individual words. For example:

www.science.com/stuff/neat_stuff/super_neat_stuff/balloons.htm

The Web address could be broken into a string of words, if the "." and "_" characters could be considered valid word separators. In that case, the single Web address would consist of 11 words: www, science, com, stuff, neat, stuff, super, neat, stuff, balloons, htm. If you were only counting words that match entries in a standard dictionary, then the split Web address would contain 8 words: science, stuff, neat, stuff, super, neat, stuff, balloons. If we defined a word as a string bounded by a space or a part-of-sentence separator (e.g., period, comma, colon, semicolon, question mark, exclamation mark, end of line

character), then the unsplit Web address would count as 1 word. If the word must match a dictionary term, then the unsplit Web address would count as zero words. So, which is it: 11 words, 8 words, 1 word, or 0 words?

This is just the start of the problem. How shall we deal with abbreviations [8,9]? Should all abbreviations be counted as one word, or as the sum of words represented by the abbreviation? Is "U.S." One word or two words? Suppose, before counting words, the text is pre-processed to expand abbreviations. All the abbreviated terms (i.e., every instance of "U.S." becomes an instance of United States, and UCLA would count as 4 words). This would yield an artificial increase in the number of words in the document. How would a word counter deal with abbreviations that look like words, such as "mumps" which could be the name of a viral disease of childhood, or it could be an abbreviation for a computer language used by medical informaticians and expanded as "Massachusetts General Hospital Utility Multi-Programming System."

How would we deal with numeric sequences appearing in the text? Should each numeric sequence be counted as a word? If not, how do we handle Roman numbers? Should "IV" be counted as a word, because it is composed of alphabetic characters, or should it be omitted as a word, because it is equivalent to the numeric value, "4"? When we encounter "IV," how can we be certain that we are parsing a Roman numeral? Could "IV," within the context of our document, represent the abbreviation for "intravenous"?

It is obvious that the number of words in a document will depend on the particular method used to count the words. If we use a commercial word counting application, how can we know which word counting rules are applied? In the field of informatics, the total number of words is an important feature of a document. The total word count often appears in the denominator of common statistical measurements. Counting words seems to be a highly specialized task. My favorite estimator of the number of words in any text file is simply the size of the file divided by 6.5, the average number of characters in a word plus one separator character.

The point here is that a simple counting task, such as word counting, can easily become complex. A complex counting task, involving subjective assessments of observations, seldom yields accurate results. When the criteria for counting change over time, then results that were merely inaccurate may devolve even further, into irreproducibility. An example of a counting task that is complex and objective is the counting of hits and errors in baseball. The rules for counting errors are subjective and based on the scorer's judgment of the intended purpose of the hit (e.g., sacrifice fly) and the expected number of bases reached in the absence of the error. The determination of an error sometimes depends on the outcome of the play after the presumptive error has occurred (i.e., on events that are not controlled or influenced by the error). Counting is also complex with rules covering specific instances of play. For example, passed balls and wild pitches are not scored as errors; they are assigned to another category of play. Plays involving catchers are exempt from certain rules for errors that apply to fielders. It would be difficult to find an example of a counting task that is more complex than counting baseball errors.

Sometimes counting criteria inadvertently exclude categories of items that should be counted. The diagnoses that appear on death certificates are chosen from a list of causes

of death included in the International Classification of Diseases (ICD). Diagnoses collected from all of the death certificates issued in the United States are aggregated by the CDC (Centers for Disease Control and Prevention) and published in the National Vital Statistics Report [10]. As it happens, "medical error" is not included as a cause of death in the ICD; hence, United States casualties of medical errors are not counted as such in the official records. Official tally notwithstanding, it is estimated that about one of every six deaths in the United States result from medical error [10].

Big Data is particularly prone to counting errors, as data is typically collected from multiple sources, each with its own method for annotating data. In addition, Big Data may extend forwards and backwards in time; constantly adding new data and merging with legacy data sets. The criteria for counting data may change over time, producing misleading results. Here are a few examples of counts that changed radically when the rules for counting changed. [Glossary Meta-analysis]

- Beachy Head is a cliff in England with a straight vertical drop and a beautiful sea-view. It is a favorite jumping off point for suicides. The suicide rate at Beachy Head dropped as sharply as the cliff when the medical examiner made a small policy change. From a certain moment onward, bodies found at the cliff bottom would be counted as suicides only if their post-mortem toxicology screen was negative for alcohol. Intoxicated subjects were pronounced dead by virtue of accident (i.e., not suicide) [11].
- Sudden Infant Death Syndrome (SIDS, also known as crib death) was formerly considered to be a disease of unknown etiology that caused infants to stop breathing, and die, often during sleep. Today, most SIDS deaths are presumed to be due to unintentional suffocation from bedclothes, often in an overheated environment, and aggravated by a prone (i.e., face down) sleeping position. Consequently, some infant deaths that may have been diagnosed as SIDS in past decades are now diagnosed as unintentional suffocations. This diagnostic switch has resulted in a trend characterized by increasing numbers of infant suffocations and a decreasing number of SIDS cases [12]. This trend is, in part, artifactual, arising from changes in reporting criteria.
- In the year 2000, nearly a half-century after the Korean War, the United States Department of State downsized its long-standing count of United States military war deaths; to 36,616 down from an earlier figure of about 54,000. The drop of 17,000 deaths resulted from the exclusion of United States military deaths that occurred during the Korean War, in countries outside Korea [13]. The old numbers reflected deaths during the Korean War; the newer number reflects deaths occurring due to the Korean War. Aside from historical interest, the alteration indicates how collected counts may change retroactively.
- Human life is flanked by two events, birth and death; both events are commemorated with a certificate. Death certificates are the single most important gauge of public health. They tell us the ages at which deaths occur, and the causes of those deaths. With this information, we can determine the most common causes of death in the population, changes in the frequency of occurrences of the different causes of death, and the effect of interventions intended to increase overall life expectancy and

reduce deaths caused by particular causes. Death certificates are collected from greater than 99% of individuals who die in the United States [14]. This data, vital to the health of every nation, is highly error prone, and the problems encountered in the U.S. seem to apply everywhere [15,16]. A survey of 49 national and international health atlases has shown that there is virtually no consistency in the way that death data are prepared [17]. Within the United States there is little consistency among states in the manner in which the causes of death are listed [18]. Death data is Big Data, as it is complex (i.e., containing detailed, non-standard information within death certificates), comes from many sources (i.e., every municipality), arrives continually (i.e., deaths occur every minute), with many records (i.e., everyone dies eventually). The rules for annotating the data change regularly (i.e., new versions of the International Classification of Diseases contain different new terms and codes). The consistency of the data decreases as the Big Data grows in size and in time. Our basic understanding of how humans die, and our ability to measure the effect of potentially life-saving public health interventions, is jeopardized by our inability to count the causes of death.

– **Dealing with Negations**

A large portion of Big Data is categorical, not quantitative. Whenever counting categorical features, you need to know whether a feature is present or absent. Unstructured text has no specific format for negative assertions (i.e., statements indicating that a feature is absent or that an assertion is false). Negations in unstructured data come into play during parsing routines wherein various features need to be counted.

If a computer program is seeking to collect, count, or annotate occurrences of a particular diagnosis included in a pathology report, or a particular type of "buy" order on a financial transaction, or the mention of a particular species of frog on a field report, there should be some way to distinguish a positive occurrence of the term (e.g., Amalgamated Widget is traded), from a negation statement (e.g., Amalgamated Widget is not traded."). Otherwise, counts of the positive occurrences of trades would include cases that are demonstrably negative. Informaticians have developed a variety of techniques that deal with negations occurring in textual data [19].

In general, negation techniques rely on finding a negation term (e.g., not present, not found, not seen) in proximity with an annotation term (e.g., a term that matches some term in a standard nomenclature, or a term that has been cataloged or otherwise indexed for the data set, onto which a markup tag is applied). A negated term would not be collected or counted as a positive occurrence of the annotation.

Examples of negation terms included in sentences are shown here:

– He cannot find evidence for the presence of a black hole.
– We cannot find support for the claim.
– A viral infection is not present.
– No presence of Waldo is noted.
– Bigfoot is not in evidence in this footprint analysis.

It is easy to exclude terms that are accompanied by an obvious negation term. When terms are negated or otherwise nullified by terms that are not consistently characterized by a negative inference, the problem becomes complex.

Here is a short list of implied negations, each lacking an unambiguous negation term, followed by the re-written sentence that contains an unambiguous negation term (i.e., "not").

- "Had this been a tin control processor, the satellite would have failed."—The satellite did not fail.
- "There is a complete absence of fungus."—Fungus is not present
- "We can rule out the presence of invasive cancer."—Invasive cancer is not present.
- "Hurricanes failed to show."—Hurricanes did not show.
- "The witness fails to make an appearance."—The witness did not appear.
- "The diagnosis is incompatible with psoriasis."—Psoriasis is not present.
- "Drenching rain is inconsistent with drought."—Drought does not occur with drenching rain.
- "There is insufficient evidence for a guilty verdict."—Not guilty.
- "Accidental death is excluded."—Not an accidental death.
- "A drug overdose is ruled out."—Not a drug overdose.
- "Neither fish nor foul."—Not fish. Not foul.
- There is zero evidence for aliens in Hoboken."—Aliens have not been found in Hoboken.

In addition to lacking outright negations, sentences may contain purposefully ambiguating terms, intended to prohibit readers from drawing any conclusion, positive or negative. For example, "The report is inconclusive for malignancy." How would this report be counted? Was a malignancy present, or was it not?

The point here is that, like everything else in the field of Big Data, the individuals who prepare and use resources must have a deep understanding of the contained data. They must also have a realistic understanding of the kinds of questions that can be sensibly asked and answered with the available data. They must have an understanding of the limits of their own precision.

Section 10.4. Normalizing and Transforming Your Data

Errors have occurred.
We won't tell you where or why.
Lazy programmers.

Computer-inspired haiku by Charlie Gibbs

When extracting data from multiple sources, recorded at different times, and collected for different purposes, the data values may not be directly comparable. The Big Data analyst must contrive a method to normalize or harmonize the data values.

– **Adjusting for population differences.**

Epidemiologists are constantly reviewing large data sets on large populations (e.g., local, national, and global data). If epidemiologists did not normalize their data, they would be in a constant state of panic. Suppose you are following long-term data on the incidence of a rare childhood disease in a state population. You notice that the number of people with the disease has doubled in the past decade. You are about to call the New York Times with the shocking news when one of your colleagues taps you on the shoulder and explains that the population of the state has doubled in the same time period. The incidence, described as cases per 100,000 population, has remained unchanged. You calm yourself down and continue your analysis to find that the reported cases of the disease have doubled in a different state that has had no corresponding increase in state population. You are about to alert the White House with the news when your colleague taps you on the shoulder and explains that the overall population of the state has remained unchanged, but the population of children in the state has doubled. The incidence as expressed as cases occurring in the affected population, has remained unchanged.

An age-adjusted rate is the rate of a disease within an age category, weighted against the proportion of persons in the age groups of a standard population. When we age-adjust rates, we cancel out the changes in the rates of disease that result from differences in the proportion of people in different age groups.

Some of the most notorious observations on non-adjusted data come from the field of baseball. In 1930 Bill Terry maintained a batting average of 0.401, the best batting average in the National league. In 1968 Carl Yastrzemski led his league with a batting average of 0.301. You would think that the facts prove that Terry's lead over his fellow players was greater than Yastr zemski's. Actually, both had averages that were 27% higher than the average of their fe llow ballplayers of the year. Normalized against all the players for the year in w hich the data was collected, Terry and Yastrzemski tied.

– **Rendering data values dimensionless.**

Histograms express data distributions by binning data into groups and displaying the bins in a bar graph. A histogram of an image may have bins (bars) whose heights consist of the number of pixels in a black and white image that fall within a certain gray-scale range (Fig. 10.1).

When comparing images of different sizes, the total number of pixels in the images is different, making it impossible to usefu lly compare the heights of bins. In this case, the number of pixels in each bin can be divided by the total number of pixels in the image, to produce a number that correspond s to the fraction of the total image pixels that are found in the bin. The normalized value (now represented as a fraction), can be compared between two images. Notice that by representing the bin size as a fraction, we have stripped the dimension from the data (i.e., a number expressed as pixels), and rendered a dimensionless data item (i.e., a purely numeric fraction).

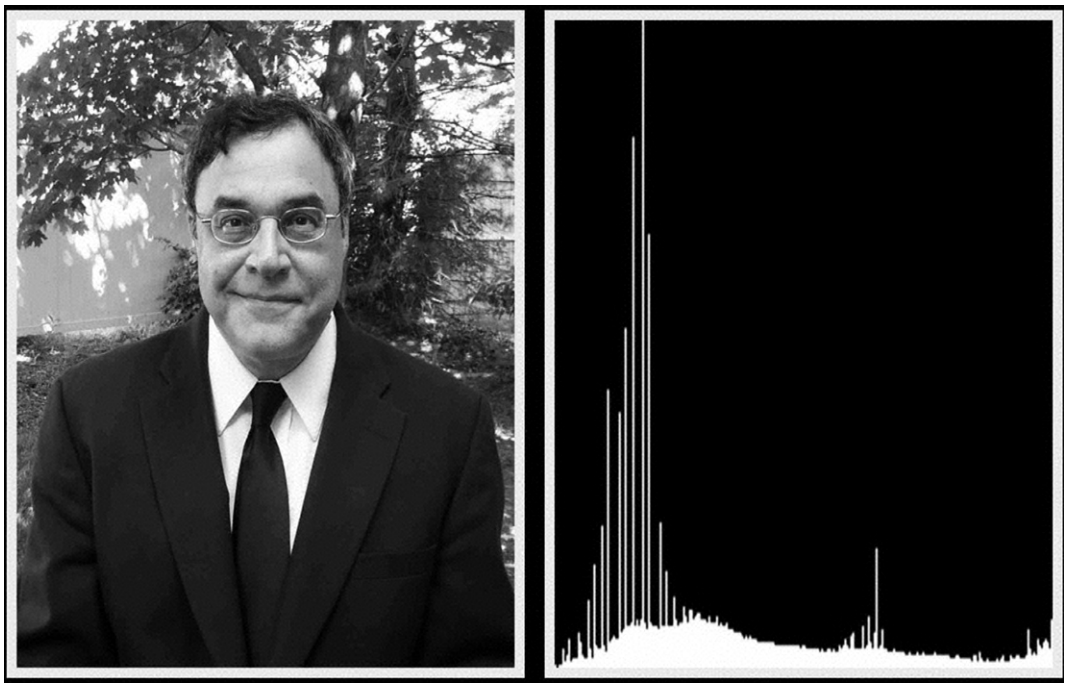

FIG. 10.1 An image of the author, left, converted into a histogram representing the number of pixels that have a gray-scale value of 0, 1, 2, 3 and so on up to the top gray-scale value of 256. Each gray-scale value is a bin.

– **Converting one data type to another, more useful, data type.**

A zip code is an example of data formed by numeric digits that lack numeric properties. You cannot add two zip codes and expect to get any useful information from the process. However, every zip code has been mapped to a specific latitude and longitude at the center of the zip code region, and these values can be used as spherical coordinates from which distances between locations can be computed. It is often useful to assign geographic coordinates to every zip code entry in a database.

– **Converting to a (0, 1) interval.**

Any set of data values can be converted into an interval between 0 and 1, wherein the original data values maintain their relative positions in the new interval. There are several simple ways to achieve the result. The most straightforward is to compute the range of the data by subtracting the smallest data value in your data set from the largest data value. To determine the location of any data value in the 0, 1 range, simply subtract from it the smallest value in the data set and then divide the result by the range of the data (Fig. 10.2). This tells you where your value is located, in a 0, 1 interval, as a fraction of the range of the data.

$$y = \frac{x - x_{min}}{x_{max} - x_{min}}$$

FIG. 10.2 A formula that will convert any value to a fraction between 0 and 1 by dividing the distance of the value from the smallest value of the attribute in the population by the full data range of the value in the population [20].

Another popular method for converting data sets to a standard interval is to subtract the mean from any data value and divide by the standard deviation. This gives you the position of the data value expressed as its deviation from the mean as a fraction of the standard deviation. The resulting value is called the z-score.

When comparing different data sets, it is frequently important to normalize all of the data points to a common interval. In the case of multi-dimensional data it is usually necessary to normalize the data in every dimension using some sensible scaling computation. This may include the methods just described (i.e., dividing by range or by standard deviation, or by substituting data with a dimensionless transformed value, such as a correlation measure).

– **Weighting.**

Weighting is a method whereby the influence of a value is moderated by some factor intended to yield an improved value. In general, when a data value is replaced by the sum of weighted factors, the weights are chosen to add to 1. For example, if you are writing your own smoothing function, in which each value in a data set is replaced by a value computed by summing contributions from itself and its immediate neighbor on the left and the right, you might multiply each number by one-third, so that the final number is scaled to a magnitude similar to your original number. Alternately, you might multiply the number to the left and to the right by one-quarter and the original by one-half, to provide a summed number weighted to favor the original number.

It is a shame that Big Data never comes with instructions. Data analysts are constantly required to choose a normalization method, and the choice will always depend on their intended use of the data. Here is an example. Three sources of data provide records on children that include an age a ttribute. Each source measures age in the same dimension; years. You would think that because the ages are all recorded in years, not months or decades, you can omit a normalization step. When you study the data, you notice that one source contai ns children up to the year 14, while another is cut off at age 12, and another stops at age 16. Suddenly, you are left with a difficult problem. Can your ignore the differences in the cut-off age in the three data sets? Should you truncate all of the data above age 12? Should you use all of the data, but weigh the data differently for the different sources? Should you divide by the available ranges for the data? Should you compute z-scores? It all depends on what you are trying to learn from the data.

Section 10.5. Reducing Your Data

> *There is something fascinating about science. One gets such a wholesale return of conjecture out of such a trifling investment of fact.*
>
> *Mark Twain*

At first glance, it seems obvious that gravitational attraction is a Big Data problem. We know that gravitation between any two bodies is proportional to the product of their masses and inversely proportional to the square of the distance between them. If we want to predict the gravitational forces on an object, we would need to know the position and mass of every body in the universe. With this data, we would compute a force vector, from which we could determine the net gravitational influence of the universe upon the mass. Of course, this is absurd. If we needed all that data for our computation, physicists would be forever computing the orbit of the earth around the sun. We are lucky to live in a universe wherein gravity follows an inverse square distance rule, as this allows us to neglect the influences of heavenly bodies that are far away from earth and sun, and of nearby bodies that have small masses compared with the sun. Any high school student can compute the orbits of the earth around the sun, predicting their relative positions millennia into the future.

Likewise, if we can see two galaxies in space and we notice that they are similar in shape, size, and have a similar star density, then we can assume that they both produce about the same amount of light. If the light received on Earth from one of those galaxies is four times that received by the other galaxy, we can apply the inverse square law for light intensity and infer that the dimmer galaxy is probably twice as far from earth as the brighter galaxy. In this short analysis, we start with our observations on every visible galaxy in the universe. Next, we compare just two galaxies and from this comparison we can develop general methods of analysis that may apply to the larger set of data.

The point here is that when Big Data is analyzed it is seldom necessary to include every point of data in your system model. In the Big Data field the most successful analysts will often be those individuals who are adept at simplifying the system model; thus eliminating unnecessary calculations.

Because Big Data is complex, you will often find that your data objects have high dimensionality; each data object is annotated with a large number of values. The types of values that are shared among all the different data objects are usually referred to as parameters. It is very difficult to make much sense of high dimensional data. It is always best to develop a filtering mechanism that expunges useless parameters. A useless parameter will often have one of these two properties:

1. Redundancy. If a parameter correlates perfectly with some other parameter, you know that you can safely drop one of the two parameters. For example, you may have some physiologic data on a collection of people, and the data may include weight, waist size, body fat index, weight adjusted by height, and density. These measurements seem to

be measuring about the same thing; are they all necessary? If several attributes closely correlate with one another, you might want to drop a few.

Association scores provide a measure of similarity between two variables. Two similar variables will rise and fall together. The Pearson correlation score is popular and can be easily implemented [18,21]. It produces a score that varies from −1 to 1. A score of 1 indicates perfect correlation; a score of −1 indicates perfect anti-correlation (i.e., one variable rises while the other falls). A Pearson score of 0 indicates lack of correlation. Other correlation measures are readily available, as discussed in Section 11.3, "The Dot Product, a Simple and Fast Correlation Method" [22,23]. Big Data analysts should not demure from developing their own correlation scores, as needed, to ensure enhanced speed, or to provide a scoring measure that best serves their particular goals.

2. Randomness. If a parameter is totally random, then it cannot tell you anything meaningful about the data object, and you can drop the parameter. There are many tests that measure randomness; most were designed to measure the quality of random number generators [24]. They can also be used to determine the randomness of data sets.

Putting your set of parameter values into a file, and compressing the file can achieve a simple but useful test for randomness. If the values of the parameter are distributed randomly, the file will not compress well, whereas a set of data that has a regular distribution (e.g., a simple curve, or a Zipf-like distribution, or a distribution with a sharp peak), will compress down into a very small file.

As a small illustration, I wrote a short program that created three files, each 10,000 bytes in length. The first file consisted of the number 1, repeated 10,000 times (i.e., 11111111...). The second file consisted of the numbers 0 through 9, distributed as a sequence of 1000 zeros followed by 1000 ones, followed by 1000 twos, and so on, up to 1000 nines. The final file consisted of the numbers 0 through 9 repeated in a purely random sequence (e.g., 285963222202186026084095527364317), extended to fill a file of 10,000 bytes. Each file was compressed with gunzip, which uses the DEFLATE compression algorithm, combining LZ77 and Huffman coding.

The uncompressed files (10,000 bytes) were compressed into the following file sizes:

```
compressed file size: 58 bytes for 10,000 consecutive "1"
compressed file size: 75 bytes for 1,000 consecutive values of 0 through 9
compressed file size: 5,092 bytes for a random sequence of 10,000 digits
```

In the third file, which consisted of a random sequence of digits, a small compression was achieved simply through the conversion from ASCII to binary representation. In general, though, a purely random sequence cannot be compressed. A data analyst can compare the compressibility of data values, parameter by parameter, to determine which parameters might be expunged, at least during the preliminary analysis of a large, multi-dimensional data set.

When random data are not omitted from the data parameters the unwary analyst may actually develop predictive models and classifiers based entirely on noise. This can occur because clustering algorithms and predictive methods, including neural networks, will

produce an outcome from random input data. It has been reported that some published diagnostic tests have been developed from random data [25]. [Glossary Classifier, Neural network]

Aside from eliminating redundant or random parameters, you might want to review the data and eliminate parameters that do not contribute in any useful way toward your analysis. For example, if you have the zip code for an individual, you will probably not need to retain the street address. If you have the radiologic diagnosis for a patient's chest X-ray, you might not need to retain the file containing the X-ray image unless you are conducting an image analysis project.

The process of reducing parameters applies to virtually all of the fields of data analysis, including standard statistical analysis. Names for this activity include feature reduction or selection, variable reduction and variable subset reduction, and attribute selection. There is sometimes a fine line between eliminating useless data parameters and cherry-picking your test set. It is important to document the data attributes you have expunged and your reason for doing so. Your colleagues should be given the opportunity of reviewing all of your data, including the expunged parameters. [Glossary Cherry-picking, Second trial bias]

An example of a data elimination method is found in the Apriori algorithm. At its simplest, it expresses the observation that a collection of items cannot occur frequently unless each item in the collection also occurs frequently. To understand the algorithm and its significance, consider the items placed together in a grocery checkout cart. If the most popular combination of purchase items is a sack of flour, a stick of butter, and a quart of milk, then you can be certain that collections of each of these items individually, and all pairs of items from the list of 3, must also occur frequently. In fact, they must occur at least as often as the combination of all three, because each of these smaller combinations are subsets of the larger set and will occur with the frequency of the larger set plus the frequency of their occurrences in any other item sets. The importance of the apriori algorithm to Big Data relates to data reduction. If the goal of the analysis is to find association rules for frequently occurring combinations of items, then you can restrict your analysis to combinations composed of single items that occur frequently [26,20].

After a reduced data set has been collected, it is often useful to transform the data by any of a variety of methods that enhance our ability to find trends, patterns, clusters or relational properties that might be computationally invisible in the untransformed data set. The first step is data normalization, described in the next section. It is critical that data be expressed in a comparable form and measure. After the data is normalized, you can further reduce your data by advanced transformative methods.

As a final caveat, data analysts should be prepared to learn that there is never any guarantee that a collection of data will be helpful, even if it meets every criterion for accuracy and reproducibility. Sometimes the data you have is not the data you need. Data analysts should be aware that advanced analytic methods may produce a result that does not take you any closer to a meaningful answer. The data analyst must understand that there is an important difference between a result and an answer. [Glossary Support vector machine]

Section 10.6. Understanding Your Control

The purpose of computing is insight, not numbers.

Richard Hamming

In the small data realm the concept of "control" is easily defined and grasped. Typically, a group is divided into treatment and control sub-groups. Heterogeneity in the population (e.g., gender, age, health status) is randomly distributed into both groups, so that the treatment and the control subgroups are, to the extent possible, indistinguishable from one another. If the treatment group receives a drug administered by syringe suspended in a saline solution, then the control group might receive an injection of saline solution by syringe, without the drug. The idea is to control the experimental groups so that they are identical in every way, save for one isolated factor. Measurable differences in the control and the treatment groups that arise after treatment are potentially due to the action of the one treatment factor.

The concept of "control" does not strictly apply to Big Data; the data analyst never actually "controls" the data. We resign ourselves to doing our best with the "uncontrolled" data that is provided. In the absence of controlling an experiment, what can the data analyst do to exert some kind of data selection that simulates a controlled experiment? It often comes down to extracting two populations, from the Big Data resource, that are alike in every respect, but one: the treatment.

Let me relate a hypothetical situation that illustrates the special skills that Big Data analysts must master. An analyst is charged with developing a method for distinguishing endometriosis from non-diseased (control) tissue using gene expression data. By way of background, endometriosis is a gynecologic condition wherein endometrial tissue that is usually confined to the endometrium (the tissue that lines the inside cavity of the uterus) is found growing outside the uterus, on the surfaces of the ovaries, pelvis, and other organs found in the pelvis. He finds a public data collection that provides gene expression data on endometriosis tissue (five samples) and on control tissues (five samples). By comparing the endometriosis samples with the control samples, he finds a set of 1000 genes that are biomarkers for endometriosis (i.e., that have "significantly" different expression in the disease samples compared with the control samples).

Let us set aside the natural skepticism reserved for studies that generate 1000 new biomarkers from an analysis of 10 tissue samples. The analyst is asked the question, "What was your control tissue, and how was it selected and prepared for analysis?" The analyst indicates that he does not know anything about the control tissues. He points out that the selection and preparation of control tissues is a pre-analytic task (i.e., outside the realm of influence of the data analyst). In this case, the choice of the control tissue was not at all obvious. If the control tissue were non-uterine tissue, taken from the area immediately adjacent to the area from which the endometriosis was sampled, then the analysis would have been comparing endometriosis with the normal tissue that covers the surface of pelvic organs (i.e., a mixture of various types of connective tissue cells unlike endometrial

cells). If the control consisted of samples of normal endometriotic tissue (i.e., the epithelium lining the endometrial canal), then the analysis would have been comparing endometriosis with its normal counterpart. In either case, the significance and rationale for the study would have been very different, depending on the choice of controls.

In this case, as in every case, the choice and preparation of the control is of the utmost importance to the analysis that will follow. In a "small data" controlled study, every system variable but one, the variable studied in the experiment, is "frozen"; an experimental luxury lacking in Big Data. The Big Data analyst must somehow invent a plausible control from the available data. This means that the data analyst, and his close co-workers, must delve into the details of data preparation and have a profound understanding of the kinds of questions that the data can answer. Finding the most sensible control and treatment groups from a Big Data resource can require a particular type of analytic mind that has been trained to cope with data drawn from many different scientific disciplines.

Section 10.7. Statistical Significance Without Practical Significance

> *The most savage controversies are those about matters as to which there is no good evidence either way.*
>
> *Bertrand Russell*

Big Data provides statistical significance without necessarily providing any practical significance. Here is an example. Suppose you have two populations of people and you suspect that the adult males in the first population are taller than the second population. To test your hypothesis, you measure the heights of a random sampling (100 subjects) from both groups. You find that the average height of group 1 is 172.7 cm, while the average height of the second group is 172.5 cm. You calculate the standard error of the mean (the standard deviation divided by the square root of the number of subjects in the sampled population), and you use this statistic to determine the range in which the mean is expected to fall. You find that the difference in the average height in the two sampled populations is not significant, and you cannot exclude the null hypothesis (i.e., that the two sampled groups are equivalent, height-wise).

This outcome really bugs you! You have demonstrated a 2 mm difference in the average heights of the two groups, but the statistical tests do not seem to care. You decide to up the ante. You use a sampling of one million individuals from the two populations and recalculate the averages and the standard errors of the means. This time, you get a slightly smaller difference in the heights (172.65 for group 1 and 172.51 for group 2). When you calculate the standard error of the mean for each population, you find a much smaller number, because you are dividing the standard deviation by the square root of one million (i.e., one thousand); not by the square root of 100 (i.e., 10) that you used for the first calculation. The confidence interval for the ranges of the averages is much smaller

now, and you find that the differences in heights between group 1 and group 2 are sufficient to exclude the null hypothesis with reasonable confidence.

Your Big Data project was a stunning success; you have shown that group 1 is taller than group 2, with reasonable confidence. However, the average difference in their heights seems to be about a millimeter. There are no real life situations where a difference of this small magnitude would have any practical significance. You could not use height to distinguish individual members of group 1 from individual members of group 2; there is too much overlap among the groups, and height cannot be accurately measured to within a millimeter tolerance. You have used Big Data to achieve statistical significance, without any practical significance.

There is a tendency among Big Data enthusiasts to promote large data sets as a cure for the limited statistical power and frequent irreproducibility of small data studies. In general, if an effect is large, it can be evaluated in a small data project. If an effect is too small to confirm in a small data study, statistical analysis may benefit from a Big Data study, by increasing the sample size and reducing variances. Nonetheless, the final results may have no practical significance, or the results may be unrepeatable in a small-scale (i.e., real life) setting, or may be invalidated due to the persistence of biases that were not eliminated when the sample size was increased.

Section 10.8. Case Study: Gene Counting

There is a chasm
of carbon and silicon
the software can't bridge.

Computer-inspired haiku by Rahul Sonnad

The Human Genome Project is a massive bioinformatics project in which multiple laboratories helped to sequence the 3 billion base pair haploid human genome. The project began its work in 1990, a draft human genome was prepared in 2000, and a completed genome was finished in 2003, marking the start of the so-called post-genomics era. There are about 2 million species of proteins synthesized by human cells. If every protein had its own private gene containing its specific genetic code, then there would be about two million protein-coding genes contained in the human genome. As it turns out, this estimate is completely erroneous. Analysis of the human genome indicates that there are somewhere between 20,000 and 150,000 genes. The majority of estimates come in at the low end (about 25,000 genes). Why are the current estimates so much lower than the number of proteins, and why is there such a large variation in the lower and upper estimates (20,000 to 150,000)? [Glossary Human Genome Project]

Counting is difficult when you do not fully understand the object that you are counting. The reason that you are counting objects is to learn more about the object, but you cannot fully understand an object until you have learned what you need to know about the object. Perceived this way, counting is a bootstrapping problem. In the case of proteins a small

number of genes can account for a much larger number of protein species because proteins can be assembled from combinations of genes, and the final form of a unique protein can be modified by so-called post-translational events (folding variations, chemical modifications, sequence shortening, clustering by fragments, etc.). The methods used to count protein-coding genes can vary [27]. One technique might look for sequences that mark the beginning and the end of a coding sequence; another method might look for segments containing base triplets that correspond to amino acid codons. The former method might count genes that code for cellular components other than proteins, and the later might miss fragments whose triplet sequences do not match known protein sequences [28]. Improved counting methods are being developed to replace the older methods, but a final number evades our grasp.

The take-home lesson is that the most sophisticated and successful Big Data projects can be stumped by the simple act of counting.

Section 10.9. Case Study: Early Biometrics, and the Significance of Narrow Data Ranges

The proper study of Mankind is Man.

Alexander Pope in "An Essay on Man," 1734.

It is difficult to determine the moment in history when we seriously began collecting biometric data. Perhaps it started with the invention of the stethoscope. Rene-Theophile-Hyacinthe Laennec (1781–1826) is credited with inventing this device, which provided us with the opportunity to listen to the sounds generated within our bodies. Laennec's 1816 invention was soon followed by his 900-page analysis of sounds, heard in health and disease, the Traite de l'Aascultation Mediate (1819). Laennec's meticulous observations were an early effort in Big Data medical science. A few decades later, in 1854, Karl Vierordt's 1854 sphygmograph was employed to routinely monitor the pulse of patients. Perhaps the first large monitoring project came in 1868 when Carl Wunderlich published Das Verhalten der Eigenwarme in Krankheiten, which collected body temperature data on approximately 25,000 patients [29]. Wunderlich associated peaks and fluctuations of body temperature with 32 different diseases. Not only did this work result in a large collection of patient data, it also sparked considerable debate over the best way to visualize datasets. Competing suggestions for the representation of thermometric data (as it was called) included time interval (discontinuous) graphs and oscillating realtime (continuous) charts. Soon thereafter, sphygmomanometry (blood pressure recordings) was invented (1896). With bedside recordings of pulse, blood pressure, respirations, and temperature (the so-called vital signs), the foundations of modern medical data collection were laid.

At the same time that surveillance of vital signs became commonplace, a vast array of chemical assays of blood and body fluids were being developed. By the third decade

of the twentieth century, physicians had at their disposal most of the common blood tests known to modern medicine (e.g., electrolytes, blood cells, lipids, glucose, nitrogenous compounds). What the early twentieth century physicians lacked was any sensible way to interpret the test results. Learning how to interpret blood tests required examination of old data collected on many thousands of individuals, and it took considerable time and effort to understand the aggregated results.

The results of blood tests, measured under a wide range of physiologic and pathologic circumstances, produced a stunning conclusion. It was shown that nearly every blood test conducted on healthy individuals fell into a very narrow range, with very little change between individuals. This was particularly true for electrolytes (e.g., Sodium and Calcium) and to a somewhat lesser extent for blood cells (e.g., white blood cells, red blood cells). Furthermore, for any individual, multiple recordings at different times of the day and on different days, tended to produce consistent results (e.g., Sodium concentration in the morning was equivalent to Sodium concentration in the evening). These finding were totally unexpected at the time [30].

Analysis of the data also showed that significant deviations from the normal concentrations of any one of these blood chemicals is always an indicator of disease. Backed by data, but lacking any deep understanding of the physiologic role of blood components, physicians learned to associate deviations from the normal range with specific disease processes. The discovery of the "normal range" revolutionized the field of physiology. Thereafter physiologists concentrated their efforts toward understanding how the body regulates its blood constituents. These early studies led to nearly everything we now know about homeostatic control mechanisms, and the diseases thereof.

To this day, much of medicine consists of monitoring vital signs, blood chemistries, and hematologic cell indices (i.e., the so-called complete blood count), and seeking to find a cause and a remedy for deviations from the normal range.

Glossary

Cherry-picking The process whereby data objects are chosen for some quality that is intended to boost the likelihood that an experiment is successful, but which biases the study. For example, a clinical trial manager might prefer patients who seem intelligent and dependable, and thus more likely to comply with the rigors of a long and complex treatment plan. By picking those trial candidates with a set of desirable attributes, the data manager is biasing the results of the trial, which may no longer apply to a real-world patient population.

Classifier As used herein, refers to algorithms that assign a class (from a pre-existing classification) to an object whose class is unknown [26]. It is unfortunate that the term classifier, as used by data scientists, is often misapplied to the practice of classifying, in the context of building a classification. Classifier algorithms cannot be used to build a classification, as they assign class membership by similarity to other members of the class; not by relationships. For example, a classifier algorithm might assign a terrier to the same class as a housecat, because both animals have many phenotypic features in common (e.g., similar size and weight, presence of a furry tail, four legs, tendency to snuggle in a lap). A terrier is dissimilar to a wolf, and a housecat is dissimilar to a lion, but the terrier and the wolf are directly related to one another; as are the housecat and the lion. **For the purposes of creating a**

classification, relationships are all that are important. Similarities, when they occur, arise as a consequence of relationships; not the other way around. At best, classifier algorithms provide a clue to classification, by sorting objects into groups that may contain related individuals. Like clustering techniques, classifier algorithms are computationally intensive when the dimension is high, and can produce misleading results when the attributes are noisy (i.e., contain randomly distributed attribute values) or non-informative (i.e., unrelated to correct class assignment).

Human Genome Project The Human Genome Project is a massive bioinformatics project in which multiple laboratories contributed to sequencing the 3 billion base pair haploid human genome (i.e., the full sequence of human DNA). The project began its work in 1990, a draft human genome was prepared in 2000, and a completed genome was finished in 2003, marking the start of the so-called post-genomics era. All of the data produced for the Human Genome Project is freely available to the public.

Meta-analysis Meta-analysis involves combining data from multiple similar and comparable studies to produce a summary result. The hope is that by combining individual studies, the meta-analysis will carry greater credibility and accuracy than any single study. Three of the most recurring flaws in meta-analysis studies are selection bias (e.g., negative studies are often omitted from the literature), inadequate knowledge of the included sets of data (e.g., incomplete methods sections in the original articles), and non-representative data (e.g., when the published data are non-representative samples of the original data sets).

Neural network A dynamic system in which outputs are calculated by a summation of weighted functions operating on inputs. The weights for the individual functions are determined by a learning process, simulating the learning process hypothesized for human neurons. In the computer model, individual functions that contribute to a correct output (based on the training data) have their weights increased (strengthening their influence to the calculated output). Over the past ten or fifteen years, neural networks have lost some favor in the artificial intelligence community. They can become computationally complex for very large sets of multidimensional input data. More importantly, complex neural networks cannot be understood or explained by humans, endowing these systems with a "magical" quality that some scientists find unacceptable.

Second trial bias Can occur when a clinical trial yields a greatly improved outcome when it is repeated with a second group of subjects. In the medical field, second trial bias arises when trialists find subsets of patients from the first trial who do not respond well to treatment, thereby learning which clinical features are associated with poor trial response (e.g., certain pre-existing medical conditions, lack of a good home support system, obesity, nationality). During the accrual process for the second trial, potential subjects who profile as non-responders are excluded. Trialists may justify this practice by asserting that the purpose of the second trial is to find a set of subjects who will benefit from treatment. With a population enriched with good responders, the second trial may yield results that look much better than the first trial. Second trial bias can be considered a type of cherry-picking that is often justifiable.

Steghide Steghide is an open source GNU license utility that invisibly embeds data in image or audio files. Windows and Linux versions are available for download from SourceForge, at:
http://steghide.sourceforge.net/download.php
A Steghide manual is available at:
http://steghide.sourceforge.net/documentation/manpage.php
After installing, you can invoke steghide at the system prompt as a command line launched from the subdirectory in which steghide.exe resides.
Here is an example of a command line invocation of Steghide. Your chosen password can be inserted directly into the commandline. For example:

```
steghide embed -cf myphoto.jpg -ef mytext.txt -p hideme
```

The command line was launched from the subdirectory that holds the steghide executable files on my computer. The command instructs steghide to embed the text file, berman_author_bio.txt into the image file, berman_author_photo.jpg, under the password "hideme".

That is all there is to it. The image file, containing a photo of myself, now contains an embedded text file, containing my short biography. No longer need I keep track of both files. I can generate my biography file, from my image file, but I must remember the password.

I could have called Steghide from a script. Here is an example of an equivalent Python script that invokes steghide from a system call.

```
import os
command_string = "steghide embed -cf myphoto.jpg -ef mytext.txt -p hideme"
os.system(command_string)
```

You can see how powerful this method can be. With a bit of tweaking, you can write a short script that uses the Steghide utility to embed a hidden text message in thousands of images, all at once. Anyone viewing those images would have no idea that they contained a hidden message, unless and until you told them so.

Support vector machine A machine learning technique that classifies objects. The method starts with a training set consisting of two classes of objects as input. The support vector machine computes a hyperplane, in a multidimensional space, that separates objects of the two classes. The dimension of the hyperspace is determined by the number of dimensions or attributes associated with the objects. Additional objects (i.e., test set objects) are assigned membership in one class or the other, depending on which side of the hyperplane they reside.

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11

Indispensable Tips for Fast and Simple Big Data Analysis

OUTLINE

Section 11.1. Speed and Scalability

It's hardware that makes a machine fast. It's software that makes a fast machine slow.
Craig Bruce

Speed and scalability are the two issues that never seem to go away when discussions turn to Big Data. Will we be able to collect, organize, search, retrieve, and analyze Big Data at the same speed that we have grown accustomed to in small data systems? Will the same algorithms, software, protocols, and systems that work well with small data scale up to Big Data?

Let us turn the question around for a moment. Will Big Data solutions scale down to provide reliable and fast solutions for small data? It may seem as though the answer is obvious. If a solution works for large data it must also work for small data. Actually, this is not the case. Methods that employ repeated sampling of a population may produce meaningless results when the population consists of a dozen data points. Nonsensical results can be expected when methods that determine trends, or analyze signals come up against small data.

The point here is that computational success is always an artifact of the way that we approach data-related issues. By customizing solutions to some particular set of circumstances (number of samples, number of attributes, required response time, required precision), we make our products ungeneralizable. We tend to individualize

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our work, at first, because we fail to see the downside of idiosyncratic solutions. Hence, we learn the hard way that solutions that work well under one set of circumstances will fail miserably when the situation changes. Desperate to adapt to the new circumstances, we often pick solutions that are expensive and somewhat short-sighted (e.g., "Let's chuck all our desktop computers and buy a supercomputer."; "Let's parallelize our problems and distribute the calculations to multiple computers", "Let's forget about trying to understand the system and switch to deep learning with neural networks."; "Let's purchase a new and more powerful information system and abandon our legacy data.")

In this book, which offers a low-tech approach to Big Data, we have been stressing the advantages of simple and general concepts that allow data to be organized at any level of size and complexity (e.g., identifiers, metadata/data pairs, triples, triplestores), and extremely simple algorithms for searching, retrieving, and analyzing data that can be accomplished with a few lines of code in any programming language. The solutions discussed in this book may not be suitable for everyone, but it is highly likely that many of the difficulties associated with Big Data could be eliminated or ameliorated, if all data were well organized.

Aside from issues of data organization, here are a few specific suggestions for avoiding some of the obstacles that get in the way of computational speed and scalability:

– **High-level programming languages (including Python) employ built-in methods that fail when the variables are large, and such methods must be avoided by programmers.**

Modern programming languages relieve programmers from the tedium of allocating memory to every variable. The language environment is tailored to the ample memory capacities of desktop and laptop computers and provides data structures (e.g., lists, dictionaries, strings) that are intended to absorb whatever data they are provided. By doing so, two problems are created for Big Data users. First, the size of data may easily exceed the loading capacity of variables (e.g., don't try to put a terabyte of data into a string variable). Second, the built-in methods that work well with small data will fail when dealing with large, multidimensional data objects, such as enormous matrices. This means that good programmers may produce terrific applications, using high-level programming languages that fail miserably in the Big Data realm.

Furthermore, the equivalent methods, in different versions of a high-level programming language, may deal differently with memory. Successive versions of a programming language, such as Python or Perl, may be written with the tacit understanding that the memory capacity of computers is increasing and that methods can be speeded assuming that memory will be available, as needed. Consequently, a relatively slow method may work quite well for a large load of data in an early version of the language. That same method, in a later version of the same language, written to enhance speed, may choke on the same data. Because the programmer is using the same named methods in her programs, run under different version of the language, the task of finding the source of consequent software failures may be daunting.

What is the solution? Should Big Data software be written exclusively in assembly language, or (worse) machine language? Probably not, although it is easy to see why programmers skilled in low-level programming languages will always be valued for their expertise. It is best to approach Big Data programming with the understanding that methods are not infinitely expandable to accommodate any size data, of any dimension. Sampling methods, such as those discussed in detail in Chapter 13, "Using Random Numbers to Knock Your Big Data Analytic Problems Down to Size" might be one solution.

– **Line-by-line reading is slow, but is always scalable.**

Years ago, I did a bit of programming in Mumps, a programming language developed in the 1960s (that will be briefly discussed in Section 11.8 of this chapter). Every variable had a maximum string size of 255 bytes. Despite this limitation, Mumps managed enormous quantities of data in hierarchical data structure (the so-called Mumps global). Efficient and reliable, Mumps was loved by a cult of loyal programmers. Every programmer of a certain age can regale younger generations with stories of magnificent software written for computers whose RAM memory was kilobytes (not Gigabytes).

A lingering residue of Mumps-like parsing is the line-by-line file read. Every file, even a file of Big Data enormity, can be parsed from beginning to end by repeated line feeds. Programmers who resist the urge to read whole files into a variable will produce software that scales to any size, but which will run slower than comparable programs that rely on memory. There are many trade-offs in life.

– **Make your data persistent.**

In Section 11.5 of this chapter, "Methods for Data Persistence" we will be discussing methods whereby data structures can be moved from RAM memory into external files, which can be retrieved in whole or in part, as needed. Doing so relieves many of the consequences of memory overload, and eliminates the necessity of rebuilding data structures each time a program or a process is called to execute.

– **Don't test your software on subsets of data**

Programs that operate with complex sets of input may behave unpredictably. It is important to use software that has been extensively tested by yourself and by your colleagues. After testing, it is important to constantly monitor the performance of software. This is especially important when using new sources of data, which may contain data values that have been formatted differently than prior data.

Here is one solution that everyone tries. If the test takes a lot of processing time, just reduce the size of the test data. Then you can quickly go through many test/debug cycles. Uh uh. When testing software, you cannot use a small subset of your data because the kinds of glitches you need to detect may only be detectable in large datasets. So, if you want to test software that will be used in large datasets, you must test the software on large datasets. How testing can be done, on Big Data, without crashing the live system, is a delicate problem. Readers are urged to consult publications in the large corpus of literature devoted to software testing.

– **Avoid turn-key applications.**

Vendors may offer Big Data solutions in the form of turn-key applications and systems that do everything for you. Often, such systems are opaque to users. When difficulties arise, including system crashes, the users are dependent upon the vendor to provide a fix. When the vendor is unreliable, or the version of the product that you are using is no longer supported, or when the vendor has gone out of business, or when the vendor simply cannot understand and fix the problem, the consequences to the Big Data effort can be catastrophic.

Everyone has his or her own opinions about vendor-provided solutions. In some cases, it may be reasonable to begin Big Data projects with an extremely simple, open source, database that offers minimal functionality. If the data is simple but identified (e.g., collections of triples), then a modest database application may suffice. Additional functionalities can be added incrementally, as needed.

– **Avoid proprietary software (when conducting scientific research)**

Proprietary software applications have their place in the realm of Big Data. Such software is used to operate the servers, databases, and communications involved in building and maintaining the Big Data resource. They are often well tested and dependable, faithfully doing the job they were designed to do. However, in the analysis phase, it may be impossible to fully explain your research methods if one of the steps is: "Install the vendor's software and mouse-click on the 'Run' button." Responsible scientists should not base their conclusion on software they cannot understand. [Glossary Black box]

– **Use small, efficient, and fast utilities**

Utilities are written to perform one task optimally. For data analysts, utilities fit perfectly with the "filter" paradigm of Big Data (i.e., that the primary purpose of Big Data is to provide a comprehensive source of small data). A savvy data analyst will have hundreds of small utilities, most being free and open source products, that can be retrieved and deployed, as needed. A utility can be tested with data sets of increasing size and complexity. If the utility scales to the job, then it can be plugged into the project. Otherwise, it can be replaced with an alternate utility or modified to suit your needs. [Glossary Undifferentiated software]

– **Avoid system calls from within iterative loops**

Many Big Data programs perform iterative loops operating on each of the elements of a large list, reading large text files line by line, or calling every key in a dictionary. Within these long loops, programmers must exercise the highest degree of parsimony, avoiding any steps that may unnecessarily delay the execution of the script, inasmuch as any delay will be multiplied by the number of iterations in the loop. System calls to external methods or utilities are always time consuming. In addition to the time spent executing the command, there is also the time spent loading and interpreting called methods, and this time is repeated at each iteration of the loop. [Glossary System call]

To demonstrate the point, let us do a little experiment. As discussed in Section 3.3, when we create new object identifiers with UUID, we have the choice of calling the Unix UUID method as a system call from a Python script; or, we can use Python's own uuid method. We will run two versions of a script. The first version will create 10,000 new UUID identifiers, using system calls to the external unix utility, uuid.gen. We will create another 10,000 UUID identifiers with Perl's own uuid method. We will keep time of how long each script runs.

Here is the script using system calls to uuidgen.exe

```
timenow = time.time()
for i in range(1, 10000):
  os.system("uuidgen.exe >uuid.out")
timenew = time.time()
print("Time for 10,000 uuid assignments: " + str(timenew - timenow))

output:
Time for 10,000 uuid assignments: 422.0238435268402
```

10,000 system calls to uuidgen.exe required 422 seconds to complete.

Here is the equivalent script using Python's built-in uuid method.

```
timenow = time.time()
for i in range(1, 10000):
  uuid.uuid4()
timenew = time.time()
print("Time for 10,000 uuid assignments: " + str(timenew - timenow))

output:
Time for 10,000 uuid assignments: 0.06850886344909668
```

Python's built-in method required 0.07 seconds to complete, a dramatic time savings.

– **Use look-up tables, and other pre-computed pointers**

Computers are very fast at retrieving information from look-up tables, and these would include concordances, indexes, color maps (for images), and even dictionary objects (known also as associative arrays). For example, the Google search engine uses a look-up table built upon the PageRank algorithm. PageRank (alternate form Page Rank) is a method, developed at Google, for displaying an ordered set of results (for a phrase search conducted over every page of the Web). The rank of a page is determined by two scores: the relevancy of the page to the query phrase; and the importance of the page. The relevancy of the page is determined by factors such as how closely the page matches the query phrase, and whether the content of the page is focused on the subject of the query. The importance of the page is determined by how many Web pages link to and from the page, and the importance of the Web pages involved in the linkages. It is easy to see that the methods for scoring relevance and importance are subject to many algorithmic variances, particularly with respect to the choice of measures (i.e., the way in which a page's focus on a particular topic is quantified),

and the weights applied to each measurement. The reasons that PageRank query responses can be completed very rapidly is that the score of a page's importance can be pre-computed, and stored with the page's Web addresses. Word matches from the query phrase to Web pages are quickly assembled using a precomputed index of words, the pages containing the words, and the locations of the words in the pages [1]. [Glossary Associative array]

– **Avoid RegEx, especially in iterative processes**

RegEx (short for Regular Expressions) is a language for describing string patterns. The RegEx language is used in virtually every modern programming language to describe search, find, and substitution operations on strings. Most programmers love RegEx, especially those programmers who have mastered its many subtleties. There is a strong tendency to get carried away by the power and speed of Regex. I have personally reviewed software in which hundreds of RegEx operations are performed on every line read from files. In one such program the software managed to parse through text at the numbingly slow rate of 1000 bytes (about a paragraph) every 4 seconds. As this rate a terabyte of data would require a 4 billion seconds to parse (somewhat more than one century). In this particular case, I developed an alternate program that used a fast look-up table and did not rely upon RegEx filters. My program ran at a speed 1000 times faster than the RegEx intense program [2]. [Glossary RegEx]

– **Avoid unpredictable software.**

Everyone thinks of software as something that functions in a predetermined manner, as specified by the instructions in its code. It may seem odd to learn that software output may be unpredictable. It is easiest to understand the unpredictability of software when we examine how instructions are followed in software that employs class libraries (C++, Java) or that employs some features of object-oriented languages (Python) or is fully object oriented (Smalltalk, Ruby, Eiffel) [3]. When a method (e.g., an instruction to perform a function) is sent to an object, the object checks to see if the method belongs to itself (i.e., if the method is an instance method for the object). If not, it checks to see if the method belongs to its class (i.e., if the method is a class method for the object's class). If not, it checks its through the lineage of ancestral classes, searching for the method. When classes are permitted to have more than one parent class, there will be occasions when a named method exists in more than one ancestral class, for more than one ancestral lineage. In these cases, we cannot predict with any certainty which class method will be chosen to fulfill the method call. Depending on the object receiving the method call, and its particular ancestral lineages, and the route taken to explore the lineages, the operation and output of the software will change.

In the realm of Big Data, you do not need to work in an object oriented environment to suffer the consequences of method ambiguity. An instruction can be sent over a network of servers as an RPC (Remote Procedure Call) that is executed in a different ways by the various servers that receive the call.

Unpredictability is often the very worst kind of programming bug because incorrect outputs producing adverse outcomes often go undetected. In cases where an adverse outcome is detected, it may be nearly impossible to find the glitch.

– **Avoid combinatorics.**

Much of Big Data analytics involves combinatorics; the evaluation, on some numeric level, of combinations of things. Often, Big Data combinatorics involves pairwise comparisons of all possible combinations of data objects, searching for similarities, or proximity (a distance measure) of pairs. The goal of these comparisons often involves clustering data into similar groups, finding relationships among data that will lead to classifying the data objects, or predicting how data objects will respond or change under a particular set of conditions. When the number of comparisons becomes large, as is the case with virtually all combinatoric problems involving Big Data, the computational effort may become massive. For this reason, combinatorics research has become somewhat of a subspecialty for Big Data mathematics. There are four "hot" areas in combinatorics. The first involves building increasingly powerful computers capable of solving combinatoric problems for Big Data. The second involves developing methods whereby combinatoric problems can be broken into smaller problems that can be distributed to many computers, to provide relatively fast solutions for problems that could not otherwise be solved in any reasonable length of time. The third area of research involves developing new algorithms for solving combinatoric problems quickly and efficiently. The fourth area, perhaps the most promising, involves finding innovative non-combinatoric solutions for traditionally combinatoric problems.

– **Pay for smart speed**

The Cleveland Clinic developed software that predicts disease survival outcomes from a large number of genetic variables. Unfortunately the time required for these computations was unacceptable. As a result, the Cleveland Clinic issued a Challenge "to deliver an efficient computer program that predicts cancer survival outcomes with accuracy equal or better than the reference algorithm, including 10-fold validation, in less than 15 hours of real world (wall clock) time" [4]. The Cleveland Clinic had its own working algorithm, but it was not scalable to the number of variables analyzed. The Clinic was willing to pay for faster service.

Section 11.2. Fast Operations, Suitable for Big Data, That Every Computer Supports

> *No one will need more than 637 kb of memory for a personal computer. 640K ought to be enough for anybody.*
>
> *Bill Gates, founder of Microsoft Corporation, in 1981*

– Random access to files

Most programming languages have a way of providing so-called random access to file locations. This means that if you want to retrieve the 2053th line of a file, you need not sequentially read lines 1 through 2052 before reaching your desired line. You can go directly to any line in the text, or any byte location, for that matter.

In Python, so-called random access to file locations is invoked by the seek() command. Here is a 9-line Python script that randomly selects twenty locations in a text file (the plain-text version of James Joyce's Ulysses in this example) for file access.

```
import os, sys, itertools, random
size = os.path.getsize("ulysses.txt")
infile = open("ulysses.txt", "r")
random_location = "0"
for i in range(20):
  random_location = random.uniform(0,size)
  infile.seek(random_location, 0)
  print(infile.readline(), end="\n")
infile.close()
```

Random access to files is a gift to programmers. When we have indexes, concordances, and other types of lookup tables, we can jump to the file locations we need, nearly instantaneously.

– Addition and multiplication

Some mathematical operations are easier than others. Addition and multiplication and the bitwise logic operations (e.g., XOR) are done so quickly that programmers can include these operations liberally in programs that loop through huge data structures.

– Time stamps

Computers have an intimate relationship with time. As discussed in Section 6.4, every computer has several different internal clocks that set the tempo for the processor, the motherboard, and for software operations. A so-called real-time clock (also known as system clock) knows the time internally as the number of seconds since the epoch. By convention, in Unix systems, the epoch begins at midnight on New Year's Eve, 1970. Prior dates are provided a negative time value. On most systems, the time is automatically updated 50–100 times per second, providing us with an extremely precise way of measuring the time between events.

Never hesitate to use built-in time functions to determine the time of events and to determine the intervals between times. Many important data analysis opportunities have been lost simply because the programmers who prepared the data neglected to annotate the times that the data was obtained, created, updated, or otherwise modified.

– One-way hashes

One-way hashes were discussed in Section 3.9. One-way hash algorithms have many different uses in the realm of Big Data, particularly in areas of data authentication and security. In some applications, one-way hashes are called iteratively, as in blockchains (Section 8.6) and in protocol for exchanging confidential information [5,6]. As previously discussed, various hash algorithms can be invoked via system calls from Python scripts to the openssl suite of data security algorithms. With few exceptions, a call to methods

from within the running programming environment, is much faster than a system call to an external program. Python provides a suite of one-way hash algorithms in the hashlib module.

```
>>> import hashlib
>>> hashlib.algorithms_available
{'sha', 'SHA', 'SHA256', 'sha512', 'ecdsa-with-SHA1', 'sha256',
'whirlpool', 'sha1', 'RIPEMD160', 'SHA224', 'dsaEncryption',
'dsaWithSHA', 'sha384', 'SHA384', 'DSA-SHA', 'MD4', 'ripemd160',
'DSA', 'SHA512', 'md4', 'sha224', 'MD5', 'md5', 'SHA1'}
```

The python zlib module also provides some one-way hash functions, including adler32, with extremely fast algorithms, producing a short string output.

The following Python command lines imports Python's zlib module and calls the adler32 hash, producing a short one-way hash for "hello world." The bottom two command lines imports sha256 from Python's hashlib module and produces a much longer hash value.

```
>>> import zlib
>>> zlib.adler32("hello world".encode('utf-8'))
436929629
>>> import hashlib
>>> hashlib.sha256(b"hello world").hexdigest()
'b94d27b9934d3e08a52e52d7da7dabfac484efe37a5380ee9088f7
ace2efcde9'
```

Is there any difference in the execution time when we compare the adler32 and sha256 algorithms. Let's find out with the hash_speed.py script that repeats 10,000 one-way hash operations with each one-way hash algorithms, testing both algorithms on a short phrase ("hello world") and a long file (meshword.txt, in this example, which happens to be 1,901,912 bytes in length).

```
import time, zlib, hashlib
timenow = time.time()
for i in range(1, 10000):
  zlib.adler32("hello world".encode('utf-8'))
timenew = time.time()
print("Time for 10,000 adler32 hashes on a short string: " + str(timenew -
timenow))
timenow = time.time()
for i in range(1, 10000):
  hashlib.sha256(b"hello world").hexdigest()
timenew = time.time()
print("Time for 10,000 sha256 hashes on a short string: " + str(timenew -
timenow))
with open('meshword.txt', 'r') as myfile:
```

```
    data=myfile.read()

timenow = time.time()
for i in range(1, 10000):
  zlib.adler32(data.encode('utf-8'))
timenew = time.time()
print("Time for 10,000 adler32 hashes on a file: " + str(timenew -
timenow))
timenow = time.time()
for i in range(1, 10000):
  hashlib.sha256(data.encode('utf-8')).hexdigest()
timenew = time.time()
print("Time for 10,000 sha256 hashes on a file: " + str(timenew -
timenow))
```

Here is the output of the hash_speed.py script

```
Time for 10,000 adler32 hashes on a short string: 0.006000041961669922
Time for 10,000 sha256 hashes on a short string: 0.014998674392700195
Time for 10,000 adler32 hashes on a file: 20.740180492401123
Time for 10,000 sha256 hashes on a file: 76.80237746238708
```

Both adler32 and SHA256 took much longer (several thousand times longer) to hash a 2 Megabyte file than a short, 11-character string. This indicates that one-way hashes can be performed on individual identifiers and triples, at high speed.

The adler32 hash is several times faster than sha256. This difference may be insignificant under most circumstances, but would be of considerable importance in operations that repeat millions or billions of times. The adler 32 hash is less secure against attack than the sha256, and has a higher chance of collisions. Hence, the adler32 hash may be useful for projects where security and confidentiality are not at issue, and where speed is required. Otherwise, a strong hashing algorithm, such as sha256, is recommended.

– Pseudorandom number generators are fast.

As will be discussed in Chapter 13, "Using Random Numbers to Knock Your Big Data Analytic Problems Down to Size," random number generators have many uses in Big Data analyses. [Glossary Pseudorandom number generator]

Let us look at the time required to compute 10 million random numbers.

```
import random, time
timenow = time.time()
for iterations in range(10000000):
  random.uniform(0,1)
timenew = time.time()
print("Time for 10 million random numbers: " + str(timenew - timenow))
```

Here is the output from the ten_million_rand.py script:

```
output:
Time for 10 million random numbers: 6.093759775161743
```

Ten million random numbers were generated in just over 6 seconds, on my refurbished home desktop running at a CPU speed of 3.40 GHz. This tells us that, under most circumstances, the time required to generate random numbers will not be a limiting factor, even when we need to generate millions of numbers. Next, we need to know whether the random numbers we generate are truly random. Alas, it is impossible for computers to produce an endless collection of truly random numbers. Eventually, algorithms will cycle through their available variations and begin to repeat themselves, producing the same set of "random" numbers, in the same order; a phenomenon referred to as the generator's period. Because algorithms that produce seemingly random numbers are imperfect, they are known as pseudorandom number generators. The Mersenne Twister algorithm, which has an extremely long period, is used as the default random number generator in Python. This algorithm performs well on most of the tests that mathematicians have devised to test randomness [7].

– Be aware that calls to external cryptographic programs may slow your scripts.

In Section 18.3, we will be discussing cryptographic protocols. For now, suffice it to say that encryption protocols can be invoked from Python scripts with a system call to the openssl toolkit. Let us look at aes128, a strong encryption standard used by the United States government. We will see how long it takes to encrypt a nearly two megabyte file, 10,000 times, with the Python crypt_speed.py script. [Glossary AES]

```
#!/usr/bin/python
import time, os
os.chdir("c:/cygwin64/bin/")
timenow = time.time()
for i in range(1, 10000):
  os.system("openssl.exe aes128 -in c:/ftp/py/meshword.txt -out
meshword.aes -pass pass:12345")
timenew = time.time()
print("Time for 10,000 aes128 encryptions on a long file:
" + str(timenew - timenow))
exit
```

```
outputtp\py>crypt_speed.py
Time for 10,000 aes128 encryptions on a long file: 499.7346260547638
```

We see that it would take take about 500 seconds to encrypt a file 10,000 times (or 0.05 seconds per encryption); glacial in comparison to other functions (e.g., random number, time). Is it faster to encrypt a small file than a large file? Let us repeat the process, using the 11 byte helloworld.txt file.

```
import time, os
os.chdir("c:/cygwin64/bin/")
timenow = time.time()
for i in range(1, 10000):
  os.system("openssl.exe aes128 -in c:/ftp/py/helloworld.txt -out
meshword.aes -pass pass:12345")
timenew = time.time()
print("Time for 10,000 aes128 encryptions on a short file:
" + str(timenew - timenow))

c:\ftp\py>crypt_speed.py
Time for 10,000 aes128 encryptions on a short file: 411.52050709724426
```

Short files encrypt faster than longer files, but the savings is not great. As we have seen, calling an external program from within Python is always a time-consuming process, and we can presume that most of the loop time was devoted to finding the openssl.exe program, interpreting the entire program and returning a value."

– **Do not insist on precision when there is no practical value in precise answers.**

Approximation methods are often orders of magnitude faster than exact methods. Furthermore, algorithms that produce inexact answers are preferable to exact algorithms that crash under the load of a gigabyte of data. Real world data is never exact, so why must we pretend that we need exact solutions?

– **Write you scripts in such a way that calculations are completed in one pass through the data.**

Programmers commonly write iterative loops through their data, calculating some particular component of an equation, only to repeat the loop to calculate another piece of the puzzle. As an example, consider the common task of calculating the variance (square of the standard deviation) of a population. The typical algorithm involves calculating the population mean, by summing all the data values in the population and dividing by the number of values summed. After the population mean is calculated, the variance is obtained by a second pass through the population and applying the formula below (Fig. 11.1):

$$\sigma^2 = \frac{1}{N}\sum_{i=1}^{N}(x_i - \mu)^2$$

FIG. 11.1 Calculating the variance (square of standard deviation) after first calculating the population mean.

The variance can be calculated in a fast, single pass through the population, using the equivalent formula, below, which does not involve precalculating the population mean (Fig. 11.2).

$$\sigma^2 = \frac{1}{n}\sum x_i^2 - \left(\frac{1}{n}\sum x_i\right)^2$$

FIG. 11.2 Calculating the variance, in a single pass through the values of a population [8].

By using the one-pass equation, after any number of data values have been processed, the running values of the average and variance can be easily determined; a handy trick, especially applicable to signal processing [8,9].

Section 11.3. The Dot Product, a Simple and Fast Correlation Method

Our similarities are different.

Yogi Berra

Similarity scores are based on comparing one data object with another, attribute by attribute. Two similar variables will rise and fall together. A score can be calculated by summing the squares of the differences in magnitude for each attribute, and using the calculation to compute a final outcome, known as the correlation score. One of the most popular correlation methods is Pearson's correlation, which produces a score that can vary from −1 to +1. Two objects with a high score (near +1) are highly similar [10]. Two uncorrelated objects would have a Pearson score near zero. Two objects that correlated inversely (i.e., one falling when the other rises) would have a Pearson score near −1. [Glossary Correlation distance, Normalized compression distance, Mahalanobis distance]

The Pearson correlation for two objects, with paired attributes, sums the product of their differences from their object means and divides the sum by the product of the squared differences from the object means (Fig. 11.3).

Python's Scipy module offers a Pearson function. In addition to computing Pearson's correlation, the scipy function produces a two-tailed *P*-value, which provides some indication of the likelihood that two totally uncorrelated objects might produce a Pearson's correlation value as extreme as the calculated value. [Glossary *P* value, Scipy]

Let us look at a short python script, sci_pearson.py, that calculates the Pearson correlation on two lists.

$$r = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n}(x_i - \bar{x})^2}\sqrt{\sum_{i=1}^{n}(y_i - \bar{y})^2}}$$

FIG. 11.3 Formula for Pearson's correlation, for two data objects, with paired sets of attributes, *x* and *y*.

```
from scipy.stats.stats import pearsonr
a = [1, 2, 3, 4]
b = [2, 4, 6, 8]
c = [1,4,6,9,15,55,62,-5]
d = [-2,-8,-9,-12,-80,14,15,2]
print("Correlation a with b: " + str(pearsonr(a,b)))
print("Correlation c with d: " + str(pearsonr(c,d)))
```

Here is the output of pearson.py

```
Correlation a with b: (1.0, 0.0)
Correlation c with d: (0.32893766587262174, 0.42628658412101167)
```

The Pearson correlation of a with b is 1 because the values of b are simply double the values of a; hence the values in a and b correlate perfectly with one another. The second number, "0.0", is the calculated P value.

In the case of c correlated with d, the Pearson correlation, 0.329, is intermediate between 0 and 1, indicating some correlation. How does the Pearson correlation help us to simplify and reduce data? If two lists of data have a Pearson correlation of 1 or of -1, this implies that one set of the data is redundant. We can assume the two lists have the same information content. If we were comparing two sets of data and found a Pearson correlation of zero, then we might assume that the two sets of data were uncorrelated, and that it would be futile to try to model (i.e., find a mathematical relationship for) the data. [Glossary Overfitting]

There are many different correlation measurements, and all of them are based on assumptions about how well-correlated sets of data ought to behave. A data analyst who works with gene sequences might impose a different set of requirements, for well-correlated data, than a data analyst who is investigating fluctuations in the stock market. Hence, there are many available correlation values that are available to data scientists, and these include: Pearson, Cosine, Spearman, Jaccard, Gini, Maximal Information Coefficient, and Complex Linear Pathway score. The computationally fastest of the correlation scores is the dot product (Fig. 11.4). In a recent paper comparing the performance of 12 correlation formulas the simple dot product led the pack [11].

Let us examine the various dot products that can be calculated for three sample vectors,

$$\sum_i x_i y_i$$

FIG. 11.4 The lowly dot product. For two vectors, the dot product is the sum of the products of the corresponding values. To normalize the dot product, we would divide the dot product by the product of the lengths of the two vectors.

```
a = [1,4,6,9,15,55,62,-5]
b = [-2,-8,-9,-12,-80,14,15,2]
c = [2,8,12,18,30,110,124,-10]
```

Notice that vector *c* has twice the value of each paired attribute in vector *a*. We'll use the Python script, numpy_dot.py to compute the lengths of the vectors *a*, *b*, and *c*; and we will calculate the simple dot products, normalized by the product of the lengths of the vectors.

```
from __future__ import division
import numpy
from numpy import linalg
a = [1,4,6,9,15,55,62,-5]
b = [-2,-8,-9,-12,-80,14,15,2]
c = [2,8,12,18,30,110,124,-10]
a_length = linalg.norm(a)
b_length = linalg.norm(b)
c_length = linalg.norm(c)
print(numpy.dot(a,b) / (a_length * b_length))
print(numpy.dot(a,a) / (a_length * a_length))
print(numpy.dot(a,c) / (a_length * c_length))
print(numpy.dot(b,c) / (b_length * c_length))
```

Here is the commented output:

```
0.0409175385118  (Normalized dot product of a with b)
1.0              (Normalized dot product of a with a)
1.0              (Normalized dot product of a with c)
0.0409175385118  (Normalized dot product of b with c)
```

Inspecting the output, we see that the normalized dot product of a vector with itself is 1. The normalized dot product of a and c is also 1, because *c* is perfectly correlated with *a*, being twice its value, attribute by attribute. We also see that the normalized dot product of *a* and *b* is equal to the normalized dot product of *b* and *c* (0.0409175385118); because *c* is perfectly correlated with a and because dot products are transitive.

Section 11.4. Clustering

Reality is merely an illusion, albeit a very persistent one.

Albert Einstein

Clustering algorithms are currently very popular. They provide a way of taking a large set of data objects that seem to have no relationship to one another and to produce a visually simple collection of clusters wherein each cluster member is similar to every other member of the same cluster.

The algorithmic methods for clustering are simple. One of the most popular clustering algorithms is the *k*-means algorithm, which assigns any number of data objects to one of *k* clusters [12]. The number *k* of clusters is provided by the user. The algorithm is easy to describe and to understand, but the computational task of completing the algorithm can be difficult when the number of dimensions in the object (i.e., the number of attributes associated with the object), is large. [Glossary *K*-means algorithm, *K*-nearest neighbor algorithm]

Here is how the algorithm works for sets of quantitative data:

1. The program randomly chooses *k* objects from the collection of objects to be clustered. We will call each of these these *k* objects a focus.
2. For every object in the collection, the distance between the object and all of randomly chosen *k* objects (chosen in step 1) is computed.
3. A round of *k*-clusters are computed by assigning every object to its nearest focus.
4. The centroid focus for each of the *k* clusters is calculated. The centroid is the point that is closest to all of the objects within the cluster. Another way of saying this is that if you sum the distances between the centroid and all of the objects in the cluster, this summed distance will be smaller than the summed distance from any other point in space.
5. Steps 2, 3, and 4 are repeated, using the *k* centroid foci as the points for which all distances are computed.
6. Step 5 is repeated until the *k* centroid foci converge on a non-changing set of values (or until the program slows to an interminable crawl).

There are some serious drawbacks to the algorithm:

- The final set of clusters will sometimes depend on the initial, random choice of *k* data objects. This means that multiple runs of the algorithm may produce different outcomes.
- The algorithms are not guaranteed to succeed. Sometimes, the algorithm does not converge to a final, stable set of clusters.
- When the dimensionality is very high the distances between data objects (i.e., the square root of the sum of squares of the measured differences between corresponding attributes of two objects) can be ridiculously large and of no practical meaning. Computations may bog down, cease altogether, or produce meaningless results. In this case the only recourse may require eliminating some of the attributes (i.e., reducing dimensionality of the data objects). Subspace clustering is a method wherein clusters are found for computationally manageable subsets of attributes. If useful clusters are found using this method, additional attributes can be added to the mix to see if the clustering can be improved. [Glossary Curse of dimensionality]
- The clustering algorithm may succeed, producing a set of clusters of similar objects, but the clusters may have no practical value. They may miss important relationships among the objects, or they might group together objects whose similarities are totally non-informative.

At best, clustering algorithms should be considered a first step toward understanding how attributes account for the behavior of data objects.

Classifier algorithms are different from clustering algorithms. Classifiers assign a class (from a pre-existing classification) to an object whose class is unknown [12]. The *k*-nearest neighbor algorithm (not to be confused with the *k*-means clustering algorithm) is a simple and popular classifier algorithm. From a collection of data objects whose class is known, the algorithm computes the distances from the object of unknown class to the objects of known class. This involves a distance measurement from the feature set of the objects of unknown class to every object of known class (the test set). The distance measure uses the set of attributes that are associated with each object. After the distances are computed, the *k* classed objects with the smallest distance to the object of unknown class are collected. The most common class in the nearest *k* classed objects is assigned to the object of unknown class. If the chosen value of *k* is 1, then the object of unknown class is assigned the class of its closest classed object (i.e., the nearest neighbor).

The k-nearest neighbor algorithm is just one among many excellent classifier algorithms, and analysts have the luxury of choosing algorithms that match their data (e.g., sample size, dimensionality) and purposes [13]. Classifier algorithms differ fundamentally from clustering algorithms and from recommender algorithms in that they begin with an existing classification. Their task is very simple; assign an object to its proper class within the classification. Classifier algorithms carry the assumption that similarities among class objects determine class membership. This may not be the case. For example, a classifier algorithm might place cats into the class of small dogs because of the similarities among several attributes of cats and dogs (e.g., four legs, one tail, pointy ears, average weight about 8 pounds, furry, carnivorous, etc.). The similarities are impressive, but irrelevant. No matter how much you try to make it so, a cat is not a type of dog. The fundamental difference between grouping by similarity and grouping by relationship has been discussed in Section 5.1. [Glossary Recommender, Modeling]

Like clustering techniques, classifier techniques are computationally intensive when the dimension is high, and can produce misleading results when the attributes are noisy (i.e., contain randomly distributed attribute values) or non-informative (i.e., unrelated to correct class assignment).

Section 11.5. Methods for Data Persistence (Without Using a Database)

A file that big?
It might be very useful.
But now it is gone.

Haiku by David J. Liszewski

Your scripts create data objects, and the data objects hold data. Sometimes, these data objects are transient, existing only during a block or subroutine. At other times, the data

objects produced by scripts represent prodigious amounts of data, resulting from complex and time-consuming calculations. What happens to these data structures when the script finishes executing? Ordinarily, when a script stops, all the data structures produced by the script simply vanish.

Persistence is the ability of data to outlive the program that produced it. The methods by which we create persistent data are sometimes referred to as marshalling or serializing. Some of the language specific methods are called by such colorful names as data dumping, pickling, freezing/thawing, and storable/retrieve. [Glossary Serializing, Marshalling, Persistence]

Data persistence can be ranked by level of sophistication. At the bottom is the exportation of data to a simple flat-file, wherein records are each one line in length, and each line of the record consists of a record key, followed by a list of record attributes. The simple spreadsheet stores data as tab delimited or comma separated line records. Flat-files can contain a limitless number of line records, but spreadsheets are limited by the number of records they can import and manage. Scripts can be written that parse through flat-files line by line (i.e ., record by record), selecting data as they go. Software programs that write data to flat-files achieve a crude but serviceable type of data persistence.

A middle-level technique for creating persistent data is the venerable database. If nothing else, databases can create, store, and retrieve data records. Scripts that have access to a database can achieve persistence by creating database records that accommodate data objects. When the script ends, the database persists, and the data objects can be fetched and reconstructed for later use.

Perhaps the highest level of data persiste nce is achieved when complex data objects are saved in toto. Flat-files and databases may not be suited to storing complex data objects, holding encapsulated data values. Most languages provide built-in methods for storing complex objects, and a number of languages designed to describe complex forms of data have been developed. Data description languages, such as YAML (Yet Another Markup Language) and JSON (JavaScr ipt Object Notation), can be adopted by any programming language.

Let us review some of the techniques for data persistence that are readily accessible to Python programmers.

Python pickles its data. Here, the Python script, pickle_up.py, pickles a string variable, in the save.p file.

```
import pickle
pumpkin_color = "orange"
pickle.dump( pumpkin_color, open("save.p","wb"))
```

The Python script, pickle_down.py, loads the pickled data, from the “save.p” file, and prints it to the screen.

```
import pickle
pumpkin_color = pickle.load(open("save.p","rb"))
print(pumpkin_color)
```

The output of the pickle_down.py script is shown here:

```
orange
```

Python has several database modules that will insert database objects into external files that persist after the script has executed. The database objects can be quickly called from the external module, with a simple command syntax [10]. Here is the Python script, lucy.py, that creates a tiny external database, using Python's most generic dbm.dumb module.

```
import dbm.dumb
lucy_hash = dbm.dumb.open('lucy', 'c')
lucy_hash["Fred Mertz"] = "Neighbor"
lucy_hash["Ethel Mertz"] = "Neighbor"
lucy_hash["Lucy Ricardo"] = "Star"
lucy_hash["Ricky Ricardo"] = "Band leader"
lucy_hash.close()
```

Here is the Python script, lucy_untie.py, that reads all of the key/value pairs held in the persistent database created for the lucy_hash dictionary object.

```
import dbm.dumb
lucy_hash = dbm.dumb.open('lucy')
for character in lucy_hash.keys():
  print(character.decode('utf-8') + " " + lucy_hash[character].
  decode('utf-8'))
lucy_hash.close()
```

Here is the output produced by the Python script, lucy_untie.py script.

```
Ethel Mertz Neighbor
Lucy Ricardo Star
Ricky Ricardo Band leader
Fred Mertz Neighbor
```

Persistence is a simple and fundamental process ensuring that data created in your scripts can be recalled by yourself or by others who need to verify your results. Regardless of the programming language you use, or the data structures you prefer, you will need to familiarize with at least one data persistence technique.

Section 11.6. Case Study: Climbing a Classification

But - once I bent to taste an upland spring
And, bending, heard it whisper of its Sea.

Ecclesiastes

Classifications are characterized by a linear ascension through a hierarchy. The parental classes of any instance of the classification can be traced as a simple, non-branched, and non-recursive, ordered, and uninterrupted list of ancestral classes.

In a prior work [10], I described how a large, publicly available, taxonomy data file could be instantly queried to retrieve any listed organism, and to compute its complete class lineage, back to the "root" class, the primordial origin the classification of living organisms [10]. Basically, the trick to climbing backwards up the class lineage involves building two dictionary objects, also known as associative arrays. One dictionary object (which we will be calling "namehash") is composed of key/value pairs wherein each key is the identifier code of a class (in the nomenclature of the taxonomy data file), and each value is its name or label. The second dictionary object (which we'll be calling "parenthash") is composed of key/value pairs wherein each key is the identifier code of a class, and each value is the identifier code of the parent class. Once you have prepared the namehash dictionary and the parenthash dictionary the entire ancestral lineage of every one of the many thousands of organisms included in the taxonomy of living species (contained in the taxonomy.dat file) can be reconstructed with just a few lines of Python code, as shown here:

```
for i in range(30):
      if id_name in namehash:
        outtext.write(namehash[id_name] + "\n")
      if id_name in parenthash:
        id_name = parenthash[id_name]
```

The parts of the script that build the dictionary objects are left as an exercise for the reader. As an example of the script's output, here is the lineage for the Myxococcus bacteria:

```
Myxococcus
Myxococcaceae
Cystobacterineae
Myxococcales
Deltaproteobacteria
delta/epsilon subdivisions
Proteobacteria
Bacteria
cellular organisms
root
```

The words in this lineage may seem strange to laypersons, but taxonomists who view this lineage instantly grasp the place of organism within the classification of all living organisms. Every large and complex knowledge domain should have its own taxonomy, complete with a parent class for every child class. The basic approach to reconstructing lineages from the raw taxonomy file would apply to every field of study. For those interested in the taxonomy of living organisms, possibly the best documented classification of any kind, the taxonomy.dat file (exceeding 350 Mbytes) is available at no cost via ftp at:

ftp://ftp.ebi.ac.uk/pub/databases/taxonomy/

Section 11.7. Case Study (Advanced): A Database Example

Experts often possess more data than judgment.

Colin Powell

For industrial strength persistence, providing storage for millions or billions of data objects, database applications are a good choice. SQL (Systems Query Language, pronounced like "sequel") is a specialized language used to query relational databases. SQL allows programmers to connect with large, complex server-based network databases. A high level of expertise is needed to install and implement the software that creates server-based relational databases responding to multi-user client-based SQL queries. Fortunately, Python provides access to SQLite, a free, and widely available spin-off of SQL [10]. The source code for SQLite is public domain. [Glossary Public domain]

SQLite is bundled into the newer distributions of Python, and can be called from Python scripts with an "import sqlite3" command. Here is a Python script, sqlite.py, that reads a very short dictionary into an SQL database.

```
import sqlite3, itertools
from sqlite3 import dbapi2 as sqlite
import string, re, os
mesh_hash = {}
entry = ()
mesh_hash["Fred Mertz"] = "Neighbor"
mesh_hash["Ethel Mertz"] = "Neighbor"
mesh_hash["Lucy Ricardo"] = "Star"
mesh_hash["Ricky Ricardo"] = "Band leader"
con=sqlite.connect('test1.db')
cur=con.cursor()
cur.executescript("""
    create table lucytable
    (
      name     varchar(64),
      term     varchar(64)
    );
    """)
for key,value in mesh_hash.items():
  entry = (key, value)
  cur.execute("insert into lucytable (name, term) values (?, ?)",
  entry)
con.commit()
```

Once created, entries in the SQL database file, test1.db, can be retrieved, as shown in the Python script, sqlite_read.py:

```
import sqlite3
from sqlite3 import dbapi2 as sqlite
import string, re, os
con=sqlite.connect('test1.db')
cur=con.cursor()
cur.execute("select * from lucytable")
for row in cur:
  print(row[0], row[1])
```

Here is the output of the sqlite_read.py script

```
Fred Mertz Neighbor
Ethel Mertz Neighbor
Lucy Ricardo Star
Ricky Ricardo Band leader
```

Databases, such as SQLite, are a great way to achieve data persistence, if you are adept at programming in SQL, and if you need to store millions of simple data objects. You may be surprised to learn that built-in persistence methods native to your favorite programming language may provide a simpler, more flexible option than proprietary database applications, when dealing with Big Data.

Section 11.8. Case Study (Advanced): NoSQL

The creative act is the defeat of habit by originality

George Lois

Triples are the basic commodities of information science. Every triple represents a meaningful assertion, and collections of triples can be automatically integrated with other triples. As such all the triples that share the same identifier can be collected to yield all the available information that pertains to the unique object. Furthermore, all the triples that pertain to all the members of a class of objects can be combined to provide information about the class, and to find relationships among different classes of objects. This being the case, it should come as no surprise that databases have been designed to utilize triples as their data structure; dedicating their principal functionality to the creation, storage, and retrieval of triples.

Triple databases, also known as triplestores, are specialized variants of the better-known NoSQL databases,; databases that are designed to store records consisting of nothing more than a key and value. In the case of triplestores, the key is the identifier of a data object, and the value is a metadata/data pair belonging associated with the identifier belonging to the data object.

Today, large triplestores exist, holding trillions of triples. At the current time, software development for triplestore databases is in a state of volatility. Triplestore databases are

dropping in an out of existence, changing their names, being incorporated into other systems, or being redesigned from the ground up.

At the risk of showing my own personal bias, as an unapologetic Mumps fan, I would suggest that readers may want to investigate the value of using native Mumps as a triplestore database. Mumps, also known as the M programming language, is one of a small handful of ANSI-standard (American National Standard Institute) languages that includes C, Ada, and Fortran. It was developed in the 1960s and is still in use, primarily in hospital information systems and large production facilities [14]. The simple, hierarchical database design of Mumps lost favor through the last decades of the twentieth century, as relational databases gained popularity. In the past decade, with the push toward NoSQL databases holding massive sets of simplified data, Mumps has received renewed interest. As it happens, Mumps can be implemented as a powerful and high performance Triplestore database.

Versions of Mumps are available as open source, free distributions [15,16]. but the Mumps installation process can be challenging for those who are unfamiliar with the Mumps environment. Stalwarts who successfully navigate the Mumps installation process may find that Mumps' native features render it suitable for storing triples and exploring their relationships [17].

Glossary

AES The Advanced Encryption Standard (AES) is the cryptographic standard endorsed by the United States government as a replacement for the old government standard, DES (Data Encryption Standard). AES was chosen from among many different encryption protocols submitted in a cryptographic contest conducted by the United States National Institute of Standards and Technology, in 2001. AES is also known as Rijndael, after its developer. It is a symmetric encryption standard, meaning that the same password used for encryption is also used for decryption.

Associative array A data structure consisting of an unordered list of key/value data pairs. Also known as hash, hash table, map, symbol table, dictionary, or dictionary array. The proliferation of synonyms suggests that associative arrays, or their computational equivalents, have great utility. Associative arrays are used in Perl, Python, Ruby and most modern programming languages.

Black box In physics, a black box is a device with observable inputs and outputs, but what goes on inside the box is unknowable. The term is used to describe software, algorithms, machines, and systems whose inner workings are inscrutable.

Correlation distance Also known as correlation score. The correlation distance provides a measure of similarity between two variables. Two similar variables will rise rise and fall together [18,19]. The Pearson correlation score is popular, and can be easily implemented [10,20]. It produces a score that varies from -1 to 1. A score of 1 indicates perfect correlation; a score of -1 indicates perfect anti-correlation (i.e., one variable rises while the other falls). A Pearson score of 0 indicates lack of correlation. Other correlation measures can be applied to Big Data sets [18,19].

Curse of dimensionality As the number of attributes for a data object increases, the distance between data objects grows to enormous size. The multidimensional space becomes sparsely populated, and the distances between any two objects, even the two closest neighbors, becomes absurdly large. When you have thousands of dimensions, the space that holds the objects is so large that distances

between objects become difficult or impossible to compute, and computational products become useless for most purposes.

K-means algorithm The *k*-means algorithm assigns any number of data objects to one of *k* clusters [12]. The algorithm is described fully in Chapter 9. The *k*-means algorithm should not be confused with the *k*-nearest neighbor algorithm.

K-nearest neighbor algorithm The *k*-nearest neighbor algorithm is a simple and popular classifier algorithm. From a collection of data objects whose class is known, the algorithm computes the distances from the object of unknown class to the objects of known class. This involves a distance measurement from the feature set of the objects of unknown class to every object of known class (the test set). After the distances are computed, the *k* classed objects with the smallest distance to the object of unknown class are collected. The most common class (i.e., the class with the most objects) among the nearest *k* classed objects is assigned to the object of unknown class. If the chosen value of *k* is 1, then the object of unknown class is assigned the class of its closest classed object (i.e., the nearest neighbor).

Mahalanobis distance A distance measure based on correlations between variables; hence, it measures the similarity of the objects whose attributes are compared. As a correlation measure, it is not influenced by the relative scale of the different attributes. It is used routinely in clustering and classifier algorithms.

Marshalling Marshalling, like serializing, is a method for achieving data persistence (i.e., saving variables and other data structures produced in a program, after the program has stopped running). Marshalling methods preserve data objects, with their encapsulated data and data structures.

Modeling Modeling involves explaining the behavior of a system, often with a formula, sometimes with descriptive language. The formula for the data describes the distribution of the data and often predicts how the different variables will change with one another. Consequently, modeling often provides reasonable hypotheses to explain how the data objects within a system will influence one another. Many of the great milestones in the physical sciences have arisen from a bit of data modeling supplemented by scientific genius (e.g., Newton's laws of mechanics and optics, Kepler's laws of planetary orbits, Quantum mechanics). The occasional ability to relate observation with causality endows modeling with greater versatility and greater scientific impact than the predictive techniques (e.g., recommenders, classifiers and clustering methods). Unlike the methods of predictive analytics, which tend to rest on a few basic assumptions about measuring similarities among data objects, the methods of data modeling are selected from every field of mathematics and are based on an intuitive approach to data analysis. In many cases, the modeler simply plots the data and looks for familiar shapes and patterns that suggest a particular type of function (e.g., logarithmic, linear, normal, Fourier series, Power law).

Normalized compression distance String compression algorithms (e.g., zip, gzip, bunzip) should yield better compression from a concatenation of two similar strings than from a concatenation of two highly dissimilar strings. The reason being that the same string patterns that are employed to compress a string (i.e., repeated runs of a particular pattern) are likely to be found in another, similar string. If two strings are completely dissimilar, then the compression algorithm would fail to find repeated patterns that enhance compressibility. The normalized compression distance is a similarity measure based on the enhanced compressibility of concatenated strings of high similarity [21]. A full discussion, with examples, is found in the Open Source Tools section of Chapter 4.

Overfitting Overfitting occurs when a formula describes a set of data very closely, but does not lead to any sensible explanation for the behavior of the data, and does not predict the behavior of comparable data sets. In the case of overfitting the formula is said to describe the noise of the system rather than the characteristic behavior of the system. Overfitting occurs frequently with models that perform iterative approximations on training data, coming closer and closer to the training data set with each iteration. Neural networks are an example of a data modeling strategy that is prone to overfitting.

***P* value** The *P* value is the probability of getting a set of results that are as extreme or more extreme as the set of results you observed, assuming that the null hypothesis is true (that there is no statistical difference between the results). The *P*-value has come under great criticism over the decades, with a growing consensus that the *P*-value is often misinterpreted, used incorrectly, or used in situations wherein it does not apply [22]. In the realm of Big Data, repeated samplings of data from large data sets will produce small *P*-values that cannot be directly applied to determining statistical significance. It is best to think of the *P*-value as just another piece of information that tells you something about how sets of observations compare with one another; and not as a test of statistical significance.

Persistence Persistence is the ability of data to remain available in memory or storage after the program in which the data was created has stopped executing. Databases are designed to achieve persistence. When the database application is turned off, the data remains available to the database application when it is re-started at some later time.

Pseudorandom number generator It is impossible for computers to produce an endless collection of truly random numbers. Eventually, algorithms will cycle through their available variations and begins to repeat themselves, producing the same set of "random" numbers, in the same order; a phenomenon referred to as the generator's period. Because algorithms that produce seemingly random numbers are imperfect, they are known as pseudorandom number generators. The Mersenne Twister algorithm, which has an extremely long period, is used as the default random number generator in Python. This algorithm performs well on most of the tests that mathematicians have devised to test randomness.

Public domain Data that is not owned by an entity. Public domain materials include documents whose copyright terms have expired, materials produced by the federal government, materials that contain no creative content (i.e., materials that cannot be copyrighted), or materials donated to the public domain by the entity that holds copyright. Public domain data can be accessed, copied, and re-distributed without violating piracy laws. It is important to note that plagiarism laws and rules of ethics apply to public domain data. You must properly attribute authorship to public domain documents. If you fail to attribute authorship or if you purposefully and falsely attribute authorship to the wrong person (e.g., yourself), then this would be an unethical act and an act of plagiarism.

Recommender A collection of methods for predicting the preferences of individuals. Recommender methods often rely on one or two simple assumptions: (1) If an individual expresses a preference for a certain type of product, and the individual encounters a new product that is similar to a previously preferred product, then he is likely to prefer the new product; (2) If an individual expresses preferences that are similar to the preferences expressed by a cluster of individuals, and if the members of the cluster prefer a product that the individual has not yet encountered, then the individual will most likely prefer the product.

RegEx Short for Regular Expressions, RegEx is a syntax for describing patterns in text. For example, if I wanted to pull all lines from a text file that began with an uppercase "B" and contained at least one integer, and ended with the a lowercase x, then I might use the regular expression: " ̂B.*[0-9].*x$". This syntax for expressing patterns of strings that can be matched by pre-built methods available to a programming language is somewhat standardized. This means that a RegEx expression in Perl will match the same pattern in Python, or Ruby, or any language that employs RegEx. The relevance of Regex to Big Data is several-fold. Regex can be used to build or transform data from one format to another; hence creating or merging data records. It can be used to convert sets of data to a desired format; hence transforming data sets. It can be used to extract records that meet a set of characteristics specified by a user; thus filtering subsets of data or executing data queries over text-based files or text-based indexes. The big drawback to using RegEx is speed: operations that call for many Regex operations, particularly when those operations are repeated for each parsed line or record, will reduce software performance. Regex-heavy programs that operate just fine on megabyte files may take hours, days or months to parse through terabytes of data.

A 12-line python script, file_search.py, prompts the user for the name of a text file to be searched, and then prompts the user to supply a RegEx pattern. The script will parse the text file, line by line, displaying those lines that contain a match to the RegEx pattern.

```
import sys, string, re
print("What is file would you like to search?")
filename = sys.stdin.readline()
filename = filename.rstrip()
print("Enter a word, phrase or regular expression to search.")
word_to_search = (sys.stdin.readline()).rstrip()
infile = open (filename, "r")
regex_object = re.compile(word_to_search, re.I)
for line in infile:
  m= regex_object.search(line)
  if m:
     print(line)
```

Scipy Scipy, like numpy, is an open source extension to Python [23]. It includes many very useful mathematical routines commonly used by scientists, including: integration, interpolation, Fourier transforms, signal processing, linear algebra, and statistics. Scipy can be downloaded as a suite of modules from: http://www.scipy.org/scipylib/download.html. You can spare yourself the trouble of downloading individual installations of numpy and scipy by downloading Anaconda, a free distribution that bundles hundreds of python packages, along with a recent version of Python. Anaconda is available at: https://store.continuum.io/cshop/anaconda/

Serializing Serializing is a plesionym (i.e., near-synonym) for marshalling and is a method for taking data produced within a script or program, and preserving it in an external file, that can be saved when the program stops, and quickly reconstituted as needed, in the same program or in different programs. The difference, in terms of common usage, between serialization and marshalling is that serialization usually involves capturing parameters (i.e., particular pieces of information), while marshalling preserves all of the specifics of a data object, including its structure, content, and code content). As you might imagine, the meaning of terms might change depending on the programming language and the intent of the serializing and marshalling methods.

System call Refers to a command, within a running script, that calls the operating system into action, momentarily bypassing the programming interpreter for the script. A system call can do essentially anything the operating system can do via a command line.

Undifferentiated software Intellectual property disputes have driven developers to divide software into two categories: undifferentiated software and differentiated software. Undifferentiated software comprises the fundamental algorithms that everyone uses whenever they develop a new software application. It is in nobody's interest to assign patents to basic algorithms and their implementations. Nobody wants to devote their careers to prosecuting or defending tenuous legal claims over the ownership of the fundamental building blocks of computer science. Differentiated software comprises customized applications that are sufficiently new and different from any preceding product that patent protection would be reasonable.

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12

Finding the Clues in Large Collections of Data

OUTLINE

Section 12.1. Denominators

The question is not what you look at, but what you see.

Henry David Thoreau in Journal, 5 August 1851

Denominators are the numbers that provide perspective to other numbers. If you are informed that 10,000 persons die each year in the United States, from a particular disease, then you might want to know the total number of deaths, from all causes. When you compare the death from a particular disease with the total number of deaths from all causes (the denominator), you learn something about the relative importance of your original count (e.g., an incidence of 10,000 deaths/350 million persons). Epidemiologists typically represent incidences as numbers per 100,000 population. An incidence of 10,000/350 million is equivalent to an incidence of 2.9 per 100,000.

Denominators are not always easy to find. In most cases the denominator is computed by tallying every data object in a Big Data resource. If you have a very large number of data objects, then the time required to reach a global tally may be quite long. In many cases a Big Data resource will permit data analysts to extract subsets of data, but analysts will be forbidden to examine the entire resource. In such cases the denominator will be computed for the subset of extracted data and will not accurately represent all of the data objects available to the resource.

If you are using Big Data collected from multiple sources, your histograms (i.e., graphic representations of the distribution of objects by some measureable attribute such as age, frequency, size) will need to be represented as fractional distributions for each source's

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data; not as value counts. The reason for this is that a histogram from one source may not have the same total number of distributed values compared with the histogram created from another source. As discussed in Section 10.4, "Normalizing and Transforming Your Data," we achieve comparability among histograms by dividing the binned values by the total number of values in a distribution, for each data source. Doing so renders the bin value as a percentage of total, rather than a sum of data values.

Big Data managers should make an effort to supply information that summarizes the total set of data available at any moment in time, and should also provide information on the sources of data that contribute to the total collection. Here are some of the numbers that should be available to analysts: the number of records in the resource, the number of classes of data objects in the resource, the number of data objects belonging to each class in the resource, and the number of data values (preferably expressed as metadata/data pairs) that belong to data objects.

Section 12.2. Word Frequency Distributions

Poetry is everywhere; it just needs editing.

James Tate

There are two general types of data: quantitative and categorical. Quantitative data refers to measurements. Categorical data is simply a number that represents the number of items that have a feature. For most purposes the analysis of categorical data reduces to counting and binning.

Categorical data typically conforms to a Zipf distribution. George Kingsley Zipf (1902–50) was an American linguist who demonstrated that, for most languages, a small number of words account for the majority of occurrences of all the words found in prose. Specifically, he found that the frequency of any word is inversely proportional to its placement in a list of words, ordered by their decreasing frequencies in text. The first word in the frequency list will occur about twice as often as the second word in the list and three times as often as the third word in the list. [Glossary Word lists]

The Zipf distribution applied to languages is a special form of Pareto's principle, or the 80/20 rule. Pareto's principle holds that a small number of causes may account for the vast majority of observed instances. For example a small number of rich people account for the majority of wealth. Likewise, a small number of diseases account for the vast majority of human illnesses. A small number of children account for the majority of the behavioral problems encountered in a school. A small number of states hold the majority of the population of the United States. A small number of book titles, compared with the total number of publications, account for the majority of book sales. Much of Big Data is categorical and obeys the Pareto principle. Mathematicians often refer to Zipf distributions as Power law distributions. A short Python script for producing Zipf distribution's is found under its Glossary item. [Glossary Power law, Pareto's principle, Zipf distribution]

Let us take a look at the frequency distribution of words appearing in a book. Here is the list of the 30 most frequent words in a sample book and the number of occurrence of each word.

```
01 003977 the
02 001680 and
03 001091 class
04 000946 are
05 000925 chapter
06 000919 that
07 000884 species
08 000580 virus
09 000570 with
10 000503 disease
11 000434 for
12 000427 organisms
13 000414 from
14 000412 hierarchy
15 000335 not
16 000329 humans
17 000320 have
18 000319 proteobacteria
19 000309 human
20 000300 can
21 000264 fever
22 000263 group
23 000248 most
24 000225 infections
25 000219 viruses
26 000219 infectious
27 000216 organism
28 000216 host
29 000215 this
30 000211 all
```

As Zipf would predict, the most frequent word, "the" occurs 3977 times, roughly twice as often as the second most frequently occurring word, "and," which occurs 1689 times. The third most frequently occurring word "class" occurs 1091 times, or very roughly one-third as frequently as the most frequently occurring word.

What can we learn about the text from which these word frequencies were calculated? As discussed in Chapter 1 "stop" words are high frequency words that separate terms and tell us little or nothing about the informational content of text. Let us look at this same list with the "stop" words removed:

```
03 001091 class
05 000925 chapter
07 000884 species
08 000580 virus
10 000503 disease
12 000427 organisms
14 000412 hierarchy
16 000329 humans
18 000319 proteobacteria
19 000309 human
21 000264 fever
22 000263 group
24 000225 infections
25 000219 viruses
26 000219 infectious
27 000216 organism
28 000216 host
```

What kind of text could have produced this list? Could there be any doubt that the list of words and frequencies shown here came from a book whose subject is related to microbiology? As it happens, this word-frequency list came from a book that I previously wrote entitled "Taxonomic Guide to Infections Diseases: Understanding the Biologic Classes of Pathogenic Organisms" [1]. By glancing at a few words from a large text file, we gain a deep understanding of the subject matter of the text. The words with the top occurrence frequencies told us the most about the book, because these words are low-frequency in most books (e.g., words such as hierarchy, proteobacteria, organism). They occurred in high frequency because the text was focused on a narrow subject (e.g., infectious diseases).

A clever analyst will always produce a Zipf distribution for categorical data. A glance at the output reveals a great deal about the contents of the data.

Let us go one more step, and produce a cumulative index for the occurrence of words in the text, arranging them in order of descending frequency of occurrence.

```
01 003977 0.0559054232618291 the
02 001680 0.0795214934352948 and
03 001091 0.0948578818634204 class
04 000946 0.108155978520622 are
05 000925 0.121158874300655 chapter
06 000919 0.134077426972926 that
07 000884 0.146503978183249 species
08 000580 0.154657145266946 virus
09 000570 0.162669740504372 with
10 000503 0.169740504371784 disease
11 000434 0.175841322499930 for
```

```
12 000427 0.181843740335686 organisms
13 000414 0.187663414771290 from
14 000412 0.193454974837640 hierarchy
15 000335 0.198164131687706 not
16 000329 0.202788945430009 humans
17 000320 0.207287244510669 have
18 000319 0.211771486406702 proteobacteria
19 000309 0.216115156456465 human
20 000300 0.220332311844584 can
21 000264 0.224043408586128 fever
22 000263 0.227740448143046 group
23 000248 0.231226629930558 most
24 000225 0.234389496471647 infections
25 000219 0.237468019904973 viruses
26 000219 0.240546543338300 infectious
27 000216 0.243582895217746 organism
28 000216 0.246619247097191 host
29 000215 0.249641541792010 this
30 000211 0.252607607748320 all
.
.
.
.
.
8957 000001 0.999873485338356 acanthaemoeba
8958 000001 0.999887542522984 acalculous
8959 000001 0.999901599707611 academic
8960 000001 0.999915656892238 absurd
8961 000001 0.999929714076865 abstract
8962 000001 0.999943771261492 absorbing
8963 000001 0.999957828446119 absorbed
8964 000001 0.999971885630746 abrasion
8965 000001 0.999985942815373 abnormalities
8966 000001 1.000000000000000 abasence
```

In this cumulative listing the third column is the fraction of the occurrences of the word along with the preceding words in the list as a fraction of all the occurrences of every word in the text.

The list is truncated after the thirtieth entry and picks up again at entry number 8957. There are a total of 8966 different, sometimes called unique, words in the text. The total number of words in the text happens to be 71,138. The last word on the list "abasence" has a cumulative fraction of 1.0, as all of the preceding words, plus the last word, account for

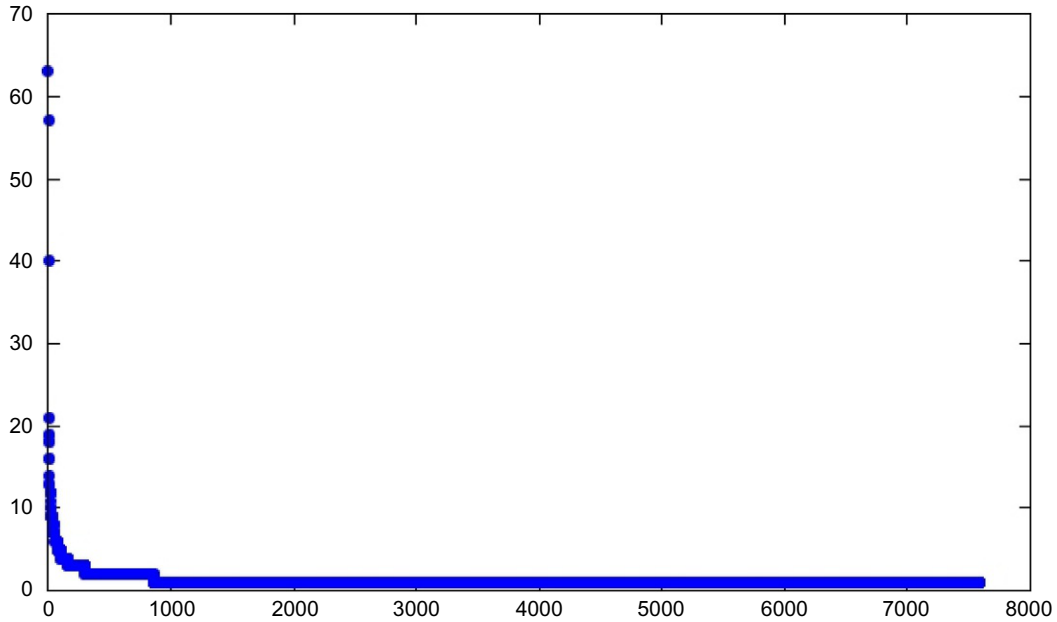

FIG. 12.1 A frequency distribution of word occurrences from a sample text. The bottom coordinates indicate that the entire text is accounted for by a list of about 9000 different words. The steep and early rise indicates that a few words account for the bulk of word occurrences. Graphs with this shape are sometimes referred to as Zipf distributions.

100% of word occurrences. The cumulative frequency distribution for the different words in the text is shown (Fig. 12.1). As an aside, the tail of the Zip distribution, which typically contains items occurring once only in a large data collection, are often "mistakes." In the case of text distributions, typographic errors can be found in the farthest and thinnest part of the tail. In this case the word "abasence" occurs just once, as the last item in the distribution. It is a misspelling for the word "absence."

Notice that though there are a total of 8957 unique words in the text, the first thirty words account for more than 25% of all word occurrences. The final ten words on the list occurred only once in the text. Common statistical measurements, such as the average of a population or the standard deviation, fail to provide any useful description of Zipf distributions. [Glossary Nonparametric statistics]

Section 12.3. Outliers and Anomalies

The mere formulation of a problem is far more essential than its solution, which may be merely a matter of mathematical or experimental skills. To raise new questions, new possibilities, to regard old problems from a new angle requires creative imagination and marks real advances in science.

Albert Einstein

On occasion the maxima or minima of a set of data will be determined by an outlier value; a value lying nowhere near any of the other values in the data set. If you could just eliminate the outlier, then you might enjoy a maxima and minima that were somewhat close to your other data values (i.e., the second-highest data value and the second-lowest data values would be close to the maxima and the minima, respectively). In these cases the data analyst must come to a decision, to drop or not to drop the outlier. There is no simple guideline for dealing with outliers, but it is sometimes helpful to know something about the dynamic range of the measurements. If a thermometer can measure temperature from −20 to 140°F, and your data outlier has a temperature of 390°F, then you know that the outlier must be an error; the thermometer does not measure above 140 degrees. The data analyst can drop the outlier, but it would be prudent to determine why the outlier was generated. [Glossary Dynamic range, Outlier, Case report, Dimensionality]

Outliers are extreme data values. The occurrence of outliers hinders the task of developing models, equations, or curves that closely fit all the available data. In some cases, outliers are simply mistakes; while in other cases, outliers may be the most important data in the data set. Examples of outliers that have advanced science are many, including: the observance of wobbly starts leading to the discovery of exoplanets; anomalous X-ray bursts from space leading to the discovery of magnetars, highly magnetized neutron stars; individuals with unusual physiological measurements leading to the discovery of rare diseases. The special importance of outliers to Big Data is that as the size of data sets increases, the number of outliers also increases.

True outliers (i.e., outliers not caused by experimental design error or errors in observation and measurement) obey the same physical laws as everything else in the universe. Therefore a valid outlier will always reveal something that is generally true about reality. Put another way, outliers are not exceptions to the general rules; outliers are the exceptions upon which the general rules are based. This assertion brings us to the sadly underappreciated and underutilized creation known as "the case report."

The case report, also known as the case study, is a detailed description of a single event or situation, often focused on a particular outlier, detail, or unique event. The concept of the case study is important in the field of Big Data because it highlights the utility of seeking general truths based on observations of outliers that can only be found in Big Data resources. Case reports are common in the medical literature, often beginning with a comment regarding the extreme rarity of the featured disease. You can expect to see phrases such as "fewer than a dozen have been reported in the literature" or "the authors have encountered no other cases of this lesion," or such and such a finding makes this lesion particularly uncommon and difficult to diagnose. The point that the authors are trying to convey is that the case report is worthy of publication specifically because the observation departs from normal experience. This is just wrong.

Too often, case reports serve merely as cautionary exercises, intended to ward against misdiagnosis. The "beware this lesion" approach to case reporting misses the most important aspect of this type of publication; namely that science, and most aspects of human understanding, involve generalizing from single observations to general rules. When Isaac

Newton saw an apple falling, he was not thinking that he could write a case report about how he once saw an apple drop, thus warning others not to stand under apple trees lest a rare apple might thump them upon the head. Newton generalized from the apple to all objects, addressing universal properties of gravity, and discovering the laws by which gravity interacts with matter. Case reports give us an opportunity to clarify the general way things work, by isolating one specific and rarely observed factor [2,3].

Section 12.4. Back-of-Envelope Analyses

Couldn't Prove, Had to Promise.

Book title, Wyatt Prunty

It is often assumed that Big Data resources are too large and complex for human comprehension. The analysis of Big Data is best left to software programs. Not so. When data analysts go straight to the complex calculations, before they perform a simple estimation, they will find themselves accepting wildly ridiculous calculations. For comparison purposes, there is nothing quite like a simple, and intuitive estimate to pull an overly-eager analyst back to reality. Often, the simple act of looking at a stripped-down version of the problem opens a new approach that can drastically reduce computation time. In some situations, analysts will find that a point is reached when higher refinements in methods yield diminishing returns. After the numerati have used their most advanced algorithms to make an accurate prediction, they may find that their best efforts offer little improvement over a simple estimator. This chapter reviews simple methods for analyzing big and complex data.

– Estimation-only analyses

The sun is about 93 million miles from the Earth. At this enormous distance, the light hitting Earth arrives as near-parallel rays and the shadow produced by the earth is nearly cylindrical. This means that the shadow of the earth is approximately the same size as the Earth itself. If the Earth's circular shadow on the moon, as observed during a lunar eclipse, appears to be about 2.5 times the diameter of the moon itself, then the moon must have a diameter approximately 1/2.5 times that of the earth. The diameter of the earth is about 8000 miles, so the diameter of the moon must be about 8000/2.5 or about 3000 miles.

The true diameter of the moon is smaller, about 2160 miles. Our estimate is inaccurate because the Earth's shadow is actually conical, not cylindrical. If we wanted to use a bit more trigonometry, we'd arrive at a closer approximation. Still, we arrived at a fair approximation of the moon's size from one, simple division, based on a casual observation made during a lunar eclipse. The distance was not measured; it was estimated from a simple observation. Credit for the first astronomer to use this estimation goes to the Greek astronomer Aristarchus of Samos (310 BCE–230 BCE). In this particular case, a direct measurement of the moon's distance was impossible. Aristarchus' only option was the rough

estimate. His predicament was not unique. Sometimes estimation is the only recourse for data analysts.

A modern-day example wherein measurements failed to help the data analyst is the calculation of deaths caused by heat waves. People suffer during heat waves, and municipalities need to determine whether people are dying from heat-related conditions. If heat-related deaths occur, then the municipality can justifiably budget for supportive services such as municipal cooling stations, the free delivery of ice, and increased staffing for emergency personnel. If the number of heat-related deaths is high, the governor may justifiably call a state of emergency.

Medical examiners perform autopsies to determine causes of death. During a heat wave the number of deceased individuals with a heat-related cause of death seldom rises as much as anyone would expect [4]. The reason for this is that stresses produced by heat cause death by exacerbating pre-existing non-heat-related conditions. The cause of death can seldom be pinned on heat. The paucity of autopsy-proven heat deaths can be relieved, somewhat, by permitting pathologists to declare a heat-related death when the environmental conditions at the site of death are consistent with hyperthermia (e.g., a high temperature at the site of death, and a high body temperature of the deceased measured shortly after death). Adjusting the criteria for declaring heat-related deaths is a poor remedy. In many cases the body is not discovered anytime near the time of death, invalidating the use of body temperature. More importantly, different municipalities may develop their own criteria for heat-related deaths (e.g., different temperature threshold measures, different ways of factoring night-time temperatures and humidity measurements). Basically, there is no accurate, reliable, or standard way to determine heat-related deaths at autopsy [4].

How would you, a data estimator, handle this problem? It is simple. You take the total number of deaths that occurred during the heat wave. Then you go back over your records of deaths occurring in the same period, in the same geographic region, over a series of years in which a heat wave did not occur. You average that number, giving you the expected number of deaths in a normal (i.e., without heat wave) period. You subtract that number from the number of deaths that occurred during the heat wave, and that gives you an estimate of the number of people who died from heat-related mortality. This strategy, applied to the 1995 Chicago heat wave, estimated that the number of heat-related deaths rose from 485 to 739 [5].

– **Mean-field averaging**

The average behavior of a collection of objects can be applied toward calculations that would exceed computational feasibility if applied to individual objects. Here is an example. Years ago, I worked on a project that involved simulating cell colony growth, using a Monte Carlo method [6]. Each simulation began with a single cell that divided, producing two cells, unless the cell happened to die prior to cell division. Each simulation applied a certain chance of cell death, somewhere around 0.5, for each cell, at each cell division. When you simulate colony growth, beginning with a single cell, the chance that

the first cell will die on the first cell division would be about 0.5; hence, there is about a 50% chance that the colony will die out on the first cell division. If the cell survives the first cell division, the cell might go through several additional cell divisions before it dies, by chance. By that time, there are other progeny that are dividing, and these progeny cells might successfully divide, thus enlarging the size of the colony. A Monte Carlo simulation randomly assigned death or life at each cell division, for each cell in the colony. When the colony manages to reach a large size (e.g., ten million cells), the simulation slows down, as the Monte Carlo algorithm must parse through ten million cells, calculating whether each cell will live or die, and assigning two offspring cells for each simulated division, and removing cells that were assigned a simulated "death." When the computer simulation slowed to a crawl, I found that the whole population displayed an "average" behavior. There was no longer any need to perform a Monte Carlo simulation on every cell in the population. I could simply multiply the total number of cells by the cell death probability (for the entire population), and this would tell me the total number of cells that survived the cycle. For a large colony of cells, with a death probability of 0.5 for each cell, half the cells will die at each cell cycle, and the other half will live and divide, produce two progeny cells; hence the population of the colony will remain stable. When dealing with large numbers, it becomes possible to dispense with the Monte Carlo simulation and to predict each generational outcome with a pencil and paper. [Glossary Monte Carlo simulation]

Substituting the average behavior for a population of objects, rather than calculating the behavior of every single object, is called mean-field approximation. It uses a physical law telling us that large collections of objects can be characterized by their average behavior. Mean-field approximation has been used with great success to understand the behavior of gases, epidemics, crystals, viruses, and all manner of large population problems. [Glossary Mean-field approximation]

Section 12.5. Case Study: Predicting User Preferences

He has no enemies, but is intensely disliked by his friends.

Oscar Wilde

Imagine you have all the preference data for every user of a large movie subscriber service, such as Netflix. You want to develop a system whereby the preference of any subscriber, for any movie, can be predicted. Here are some analytic options, listed in order of increasing complexity; omitting methods that require advanced mathematical skills.

1. Ignore your data and use experts.

Movie reviewers are fairly good predictors of a movie's appeal. If they were not good predictors, they would have been replaced by people with better predictive skills. For any movie, go to the newspapers and magazines and collect about ten movie reviews. Average the review scores and use the average as the predictor for all of your subscribers.

You can refine this method a bit by looking at the average subscriber scores, after the movie has been released. You can compare the scores of the individual experts to the average score of the subscribers. Scores from experts that closely matched the scores from the subscribers can be weighted a bit more heavily than experts whose scores were nothing like the average subscriber score.

2. Use all of your data, as it comes in, to produce an average subscriber score.

Skip the experts; go straight to your own data. In most instances, you would expect that a particular user's preference will come close to the average preference of the entire population in the data set for any given movie.

3. Lump people into preference groups based on shared favorites.

If Ann's personal list of top-favored movies is the same as Fred's top-favored list, then it is likely that their preferences will coincide. For movies that Ann has seen but Fred has not, use Ann's score as a predictor.

In a large data set, find an individual's top ten movie choices and add the individual to a group of individuals who share the same top-ten list. Use the average score for members of the group, for any particular movie as that movie's predictor for each of the members of the group.

As a refinement, find a group of people who share the top-ten and the bottom-ten scoring movies. Everyone in this group shares a love of the same top movies and a loathing for the same bottom movies.

4. Focus your refined predictions.

For many movies, there really is not much of a spread in ratings. If just about everyone loves "Star Wars" and "Raiders of the Lost Arc" and "It's a Wonderful Life," then there really is no need to provide an individual prediction for such movies. Likewise, if a movie is universally loathed, or universally accepted as an "average" flick, then why would you want to use computationally intensive models for these movies?

Most data sets have a mixture of easy and difficult data. There is seldom any good reason to develop predictors for the easy data. In the case of movie predictors, if there is very little spread in a movie's score, then you can safely use the average rating as the predicted rating for all individuals. By removing all of the "easy" movies from your group-specific calculations, you reduce the total number of calculations for the data collection.

This method of eliminating the obvious has application in many different fields. As a program director at the National Cancer Institute, I was peripherally involved in efforts to predict cancer treatment options for patients diagnosed in different stages of disease. Traditionally, large numbers of patients, at every stage of disease, were included in a prediction model that employed a list of measurable clinical and pathological parameters (e.g., age and gender of patient, size of tumor, the presence of local or distant metastases, and so on). It turned out that early models produced predictions where none were

necessary. If a patient had a tumor that was small, confined to its primary site of growth, and minimally invasive at its origin, then the treatment was always limited to surgical excision; there were no options for treatment, and hence no reason to predict the best option for treatment. If a tumor was widely metastatic to distant organs at the time of diagnosis, then there were no available treatments known, at that time, that could cure the patient. By focusing their analyses on the subset of patients who could benefit from treatment and for whom the best treatment option was not predetermined, the data analysts reduced the size and complexity of the data and simplified the problem.

The take-away lesson from this section is that predictor algorithms, so popular now among marketers, are just one of many different ways of determining how individuals and subgroups may behave, under different circumstances. Big Data analysts should not be reluctant to try several different analytic approaches, including approaches of their own invention. Sometimes the simplest algorithms, involving nothing more than arithmetic, are the best.

Section 12.6. Case Study: Multimodality in Population Data

What is essential is invisible to the eye.

Antoine de saint-exupery

Big Data distributions are sometimes multi-modal with several peaks and troughs. Multimodality always says something about the data under study. It tells us that the population is somehow non-homogeneous. Hodgkin lymphoma is an example of a cancer with a bimodal age distribution. There is a peak in occurrences at a young age, and another peak of occurrences at a more advanced age. This two-peak phenomenon can be found whenever Hodgkin Lymphoma is studied in large populations [7,8].

In the case of Hodgkin lymphoma, lymphomas occurring in the young may share diagnostic features with the lymphomas occurring in the older population, but the occurrence of lymphomas in two separable populations may indicate that some important distinction may have been overlooked: a different environmental cause, or different genetic alterations of lymphomas in the two age sets, or two different types of lymphomas that were mistakenly classified under one name, or there may be something wrong with the data (i.e., misdiagnoses, mix-ups during data collection). Big Data, by providing large numbers of cases, makes it easy to detect data incongruities (such as multimodality), when they are present. Explaining the causes for data incongruities is always a scientific challenge.

Multimodality in the age distribution of human diseases is an uncommon but well-known phenomenon. In the case of deaths resulting the Spanish flu of 1918, a tri-modal distribution was noticed (i.e., a high death rate in young, middle aged, and old individuals). In such cases, the observation of multimodality has provoked scientific interest, leading to fundamental discoveries in disease biology [9].

Section 12.7. Case Study: Big and Small Black Holes

If I didn't believe it, I would never have seen it.

Anon

The importance of inspecting data for multi-modality also applies to black holes. Most black holes have mass equivalents under 33 solar masses. Another set of black holes are supermassive, with mass equivalents of 10 or 20 billion solar masses. When there are objects of the same type, whose masses differ by a factor of a billion, scientists infer that there is something fundamentally different in the origin or development of these two variant forms of the same object. Black hole formation is an active area of interest, but current theory suggests that lower-mass black holes arise from pre-existing heavy stars. The supermassive black holes presumably grow from large quantities of matter available at the center of galaxies. The observation of bimodality inspired astronomers to search for black holes whose masses are intermediate between black holes with near-solar masses and the supermassive black holes. Intermediates have been found, and, not surprisingly, they come with a set of fascinating properties that distinguish them from other types of black holes. Fundamental advances in our understanding of the universe may sometimes follow from simple observations of multimodal data distributions.

Glossary

Case report The case report, also known as the case study, is a detailed description of a single event or situation, often devoted to an outlier, or a detail, or a unique occurrence of an observation. The concept of the case study is important in the field of data simplification because it highlights the utility of seeking general truths based on observations of rare events. Case reports are common in the biomedical literature, often beginning with a comment regarding the extreme rarity of the featured disease. You can expect to see phrases such as "fewer than a dozen have been reported in the literature" or "the authors have encountered no other cases of this lesion," or such and such a finding makes this lesion particularly uncommon and difficult to diagnose; and so on. The point that the authors are trying to convey is that the case report is worthy of publication specifically because the observation is rare. Too often, case reports serve merely as a cautionary exercise, intended to ward against misdiagnosis. The "beware this lesion" approach to case reporting misses the most important aspect of this type of publication; namely that science, and most aspects of human understanding, involve generalizing from the specific. When Isaac Newton saw an apple falling, he was not thinking that he could write a case report about how he once saw an apple drop, thus warning others not to stand under apple trees lest a rare apple might thump them upon the head. Newton generalized from the apple to all objects, addressing universal properties of gravity, and discovering the laws by which gravity interacts with matter. The case report gives us an opportunity to clarify the general way things work, by isolating one specific and rarely observed factor [2]. Data scientists must understand that rare cases are not exceptions to the general laws of reality; they are the exceptions upon which the general laws of reality are based.

Dimensionality The dimensionality of a data objects consists of the number of attributes that describe the object. Depending on the design and content of the data structure that contains the data object (i.e., database, array, list of records, object instance, etc.), the attributes will be called by different names, including field, variable, parameter, feature, or property. Data objects with high dimensionality create computational challenges, and data analysts typically reduce the dimensionality of data objects wherever possible.

Dynamic range Every measuring device has a dynamic range beyond which its measurements are without meaning. A bathroom scale may be accurate for weights that vary from 50 to 250 pounds, but you would not expect it to produce a sensible measurement for the weight of a mustard seed or an elephant.

Mean-field approximation A method whereby the average behavior for a population of objects substitutes for the behavior of each and every object in the population. This method greatly simplifies calculations. It is based on the observation that large collections of objects can be characterized by their average behavior. Mean-field approximation has been used with great success to understand the behavior of gases, epidemics, crystals, viruses, and all manner of large population phenomena.

Monte Carlo simulation This technique was introduced in 1946 by John von Neumann, Stan Ulam, and Nick Metropolis [10]. For this technique, the computer generates random numbers and uses the resultant values to simulate repeated trials of a probabilistic event. Monte Carlo simulations can easily simulate various processes (e.g., Markov models and Poisson processes) and can be used to solve a wide range of problems [6,11]. The Achilles heel of the Monte Carlo simulation, when applied to enormous sets of data, is that so-called random number generators may introduce periodic (non-random) repeats over large stretches of data [12]. What you thought was a fine Monte Carlo simulation, based on small data test cases, may produce misleading results for large data sets. The wise Big Data analyst will avail himself of the best possible random number generators, and will test his outputs for randomness. Various tests of randomness are available [13].

Nonparametric statistics Statistical methods that are not based on assumptions about the distribution of the sample population (e.g., not based on the assumption that the sample population fits a Gaussian distribution). Median, mode, and range are examples of common nonparametric statistics.

Outlier The term refers to a data point that lies far outside the value of the other data points in a distribution. The outlier may occur as the result of an error, or it may represent a true value that needs to be explained. When computing a line that is the "best fit" to the data, it is usually prudent to omit the outliers; otherwise, the best fit line may miss most of the data in your distribution. There is no strict rule for identifying outliers, but by convention, statisticians may construct a cut-off that lies 1.5 times the range of the lower quartile of the data, for small outliers, or 1.5 times the upper quartile range for large values.

Pareto's principle Also known as the 80/20 rule, Pareto's principle holds that a small number of items account for the vast majority of observations. For example, a small number of rich people account for the majority of wealth. Just 2 countries, India plus China, account for 37% of the world population. Within most countries, a small number of provinces or geographic areas contain the majority of the population of a country (e.g., East and West coastlines of the United States). A small number of books, compared with the total number of published books, account for the majority of book sales. Likewise, a small number of diseases account for the bulk of human morbidity and mortality. For example, two common types of cancer, basal cell carcinoma of skin and squamous cell carcinoma of skin account for about 1 million new cases of cancer each year in the United States. This is approximately the sum total of for all other types of cancer combined. We see a similar phenomenon when we count causes of death. About 2.6 million people die each year in the United States [14]. The top two causes of death account for 1,171,652 deaths (596,339 deaths from heart disease and 575,313 deaths from cancer [15]), or about 45% of all United States deaths. All of the remaining deaths are accounted for by more than 7000 conditions. Sets of data that follow Pareto's principle are often said to follow a Zipf distribution, or a power law distribution. These types of distributions are not tractable by standard statistical descriptors because they do not produce a symmetric bell-shaped curve. Simple measurements such as average and standard deviation have virtually no practical meaning when applied to Zipf distributions. Furthermore, the Gaussian distribution does not apply, and none of the statistical inferences built upon an assumption of a Gaussian distribution will hold on data sets that observe Pareto's principle [16].

Power law A mathematical formula wherein a particular value of some quantity varies as an inverse power of some other quantity [17,18]. The power law applies to many natural phenomena and describes the Zipf distribution or Pareto's principle. The power law is unrelated to the power of a statistical test.

Word lists Word lists are collections, usually in alphabetic order, of the different words that might appear in a corpus of text or a language dictionary. Such lists are easy to create. Here is a short Python script, words.py, that prepares an alphabetized list of the words occurring in a line of text. This script can be easily modified to create word lists from plain-text files.

```
import string
line = "a way a lone a last a loved a long the riverrun past eve and adam's from swerve of
   shore to bend of bay brings us by a commodius vicus"
linearray = sorted(set(line.split(" ")))
for item in linearray:
  print(item)
```

Here is the output:

```
a
adam's
and
bay
bend
brings
by
commodius
eve
from
last
lone
long
loved
of
past
riverrun
shore
swerve
the
to
us
vicus
way
```

Aside from word lists you create for yourself, there are a wide variety of specialized knowledge domain nomenclatures that are available to the public [19–24]. Linux distributions often bundle a wordlist, under filename "words," that is useful for parsing and natural language processing applications. A copy of the Linux wordlist is available at: http://www.cs.duke.edu/~ola/ap/linuxwords

Curated lists of terms, either generalized or restricted to a specific knowledge domain, are indispensable for a variety of applications (e.g., spell-checkers, natural language processors, machine translation, coding by term, indexing.) Personally, I have spent an inexcusable amount of time creating my own lists, when no equivalent public domain resource was available.

Zipf distribution George Kingsley Zipf (1902–50) was an American linguist who demonstrated that, for most languages, a small number of words account for the majority of occurrences of all the words found in prose. Specifically, he found that the frequency of any word is inversely proportional to its placement in a list of words, ordered by their decreasing frequencies in text. The first word in the frequency list will occur about twice as often as the second word in the list, three times as often as the third word in the list, and so on. Many Big Data collections follow a Zipf distribution (income distribution in a population, energy consumption by country, and so on). Zipf distributions within Big Data cannot be sensibly described by the standard statistical measures that apply to normal distributions. Zipf distributions are instances of Pareto's principle.

Here is a short Python script, zipf.py, that produces a Zipf distribution for a few lines of text.

```
import re, string
word_list=[];freq_list=[];format_list=[];freq={}
my_string = "Peter Piper picked a peck of pickled \
peppers. A peck of pickled peppers Peter Piper picked. \
If Peter Piper picked a peck of pickled peppers, \
Where is the peck of pickled peppers that Peter Piper \
picked?".lower()
word_list = re.findall(r'(\b[a-z]{1,}\b)', my_string)
for item in word_list:
  count = freq.get(item,0)
  freq[item] = count + 1
for key, value in freq.items():
  value = "000000" + str(value)
  value = value[-6:]
  format_list += [value + " " + key]
format_list = reversed(sorted(format_list))
print("\n".join(format_list))
```

Here is the output of the zipf,py script:

```
000004 piper
000004 pickled
000004 picked
000004 peter
000004 peppers
000004 peck
000004 of
000003 a
000001 where
000001 the
000001 that
000001 is
000001 if
```

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13

Using Random Numbers to Knock Your Big Data Analytic Problems Down to Size

OUTLINE

Section 13.1. The Remarkable Utility of (Pseudo)Random Numbers

Chaos reigns within.
Reflect, repent, and reboot.
Order shall return.

Computer haiku by Suzie Wagner

As discussed in Section 11.1, much of the difficulty that of Big Data analysis comes down to combinatorics. As the number of data objects increases, along with the number of attributes that describe each object, it becomes computationally difficult, or impossible, to compute all the pairwise comparisons that would be necessary for analytics tasks (e.g., clustering algorithms, predictive algorithms). Consequently, Big Data analysts are always on the lookout for innovative, non-combinatoric approaches to traditionally combinatoric problems.

There are many different approaches to data analysis that help us to reduce the complexity of data (e.g., principal component analysis) or transform data into a domain that facilitates various types of analytic procedures (e.g., the Fourier transform). In this chapter, we will be discussing an approach that is easy to learn, easy to implement, and which is

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particularly well-suited to enormous data sets. The techniques that we will be describing fall under different names, depending on how they are applied (e.g., resampling, Monte Carlo simulations, bootstrapping), but they all make use of random number generators, and they all involve repeated sampling from a large population of data, or from infinite points in a distribution. Together, these heuristic techniques permit us to perform nearly any type of Big Data analysis we might imagine in a few lines of Python code [1–4]. [Glossary Heuristic technique, Principal component analysis]

In this chapter, we will explore:

- Random numbers (strictly, pseudorandom numbers) [Glossary Pseudorandom number generator]
- General problems of probability
- Statistical tests
- Monte Carlo simulations
- Bayesian models
- Methods for determining whether there are multiple populations represented in a data set
- Determining the minimal sample size required to test a hypothesis [Glossary Power]
- Integration (calculus)

Let us look at how a random number generator works in Python, with a 3-line random.py script.

```
import random
for iterations in range(10):
  print(random.uniform(0,1))
```

Here is the sample output, listing 10 random numbers in the range 0–1:

```
0.594530508550135
0.289645594799927
0.393738321195123
0.648691742041396
0.215592023796071
0.663453594144743
0.427212189295081
0.730280586218356
0.768547788018729
0.906096189758145
```

Had we chosen, we could have rendered an integer output by multiplying each random number by 10 and rounding up or down to the closest integer.

Now, let us perform a few very simple simulations that confirm what we already know, intuitively. Imagine that you have a pair of dice and you would like to know how often you might expect each of the numbers (from one to six) to appear after you've thrown one die [5].

Let us simulate 60,000 throws of a die using the Python script, randtest.py:

```
import random, itertools
one_of_six = 0
for i in itertools.repeat(None, 60000):
  if (int(random.uniform(1,7))) > 5:
    one_of_six = one_of_six + 1
print(str(one_of_six))
```

The script, randtest.pl, begins by setting a loop that repeats 60,000 times, each repeat simulating the cast of a die. With each cast of the die, Python generates a random integer, 1 through 6, simulating the outcome of a throw.

The script yields the total number die casts that would be expected to come up "6." Here is the output of seven consecutive runs of the randtest.py script

```
10020
10072
10048
10158
10000
9873
9899
```

As one might expect, a "6" came up about 1/6th of the time, or about 10,000 times in the 60,000 simulated roles. We could have chosen any of the other five outcomes of a die role (i.e., 1, 2, 3, 4, or 5), and the outcomes would have been about the same.

Let us use a random number generator to calculate the value of pi, without measuring anything, and without resorting to summing an infinite series of numbers. Here is a simple python script, pi.py, that does the job.

```
import random, itertools
from math import sqrt
totr = 0; totsq = 0
for i in range(10000000):
  x= random.uniform(0,1)
  y= random.uniform(0,1)
  r= sqrt((x*x) + (y*y))
  if r < 1:
    totr = totr + 1
  totsq = totsq + 1
print(float(totr)*4.0/float(totsq))
```

The script returns a fairly close estimate of pi.

```
output: 3.1414256
```

The value of pi is the ratio of a circle of unit radius (pi * r^2) divided by the area of a square of unit radius (r^2). When we randomly select points within a unit distance in the x or the y dimension, we are filling up a unit square. When we count the number of randomly selected points within a unit radius of the origin, and compare this number with the number of points in the unit square, we are actually calculating a number that comes fairly close to pi. In this simulation, we are looking at one quadrant, but the results are equivalent, and we come up with a number that is a good approximation of pi (i.e., 3.1414256, in this simulation).

With a few extra lines of code, we can send the output to a to a data file, named pi.dat, that will helps us visualize how the script works. The data output (held in the pi.dat file) contains the *x*, *y* data points, generated by the random number generator, meeting the "if" statement's condition that the hypotenuse of the *x*, *y* coordinates must be less than one (i.e., less than a circle of radius 1). We can plot the output of the script with a few lines of Gnuplot code:

```
gnuplot > set size square
gnuplot > unset key
gnuplot > plot 'c:\ftp\pi.dat'
```

The resulting graph is a quarter-circle within a square (Fig. 13.1).

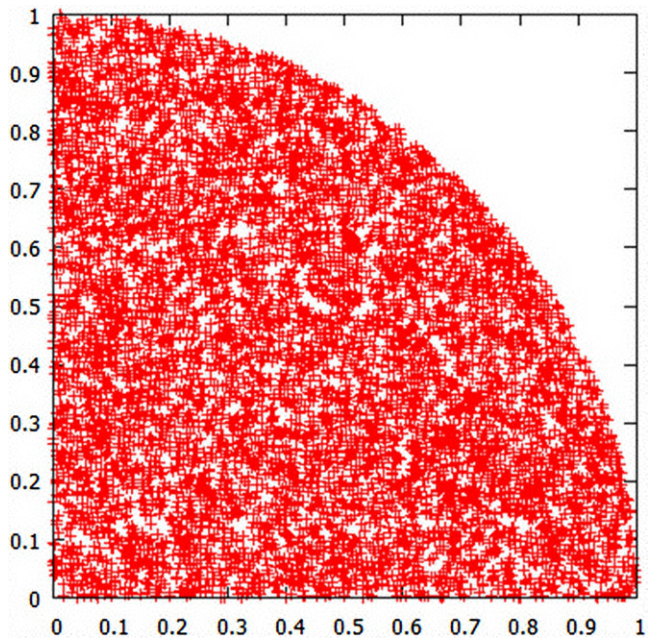

FIG. 13.1 The data points produced by 10,000 random assignments of *x* and *y* coordinates in a range of 0–1. Randomly assigned data points whose hypotenuse exceeds "1" are excluded.

Let us see how we can simulate calculus operations, using a random number generator. We will integrate the expression f(x) = x^3 − 1. First, let us visualize the relationship between f(x) and x, by plotting the expression. We can use a very simple Python script, plot_funct.py, that can be trivially generalized to plot almost any expression we choose, over any interval.

```
import math, random, itertools
import numpy as np
import matplotlib.pyplot as plt
x=0.000

def f(x):
  return (x*x*x -1)

x = np.arange(0.7, 1.5, 0.01)
plt.plot(x, f(x))
plt.show()
```

The output is a graph, produced by Python's matplotlib module (Fig. 13.2).

Let us use a random number generator, in the Python script integrator.py, to perform the integration and produce an approximate evaluation of the integral (i.e., the area under the curve of the equation).

```
import math, random, itertools
def f(x):
  return (x*x*x -1)
```

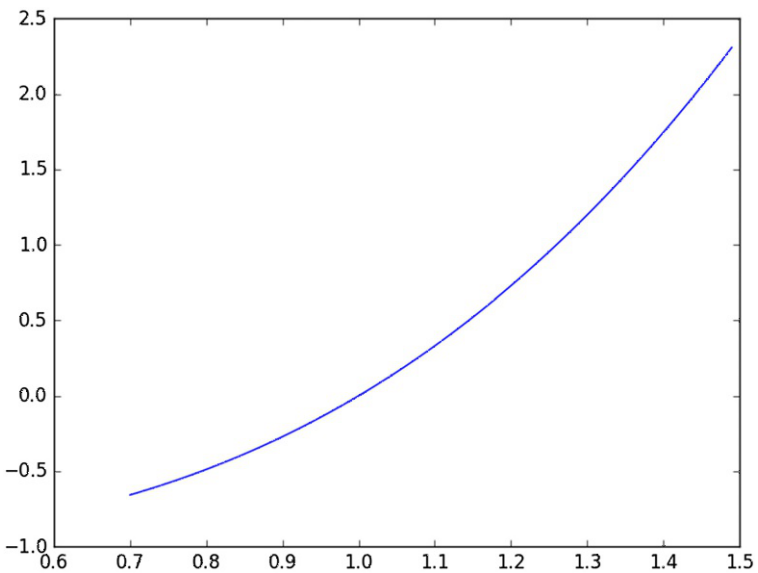

FIG. 13.2 The plot of the function x^3 − 1, in the interval 0.7–1.5.

```
range = 2     #let's evaluate the integral from x=1 to x=3
running_total = 0
for i in itertools.repeat(None, 1000000):
  x = float(random.uniform(1,3))
  running_total = running_total + f(x)
integral = (running_total / 1000000) * range
print(str(integral))
```

Here is the output:

```
18.001426696174935
```

The output comes very close to the exact integral, 18, calculated for the interval between 1 and 3. How did our short Python script calculate the integral? The integral of a function is equivalent to the area under of the curve of the function, in the chosen interval. The area under the cover is equal to the size of the interval (i.e., the x coordinate range) multiplied by the average value of the function in the interval. By calculating a million values of the function, from randomly chosen values of x in the selected interval, and taking the average of all of those values, we get the average value of the function. When we multiply this by the interval, we get the area, which is equal to the value of the integral.

Let us apply our newfound ability to perform calculus with a random number generator and calculate one of the most famous integrals in mathematics.

The integral of $1/x$ equals the natural logarithm of x (Fig. 13.3). This tells us that the integral of $(1/x)\mathrm{d}x$ evaluated in the integral from 5 to 105 will be equal to ln(105) minus ln(5). Let us evaluate the integral in the range from $x = 5$ to $x = 105$, using our random number generator, alongside the calculation performed with Python's numpy (math) module, to see how close our approximation came. We will use the Python script, natural.py

```
import math, random, itertools
import numpy as np
def f(x):
  return (1 / x)
range = 100
running_total = 0
for i in itertools.repeat(None, 1000000):
  x = float(random.uniform(5,105))
  running_total = float(running_total + f(x))
```

$$\ln(x) = \int \frac{1}{x} dx$$

FIG. 13.3 The integral of the inverse of *x* is equal to the natural logarithm of *x*.

```
integral = (running_total / 1000000) * range
print("The estimate produced with a random number generator is: " + str
   (integral))
print("The value produced with Python's numpy function for ln(x) is: " +
   str(np.log(105) - np.log(5)))
```

Here is the output of the natural.py script.

```
The estimate produced with a random number generator
   is:   3.04209561069317
The value produced with Python's numpy function for ln(x)
   is: 3.04452243772
```

Not bad. Of course, python programmers know that they do not need to use a random number generator to solve calculus problems in python. The numpy and sympy modules seem to do the job nicely. Here is a short example wherein the a classic integral equation is demonstrated:

```
>>> import sympy as sy
>>> import numpy as np
>>> x = sy.Symbol('x')
>>> sy.integrate(1/x,x)
log(x)
```

Or, as any introductory calculus book would demonstrate: $\ln x =$ integral $1/x\ \mathrm{d}x$

Why would anyone bother to integrate using a random number generator when they can produce an exact solution using elementary calculus? It happens that integration by repeated sampling using a random number generator comes in handy when dealing with multi-dimensional functions, particularly when the number of dimensions exceeds 8 (i.e., when there are 8 or more quantitative attributes describing each variable). In Big Data, where the variables have many attributes, standard computational approaches may fail. In these cases the methods described in this section may provide the most exact and the most practical solutions to a large set of Big Data computations. [Glossary Curse of dimensionality]

Section 13.2. Repeated Sampling

Every problem contains within itself the seeds of its own solution.

Stanley Arnold

In Big Data analytics, we can use a random number generator to solve problems in the areas of clustering, correlations, sample size determination, differential equations, integral equations, digital signals processing, and virtually every subdiscipline of physics [3,1,6,5]. Purists would suggest that we should be using formal, exact, and robust

mathematical techniques for all these calculations. Maybe so, but there is one general set of problems for which the random number generator is the ideal tool; requiring no special assumptions about the data being explored, and producing answers that are as reliable as anything that can be produced with computationally intensive exact techniques. This set of problems typically consists of hypothesis testing on sets of data of uncertain distribution (i.e., not Gaussian) that are not strictly amenable to classic statistical analysis. The methods by which these problems are solved are the closely related techniques of resampling (from a population or data set) and permutating, both of which employ random number generators. [Glossary Resampling statistics, Permutation test, Resampling versus Repeated Sampling, Modified random sampling]

Resampling methods are not new. The resampling methods that are commonly used today by data analysts have been around since the early 1980s [3,1,2]. The underlying algorithms for these methods are so very simple that they have certainly been in use, using simple casts of dice, for thousands of years.

The early twentieth century saw the rise of mathematically rigorous statistical methods, that enabled scientists to test hypotheses and draw conclusions from small or large collections of data. These tests, which required nothing more than pencil and paper to perform, dominated the field of analysis and are not likely to be replaced anytime soon. Nonetheless, the advent of fast computers provides us with alternative methods of analysis that may lack the rigor of advanced statistics, but have the advantage of being easily comprehensible. Calculations that require millions of operations can be done essentially instantly, and can be programmed with ease. Never before, in the history of the world, has it been possible to design and perform resampling exercises, requiring millions or billions of iterative operations, in a matter of seconds, on computers that are affordable to a vast number of individuals in developed or developing countries. The current literature abounds with resources for scientists with rudimentary programming skills, who might wish to employ resampling techniques [7,8].

For starters, we need to learn a new technique: shuffling. Python's numpy module provides a simple method for shuffling the contents of a container (such as the data objects listed in an array) to produce a random set of objects. Here is Python's shuffle_100.py script, that produces a shuffled list of numbers ranging from 0 to 99:

```
import numpy as np
sample = np.arange(100)
gather = []
for i in sample:
  np.random.shuffle(sample)
print(sample)
```

Here is the output of the shuffle_100.py script:

```
[27 60 21 99 17 79 49 62 81  2 88 90 45 61 66 80 50 31 59 24 53 29 64 33 30
 41 13 23  0 67 78 70  1 35 18 86 25 93  6 98 97 84  9 12 56 48 74 96  4 32
```

```
44 11 19 38 26 52 87 77 39 91 92 76 65 75 63 57  8 94 51 69 71  7 73 34 20
40 68 22 82 15 37 72 28 47 95 54 55 58  5  3 89 46 85 16 42 36 43 10 83 14]
```

We will be using the shuffle method to help us answer a question that arises often, whenever we examine sets of data: "Does my data represent samples from one homogeneous population of data objects, or does my data represent samples from different classes of data objects that have been blended together in one collection?" The blending of distinctive classes of data into one data set is one of the most formidable biases in experimental design, and has resulted in the failures of many clinical trials, the misclassification of diseases, and the misinterpretation of the significance of outliers. How often do we fail to understand our data, simply because we cannot see the different populations lurking within? In Section 12.6, we discussed the importance of finding multimodal peaks in data distributions. Our discussion of multimodal peaks and separable subpopulations begged the question as to how we can distinguish peaks that represent subpopulations from peaks that represent random perturbations in our data. [Glossary Blended class]

Let us begin by using a random number generator to make two separate populations of data objects. The first population of data objects will have values that range uniformly between 1 and 80. The second population of data objects will have values that range uniformly between 20 and 100. These two populations will overlap (between 20 and 80), but they are different populations, with different population means, and different sets of properties that must account for their differences in values. We'll call the population ranging from 1 to 80 our low_array and the population ranging from 20 to 100 as high_array.

Here is a Python script, low_high.py, that generates the two sets of data, representing 50 randomly selected objects from each population:

```
import numpy as np
from random import randint
low_array = []; high_array = []
for i in range(50):
  low_array.append(randint(1,80))
print("Here's the low-skewed data set " + str(low_array))
for i in range(50):
  high_array.append(randint(21,100))
print("\nHere's the high-skewed data set " + str(high_array))
av_diff = (sum(high_array)/len(high_array)) - (sum(low_array)/len
   (low_array))
print("\nThe difference in average value of the two arrays is:
   " + str(av_diff))
```

Here is the output of the low_high.py script:

```
Here is the low-skewed data set [31, 8, 60, 4, 64, 35, 49, 80, 6, 9, 14, 15,
50, 45, 61, 77, 58, 24, 54, 45, 44, 6, 78, 59, 44, 61, 56, 8, 30, 34, 72, 33,
14, 13, 45, 10, 49, 65, 4, 51, 25, 6, 37, 63, 19, 74, 78, 55, 34, 22]
```

```
Here is the high-skewed data set [36, 87, 54, 98, 33, 49, 37, 35, 100, 48,
71, 86, 76, 93, 98, 99, 92, 68, 29, 34, 64, 30, 99, 76, 71, 32, 77, 32, 73,
54, 34, 44, 37, 98, 42, 81, 84, 56, 55, 85, 55, 22, 98, 72, 89, 24, 43, 76,
87, 61]

The difference in average value of the two arrays is: 23.919999999999995
```

The low-skewed data set consists of 50 random integers selected from the interval 1–80. The high-skewed data set consists of 50 random numbers selected from the interval between 20 and 100. Notice that not all possible outcomes in these two intervals are represented (i.e., there is no number 2 in the low-skewed data set and there is no number 25 in the high-skewed data set). If we were to repeat the low_high.py script, we would generate two different sets of numbers. Also, notice that the two populations have different average values. The difference between the average value of the low-skewed data population and the high-skewed data population is 23.9, in this particular simulation.

Now, we are just about ready to determine whether the two populations are statistically different. Let us repeat the simulation. This time, we will combine the two sets of data into one array that we will call "total_array," containing 100 data elements. Then we will shuffle all of the values in total_array and we will create two new arrays: a left array consisting of the first 50 values in the shuffled total_array and a right array consisting of the last 50 values in the total_array. Then we will find the difference between the average of the 50 values of the left array of the right array. We will repeat this 100 times, printing out the lowest five differences in averages and the highest five differences in averages. Then we will stop and contemplate what we have done.

Here is the Python script, pop_diff.py

```
import numpy as np
from random import randint
low_array = []
high_array = []
gather = []
for i in range(50):
  low_array.append(randint(1,80))
for i in range(50):
  high_array.append(randint(21,100))
av_diff = (sum(high_array)/len(high_array)) - (sum(low_array)/len
   (low_array))
print("The difference in the average value of the high and low arrays is:
   " + str(av_diff))
sample = low_array + high_array
for i in sample:
  np.random.shuffle(sample)
  right = sample[50:]
```

```
    left = sample[:50]
    gather.append(abs((sum(left)/len(left)) - (sum(right)/len
     (right))))
sorted_gather = sorted(gather)
print("The 5 largest differences of averages of the shuffled arrays
    are:")
print(str(sorted_gather[95:]))

output:
The difference in the average value of the high and low arrays is:
    19.580000000000005
The 5 largest differences of averages of the shuffled arrays are:
    [8.780000000000001, 8.899999999999999, 9.46, 9.82,
     9.899999999999999]
```

Believe it or not, we just demonstrated that the two arrays that we began with (i.e., the array with data values randomly distributed between 0 and 80; and the array with data values randomly distributed between 20 and 100) represent two different populations of data (i.e., two separable classes of data objects). Here is what we did and how we reached our conclusion.

1. We recomputed two new arrays, with 50 items each, with data values randomly distributed between 0 and 80; and the array with data values randomly distributed between 20 and 100.
2. We calculated the difference of the average size of an item in the first array, compared with the average size of an item in the second array. This came out to 19.58 in this simulation.
3. We combined the two arrays into a new array of 100 items, and we shuffled these items 100 times, each time splitting the shuffle in half to produce two new arrays of 50 items each., We calculated the difference in the average value of the two arrays (produced by the shuffle).
4. We found the five sets of shuffled arrays (the two arrays produced by a shuffle of the combined array) that had the largest differences in their values (corresponding to the upper 5% of the combined and shuffled populations) and we printed these numbers.

The upper 5 percentile differences among the shuffled arrays (i.e., 8.78, 8.89, 9.46, 9.82, 9.89) came nowhere close to the difference of 19.58 we calculated for the original two sets of data. This tells us that whenever we shuffle the combined array, we never encounter differences anywhere near as great as what we observed in the original arrays. Hence, the original two arrays cannot be explained by random selection from one population (obtained when we combined the two original arrays). The two original arrays must represent two different populations of data objects.

A note of caution regarding scalability. Shuffling is not a particularly scalable function [9]. Shuffling a hundred items is a lot easier than shuffling a million items. Hence, when

writing short programs that test whether two data arrays are statistically separable, it is best to impose a limit to the size of the arrays that you create when you sample from the combined array. If you keep the shuffling size small, you can compensate by repeating the shuffle nearly as often as you like.

– **Sample Size and Power Estimates**

In the prior exercise, we generated two populations, of 50 samples each, and we determined that the two populations were statistically separable from one another. Would we have been able to draw the same conclusion if we had performed the exercise using 25 samples in each population in each population? How about 10 samples? We would expect that as the population sizes of the two populations shrinks, the likelihood that we could reliably distinguish one population from another will fall. How do we determine the minimal population size necessary to perform our experiment?

The power of a trial is the likelihood of detecting a difference in two populations, if the difference actually exists. The power is related to the sample size. At a sufficiently large sample size, you can be virtually certain that the difference will be found, if the difference exists. Resampling permits the experimenter to conduct repeated trials, with different sample sizes, and under conditions that simulate the population differences that are expected. For example, an experimenter might expect that a certain drug produces a 15% difference in the measured outcomes in the treated population compared with the control population. By setting the conditions of the trials, and by performing repeated trials with increasing sizes of simulated populations, the data scientist can determine the minimum sampling size that consistently (e.g., in greater than 95% of the trials), demonstrates that the treated population and the control population are separable. Hence, using a random number generator and a few short scripts, the data scientist can determine the sampling size required to yield a power that is acceptable for a "real" experiment. [Glossary Sample size, Sampling theorem]

Section 13.3. Monte Carlo Simulations

One of the marks of a good model - it is sometimes smarter than you are.
Paul Krugman, Nobel prize-winning economist

Random number generators are well suited to Monte Carlo simulations, a technique described in 1946 by John von Neumann, Stan Ulam, and Nick Metropolis [10]. For these simulations, the computer generates random numbers and uses the resultant values to represent outcomes for repeated trials of a probabilistic event. Monte Carlo simulations can easily simulate various processes (e.g., Markov models and Poisson processes) and can be used to solve a wide range of problems [11,12].

For example, consider how biologists may want to model the growth of clonal colonies of cells. In the simplest case, wherein cell growth is continuous, a single cell divides, producing two cells. Each of the daughter cells divides, producing a total of four cells. The size

of the colony increases as powers of 2. A single liver cancer cell happens to have a volume of about 30,000 cubic microns [13]. If the cell cycle time is one day, then the volume of a liver cell colony, grown for 45 days, and starting at day 1 with a single cell, would be 1 m^3. In 55 days, the volume would exceed 1000 m^3. If an unregulated tumor composed of malignant liver cells were to grow for the normal lifetime of a human, it would come to occupy much of the measured universe [14]. Obviously, unregulated cellular growth is unsustainable. In tumors, as in all systems that model the growth of cells and cellular organisms, the rate of cell growth is countered by the rate of cell death.

With the help of a random number generator, we can model the growth of colonies of cells by assigning each cell in the colony a probability of dying. If we say that the likelihood that a cell will die is 50%, then we are saying that its chance of dividing (i.e., producing two cells) is the same as its chance of dying (i.e., producing zero cells and thus eliminating itself from the population). We can create a Monte Carlo simulation of cell growth by starting with some arbitrary number of cells (let us say three), and assigning each cell an arbitrary chance of dying (let us say 49%). We can assign each imaginary cell to an array, and we can iterate through the array, cell by cell. As we iterate over each cell, we can use a random number generator to produce a number between 0 and 1. If the random number is less than 0.49, we say that the cell must die, dropping out of the array. If a cell is randomly assigned a number that is greater than 0.49, then we say that the cell can reproduce, to produce two cells that will take their place in the array. Every iteration over the cells in the array produces a new array, composed of the lucky winners and their offspring, from the prior array. In theory, we can repeat this process forever. More practically, we can repeat this process until the size of the colony reduces to zero, or until the colony becomes so large that additional iterations become tedious (even for a computer).

Here is the Python script, clone.py, that creates a Monte Carlo simulation for the growth of a colony, beginning with three cells, with a likelihood of cell death for all cells, during any generation, of 0.41. The script exits if the clone size dwindles to zero (i.e., dies out) or reaches a size exceeding 800 (presumably on the way to growing without limit).

```
import numpy.random as npr
import sys
death_chance = 0.41; cell_array = [1, 1, 1]; cell_array_incremented =
[1,1,1]
while(len(cell_array) > 0):
  for cell in cell_array:
       randnum = npr.randint(1,101)
       if randnum > 100 * death_chance:
         cell_array_incremented.append(1)
       else:
        cell_array_incremented.remove(1)
  if len(cell_array_incremented) < 1:
    sys.exit()
```

```
    if len(cell_array_incremented) > 800:
      sys.exit()
    cell_array = cell_array_incremented
    print(len(cell_array_incremented), end = ", ")
```

For each cell in the array, if the random number generated for the cell exceeds the likelihood of cell death, then the colony array is incremented by one. Otherwise, the colony array is decremented by 1. This simple step is repeated for every cell in the colony array, and is repeated for every clonal generation.

Here is a sample output when death_chance = 0.49

```
multiple outputs:

First trial:
2, 1, 1, 1,

Second trial:
4, 3, 3, 1,

Third trial:
6, 12, 8, 15, 16, 21, 30, 37, 47, 61, 64, 71, 91, 111, 141, 178, 216, 254,
310, 417, 497, 597, 712,

Fourth trial:
2, 4, 4, 4, 3, 3, 4, 4, 8, 5, 6, 4, 4, 6, 4, 10, 19, 17, 15, 32, 37, 53, 83, 96,
128, 167, 188, 224, 273, 324, 368, 416, 520, 642,

Fifth trial
4, 3, 7, 9, 19, 19, 26, 36, 45, 71, 88, 111, 119, 157, 214, 254, 319, 390,
480, 568, 675,

Sixth trial:
2, 1, 2, 2, 1,

Seventh trial:
2, 1,

Eighth trial:
2, 1, 1, 1, 4, 8, 10, 8, 10, 9, 10, 15, 11, 12, 16, 15, 21, 21, 35, 44, 43, 41,
47, 68, 62, 69, 90, 97, 121, 181, 229, 271, 336, 439, 501, 617, 786,
```

In each case the clone increases or decreases with each cell cycle until the clone reaches extinction or exceeds our cut off limit. These simulations indicate that clonal growth is precarious, under conditions when the cell death probability is approximately 50%. In these two simulations the early clones eventually die out. Had we repeated the simulation hundreds of times, we would have seen that most clonal simulations end in the extinction of the clone; while a few rare simulations yield a large, continuously

expanding population, with virtually no chance of reaching extinction. In a series of papers by Dr. William Moore and myself, we developed Monte Carlo simulations of tumor cell growth. Those simulations suggested that very small changes in a tumor cell's death probability (per replication generation) profoundly affected the tumor's growth rate [11,12,15]. This simulation suggested that chemotherapeutic agents that can incrementally increase the death rate of tumor cells may have enormous treatment benefit. Furthermore, simulations showed that if you simulate the growth of a cancer from a single abnormal cancer cell, most simulations result in the spontaneous extinction of the tumor, an unexpected finding that helps us to understand the observed high spontaneous regression rate of nascent growths that precede the development of clinically malignant cancers [16,17].

This example demonstrates how simple Monte Carlo simulations, written in little more than a dozen lines of Python code, can simulate outcomes that would be difficult to compute using any other means.

Section 13.4. Case Study: Proving the Central Limit Theorem

The solution to a problem changes the nature of the problem.

John Peers ("Peer's Law" 1,001 Logical Laws)

The Central Limit Theorem is a key concept in probability theory and statistics. It asserts that when independent random variables are added, their sum tends toward a normal distribution (i.e., a "bell curve"). The importance of this theorem is that statistical methods designed for normal distributions will also apply in some situations wherein variables are chosen randomly from non-normal distributions.

For many years, the Central Limit Theorem was a personal stumbling block for me; I simply could not understand why it was true. It seemed to me that if you randomly select numbers in an interval, you would always get a random number, and if you summed and averaged two random numbers, you'll get another random number that is equally likely to by anywhere within the interval (i.e., not distributed along a bell curve with a central peak). According to the Central Limit Theorem, the sum of repeated random samplings will produce lots of numbers in the center of the interval, and very few or no numbers at the extremes.

As previously mentioned, repeated sampling allows us to draw inferences about a population, without examining every member of the population; a handy trick for Big Data analyses. In addition, repeated sampling allows us to test hypotheses that we are too dumb to understand (speaking for myself). In the case of the Central Limit Theorem, we can simulate a proof of the Central Limit Theorem by randomly selecting numbers in an interval (between 0 and 1) many times (say 10,000), and averaging their sum. We can repeat each of these trials 10,000 times, and then plot where the 10,000 values lie. If we get a Bell curve, then the Central Limit Theorem must be correct. Here is the Python script, central.py, that computes the results of the simulation, and plots the points as a graph.

```
import random, itertools
from matplotlib import numpy
import matplotlib.pyplot as plt
out_file = open('central.dat',"w")
randhash = {}
for i in itertools.repeat(None, 10000):
  product = 0
  for n in itertools.repeat(None, 10000):
    product = product + random.uniform(0,1)
  product = int(product)
  if product in randhash:
    randhash[product] = randhash[product] + 1
  else:
    randhash[product] = 1
lists = sorted(randhash.items())
x, y = zip(*lists)
plt.plot(x, y)
plt.show()
```

Here is the resultant graph (Fig. 13.4).

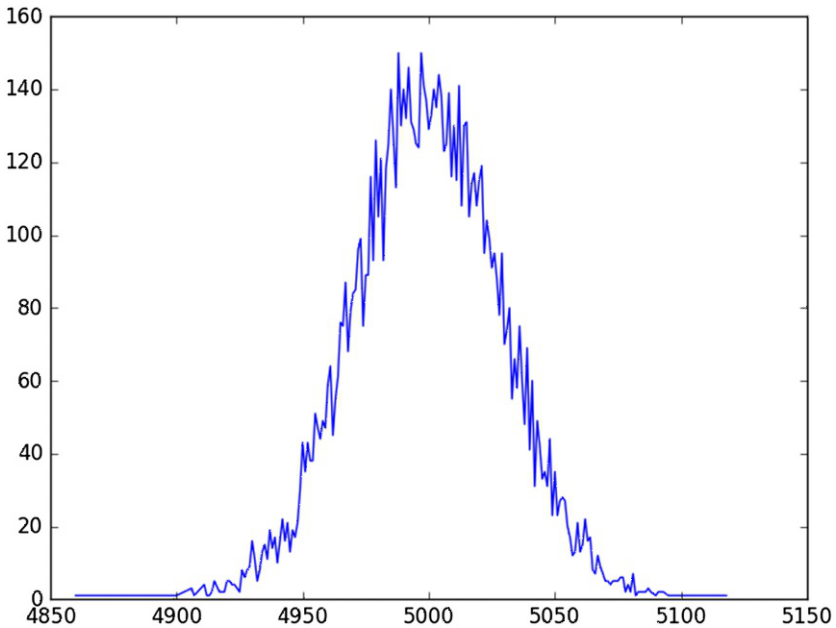

FIG. 13.4 The results of the simulation of the Central Limit Theorem (as executed in the Python script central.py), is a bell-shaped curve.

Without bludgeoning the point, after performing the simulation, and looking at the results, the Central Limit Theorem suddenly makes perfect sense to me. The reader can draw her own conclusion.

Section 13.5. Case Study: Frequency of Unlikely String of Occurrences

Luck is believing you're lucky.

Tennessee Williams

Imagine this scenario. A waitress drops a serving tray three times while serving each of three consecutive customers on the same day. Her boss tells her that she is incompetent, and indicates that he should fire her on the spot. The waitress objects, saying that the other staff drops trays all the time. Why should she be singled out for punishment simply because she had the bad luck of dropping three trays in a row. The manager and the waitress review the restaurant's records and find that there is a 2% drop rate, overall (i.e., a tray is dropped 2% of the time when serving customers), and that the waitress who dropped the three trays in one afternoon had had a low drop rate prior to this day's performance. She cannot explain why three trays dropped consecutively, but she supposes that if anyone works the job long enough, the day will come when they drop three consecutive trays.

We can resolve this issue, very easily, with the Python script runs.py, that simulates a million customer wait services and determines how often we are likely to see a string of three consecutive dropped trays.

```
import random, itertools
errorno = 0;
for i in itertools.repeat(None, 1000000): #let's do 1 million table
   services
   x = int(random.uniform(0,100))     #x any integer from 0 to 99
   if (x < 2):              #x simulates a 2% error rate
      errorno = errorno + 1
   else:
      errorno = 0
   if (errorno == 3):
      print("Uh oh. 3 consecutive errors")
      errorno = 0
```

Here is the output from one execution of runs.py

```
Uh oh. 3 consecutive errors
Uh oh. 3 consecutive errors
Uh oh. 3 consecutive errors
Uh oh. 3 consecutive errors
```

```
Uh oh. 3 consecutive errors
Uh oh. 3 consecutive errors
Uh oh. 3 consecutive errors
Uh oh. 3 consecutive errors
```

The 11-line Python script simulates 1 million table services. Each service is assigned a random number between 0 and 100. If the randomly assigned number is less than 2 the simulation counts as a dropped tray (because the drop rate is 2%). Now we watch to see the outcome of the next two served trays. If three consecutive trays are dropped, we print out "Uh oh. 3 consecutive errors") and we resume our simulations.

In this trial of 1 million table services, using a 2% error rate, the modeled waitress had eight runs of three consecutive tray drops. Since a million table services might possibly represent the total number of customers served by a waitress in her entire career, one can say that she should be allowed at least eight episodes of three consecutive tray drops, in her lifetime.

Section 13.6. Case Study: The Infamous Birthday Problem

I want to thank you for making this day necessary.

Yogi Berra

Let us use our random number generator to tackle the infamous birthday problem. It may seem unintuitive, but if you have a room holding 23 people, the odds are about even that two or more of the group will share the same birth date. The solution of the birthday problem has become a popular lesson in introductory probability courses. The answer involves an onerous calculation, involving lots of multiplied values, divided by an enormous exponential (Fig. 13.5).

If we wanted to know the probability of finding two or more individuals with the same birthday, in a group of 30 individuals, we could substitute 365 for n and 30 for k, and we would learn that the odds are about 70%. Or, we could design a simple little program, using a random number generator, to create an intuitively obvious simulation of the problem.

Here is the Python script, birthday.py, that conducts 10,000 random simulations of the birthday problem:

```
import random, itertools
success = 0
for i in itertools.repeat(None, 10000):
```

$$\frac{n(n-1)(n-2)(n-k+1)}{n^k}$$

FIG. 13.5 Calculating the general solution of the birthday problem. "n" is the number of days in a year. "k" is the number of people.

```
    date_hash = {}
    for j in itertools.repeat(None, 30):
      date = int(random.uniform(1,365))
      if date in date_hash:
        date_hash[date] = date_hash[date] + 1
      else:
        date_hash[date] = 1
      if (date_hash[date] == 2):
        success = success + 1
        break
print(str(success / 10000))
```

Here is the output from six consecutive runs of birthday.py, with 10,000 trials in each run:

```
0.7076
0.7083
0.7067
0.7101
0.7087
0.7102
```

The calculated probability is about 70%. The birthday.py script created variables, assigning each variable a birth date selected at random from a range of 1–365 (the number of days in the year). The script then checked among the 30 assigned variables, to see if any of them shared the same birthday (i.e., the same randomly assigned number). If so, then the set of 30 assigned variables was deemed a success. The script repeated this exercise 10,000 times, incrementing, by one, the number of successes whenever a match was found in the 30 assignments. At the end of it all, the total number of successes (i.e., instances where there is a birthday match in the group of 30) divided by the total number of simulations (10,000 in this case) provides the likelihood that any given simulation will find a birthday match. The answer, which happens to be about 70%, is achieved without the use of any knowledge of probability theory.

Section 13.7. Case Study (Advanced): The Monty Hall Problem

> *Of course I believe in luck. How otherwise to explain the success of some people you detest?*
>
> *Jean Cocteau*

This is the legendary Monty Hall problem, named after the host of a televised quiz show, where contestants faced a similar problem: "The player faces three closed containers, one containing a prize and two empty. After the player chooses, s/he is shown that one of the other two containers is empty. The player is now given the option of switching from

her/his original choice to the other closed container. Should s/he do so? Answer: Switching will double the chances of winning."

Marilyn vos Savant, touted by some as the world's smartest person, correctly solved the Monty Hall problem in her newspaper column. When she published her solution, she received thousands of responses, many from mathematicians, disputing her answer.

Basically, this is one of those rare problems that seems to defy common sense. Personally, whenever I have approached this problem using an analytic approach based on probability theory, I come up with the wrong answer.

In desperation, I decided to forget everything I thought I knew about probability, in favor of performing the Monty Hall game, with a 10-line Python script, montyhall.py, that uses a random number generator to simulate outcomes.

```
import random, itertools
winner = 0; box_array = [1,2,3]
for i in itertools.repeat(None, 10000):
  full_box=int(random.uniform(1,4))  #randomly picks 1,2,or 3 as prize box
   guess_box=int(random.uniform(1,4))#represents your guess, for prize box
  del box_array[full_box - 1]          #prize box deletes itself from array
  if guess_box in box_array:           #if your first guess is in the remaining array
                                       #(which excludes prize and includes the second
                                       #empty box), then you must have won
                                       #when you chose to switch your choice
    winner = winner + 1
  box_array = [1,2,3]
print(winner)
```

Here are the outputs of nine consecutive runs of montyhall.py script:

```
6710
6596
6657
6698
6653
6684
6661
6607
6674
```

The script simulates the Monty Hall strategy where the player takes the option of switching her selection. By taking the switch option, she wins nearly two thirds of the time (about 6600 wins in 10,000 simulations), twice as often as when the switch option is declined. The beauty of the resampling approach is that the programmer does not need to understand why it works. The programmer only needs to know how to use a random number generator to create an accurate simulation of the Monte Hall problem that can be repeated thousands and thousands of times.

How does the Monty Hall problem relate to Big Data? Preliminary outcomes of experimental trials are often so dramatic that the trialists choose to re-design their protocol mid-trial. For example, a drug or drug combination may have demonstrated sufficient effectiveness to justify moving control patients into the treated group. Or adverse reactions may necessitate switching patients off a certain trial arm. In either case, the decision to switch protocols based on mid-trial observations is a Monty Hall scenario.

Section 13.8. Case Study (Advanced): A Bayesian Analysis

It's hard to detect good luck - it looks so much like something you've earned.
Frank A. Clark

The Bayes theorem relates probabilities of events that are conditional upon one another (Fig. 13.6). Specifically, the probability of A occurring given that B has occurred multiplied by the probability that B occurs is equal to the probability of B occurring, given that A has occurred multiplied by the probability that A occurs. Despite all the hype surrounding Bayes theorem, it basically indicates the obvious: that if A and B are conditional, then A won't occur unless B occurs and B won't occur unless A occurs.

Bayesian inferences involve computing conditional probabilities, based on having information about the likelihood of underlying events. For example, the probability of rain would be increased if it were known that the sky is cloudy. The fundamentals of Bayesian analysis are deceptively simple. In practice, Bayesian analysis can easily evade the grasp of intelligent data scientists. By simulating repeated trials, using a random number generator, some of the toughest Bayesian inferences can be computed in a manner that is easily understood, without resorting to any statistical methods.

Here is a problem that was previously posed by William Feller, and adapted for resampling statistics by Julian L. Simon [1]. Imagine a world wherein there are two classes of drivers. One class, the good drivers, comprise 80% of the population, and the likelihood that a member of this class will crash his car is 0.06 per year. The other class, the bad drivers, comprise 20% of the population, and the likelihood that a member of this class will crash his car is 0.6 per year. An insurance company charges clients $100 times the likelihood of having an accident, as expressed as a percentage. Hence, a member of the good driver class would pay $600 per year; a member of the bad driver class would pay $6000 per year. The question is: If nothing is known about a driver other than that he had an accident in the prior year, then what should he be charged for his annual car insurance payment?

The Python script, bayes.py, calculates the insurance cost, based on 10,000 trial simulations:

$$P(A \mid B) * P(B) = P(B \mid A) * P(A)$$

FIG. 13.6 Bayes' theorem relating probabilities of event that are conditional upon one another.

```
import random, itertools
accidents_next_year = 0
no_accidents_next_year = 0
for i in itertools.repeat(None, 10000):
  group_likelihood = random.uniform(0,1)
  if (group_likelihood<0.2):            #puts trial in poor-judgment group
    bad_likelihood=random.uniform(0,1) #roll the dice to see if accident occurs
    if (bad_likelihood<0.6):            #an accident occurred, simulating an initial
                                        #condition of poor-judgment with accident
      next_bad_likelihood = random.uniform(0,1)
      if (next_bad_likelihood < 0.6):
        accidents_next_year = accidents_next_year + 1
      else:
        no_accidents_next_year = no_accidents_next_year + 1
  else: #othwerwise we bump the trial into the good-judgment group
    bad_likelihood=random.uniform(0,1) #simulates an accident accident
    if (bad_likelihood < 0.06):          #an accident with good-judgment
      next_bad_likelihood = random.uniform(0,1)
      if (next_bad_likelihood < 0.06):
         accidents_next_year = accidents_next_year + 1
      else:
         no_accidents_next_year = no_accidents_next_year + 1
cost=int(((accidents_next_year)/(accidents_next_year+no_accidents_next_year)
*100*100))

print("Insurance cost is $" + str(cost))

outputs of 7 executions of bayes.py script:
Insurance cost is 4352
Insurance cost is 4487
Insurance cost is 4406
Insurance cost is 4552
Insurance cost is 4454
Insurance cost is 4583
Insurance cost is 4471
```

In all eight executions of the script, each having 10,000 trials, we find that the insurance cost, based on initial conditions, should be about $4500.

What does our bayes.py do? First, it creates a loop for 10,000 trial simulations. Within each simulation, it begins by choosing a random number between 0 and 1. If the random number is less than 0.2, then this simulates an encounter with a member of the bad-driver class (i.e., the bottom 20% of the population). In this case the random number generator produces another number between 0 and 1. If this number is less than 0.6 (the annual likelihood of a bad driver having an accident), then this would be simulate a member of the bad-driver class who had an accident and who is applying for car insurance. Now, we run

the random number generator one more time, to simulate whether the bad driver will have an accident during the insurance year. If the generated random number is less than 0.6, we will consider this a simulation of a bad-driver, who had an accident prior to asking for applying for car insurance, having an accident in the subsequent year. We will do the same for the simulations that apply to the good drivers (i.e., the trials for which our group likelihood random number was greater than 0.2). After the simulations have looped 10,000 times, all that remains is to use our tallies to calculate the likelihood of an accident, which in turn gives us the insurance cost. In this example, as in all our other examples, we really did not need to know any statistics. We only needed to know the conditions of the problem, and how to simulate those conditions as Monte Carlo trials.

Glossary

Blended class Also known as class noise. Blended class refers to inaccuracies (e.g., misleading results) introduced in the analysis of data due to errors in class assignments (e.g., inaccurate diagnosis). If you are testing the effectiveness of an antibiotic on a class of people with bacterial pneumonia, the accuracy of your results will be forfeit when your study population includes subjects with viral pneumonia, or smoking-related lung damage. Errors induced by blending classes are often overlooked by data analysts who incorrectly assume that the experiment was designed to ensure that each data group is composed of a uniform and representative population. A common source of class blending occurs when the classification upon which the experiment is designed is itself blended. For example, imagine that you are a cancer researcher and you want to perform a study of patients with malignant fibrous histiocytomas (MFH), comparing the clinical course of these patients with the clinical course of patients who have other types of tumors. Let us imagine that the class of tumors known as MFH does not actually exist; that it is a grab-bag term erroneously assigned to a variety of other tumors that happened to look similar to one another. This being the case, it would be impossible to produce any valid results based on a study of patients diagnosed as MFH. The results would be a biased and irreproducible cacophony of data collected across different, and undetermined, classes tumors. Believe it or not, this specific example, of the blended MFH class of tumors, is selected from the real-life annals of tumor biology [18–20]. The literature is rife with research of dubious quality, based on poorly designed classifications and blended classes. One caveat; efforts to reduce class blending can be counterproductive if undertaken with excess zeal. For example, in an effort to reduce class blending, a researcher may choose groups of subjects who are uniform with respect to every known observable property. For example, suppose you want to actually compare apples with oranges. To avoid class blending, you might want to make very sure that your apples do not included any cumquats, or persimmons. You should be certain that your oranges do not include any limes or grapefruits. Imagine that you go even further, choosing only apples and oranges of one variety (e.g., Macintosh apples and Navel oranges), size (e.g., 10 cm), and origin (e.g., California). How will your comparisons apply to the varieties of apples and oranges that you have excluded from your study? You may actually reach conclusions that are invalid and irreproducible for more generalized populations within each class. In this case, you have succeeded in eliminated class blending at the expense of having representative populations of the classes.

Curse of dimensionality As the number of attributes for a data object increases, the distance between data objects grows to enormous size. The multidimensional space becomes sparsely populated, and the distance between any two objects, even the two closest neighbors, becomes absurdly large. When you have thousands of dimensions, the space that holds the objects is so large that distances between objects become difficult or impossible to compute, and computational products become useless for most purposes.

Heuristic technique A way to solve problems with inexact but quick methods, sufficient for most practical purposes.

Modified random sampling When we think of random sampling, we envision a simple, unbiased random selection from all the data objects within a collection. Consider a population of 7 billion people, where the number of individuals aged 60 and above account for 75% of the population. A random sampling of this population would be skewed to select senior citizens, and might yield very few children in kindergarten. Depending on the study, the data analyst may want to change the sampling rules to attain a random sampling that produces a population that fits the study goals. In this example the population might be partitioned into age groups (by decade), with an individual in any partitioned group having the same chance of being randomly selected as an individual in any other partitioned age group.

There are many different ways in which the rules of random sampling can be modified to accommodate an analytic approach [21]. Here are a few:

– Event-based sampling, in which data are collected only at specific moments, when the data being received meet particular criteria or exceed a preset threshold
– Adaptive random sampling, in which the rules for selection are determined by prior observations on the selected samples
– Attribute-based sampling, in which the probability of selection is weighted by a feature attribute of a data object

Of course, when we introduce a modification to the simple process of random selection, we risk introducing new and unexpected biases and confounders, and we open ourselves to criticism and the possibility that our conclusions cannot be repeated in other populations. It is another of those damned if you do and damned if you don't scenarios that we can expect in nearly every Big Data analysis.

Permutation test A method whereby the null hypothesis is accepted or rejected after testing all possible outcomes under rearrangements of the observed data elements.

Power In statistics, power describes the likelihood that a test will detect an effect, if the effect actually exists. In many cases, power reflects sample size. The larger the sample size, the more likely that an experiment will detect a true effect; thus correctly rejecting the null hypothesis.

Principal component analysis One popular methods for transforming data to reduce the dimensionality of data objects is multidimensional scaling, which employs principal component analysis [22]. Without going into the mathematics, principal component analysis takes a list of parameters and reduces it to a smaller list, with each component of the smaller list constructed from variables in the longer list (as a sum of variables multiplied by weighted coefficients). Furthermore, principal component analysis provides an indication of which variables are least correlated with the other variables (as determined by the size of the coefficients). Principal component analysis requires operations on large matrices. Such operations are computationally intensive and can easily exceed the capacity of most computers [22].

Pseudorandom number generator It is impossible for computers to produce an endless collection of truly random numbers. Eventually, algorithms will cycle through their available variations and begins to repeat themselves, producing the same set of "random" numbers, in the same order; a phenomenon referred to as the generator's period. Because algorithms that produce seemingly random numbers are imperfect, they are known as pseudorandom number generators. The Mersenne Twister algorithm, which has an extremely long period, is used as the default random number generator in Python. This algorithm performs well on most of the tests that mathematicians have devised to test randomness.

Resampling statistics A technique whereby a sampling of observations is artifactually expanded by randomly selecting observations and adding them to the original data set; or by creating new sets of data by randomly selecting, without removing, data elements from the original data.

Resampling versus Repeated Sampling In resampling statistics, a limited number of data measurements is expanded by randomly selecting data and adding them back to the original data. In Big Data, there are so many data points that statistical tools cannot quickly evaluate them. Repeated sampling

involves randomly selecting subpopulations of enormous data sets, over and over again, and performing statistical evaluations on these multiple samplings, to arrive at some reasonable estimate of the behavior of the entire set of data. Although random sampling is involved in resampling statistics and repeated sampling statistics, the latter does not resample the same data points.

Sample size The number of samples used in a study. Methods are available for calculating the required sample size to rule out the null hypothesis, when an effect is present at a specified significance level, in a population with a known population mean, and a known standard deviation [23]. The sample size formula should not be confused with the sampling theorem, which deals with the rate of sampling that would be required to adequately digitize an analog (e.g., physical or electromagnetic) signal.

Sampling theorem A foundational principle of digital signal processing, also known as the Shannon sampling theorem or the Nyquist sampling theorem. The theorem states that a continuous signal can be properly sampled, only if it does not contain components with frequencies exceeding one-half of the sampling rate. For example, if you want to sample at a rate of 4000 samples per second, you would prefer a signal containing no frequencies greater than 2000 cycles per second.

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14

Special Considerations in Big Data Analysis

OUTLINE

Section 14.1. Theory in Search of Data

If triangles had a god, they would give him three sides.

Voltaire

Here is a riddle: "Which came first, the data, or the data analyst?" The intuitive answer would be that data precedes the data analyst. Without data, there really is no reason for the data analyst to exist. In the Big Data universe nothing is as it seems, and the data analyst commonly precedes the data. All too often the analyst develops a question or a hypothesis or a notion of what the facts "should be," and then goes about rummaging through the Big Data resource until he or she has created a data set that proves the point.

Several intrinsic flaws plague Big Data statistics. When the amount of data is sufficiently large, you can find almost anything you seek lurking somewhere within. Such findings may have statistical significance without having any practical significance. Also, whenever you select a subset of data from an enormous collection, you may have no way of knowing the relevance of the data that you excluded. Most importantly, Big Data resources cannot be designed to examine every conceivable hypothesis. Many types of analytic errors ensue when a Big Data resource is forced to respond to questions that it cannot possibly answer. The purpose of this chapter is to provide general recommendations for the responsible use of analytic methods, while avoiding some of the pitfalls in Big Data analysis.

We cannot escape the dangerous practice of imposing models on selected sets of data. Historians, who have the whole of human history to study, are just as guilty as technical data analysts in this regard. Consider this hypothetical example: the United States is on the

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brink of a military intervention against entrenched and hostile revolutionaries on the other side of the globe. Two historians are asked to analyze the situation and render their opinions. The first historian compares the current crisis to the entrance of the United States into World War II. World War II worked out well for the United States. The first historian insists that World War II is a useful model for today's emergency and that we should engage our military against the current threat. The second historian says that the current crisis is very much like the crisis that preceded the Vietnam War. The Vietnam War did not turn out well for United States interests, and it would be best if we avoided direct military involvement in the current emergency. When you have all of history from which to choose, you can select any set of data that supports your biases. As humans, we do this all the time, whenever we make decisions.

Scientists have accused their peers of developing models for the purpose of reinforcing belief in their own favorite paradigms [1]. Big Data will not help advance science if analysts preferentially draw data to support their previously held biases. One of the important tasks for Big Data analysts will involve developing methods for creating unbiased models from Big Data. In the meantime, there is no practical way to validate conclusions drawn from Big Data, other than to test the hypothesis on additional data sets.

Section 14.2. Data in Search of Theory

> *Without highly specified a-priori hypotheses, there are hundreds of ways to analyse the dullest data set.*
>
> *John P A Ioannidis [2]*

In the prior section the point was made that data analysts can abuse Big Data if data is selected to confirm a hypothesis. In this section the point is made that scientists must enter their analysis with a model theory; otherwise they will choose a hypothesis to fit their data, even if the hypothesis makes no sense. [Glossary Multiple comparisons bias]

Here is a good example. Suppose I am at a shooting range and shoot ten shots at a bull's eye target. I can measure the distance of each bullet from the center of the target, from which I would develop some type of score with which I could compare my marksmanship against that of others. Now, imagine shooting ten shots at a wall that has no target. I may find that six of the bullets clustered very close together. I could then superimpose the bullet holes with a bull's eye target, placing the center of the target over the center of the tight clusters of bullet holes. A statistician analyzing the data might find that the six tightly clustered bullet holes at the center of the bull's eye indicated that I scored very well and that it was highly likely that I had better aim than others (who had actually aimed at the target). Scientists who troll large data sets will always find clusters of data upon which they can hang a bull's eye. Statisticians provided with such data can be tricked into confirming a ridiculous hypothesis that was contrived to fit the data. This deceptive practice is referred to as moving the target to the bullet hole.

Big Data analysts walk a thin line. If they start their project with a preconceived theory, then they run the risk of choosing a data set that confirms their bias. If they start their

project without a theory, then they run the risk of favoring a false hypothesis that happens to fit their data. [Glossary Type errors]

Is there a correct approach to Big Data analysis? It is important to remember that a scientific theory is a plausible explanation of observations. Theories are always based on some set of pre-existing principles that are generally accepted as truth. When a scientist approaches a large set of data, he or she asks whether a set of commonly held principles will extend to the observations in the current set of data. Reconciling what is known with what is observed accounts for much of the activity of scientists.

For Big Data projects, holding an a prior theory or model is almost always necessary; otherwise, the scientist is overwhelmed by the options. Adequate analysis can be ensured if three conditions are met:

1. All of the available data is examined, or a subset is prepared from a random sampling (i.e., no cherry-picking data to fit the theory).
2. The analyst must be willing to modify or abandon the theory, if it does not fit the data.
3. The analyst must not believe that fitting the theory to the data validates the theory. Theories must be tested against multiple sets of data.
4. The analyst must accept that the theory may be wrong, even if it is validated. Validation is not proof that a theory is correct. It is proof that the theory is consistent with all of the observed data. A better theory may also be consistent with the observed data and may provide a true explanation of the observations.

One of the greatest errors of Big Data analysts is to believe that data models are tethered to reality; they seldom are. Models are made to express data sets as formulas or as a system that operates under a set of rules. When the data are numeric representations of physical phenomenon, it may sometimes be possible to link the model to a physical law. For example, repeated measurements of force, mass, and acceleration observed on moving bodies might produce a formula that applies consistently, at any time, any place, and with any object (i.e., $f = ma$). Most mathematical models are abstract, and cannot be ranked as physical laws. At best, they provide a quick glimpse of an ephemeral reality.

Section 14.3. Bigness Biases

Every increased possession loads us with new weariness.

John Ruskin

Because Big Data methods use enormous sets of data, there is a tendency to give the results more credence than would be given to a set of results produced from a small set of data. This is almost always a mistaken belief. In fact, Big Data is seldom a complete or accurate data collection. You can expect most Big Data resources to be selective, intentionally or not, for the data that is included and excluded from the resource. When dealing with Big Data, expect missing values, missing records, "noisy" data, huge variations in the quality of records, plus any and all of the inadequacies found in small data resources.

Nevertheless, the belief that Big Data is somehow more reliable, and more useful than smaller data is pervasive in the science community.

When a study is done on a very large number of human subjects (or with a very large number of samples), each annotated with a large number of observations, there is a tendency to accept the results, even when the results defy intuition. In 2007, a study using the enormous patient data set held by the U.S. Veterans Administration Medical Centers reported that the use of statins reduced the risk of developing lung cancer by about half [3]. The study, which involved nearly half a million patients, showed that the reduction in cancer risk held whether patients were smokers or non-smokers. The highest reduction in lung cancers (77%) occurred in people who had taken statins for four years or longer [3].

The potential importance of this study cannot be overestimated. Lung cancer is the most common cause of cancer deaths in the United States. A 77% reduction in lung cancer incidence would prevent the cancer deaths of about 123,000 U.S. residents each year. This number is equivalent to the total number of cancer deaths attributed each year to prostate cancer, breast cancer and colon cancer combined [4]!

As it happens these marvelous findings were as unintuitive as they were exciting. Statins are a widely used drugs that reduce the blood levels of cholesterol and various other blood lipids. There is absolutely nothing known about the biology of statins that would lead anyone to suspect that this drug would lower the incidence of lung cancer, or any other cancer, for that matter. It is always risky to accept a scientific conclusion without some sort of biological mechanism to explain the results.

In 2011, a second study, by another group of researchers, was published on the effect of statins on lung cancer incidence. This study was also big, using about 133,000 patients. The results failed to show any effect of statins on lung cancer incidence [5]. That same year, a third study, using a population of about 365,000 people, also failed to find any influence of statins on the incidence of lung cancer [6]. The authors of the negative studies blamed time-window bias on the misleading results of the first study.

To understand time-window bias, consider the undisputed observation that Nobel prize laureates live longer than other scientists. It would seem that scientists who want to live a long life should try their utmost to win a Nobel prize. Likewise, Popes live longer than other clergymen. If you are a priest, and you want to live long, aim for the Papacy. Both these biases are based on time-window conditions. The Nobel prize committee typically waits decades to determine whether a scientific work is worthy of the Nobel prize, and the prize is only awarded to living scientists. Would-be Nobelists who die before their scientific career begins, and accomplished scientists who die before their works are deemed Nobel-worthy, are omitted from the population of potential winners. Similarly, the Vatican seldom confers the Papacy on its junior clergy. The time-window surrounding Nobel winners and Popes skews their observed longevities upwards. Time-window bias is just one of a general class of biases wherein studies are invalidated by the pre-conditions imposed on the studies [7]. [Glossary Time-window bias]

Time-window bias affected the original large patient-based study because a population that had taken a statin for four years, without dying in the interim, was compared to a

general population. Basically, the study imposed a cancer-free 4-year window for the treated population, artifactually conferring a lower cancer incidence on the statin-treated group.

The point here is simply that analytic errors occur just as easily in studies of large populations as they do in studies involving a small number of individuals. Because Big Data analysis tends to be complex, and difficult for anyone to thoroughly review, the chances of introducing Big Data errors is larger than the chances of introducing small data errors.

In the late 1990s, interest was growing in the medical research community and in biomarkers for cancers. It was believed then, as it is believed now, that the different types of cancers must contain biological markers to tell us everything we need to know about their clinical behaviors. Such biomarkers would be used to establish the presence of a cancer, the precise diagnosis of the cancer, the stage of the cancer (i.e., the size and the extent of spread of the cancer), and to predict the response of the cancer to any type of treatment. By the turn of the century, there was a sense that useful cancer biomarkers were not forthcoming; the pipeline for new biomarkers had apparently dried up [8–11]. What was the problem? A gnawing suspicion held that biomarkers failed because we weren't collecting enough data. A consensus had grown that we were wasting cancer research funds on small-scale studies that were irreproducible. What we needed, or so everyone thought, were Big Data studies, producing lots of data, yielding trustworthy results based on many observations. If researchers abandoned their small studies, in favor of large studies, then the field would surely move forward at a rapid pace.

In the past two decades, biomarker studies have seen enormous successes. Surprisingly, though, much of the recent progress has come from relatively small genomic studies, on very rare cancers, with limited numbers of specimens [2,12–14]. Why has Big Data not yielded the kind of progress that nearly everyone expected?

When a new potential biomarker is discovered using large and complex sets of data and advanced analytic tools, it needs to be validated; and validation involves repeating the original study, and drawing the same set of conclusions [15,16]. As a general rule the more complex the experiment, the data, and the analysis, the less likely that it can be reproduced. In addition to these basic limitations on conclusions drawn from Big Data, we must remember that it can be very difficult to analyze systems whose complexity exceeds our comprehension. We assume, quite incorrectly, that given sufficient data, we can understand complex systems. There is nothing to support this kind of self-confidence. Biological systems are highly complex, and we do not, at this time, have a deep understanding of their workings. For that matter, we have very little understanding of the kinds of data that ought to be collected. We are slowly learning that it seldom helps to throw Big Data at a problem, before we have a thorough understanding of what we need to find. In the case of cancer biomarkers, it was much easier to find the key mutations that accounted for rare tumors than it was to find common biomarkers in a general population [12,13].

Still unconvinced that Bigness bias is a real concern for Big Data studies? In the United States, our knowledge of the causes of death in the population is based on death certificate data collected by the Vital Statistics Program of the National Center for Health Statistics.

Death certificate data is notoriously faulty [17–19]. In most cases, the data in death certificates is supplied by clinicians, at or near the time of the patient's death, without benefit of autopsy results. In many cases, the clinicians who fill out the death certificate are not well trained for the task, often mistaking the mode of death (e.g., cardiac arrest, cardiopulmonary arrest), with cause of death (e.g., the disease process leading to cardiac arrest or cardiopulmonary arrest), thus nullifying the intended purpose of the death certificate. Thousands of instructional pages have been written on the proper way to complete a death certificate. Nonetheless, these certificates are seldom completed in a consistent manner. Clinicians become confused when there are multiple, sometimes unrelated, conditions that contribute to the patient's death. Though the death certificates are standardized throughout the United States, there are wide variations from state to state in the level of detail provided on the forms [20]. Despite all this the venerable death certificate is the bedrock of vital statistics. What we know, or think we know, about the causes of death in the United States population, is based on an enormous repository, collected since 1935, of many millions of death certificates.

Why do we believe death certificate data when we know that death certificates are highly flawed? Again, it is the bigness factor that prevails. There seems to be a belief, based on nothing but wishful thinking, that if you have a very large data set, bad measurements will cancel themselves out, leaving a final result that comes close to a fair representation of reality. For example, if a clinician forgets to list a particular condition as a cause of death, another physician will mistakenly include the condition on another death certificate, thus rectifying the error.

The cancel-out hypothesis puts forward the delightful idea that whenever you have huge amounts of data, systemic errors cancel out in the long run, yielding conclusions that are accurate. Sadly, there is neither evidence nor serious theory to support this hypothesis. If you think about it, you will see that it makes no sense. One of the most flagrant weaknesses is the fact that it is impossible to balance something that must always be positive. Every death certificate contains a cause of death. You cannot balance a false positive cause of death with a false negative cause of death (i.e., there is no such thing as a negative cause of death). The same applies to numeric databases. An incorrect entry for 5000 pairs of shoes cannot be balanced by a separate incorrect entry for negative 5000 pairs of shoes; there is no such thing as a negative shoe. [Glossary Negative study bias]

Perhaps the most prevalent type of bigness bias relates to the misplaced faith that complete data is representative data. Certainly, you might think that if a Big Data resource contains every measurement for a data domain, then biases imposed by insufficient sampling are eliminated. Danah Boyd, a social media researcher, draws a sharp distinction between Big-ness and Whole-ness [21]. She gives the example of a scientist who is exploring a huge data set of tweets collected by Twitter. If Twitter removes tweets containing expletives, or tweets composed of non-word character strings, or containing certain types of private information, then the resulting data set, no matter how large it may be, is not representative of the population of senders. If the tweets are available as a stripped-down set of messages, without any identifier for senders, then the compulsive tweeters (those

who send hundreds or thousands of tweets) will be over-represented, and the one-time tweeters will be under-represented. If each tweet were associated with an account and all the tweets from a single account were collected as a unique record, then there would still be the problem created by tweeters who maintain multiple accounts. Basically, when you have a Big Data resource, the issue of sample representation does not disappear; it becomes more complex and less controlled. For Big Data resources lacking introspection and identifiers, data representation becomes an intractable problem.

– **Too Much Data**

Intuitively, you might think that the more data we have at our disposal, the more we can learn about the system that we are studying. This is not always the case. There are circumstances when more data simply takes you further and further from the solution you seek. As a trivial example, consider the perennial task of finding a needle in a haystack. As you add more hay, you make the problem harder to solve. You would be much better off if the haystack were small, consisting of a single straw, behind which lies your sought-after needle [22].

In the field of molecular biology the acquisition of whole genome sequencing on many individual organisms, representing hundreds of different species, has brought a flood of data, but many of the most fundamental questions cannot be answered when the data is complex and massive. Evolutionary biologists have invented a new term for a certain type of sequence data: "non-phylogenetic signal." The term applies to DNA sequences that cannot yield any useful conclusions related to the classification of an organism, or its evolutionary relationships to other organisms.

Evolutionary geneticists draw conclusions by comparing DNA sequences in organism, looking for similar, homologous regions (i.e., sequences that were inherited from a common ancestor). Because DNA mutations arise stochastically over time (i.e., at random locations in the gene, and at random times), unrelated organisms may attain the same sequence in a chosen stretch of DNA, without inheritance through a common ancestor. Such occurrences could lead to false inferences about the relatedness of different organisms. When mathematical phylogeneticists began modeling inferences for gene data sets, they assumed that most class assignment errors would be restricted to a narrow range of situations. This turned out not to be the case. In practice, errors due to non-phylogenetic signal occur due to just about any mechanism that causes DNA to change over time (e.g., random mutations, adaptive convergence) [23,24]. At the moment, there seems to be an excess of genetic information. The practical solution seems to involve moving away from purely automated data analyses and using a step-by-step approach involving human experts who take into account independently acquired knowledge concerning the relationships among organisms and their genes.

– **Overfitting**

Overfitting occurs when a formula describes a set of data very closely, but does not predict the behavior of comparable data sets. In overfitting, the formula is said to describe the noise of the system, rather than the characteristic behavior of the system. Overfitting

commonly occurs with models that perform iterative approximations on training data. Neural networks are an example of a data modeling strategy that is prone to overfitting. In general, the bigger the data set, the easier it is to overfit the model.

Overfitting is discovered by testing your predictor or model on one or several new sets of data [25]. If the data is overfitted the model will fail with the new data. It can be heartbreaking to spend months or years developing a model that works like a charm for your training data and for your first set of test data (collected from the same data set as your training data), but fails completely for a new set of data.

Overfitting can sometimes be avoided by evaluating the model before it has been fitted to a mathematical formula, often during the data reduction stage. There are a variety of techniques that will produce a complex formula fitted to all your variables. It might be better to select just a few variables from your data that you think are most relevant to the model. You might try a few mathematical relationships that seem to describe the data plotted for the subset of variables. A formula built from an intuitive understanding of the relationships among variables may sometimes serve much better than a formula built to fit a multi-dimensional data set. [Glossary Data reduction]

Section 14.4. Data Subsets in Big Data: Neither Additive Nor Transitive

> *If you're told that a room has 3 people inside, and you count 5 people exiting the room, a mathematician would feel compelled to send in 2 people to empty it out.*
>
> *Anon*

It is often assumed that Big Data has one enormous advantage over small data: that sets of Big Data can be merged to create large populations that reinforce or validate conclusions drawn from small studies. This assumption is simply incorrect. In point of fact, it is possible to draw the same conclusion from two sets of data, only to draw an opposite conclusion when the two sets of data are combined. This phenomenon, well known to statisticians as Simpson's paradox, has particular significance when Big Data resources combine observations collected from multiple populations.

One of the most famous examples of Simpson's paradox was demonstrated in the 1973 Berkeley gender bias study [26]. A preliminary review of admissions data indicated that women had a lower admissions rate than men:

```
Men   Number of applicants..   8,442  Percent applicants admitted.. 44%
Women Number of applicants.. 4,321  Percent applicants admitted.. 35%
```

A nearly 10% lower overall admission rate for women, compared with men, seemed significant, but what did it mean? Was the admissions office guilty of gender bias?

A look at admissions department-by-department (in distinction to admissions for the total number of applicants to the university, by gender) showed a very different story. Women were being admitted at higher rates than men, in almost every department.

The department-by-department data seemed incompatible with the data obtained when the admissions from all the departments were combined.

The explanation was simple. Women tended to apply to the most popular and oversubscribed departments, such as English and History, that had a high rate of admission denials. Men tended to apply to departments that the women of 1973 avoided, such as mathematics, engineering, and physics, that had high relatively few applicants and high acceptance rates. Though women had an equal footing with men in departmental admissions, the high rate of rejections in the large departments, accounted for an overall lower acceptance rate for women at Berkeley.

Simpson's paradox demonstrates that data is not additive. It also shows us that data is not transitive; you cannot make inferences based on subset comparisons. For example in randomized drug trials, you cannot assume that if drug A tests better than drug B, and drug B tests better than drug C, then drug A will test better than drug C [27]. When drugs are tested, even in well-designed trials, the test populations are drawn from a general population specific for the trial. When you compare results from different trials, you can never be sure whether the different sets of subjects are comparable. Each set may contain individuals whose responses to a third drug are unpredictable. Transitive inferences (i.e., if A is better than B, and B is better than C, then A is better than C), are unreliable.

Simpson's paradox has particular significance for Big Data research, wherein data samples are variously recombined and reanalyzed at different stages of the analytic process.

Section 14.5. Additional Big Data Pitfalls

Any problem in Computer Science can be solved with another level of indirection.

Butler Lampson

...except the problem of indirection complexity.

Bob Morgan

There is a large literature devoted to the pitfalls of data analysis. It would seem that all of the errors associated with small data analysis will apply to Big Data analysis. There are, however, a collection of Big Data errors that do not apply to small data, such as:

– **The misguided belief that Big Data is good data**

For decades, it was common for scientists to blame their failures on the paucity of their data. You would often here, at public meetings and in private, statements such as "It was a small study, using just a few samples and limited number of measurements on each sample. We really should not generalize at the moment. Let us wait for a definitive study based on a large group of samples."

There has always been the sense, based on nothing in particular, that a small study cannot be validated by another small study. A small study must be validated by a big study.

Anyone who has ever worked on a project that collects large, complex, quickly streaming data knows that such efforts are much more prone to systemic flaws in data collection than are smaller projects. In Section 16.1, "First Analysis (Nearly) Always Wrong," we will see why conclusions drawn from Big Data are notoriously misleading.

Big Data comes from many different sources, produced by many different protocols, and must undergo a series of tricky normalizations, transformation, and annotations, before it has any value whatsoever. Data analysts can never assume that Big Data is accurate. Competent analysts will always validate their conclusions based on alternate, independently collected data; big or small.

– **Blending bias**

If you are studying the properties of a class of records (e.g., records of individuals with a specific disease or data collected on a particular species of fish), then any analysis of the data, no matter how large the data set, will be biased if your class assignments are erroneous (e.g., if the disease was misdiagnosed, or if you mistakenly included other species of fish in your collection). Classifications can be deeply flawed when individual classes are poorly defined, or not based on a well-understood set of scientific principles, or are assembled through the use of poor analytic techniques.

Let us look at one example in some depth. Suppose you are a physician living in Southern Italy, in the year 1640, where people are dying in great number, from a mysterious disease characterized by recurring fevers, delirium, and pain. You are approached by an explorer who has just returned from a voyage to South America, in an area corresponding to modern-day Brazil. He holds a bag containing an herbal extract, and says "Give this to your patients, and they will quickly recover."

It happens that the drug is extracted from the bark of the Cinchona tree. It is a sure-fire cure for malaria. Unknown to you, many of your patients are suffering from malaria, and would benefit greatly from this miraculous drug. Nonetheless, you are skeptical and would like to test this new drug before subjecting your patients to any unanticipated horrors. Though you are not a statistician, you do know something about designing clinical trials. In short order, you collect 100 patients, all of whom have the symptoms of fever and delirium. You administer the cinchona powder, also known as quinine, to all the patients. A few improve, but most do not. Knowing that some patients recover without any medical assistance, you call the trial a wash-out. In the end, you decide not to administer quinine to your patients.

What happened? We know that quinine arrived as a miracle cure for malaria. It should have been effective in a population of 100 malarial patients. The problem with this hypothetical clinical trial is that the patients under study were assembled based on their mutual symptoms: fever and delirium. These same symptoms could have been accounted for by any of hundreds of other diseases that were prevalent in England at the time. The criterion employed at the time to classify diseases was imprecise, and the trial population was diluted with non-malarial patients who were guaranteed to be non-responders. Consequently, the trial failed, and you missed a golden opportunity to treat your malaria patients with quinine, a new, highly effective, miracle drug.

Back in Section 5.5, we discussed Class Blending, an insidious flaw found in many classifications, that virtually guarantees that any analysis will yield misleading results. Having lots and lots of data will not help you. The only way to overcome the bias introduced by class blending is to constantly test and refine your classification.

– **Complexity bias**

The data in Big Data resources comes from many different sources. Data from one source may not be strictly comparable to data from another source. The steps in data selection, including data filtering, and data transformation, will vary among analysts. Together, these factors create an error-prone analytic environment for all Big Data studies that does not apply to small data studies.

– **Statistical method bias**

Statisticians can apply different statistical methods to one set of data, and arrive at any of several different, even contradictory, conclusions. Statistical method biases are particularly dangerous for Big Data. The standard statistical tests that apply to small data and to data collected in controlled experiments, may not apply to Big Data. Analysts are faced with the unsatisfying option of applying standard methods to non-standard data, or of developing their own methodologies for their Big Data project. History suggests that given a choice, scientists will adhere to the analysis that reinforces their own scientific prejudices [28].

– **Ambiguity of system elements**

Big Data analysts want to believe that complex systems are composed of simple elements, having well-defined attributes and functions. Clever systems analysts, using advanced techniques, enjoy believing that algorithms can predict the behavior of complex systems, when the elements of the system are understood. We learn from biological systems that the components of complex systems have ambiguous functionalities, changing from one moment to the next, rendering our best predictions tentative, at best. [Glossary Deep analytics]

For example, living cells are complex systems in which many different metabolic pathways operate simultaneously. A metabolic pathway is a multi-step chemical process involving more than one enzyme and various additional substrate and non-substrate chemicals. Depending on the conditions within a cell, a single enzyme may participate in several different metabolic pathways; and any given pathway may exert any of a number of different biological effects [29–32]. As we learn more and more about cells, we are stunned by their complexities [33,13]. Big Data analysts, working with highly complex systems, cannot assume that any of the elements of their system have a single, defined function. This tells us that all Big Data analyses on living systems (e.g., all biomedical systems and all non-biomedical data that depends in any way on the predictability or reproducibility of biomedical data) may be intractable to the kinds of systems analysis techniques that we have come to understand.

Despite all the potential biases, at the very least Big Data offers us an opportunity to validate predictions based on small data studies. As a ready-made source of observations, Big Data resources may provide the fastest, most economical, and easiest method to "reality test" limited experimental studies. Testing against large, external data sets, on independently collected data, and coming up with the equivalent conclusions, is a reasonable way to validate scientific assertions [34,35].

Section 14.6. Case Study (Advanced): Curse of Dimensionality

As the number of spatial dimensions goes up, finding things or measuring their size and shape gets harder.

The Curse of Dimensionality, attributed to Richard Bellman, and sometimes called Bellman's curse

Any serious student of Big Data will eventually fall prey to the dreadful Curse of Dimensionality. This curse cannot be reversed, and cannot be fully fathomed by 3-dimensional entities. Luckily, we can see the tell-tale signs that indicate where the curse is strongest, and thus avoid the full force of its evil power.

First, let's understand what we mean when we talk about n-dimensional data objects. Each attribute of an object is a dimension. The object might have three attributes: height, width, and depth; and these three attributes would correspond to the familiar three dimensional measurements that we are taught in geometry. The object in a Big Data collection might have attributes of age, length of left foot, width of right foot, hearing acuity, time required to sprint 50 yards, and yearly income. In this case the object is described by 6 attributes and would occupy 6 dimensions of Big Data space.

Let us say that we have normalized the values of every attribute so that each attribute value lies between zero and two (i.e., the age is between 0 and 2; the length of the left foot is between 0 and 2; the width of the right foot is between 0 and 2, and so on for every dimension in the object.

The 6-dimensional cube that encloses the set of data objects with attributes measuring between 0 and 2 will have sides measuring 2 units in length. The general formula for the volume of an n-dimensional cube is the length of a side raised to the nth power. In the case of a 260 dimensional cube, this would give us a volume of 2 ^260. Just to give you some idea of the size of this number, 2 ^260 is roughly the estimated number of atoms contained in our universe. So the volume of the 260-dimensional cube, of side 2 units, is large enough to hold the total number of atoms in the universe, spaced one unit apart in every dimension. Because there are many more atoms in the universe than there are data objects in our Big Data resources, we can infer that all high-dimensional volumes of data will be sparsely populated (i.e., lots of space separating data objects from one another). In our physical universe, there is much more empty space than there is matter; in the infoverse, it's much the same thing, only moreso. [Glossary Euclidean distance]

So what? What does it matter that n-dimensional data space is mostly empty, so long as every data object has an n-coordinate location somewhere within the hypervolume?

Let us consider the problem of finding a data object that lies within one unit of a reference object located in the exact center of the data space. As an example, we will continue to use an n-dimensional data object composed of attributes with normalized values between 0 and 2. We will begin by looking at a two dimensional data space.

If the data objects in the 2-dimensional data space are uniformly distributed in the space, then the chances of finding a data object within one unit of the center of the space (i.e., at coordinate 1,1) will be the ratio of the circle of radius one unit around the center divided by the area of the square that contains the data space (i.e., a square whose sides have length of 2). This works out to pi/4, or 0.785. This tells us that in two dimensions, we'll have an excellent chance of finding an object within 1 unit of the center (Fig. 14.1).

We can easily imagine that as the number of the dimensions of our data space increases, with an exponentially increasing n-dimensional volume, so too will the volume of the hypersphere that accounts for all the objects lying within 1 radial unit from the center. Regardless of how fast the volume of the space is growing, our hypersphere will keep apace, and we will always be able to find data objects in a 1-radial unity vicinity. Actually, no. Here is where the Curse of Dimensionality truly kicks in.

The general formula for the volume of an n-dimensional sphere is shown in Fig. 14.2.

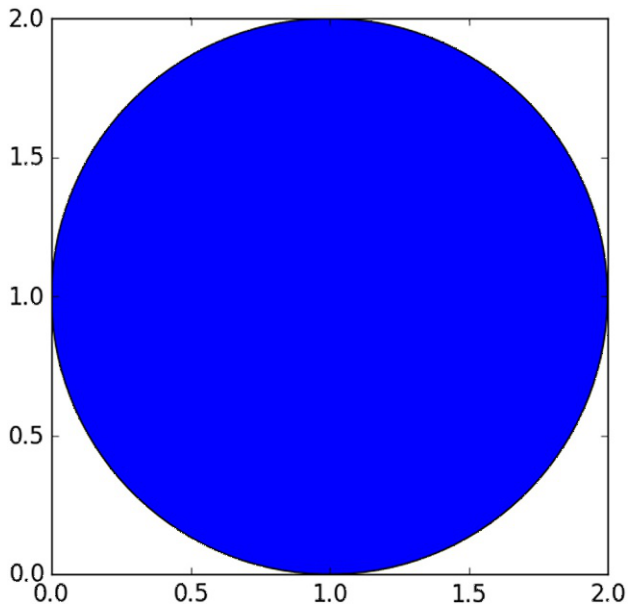

FIG. 14.1 A two-dimensional representation of the a circle, of radius length 1, in a square, of side length 2. The fraction of the square's area occupied by the circle is (pi * *r*^2)/4 or 3.1416/4 or 0.7854.

$$V_n(R) = \frac{\pi^{\frac{n}{2}}}{\Gamma(\frac{n}{2}+1)} R^n$$

FIG. 14.2 General formula for the volume of sphere of radius *R*, in *n* dimensions.

Let's not get distracted by the lambda function in the denominator. It suffices to know that the volume of a hypersphere in n dimensions is easily computable. Using the formula, here are the volumes of a 1 radial unit sphere in multiple dimensions [36].

```
Hypersphere volumes when radius = 1, in higher dimensions
n=1, V = 2
n=2, V = 3.1416
n=3, V = 4.1888
n=4, V = 4.9348
n=5, V = 5.2638
n=6, V = 5.1677
n=7, V = 4.7248
n=8, V = 4.0587
n=9, V = 3.2985
n=10, V = 2.5502
```

As the dimensionality increases, the volume of the sphere increases until we reach the fifth dimension. After that, the volumes of the 1-unit radius sphere begin to shrink. At 10 dimensions, the volume is down to 2.5502. From there on, the volume decreases faster and faster. The 20-dimension 1-radial unit sphere has a volume of only 0.0285, while the volume of the sphere in 100 dimensions is on the order of 10^-40 [36].

How is this possible? If the central hypersphere has a radius of one unit, and the coordinate space is a hypercube that is 2 units on each side, then we know that, for any dimension, the hypersphere touches each and every face of the hypersphere at one point. In the two dimensional example shown above, the inside circle touches the enclosing square on all four sides: at points (1,0), (1, 2), (1, 2), and (0,1). If an n-dimensional sphere touches one point on every face of the enclosing hypercube, then how could the sphere be infinitesimally small while the hypercube is immensely large?

The secret of the curse is that as the dimensionality of the space increases, most of the volume of the hypercube comes to lie in the corners, outside the central hypersphere. The hypersphere misses the corners, just like the 2-dimensional circle misses the corners of the square. This means that as the dimensionality of data objects increases, the likelihood of finding similar objects (i.e., object at a close n-dimensional proximity from one another) drops to about zero. When you have thousands of dimensions, the space that holds the objects is so large that distances between objects become difficult or impossible to compute. Basically, you can't find similar objects if the likelihood of finding two objects in close proximity is always zero.

Glossary

Data reduction When a very large data set is analyzed, it may be impractical or counterproductive to work with every element of the collected data. In such cases, the data analyst may choose to eliminate some of the data, or develop methods whereby the data is approximated. Some data scientists reserve the term "data reduction" for methods that reduce the dimensionality of multivariate data sets.

Deep analytics Insipid jargon occasionally applied to the skill set needed for Big Data analysis. Statistics and machine learning are often cited as two of the most important areas of deep analytic expertise. In a recent McKinsey report, entitled "Big data: The next frontier for innovation, competition, and productivity," the authors asserted that the United States "faces a shortage of 140,000 to 190,000 people with deep analytical skills" [37].

Euclidean distance Two points, $(x1, y1)$, $(x2, y2)$ in Cartesian coordinates are separated by a hypotenuse distance, that being the square root of the sum of the squares of the differences between the respective x-axis and y-axis coordinates. In n-dimensional space, the Euclidean distance between two points is the square root of the sum of the squares of the differences in coordinates for each of the n dimensional coordinates. The significance of the Euclidean distance for Big Data is that data objects are often characterized by multiple feature values, and these feature values can be listed as though they were coordinate values for an n-dimensional object. The smaller the Euclidian distance between two objects, the higher the similarity to each other. Several of the most popular correlation and clustering algorithms involve pairwise comparisons of the Euclidean distances between data objects in a data collection.

Multiple comparisons bias When you compare a control group against a treated group using multiple hypotheses based on the effects of many different measured parameters, you will eventually encounter statistical significance, based on chance alone. For example, if you are trying to determine whether a population that has been treated with a particular drug is likely to suffer a serious clinical symptom, and you start looking for statistically significant associations (e.g., liver disease, kidney disease, prostate disease, heart disease, etc.), then eventually you will find an organ in which disease is more likely to occur in the treated group than in the untreated group. Because Big Data tends to have high dimensionality, biases associated with multiple comparisons must be carefully avoided. Methods for reducing multiple comparison bias are available to Big Data analysts. They include the Bonferroni correction, the Sidak correction and the Holm-Bonferroni correction.

Negative study bias When a project produces negative results (fails to confirm a hypothesis), there may be little enthusiasm to publish the work [38]. When statisticians analyze the results from many different published manuscripts (i.e., perform a meta-analysis), their work is biased by the pervasive absence of negative studies [39]. In the field of medicine, negative study bias creates a false sense that every kind of treatment yields positive results.

Time-window bias A bias produced by the choice of a time measurement. In medicine, survival is measured as the interval between diagnosis and death. Suppose a test is introduced that provides early diagnoses. Patients given the test will be diagnosed at a younger age than patients who are not given the test. Such a test will always produce improved survival simply because the interval between diagnosis and death will be lengthened. Assuming the test does not lead to any improved treatment, the age at which the patient dies is unchanged by the testing procedure. The bias is caused by the choice of timing interval (i.e., time from diagnosis to death). Survival is improved without a prolongation of life beyond what would be expected without the test. Some of the touted advantages of early diagnosis are the direct result of timing bias.

Type errors Statistical tests should not be confused with mathematical truths. Every statistician understands that conclusions drawn from statistical analyses are occasionally wrong. Statisticians, resigned to accept their own fallibilities, have classified their errors into five types: Type 1 error—Rejecting the null hypothesis when the null hypothesis is correct (i.e., seeing an effect when there was none). Type 2 error—Accepting the null hypotheses when the null hypothesis is false (i.e., seeing no effect when there was one). Type 3 error—Rejecting the null hypothesis correctly, but for the wrong reason, leading to an erroneous interpretation of the data in favor of an incorrect affirmative statement. Type 4 error—Erroneous conclusion based on performing the wrong statistical test. Type 5 error—Erroneous conclusion based on bad data.

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15

Big Data Failures and How to Avoid (Some of) Them

OUTLINE

Section 15.1. Failure Is Common

As a rule, software systems do not work well until they have been used, and have failed repeatedly, in real applications.

Dave Parnas

There are many ways in which a complex system can be broken. In 2000, a Concorde crashed on take-off from Charles de Gaulle Airport, Paris. The Concorde was a supersonic transport jet, one of the most advanced and complex planes ever built. Some debris left on the runway had flipped up and tore a tire and some of the underside of the hull. All passengers were killed.

Big Data resources are complex; they are difficult to build and easy to break. After they break, they cannot be easily fixed.

Most Big Data failures do not result from accidents. Most failures occur when the Big Data resource is never completed, or never attains an acceptable level of performance. What goes wrong? Let us run down the reasons for failure that have been published in blogs, magazine articles and books on the subject of Big Data disappointments: Inappropriate selection and use of human resources (wrong leadership, wrong team, wrong people, wrong direction, wrong milestones, wrong deadlines); Incorrect funding (too little funding, too much funding, incorrect allocation of resources, wrong pay scales, wrong incentives); Legal snags (patent infringements, copyright infringements, inept technology transfer, wrong legal staff, inadequate confidentiality and privacy measures, untenable

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consent forms, poor contracts with unhelpful non-compete clauses, non-compliance with applicable laws and regulations, inadequate financial records and poor documentation of protocol compliances); Bad data (inaccurate and imprecise data, data obtained without regard to established protocols, data that is not fully specified, un-representative data, data that is not germane to the purpose of the resource), poor data security (purposely corrupted data, data stolen by malevolent entities, data inadvertently copied and distributed by staff, non-compliance with internal security policies, poor internal security policies). The list goes on. Generally, we see failure in terms of our own weaknesses: funders see failure as the result of improper funding; managers see failure as the result of poor management; programmers see deficiencies in programming methods, informaticians see deficiencies in metadata annotations, and so on. The field of Big Data is still young; the most senior members of a Big Data team are little more than newbies, and there's plenty of room for self-doubt. [Glossary Fair use]

It may be useful to accept every imaginable defect in a Big Data project as a potential cause of failure. For convenience sake, these defects can be divided into two general categories: (1) failures due design and operation flaws in Big Data resource, and (2) failures due to improper analysis and interpretation of results. Analytic and interpretive errors were discussed in Chapter 14. This chapter deals with the problems that arise when Big Data resources are poorly planned and operated.

Big Data resources are new arrivals to the information world. With rare exceptions, database managers are not trained to deal with the layers of complexity of Big Data resources. It is hard to assemble a team with the composite skills necessary to build a really good Big Data resource. At this time, all data managers are reflexively acquiring new software applications designed to deal with Big Data collections. Far fewer data managers are coming to grips with the fundamental concepts discussed in earlier chapters (e.g., identifier systems, introspection, metadata annotation, immutability, and data triples). It may take several decades before these fundamental principles sink in, allowing Big Data resources to reach their highest potential.

In the field of hospital informatics, costs run very high. It is not unusual for large, academic medical centers to purchase information systems that cost in excess of $500 million. Bad systems are costly and failures are frequent [1–3]. About three quarters of hospital information systems are failures [4]. Successfully implemented electronic health record systems have not been shown to improve patient outcomes [5]. Based on a study of the kinds of failures that account for patient safety errors in hospitals, it has been suggested that hospital information systems will not greatly reduce the incidence of safety-related incidents [6]. Clinical decision support systems, built into electronic health record systems, have not had much impact on physician practice [7]. These systems tend to be too complex for the hospital staff to master and are not well utilized.

The United Kingdom's National Health Service embarked on a major overhaul of its information systems, with the goal of system-wide interoperability and data integration. After investing $17 billion dollars, the project was ditched when members of Parliament called the effort "unworkable" [8–10].

It is difficult to determine the failure rate of Big Data projects. Organizations herald their triumphs but hide their misadventures. There is no registry of Big Data projects that can be followed to determine which projects fail over time. There is no formal designation "Big Data project" that is bestowed on some projects and withheld from others. Furthermore, we have no definition for failure, as applied to Big Data. Would we require a project to be officially disbanded, with all funds withdrawn, before we say that it is defunct? Or would we say that a Big Data project has failed if it did not meet its original set of goals? If a Big Data resource is built, and operates as planned, can we say that it has failed if nobody actually uses the resource? With these caveats in mind, it is believed that the majority of information technology projects fail, and that failure is positively correlated with the size and cost of the projects [11]. We know that public projects costing hundreds of billions of dollars have failed quietly, without raising much attention [12]. Big Data projects are characterized by large size, high complexity, and novel technology, all of which aggravate any deficiencies in management, personnel, or process practices [11].

Section 15.2. Failed Standards

> *Don't be afraid of missing opportunities. Behind every failure is an opportunity somebody wishes they had missed.*
>
> *Lily Tomlin*

Most standards fail. Examples are easy to find. OSI (Open Systems Interconnection) was a seven-layer protocol intended as the Internet standard. It was backed by the U.S. government and approved by the ISO/IEC (International Organization for Standardization) and the International Electrotechnical Commission). It has been supplanted by TCP/IP (Transmission Control Protocol/Internet Protocol), preferred by Unix. Simply because a standard has been developed by experts, backed by the U.S. government, and approved by an international standards organization, there is no guarantee that it will be accepted by its intended users.

In the realm of format standards (e.g., for documents, images, sound, movies), there are hundreds of standards. Some of these standards were developed for specific devices (e.g., cameras, image grabbers, word processors), and served a specific purpose in a small window of time. Today, most of these standard formats are seldom used. A few dozen remain popular. There is an on-going effort to incorporate all of the various image and media formats under one standard and one horrifying term: the BLOB (Binary Large OBject). [Glossary BLOB]

Every new programming language is born with the hope that it will be popular and immortal. In the past half century, well over 2000 programming languages have been devised. Most of these languages are seldom used and often forgotten. In 1995, Ada 95 became an ANSI/ISO standard programming language, a distinction held by only a few programming languages. The U.S. National Institute of Standards announced that Ada would be used by Federal departments and agencies in software applications that involve

control of real-time or parallel processes, very large systems, and systems with requirements for very high reliability [13]. The official announcement was entitled, Announcing the Standard for ADA. The programming language, Ada, was named for Ada Lovelace (1815–52), who wrote the first computer program (an algorithm for computing Bernoulli numbers) for Charles Babbage's prototype computer (the so-called analytic engine). Every Ada programmer knows that Ada is not an acronym; they bristle whenever Ada is spelled with all-uppercase letters. The federal government's announcement of the new "ADA" standard did not bode well. Ada is a fine programming language, but declaring it a government standard could not guarantee error-free implementations; nor could it guarantee its popularity among programmers. Following its ascension to standards status, the popularity of Ada declined rapidly. Today, it is rare to find an Ada programmer.

Even the best standards seldom meet expectations. Consider the metric system. It is used throughout the world, and it is generally acknowledged as a vast improvement over every preceding measurement standard. Nonetheless, in the United States our height is measured in feet and inches, not meters and centimeters, and our weight is measured in pounds, not kilograms. Here in the United States, it would be difficult to find a bathroom scale marked with metric graduations. The next time you look at your calendar, remember that about half the world uses a solar calendar. Most other earthlings follow a lunar calendar. Some base their calendars on a combination of solar and lunar observations.

When a standard is ignored, or improperly implemented, the results may be catastrophic. On June 4, 1996, the maiden flight of the French Ariane 5 exploded 37 seconds after launch. A software exception occurred during a data conversion from a 64-bit floating point to 16-bit signed integer value. The data conversion instructions (in Ada code) were not protected from causing an Operand Error [14].

On September 23, 1999, the United States launched the Mars Climate Orbiter, which crashed on impact on the red planet. An official investigation, by the Mars Climate Orbiter Mishap Investigation Board, concluded that the crash occurred due to a software glitch that arose when English units of measurement were used in the software when Metric units were supplied as input [15]. The flight software was coded in Ada.

The most successful standards are specifications that achieved popularity before they achieved the status of "standard." The best of these filled a need, enjoyed broad use, had few or no barriers to implementation (e.g., free and easy to use), and had the bugs ironed out (i.e., did not require excessive modifications and version updates). The most unsuccessful standards are those prepared by a committee of special interests who create the standard ab initio (i.e., without a pre-existing framework), without a user community, and without a proven need. The altogether worst standards seem to be those that only serve the interests of the standards committee members.

Robert Sowa has written a useful essay entitled "The Law of Standards" [16]. His hypothesis is, "Whenever a major organization develops a new system as an official

standard for X, the primary result is the widespread adoption of some simpler system as a de facto standard for X." He gives many examples. The PL/I standard, developed by IBM was soon replaced by Fortran and COBOL. The Algol 68 standard was replaced by Pascal. Ada, promoted by the U.S. Department of Defense, was replaced by C. The OS/2 operating system produced by IBM was replaced by Windows.

For small data projects and for software applications, the instability of data standards is not a major problem. Small data projects are finite in length and will seldom extend beyond the life span of the standards implemented within the project. For software designers, a standard implemented within an application can be replaced in the next upgrade. Any costs are passed onto the licensed user. Instability in standards serves the interests of software developers by coercing customers to purchase upgrades that comply with the new versions of included standards.

For Big Data resources, instability in standards is always bad news. A failed standard may invalidate the data model for the resource; undoing years of work. How can the data manager cope with failed standards? Over twenty years ago, I was approached by a pathologist who was tasked with annotating his diagnostic reports with a standard vocabulary of diseases. The principal options at the time were ICD (International Classification of Diseases), SNOMED (Systematized Nomenclature of Medicine) and MeSH (Medical Subject Headings produced by the National Library of Medicine). The ICD seemed too granular (i.e., not enough names of diseases). SNOMED was constantly changing; newer versions were incompatible with older versions, and he worried that annotations under an old version of SNOMED could not be integrated into the newer hospital information systems. MeSH was a well-curated public nomenclature, analogous to the Dewey Decimal System for the health informatics community, but it was not widely adopted by the pathology community.

I suggested all of his options were untenable. His best bet, under the circumstances, was to write his reports in simple, declarative sentences, using canonical diagnostic terms (i.e., terms expressed in a form suitable for a nomenclature). Reduced sentences could be easily parsed into constituent parts and accurately translated or mapped to any chosen vocabulary, as needed [17].

Consider the following sentence:

> *The patient has an scc, and we see invasion to the subcutaneous tissue, all the way to the deep margins, but the lateral margins are clear.*

This sentence, which is understandable to clinicians, would not be understandable to a computer program that parsed text. Among other impediments, a computer would not know that the abbreviation "scc" corresponds to the diagnostic term "squamous cell carcinoma." A computer that has an index list matching abbreviations to terms may falsely map the abbreviation to the wrong expansion term (e.g., small cell carcinoma rather than squamous cell carcinoma).

The complex sentence could be rewritten as six declarative statements:

Diagnosis: squamous cell carcinoma.
Invasion is present.
Invasion extends to subcutaneous tissue.
Margin is involved.
Tumor extends to deep margin.
Tumor does not extend to lateral margins.

It would be relatively easy to write a computer program that could autocode these very simple sentences. Every surgical pathology case entered in the hospital information system could be coded again and again, using any new version of any nomenclature. [Glossary Autocoding, Autoencoding]

We could go one step further, expressing every statement as a triple consisting of an identifier, a metadata term, and a data value. As discussed in Section 4.3, "Semantics and Triples," if all of the data in the resource is available as simple triples, and if the model provides a method whereby data objects can be assigned to classes, then every data object can be fully specified. Specified data objects, expressed as a simple triples, can be ported into any old or new data standard, as needed. [Glossary Class-oriented programming]

It is best to keep in mind two general principles of data management:

1. Data objects can be well specified, without a standard. You do not need to store your data in a format that is prescribed by a standard.
2. Data standards are fungible. If you know the rules for standards, you can write a program that converts to the standard, as needed.

In many instances, a simple, generic data model may free the Big Data manager from the problems that ensue when a data standard becomes obsolete.

Section 15.3. Blaming Complexity

Complexity is the worst enemy of security.

Bruce Schneier [18]

Big Data is complex, and complexity is dangerous. It is easy to write software that attains a level of complexity that exceeds anything encountered in the physical realm. Likewise, there is no limit to the complexity of operational methods, security standards, data models, and virtually every component of a Big Data resource. When a Big Data resource somehow manages to cope with complexity, it can be just a matter of time before key personnel depart to follow other opportunities, errors are introduced into the system, and a once-great resource grinds to a halt.

When errors occur in complex systems, even catastrophic errors, they can be very difficult to detect. A case in point is the Toyota Lexus ES 350 Sedan. Thousands of vehicle owners experienced unintended vehicle acceleration; the complex electronic control system was the chief suspect [19]. Over the years, Toyota expended enormous

resources trying to understand and solve the problem [20]. A host of agencies and authorities were involved in the investigation; first came the Department of Transportation and the National Highway Traffic Safety Administration. Then, owing to its expertise in software integrity, computer control systems, and electromagnetic interference, the National Aeronautics and Space Administration was called into the fray. Later, the National Academy of Sciences launched its own study of unintended acceleration in the auto industry. During these investigations, Toyota paid about $50 million in fines and recalled about 9 million cars. The dust may never settle completely on this problem, but it now appears that most, if not all, problems were due to sticky pedals, driver error, or improperly placed floor mats; no errors were uncovered in the complex electronic control system.

The most vexing problems in software engineering involve "sometimes" errors; software that runs perfectly under most circumstances, but fails at apparently random intervals. Finding the source of the problem is virtually impossible, because the most thorough evaluations will indicate that everything is working well. Sometimes the mistake occurs because of the chaotic and unpredictable quality of complex systems. Sometimes mistakes occur because the numbers get too big, or too small, or too impossible (division by zero); sometimes the order by which events occur are unexpected, causing the system to behave oddly. In all these situations, finding the problem is very difficult and could have been avoided if the system had been less complex. Knowing this, you might expect that data managers try their best to reduce the complexity of their resources. Actually, no. For most resources, increasing complexity is the normal state because it is easier to solve problems with more complexity than with more simplicity.

Every Big Data project should be designed for simplicity. The design team should constantly ask "Can we achieve this functionality with less complexity?" When the complexity cannot be reduced for a desired level of functionality, a trade-off might be reached. The team is justified in asking, "Do we need this level of functionality? Might we achieve a reduced but adequate level of functionality with a less complex system?" After the design phase, every addition, and every modification to the system should be examined for complexity. If complexity needs to be added to the system, then the team must analyze the consequences of the increased complexity.

– **When does complexity help?**

There are times when complexity is necessary. Think of the human mind and the human body. Our achievements as individuals and as a species come as the result of our complexity. This complexity was achieved over 4 billion of years of evolution, during which time disadvantageous traits were lost and advantageous traits were retained. The entire process was done incrementally. The complexity of a Big Data resource is created in a moment. We do not have four billion years to debug the system. When can complexity be permitted in a Big Data resource? There are several scenarios:

– When approximate or locally accurate solutions are not acceptable.

In the case of weather forecasting, the purpose is to attain predictions of ever-increasing accuracy. Each new forecasting model contains more parameters than the prior model,

requires more computing power, and is expected to provide accurate forecasts that extend further and further into the future. Complex models that do not yield greater accuracy than simpler models are abandoned. The whole process mimics evolution.

– When complexity is achieved incrementally.

Many of the most important devices implemented in society are complex (televisions, computers, smartphones, jet airplanes, magnetic resonance imaging devices). They all started as simpler devices, with complexity added incrementally. These complex devices did not require 4 billion years to evolve, but they did require the intense participation of many different individuals, teams, corporations, and users to attain their current utility.

The venerable U-2 U.S. spy plane is an example of incrementally achieved complexity. The U-2 was born in the 1950s and designed as a cold war spy plane. Despite its advanced age, the U-2 has stubbornly resisted obsolescence by incrementally increasing in complexity and utility. Today, it is still in service, with a functionality far greater than anything imaginable when it was created [21]. The value of incremental complexity has been emulated in some modern Big Data technologies [22].

– When your model really needs to match, item by item, the complexity of the real system that it is modeling.

Biologists have learned, in the past decade, that cellular processes are much more complex than they had originally imagined. Genes are controlled by interactions with other genes, with RNA, with proteins, and with chemical modifications to DNA. Complex chemical interactions that occur in the cell's nucleus and the cytoplasm have made it impossible to find simple genetic variants that account for many biologic processes. The entire field of genetic research has shifted to accommodate previously unanticipated complexities that have thwarted our earlier analyses [23]. Our progress in disease biology, developmental biology, and aging seems to hinge on our willingness to accept that life is complex, and cannot be reduced to a sequence of nucleotides in a strand of DNA.

There are occasions when we cannot "wish away" complexity. The best we can do is to prepare a model that does not amplify the irreducible complexity that exists in reality.

Section 15.4. An Approach to Big Data That May Work for You

> *The most likely way for the world to be destroyed, most experts agree, is by accident. That's where we come in; we're computer professionals. We cause accidents.*
>
> *Nathaniel Borenstein*

The old saying, "You can bring a horse to water, but you can't make it drink," aptly describes the situation for many Big Data resources. Sometimes Big Data projects fail because the intended users simply do not know what to do with the data. They have no approach that matches the available data, and they blame the Resource for their

inability to succeed. After a few would-be data miners give up, the Resource gets a reputation of being useless. Funding is withdrawn, and the Resource dies.

At this point, you may feel completely overwhelmed by the complexities of Big Data resources. It may seem that analysis is humanly impossible. The best way to tackle a large and complex project is to divide it into a smaller, less intimidating tasks. The approach to data analysis described in this chapter involves nine sequential steps.

– **Step 1. A question is formulated**

It takes a certain talent to ask a good question. Sometimes, a question, even a brilliant question, cannot be answered until it is phrased in a manner that clarifies the methods by which the question can be solved. For example, suppose I am interested in how much money is spent, each year, on military defense, in the United States. I could probably search the Internet and find the budget for the Department of Defense, in the year 2011. The budget for the Department of Defense would not reflect the costs associated with other agencies that have a close relationship with the military, such as intelligence agencies and the State Department. The Department of Defense budget would not reflect the budget of the Veterans Administration (an agency that is separate from the Department of Defense). The budget for the Department of Defense might include various items that have no obvious relationship to military defense. Because I am asking for the "annual" budget, I might need to know how to deal with projects whose costs are annualized over 5, 10, or 15 years. If large commitments were made, in 2005, to pay for long-term projects, with increasing sums of money paid out over the next decade, then the 2018 annual budget may reflect payouts on 2010 commitments. A 2018 budget may not provide a meaningful assessment of costs incurred by 2018 activities. After a little thought, it becomes obvious that the question: "How much money is spent, each year, on military defense, in the United States?" is complex, and probably cannot be answered by any straightforward method.

At this point, it may be best to table the question for a while, and to think deeply about what you can reasonably expect from Big Data. Many analysts start with the following general question: "How can this Big Data resource provide the answer to my question?" A more fruitful approach may be: "What is the data in this resource trying to tell me?" The two approaches are quite different, and I would suggest that data analysts begin their analyses with the second question.

– **Step 2. Resource evaluation**

Every good Big Data resource provides users with a detailed description of its data contents. This might be done through a table of contents or an index, or through a detailed "readme" file, or a detailed user license. It all depends on the type of resource and its intended purposes. Resources should provide detailed information on their methods for collecting and verifying data, and their protocols supporting outsider queries and data extractions. Big Data resources that do not provide such information generally fall into two categories: (1) highly specialized resources with a small and devoted user base who are thoroughly familiar with every aspect of the resource and who do not require guidance; or (2) bad resources.

Before developing specific queries related to your research interest, data analysts should develop queries designed to evaluate the range of information contained in the resource (discussed in detail in Chapter 9, "Assessing the Adequacy of a Big Data Resource". Even the best Big Data resources may contain systemic biases. For example, PubMed contains abstracted data on about 20 million research articles. Research articles are published on positive findings. It is very difficult for a scientist to publish a paper that reports on the absence of an effect or the non-occurrences of a biological phenomenon. PubMed has a positive result bias. The preferential exclusion or inclusion of specific types of data is very common, and data analysts must try to identify such biases.

Every Big Data resource has its blind spots; areas in which data is missing or scarce, or otherwise unrepresentative of the data domain. Often, the Big Data managers are unaware of such deficiencies. In some cases, Big Data managers blame the data analyst for "inventing" a deficiency that pertains exclusively to unauthorized uses of the resource. When a data analyst wishes to use a Big Data resource for something other than its intended purposes (e.g., using PubMed to predict NIH funding priorities over the next decade, using the Netflix query box to determine what kinds of actors appear in zombie movies), then the Big Data manager may be reluctant to respond to the analyst's complaints.

Simply having access to large amounts of subject data does not guaranteed that you have all the data you would need to draw a correct conclusion.

– **Step 3. A question is re-formulated**

"If you can dream - and not make dreams your master"

From If (poem), by Rudyard Kipling

The available data cannot always answer the exact question you started with. After you have assessed the content and design of your Big Data resource(s), you will want to calibrate your question to your available data sources. In the case of our original question, from Step 1, we wanted to know how much money is spent, each year, on military defense, in the United States. If we are unable to answer this question, we may be able to answer questions related to the budget sizes of individual government agencies that contribute to military spending. If we knew the approximate portion of each agency budget that is devoted to military spending, we might be able to produce a credible total for the amount devoted to military activities, without actually finding the exact answer.

After exploring the resource, the data analyst learns the kinds of questions that can best be answered with the available data. With this insight, he or she can re-formulate the original set of questions.

– **Step 4. Determine the adequacy of your query's returned output**

Big Data resources can often produce an enormous output in response to a data query. When a data analyst receives a large amount of data, he or she is likely to assume that

the query output is complete and valid. A query output is complete when it contains all of the data held in the Big Data resource that answers the query, and a query output is valid if the data in the query output yields a correct and repeatable answer.

A Google query is an example of an instance wherein query output is seldom seriously examined. When you enter a search term and receive millions of "hits", you may tend to assume that your query output is adequate. When you're looking for a particular Web page, or an answer to a specific question, the first output page on your initial Google query may meet all your needs. A thoughtful data analyst will want to submit many related queries to see which queries produce the best results. The analyst may want to combine the query outputs from multiple related queries, and will almost certainly want to filter the combined outputs to discard response items that are irrelevant. The process of query output examination is often arduous, requiring many aggregation and filtering steps.

After satisfying yourself that you've taken reasonable measures to collect a complete query output, you will still need to determine whether the output you have obtained is fully representative of the data domain you wish to analyze. For example, you may have a large query output file related to the topic of poisonous mushrooms. You've aggregated query outputs on phrases such as "mushroom poisoning", "mushroom poisons", "mushroom poison", "mushroom toxicity", and "fungal toxins". You pared down queries on "food poisoning," to include only mushroom-related entries. Now you want to test the output file to see if it has a comprehensive collection of information related to your topic of interest. You find a nomenclature of mushrooms, and you look for the occurrence of each nomenclature term in your aggregated and filtered output file. You find that there are no occurrences of many of the mushrooms found in the mushroom nomenclature, including mushrooms known to be toxic. In all likelihood, this means that the Big Data resource simply does not contain the level of detail you will need to support a thorough data analysis on topics related to poisonous mushrooms.

There is no standard way of measuring the adequacy of a query output; it depends on the questions you want to answer, and the analytic methods you will employ. In some cases, a query output will be inadequate because the Big Data resource simply does not contain the information you need; at least not in the detail you require. In other cases, the Big Data resource will contain the information you need, but does not provide a useful pathway by which your query can access the data. Queries cannot thoroughly access data that is not fully annotated, assigned to classes, and constructed as identified data objects.

Data analysts must be prepared to uncover major flaws in the organization, annotation, and content of Big Data resources. When a flaw is found, it should be promptly reported to the data manager for the resource. A good data manager will have a policy for accepting error reports, conducting investigations, instituting corrections as necessary, and documenting every step in the process.

– **Step 5. Describe your data**

Is the output data numeric or is it categorical? If it is numeric, is it quantitative? For example, telephone numbers are numeric, but not quantitative. If the data is numeric and

quantitative, then your analytic options are many. If the data is categorical information (e.g., male or female, true or false), then the analytic options are limited. The analysis of categorical data is first and foremost an exercise in counting; comparisons and predictions are based on the occurrences of features.

Are all of your data objects comparable? Big Data collects data objects from many different sources, and the different data objects may not be directly comparable. The objects themselves may be annotated with incompatible class hierarchies (e.g., one data object described as a "chicken" may be classed as "Aves", while another "chicken" object may be classed as "Food." One data object described as "child" may have the "age" property divided into three-year increments up to age 21. Another "child" object may have "age" divided into 4-year increments up to age 16. The data analyst must be prepared to normalize assigned classes, ranges of data, subpopulations of wildly different sizes, different nomenclature codes, and so on.

After the data is normalized and corrected for missing data and false data, you will need to visualize data distributions. Be prepared to divide your data into many different groupings, and to plot and re-plot your data with many different techniques (e.g., histograms, smoothing convolutions, cumulative plots, etc.). Look for general features (e.g., linear curves, non-linear curves, Gaussian distributions, multi-modal curves, convergences, non-convergences, Zipf-like distributions). Visualizing your data with numerous alternate plotting methods may provide fresh insights and will reduce the likelihood that any one method will bias your objectivity.

– **Step 6. Data reduction**

An irony of Big Data analysis is that the data analyst must make every effort to gather all of the data related to a project, followed by an equally arduous phase during which the data analyst must cull the data down to its bare essentials.

There are very few situations wherein all of the data contained in a Big Data resource is subjected to analysis. Aside from the computational impracticalities of analyzing massive amounts of data, most real-life problems are focused on a relatively small set of local observations drawn from a large number of events. The process of extracting a small set of relevant data from a Big Data resource is referred to by a variety of names, including data reduction, data filtering, and data selection. The reduced data set that you will use in your project should obey the courtroom oath "the whole truth, and nothing but the truth."

Methods for reducing the dimensionality of data are described in Section 10.5 "Reducing Your Data". As a practical point, when the random and redundant variables have been expunged, the remaining data set may still be too large for a frontal computational attack using advanced methods. A good data analyst knows when to retreat and regroup. If something can be calculated to great precision on a large number of variables and data points, then it should be calculated with somewhat less precision with somewhat fewer variables and fewer data points. Why not try the small job first, and see what it tells you?

– **Step 7. Select analytic algorithms (if absolutely necessary)**

Algorithms are perfect machines. They work to produce consistent solutions; they never make mistakes; they need no fuel; they never wear down; they are spiritual, not physical.

Every computer scientist loves algorithms; if they could be re-assigned to their favorite position, most computer scientists would devote their careers to writing new algorithms.

If you peruse the titles of books in the Big Data field, you will find that most of these books emphasize data analysis. They focus on parallel processing, cloud computing, high-power predictive analytics, combinatorics methods, and the like. It is very easy to believe that the essential feature of Big Data, that separates it from small data, relates to analytic algorithms. [Glossary Cloud computing, Grid]

As algorithms become more and more clever, they become more and more enigmatic. Some of the most popular statistical methods can be used injudiciously, and these include p values and linear regression [24,25]. Journal editors know this. Consequently, when a scientist submits an article to a journal, he or she can expect the editor to insist that a statistician be included as a co-author. The editors have a valid point, but is it really helpful to forcibly insert a statistician into an unfamiliar project? Isn't there some risk that the inclusion of a statistician will provide a thin veneer of scientific credibility, without necessarily attaining a valid scientific conclusion? [Glossary *P* value, Linear regression]

The field of Big Data comes with a dazzling assortment of advanced analytic options. Who is really qualified to judge whether the correct method is chosen; whether the chosen method is implemented properly; and whether the results are interpreted correctly?

Analysts in search of analytic algorithms should consider these simple options:

– Stick with simple estimates.

If you have taken to heart the suggestion in Section 12.4, "Back-of-Envelope Analyses", to estimate your answers early in project development, then you have already found simple estimators for your data. Consider this option: keep the estimators, and forget about advanced algorithms. For many projects, estimators can be easily understood by project staff, and will provide a practical alternative to exact solutions that are difficult to calculate and impossible to comprehend.

– Pick better metrics, not better algorithms.

Sabermetrics is a sterling example of analysis using simple metrics that are chosen to correlate well with a specific outcome; a winning ball game. In the past several decades, baseball analysts have developed a wide variety of new performance measurements for baseball players. These include: base runs, batting average on balls in play, defense independent pitching statistics, defense-independent earned run average, fielding independent pitching, total player rating, or batter-fielder wins, total pitcher index, and ultimate zone rating. Most of these metrics were developed empirically, tested in the field, literally, and optimized as needed. They are all simple linear metrics that use combinations of weighted measures on data collected during ballgames. Though sabermetrics has its detractors, everyone would agree that it represents a fascinating and largely successful effort to bring objective numeric techniques to the field of baseball. Nothing in sabermetrics involves advanced algorithms. It is all based on using a deep understanding of the game of baseball to develop a set of simple metrics that can be easily calculated and validated.

– Micromanage your macrodata.

Much of the success of Big Data is attained by making incremental, frequent changes to your system in response to your metrics. An example of successful micromanagement for Big Data is the municipal CompStat model, used by Police Departments and other government agencies [26,27]. A promising metric is chosen, such as 911 response time, and a team closely monitors the data on a frequent basis, sometimes several times a day. Slow 911 response times are investigated, and the results of these investigations typically generate action items intended to correct systemic errors. When implemented successfully, the metric improves (e.g., the 911 response time is shortened), and a wide range of systemic problems are solved. Micromanaging a single metric can improve the overall performance of a department.

Departments with imagination can choose very clever metrics upon which to build an improvement model (e.g., time from license application to license issuance, number of full garbage cans sitting on curbs, length of toll booth lines, numbers of broken street lights, etc.) It is important to choose useful metrics, but the choice of the metric is not as important as the ability to effectively monitor and improve the metric.

As a personal aside, I have used this technique in the medical setting and found it immensely effective. During a period of about 5 years at the Baltimore VA Medical center, I had access to all the data generated in our Pathology Department. Using a variety of metrics such as case turn-around time, cases requiring notification of clinician, cases positive for malignancy, and diagnostic errors, our pathologists were able to improve the measured outcomes. More importantly, the process of closely monitoring for deficiencies, quickly addressing the problem, and reporting on the outcome of each correction produced a staff that was sensitized to the performance of the department. There was an overall performance improvement.

Like anything in the Big Data realm, the data micromanagement approach may not work for everyone, but it serves to show that great things may come when you carefully monitor your Big Data resource.

– Let someone else find an algorithm for you; crowd-source your project.

There is a lot of analytic talent in this world. Broadcasting your project via the Web may attract the attention of individuals or teams of researchers who have already solved a problem isomorphic to your own, or who can rapidly apply their expertise to your specific problem [28].

– Offer a reward.

Funding entities have recently discovered that they can solicit algorithmic solutions, offering cash awards as an incentive. For example, the InnoCentive organization issues challenges regularly, and various sponsors pay awards for successful implementations [29]. [Glossary Predictive modeling contests]

– Develop your own algorithm that you fully understand. You should know your data better than anyone else. With a little self-confidence and imagination, you can develop an analytic algorithm tailored to your own needs.

– **Step 8. Results are reviewed and conclusions are asserted**

When the weather forecaster discusses the projected path of a hurricane, he or she will typically show the different paths projected by different models. The forecaster might draw a cone-shaped swath bounded by the paths predicted by the several different forecasts. A central line in the cone might represent the composite path produced by averaging the forecasts from the different models. The point here is that Big Data analyses never produce a single, undisputed answer. There are many ways of analyzing Big Data, and they all produce different solutions.

A good data analyst should interpret results conservatively. Here are a few habits that will keep you honest and will reduce the chances that your results will be discredited.

– Never assert that your analysis is definitive.

If you have analyzed the Big Data with several models, include your results for each model. It is perfectly reasonable to express your preference for one model over another. It is not acceptable to selectively withhold results that could undermine your conclusions.

– Avoid indicating that your analysis provides a causal explanation of any physical process.

In most cases, Big Data conclusions are descriptive, and cannot establish physical causality. This situation may improve as we develop better methods to make reasonable assertions for causality based on analyses of large, retrospective data sets [30,31]. In the meantime, the primary purpose of Big Data analysis is to provide a hypothesis that can be subsequently tested, usually through experimentation, and validated.

– Disclose your biases.

It can be hard to resist choosing an analytic model that supports your pre-existing opinion. When your results advance your own agenda, it is important to explain that you have a personal stake in the outcome or hypothesis. It is wise to indicate that the data can be interpreted by other methods and that you would be willing to cooperate with colleagues who might prefer to conduct an independent analysis of your data. When you offer your data for re-analysis, be sure to include all of your data: the raw data, the processed data, and step-by-step protocols for filtering, transforming, and analyzing the data.

– Do not try to dazzle the public with the large number of records in your Big Data project.

Large studies are not necessarily good studies, and the honest data analyst will present the facts and the analysis, without using the number of data records as a substitute for analytic rigor.

– **Step 9. Conclusions are examined and subjected to validation**

"Sometimes you gotta lose 'til you win"

From "Little Miss" (song) by Sugarland

Validation involves demonstrating that the conclusions that come from data analyses are reliable. You validate conclusions by showing that you draw the same conclusion repeatedly in comparable data sets.

Real science can be validated, if true, and invalidated, if false. Pseudoscience is a pejorative term that applies to scientific conclusions that are consistent with some observations, but which cannot be confirmed or tested. For example, there is a large body of information that would suggest that earth has been visited by flying saucers. The evidence comes in the form of many eyewitness accounts, numerous photographs, and cover-up conspiracy theories. Without commenting on the validity of UFO claims, it is fair to say that these assertions fall into the realm of pseudoscience because they are untestable (i.e., there is no way to prove that flying saucers do not exist), and there is no definitive data to prove their existence (i.e., the "little green men" have not been forthcoming).

Big Data analysis always stands on the brink of becoming a pseudoscience. Our finest Big Data analyses are only valid to the extent that they have not been disproven. A good example of a tentative and clever conclusion drawn from data is the Titius-Bode Law. Titius and Bode developed a simple formula that predicted the locations of planets orbiting a star. It was based on data collected on all of the planets known to Johann Daniel Titius and Johann Elert Bode, two eighteenth century scientists. These planets included Mercury through Saturn. In 1781, Uranus was discovered. Its position fit almost perfectly into the Titius-Bode series, thus vindicating the predictive power of their formula. The law predicted a fifth planet, between Mars and Jupiter. Though no fifth planet was found, astronomers found a very large solar-orbiting asteroid, Ceres, at the location predicted by Titius and Bode. By this time, the Titius-Bode Law was beyond rational disputation. Then came the discoveries of Neptune and Pluto, neither of which remotely obeyed the Law. The data had finally caught up to the assertion. The Titius-Bode Law was purely descriptive; not based on any universal physical principles. It served well for the limited set of data to which it was fitted, but was ultimately discredited.

Let us look at a few counter-examples. Natural selection is an interesting theory, published by Charles Darwin, in 1859. It was just one among many interesting theories aimed at explaining evolution and the origin of species. The Lamarckian theory of evolution preceded Darwin's natural selection by nearly 60 years. The key difference between Darwin's theory and Lamarck's theory comes down to validation. Darwin's theory has withstood

every test posed by scientists in the fields of geology, paleontology, bacteriology, mycology, zoology, botany, medicine, and genetics. Predictions based on Darwinian evolution dovetail perfectly with observations from diverse fields. The Lamarckian theory of evolution, proposed well before DNA was established as the genetic template for living organisms, held that animals passed experiences to succeeding generations through germ cells; thus strengthening intergenerational reliance on successful behaviors of the parent. This theory was groundbreaking in its day, but subsequent findings failed to validate the theory. Neither Darwin's theory nor Lamarck's theory could be accepted on their own merits. Darwin's theory is correct, as far as we can know, because it was validated by careful scientific observations collected over the ensuing 150 years. Lamarck's theory is incorrect, because it failed the validation process.

The value of big data is not so much to make predictions, but to test predictions on a vast number of data objects. Scientists should not be afraid to create and test their prediction models in a Big Data environment. Sometimes a prediction is invalidated, but an important conclusion can be drawn from the data anyway. Failed predictions often lead to new, more successful predictions.

Of course, every analysis project is unique, and the steps involved in a successful project will vary. Nonetheless, a manageable process, built on techniques introduced in preceding chapters, might be helpful. My hope is that as Big Data resources mature and the methods for creating meaningful, well annotated, and verified data become commonplace, some of the steps listed in this chapter can be eliminated. Realistically, though, it is best to assume that the opposite will occur; more steps will be added.

Section 15.5. After Failure

> *Programming can be fun, so can cryptography; however they should not be combined.*
>
> *Charles B. Kreitzberg and Ben Shneiderman*

In 2001, funds were appropriated to develop the National Biological Information Infrastructure. This Big Data project was a broad cooperative effort intended to produce a federated system containing biological data from many different sources, including Federal and State government agencies, universities, natural history museums, private organizations, and others. The data would be made available for studies in the field of resources management. On January 15, 2012, the resource was officially terminated, due to budget cuts. A Website announcement sits vigil, like a tombstone, marking the passage of an ambitious and noble life (Fig. 15.1).

Like the humans who create the resources, Big Data lives for a time, and then it dies. Humans often carry life insurance, or savings, to pay the costs of burial and to manage the distribution of an estate. In most cases, no preparations are made for the death of Big Data. One day it is there, and the next day it is gone.

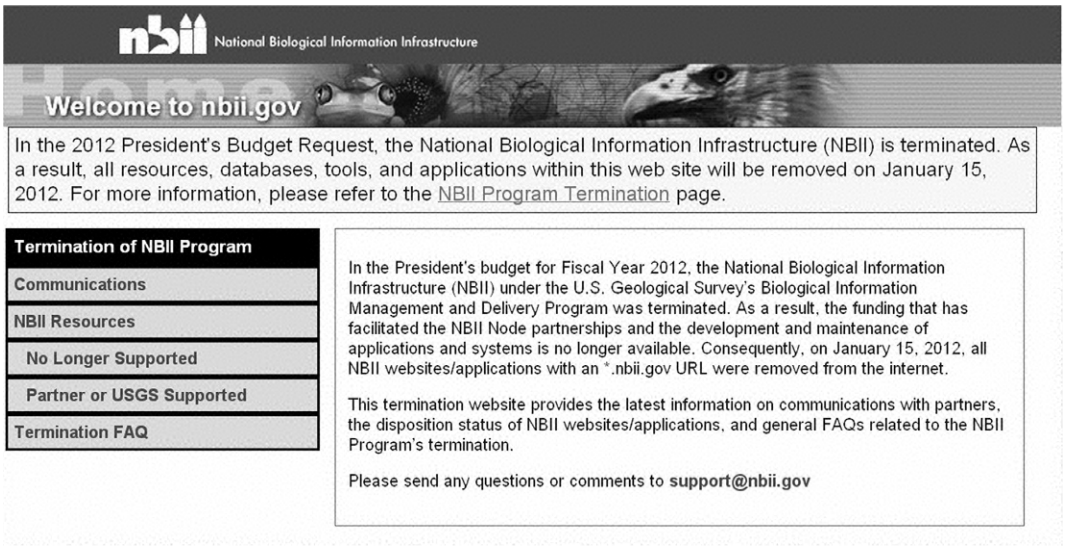

FIG. 15.1 A U.S. government website announcing the demise of the National Biological Information Infrastructure project, in 2012.

Abandonware is a term that is often applied to software developed under a grant. When the grant funding ceases, the software is almost always abandoned. Nobody assumes the responsibility of tying up loose ends, finding and removing bugs, distributing the software, or using the software in new projects. Similarly, when a Big Data project dies, the programmers and staff scrabble to find new jobs; nobody remains to clean up the leftovers. The software is abandoned. The identifier system and the data model for the resource are almost always lost to posterity. All those charts and all those registration numbers simply disappear. The data in the failed resource either slips into the bit-void or becomes legacy data; stored on disks, shelved, and forgotten. Legacy data can be resurrected, but it seldom happens.

Here are a two precautions that can salvage some of the pieces of a failed Big Data project.

– **Write utilities, not applications.**

Software applications can be envisioned as utilities with a graphic user interface. One software application may have the functionality of three or four utilities (e.g., spreadsheet plus graph plotter plus statistics suite, with the graphic user interface of a word processor). When a Big Data Resource is built, it will usually be accessed under an umbrella application. This application will support user queries, while shielding the user from the complexities of the data and the mechanics of passing the query over multiple, networked servers. When a Big Data resource is terminated, applications with a user interface to the resource retain no value. However, the small utility programs built into the application,

may have enormous value to the builders of related Big Data resources. The best applications are modularized; built from working parts that can be extracted and used as modules or utilities. Utilities that apply generally to many data-related projects are valuable assets.

When you write code, employ responsible coding practices. There is a vast literature on coding etiquette. Programmers are always advised to write simple code, to comment their code (i.e., explain the software steps and algorithms within the programs, as well as any modifications to the software), and to avoid using variable names that have no obvious meaning. This book will not dwell on good programming practices, but suffice it to say that as programs become more and more complex, good software practices become essential.

– **Pay up-front to preserve your legacy data and your identifiers.**

Big Data resources are very expensive. It makes sense to put aside funds to preserve the data, in the event of failure. Data means nothing unless it is properly identified; hence, the data held in a Big Data resource must be preserved with its identifiers. If the data is identified and well annotated, it will be possible to re-integrate the data objects into a successor resource.

Preserving legacy data is particularly important in hospital information systems, which have a very high failure rate [3]. It is unacceptable to lose patient histories, just because the hospital bought bad software. Hospitals, medical centers and all Big Data systems that serve critical missions should set aside money, in an escrow fund, for this purpose.

Section 15.6. Case Study: Cancer Biomedical Informatics Grid, a Bridge Too Far

> *In a software project team of 10, there are probably 3 people who produce enough defects to make them net negative producers.*
>
> *Gordon Schulmeyer*

Some governments do an excellent job at analyzing their own failures. After the Ariane 5 exploded 37-post launch on its maiden space flight, the French government issued the results of their investigation [14]. When the Mars Climate Orbiter crashed on Mars, the U.S. government issued a report on their investigation [15]. The world might be a better place if we, as individuals, published our own investigative reports when we disappoint our friends and co-workers or fail to meet our personal goals; but self-accountability has never been a human strength.

In 2004, the National Cancer Institute launched an ambitious project, known as the Cancer Biomedical Informatics Grid (CaBig™), aimed at developing standards for annotating and sharing biomedical data, and tools for data analysis. An unusual aspect of this government project was that it had its own business model, "to create a front end that will make caBIG attractive for others to invest in and take on responsibility for downstream

events" [32]. Further, it was "anticipated at the time that the caBIG effort would evolve into a self-sustaining community" [32].

When the effort began, its goals seemed relatively focused, but over the next 6 years, the scope of the project grew; it eventually covered software interoperability and Web-based services for sharing and analyzing data produced by virtually every biomedical specialty, from gene sequencing to radiology imaging to tissue specimens.

For a time, the project received generous support from academia and industry. In 2006, the Cancer Biomedical Informatics Grid was selected as a laureate in ComputerWorld's honors program [33]. ComputerWorld described the project as "Effectively forming a World Wide Web of cancer research," with "promises to speed progress in all aspects of cancer research and care." The laudable ambitions of the project came with a hefty price tag. By 2010, the National Cancer Institute had sunk at least 350 million dollars into the effort [32]. Though the project was ambitious, there were rumblings in the cancer informatics community that very little had been achieved. In view of past and projected costs, an ad hoc committee was assigned to review the program.

In the report issued to the public, in 2011, the committee found that the project had major deficiencies and suggested a yearlong funding moratorium [32]. Soon thereafter, the project leader left the National Cancer Institute, and the Cancer Bioinformatics Grid was terminated [34].

The ad hoc committee report went into considerable detail to explain the deficiencies of the program. Their observations serve as a general warning for overly ambitious Big Data efforts.

> *The caBIG program has grown rapidly without adequate prioritization or a cost-effective business model, has taken on a continuously increasing and unsustainable portfolio of development and support activities, and has not gained sufficient traction in supporting critical cancer research community needs. The working group interviews indicate that the program has developed some extremely expensive software solutions that have not been adopted in a meaningful way by the NCI designated Cancer Centers, have competed unnecessarily with existing solutions produced by industry leaders that hold a 60% to 70% market share in the NCI-designated Cancer Centers, and ultimately have created an enormous long-term maintenance, administration, and deployment load for the NCI that is financially unsustainable [32].*

Regarding analysis tools, the working group found that "the level of impact for most of the tools has not been commensurate with the level of investment. For example, many tools, such as caArray ($9.3M), have been developed at significant expense and without a clear justification, particularly since a number of similar commercial and open software tools already existed. It is indeed noteworthy and a lesson for the future that the more widely adopted Life Sciences tools have their roots in projects that were already fairly successfully developed by academic research institutions, whereas most of the caBIG™-initiated

projects have been less successful and, ironically, much more expensive. Similarly, enormous effort was devoted to the development of caGRID ($9.8M), an environment for grid-based cloud computing, but the working group did not find evidence that it has empowered a new class of tools to 'accelerate the discovery of new approaches for the detection, diagnosis, treatment, and prevention of cancer' as envisioned" [32].

The working group found that the project participants were attracted to new technological innovations, even when those innovations provided no advantages. "In particular, the interviews suggest that the strategic goals of the program were determined by technological advances rather than by key, pre-determined scientific and clinical requirements. Thus, caBIG™ ended up developing powerful and far-reaching technology, such as caGRID, without clear applications to demonstrate what these technologies could and would do for cancer research." Regarding the value of new technology, the working group "struggled to find projects that could not have been implemented with alternative less expensive or existing technologies and software tools" [32].

I was a program director at the National Cancer Institute during the first two years of the project and had a front-row seat for the CaBig pageant. At the time, I thought that the project was too big, too complex, too ambitious, that it served too many interests (the intramural community at NIH, the extramural community of academic researchers, a profusion of industry contractor, and the Office of the Director at the National Cancer Institute), enlisted the assistance of too many people, had too much money, was lavished with too much hype, had initiated too many projects, and that the program directors operated with insufficient accountability. In a word, I was envious.

In the case of the Cancer Biomedical Informatics Grid, hindsight would suggest that the project may have benefited from the following:

1. Start small [35].

Projects should begin with a relatively small number of highly dedicated and energetic people. Studies have shown that as more and more money and personnel are added to a software project, the chances of success drop precipitously [36]. When you stop and think about it, most of the great programming languages, some of the most important operating systems, the design of the Internet, the language of the world wide Web, computer hardware advances, innovational corporations, and virtually all of the great algorithms in computer science, were created by one individual, or a small group of people (usually less than 5).

Some Big Data projects are necessarily large. The Human Genome project, touted as one of the largest and most successful Big Data projects in human history, involved hundreds of scientists. But when it came down to organizing the pieces of data into a coherent sequence, the job fell to one man. In a report published by the Center for Biomolecular Science and Engineering at UC Santa Cruz, Jim Kent "developed in just 4 weeks a 10,000-line computer program that assembled the working draft of the human genome" [37]. "Kent's assembly was celebrated at a White House ceremony on June 26, 2000" [37].

The Cancer Biomedical Informatics Grid began with teams of workers: contractors, government employees, academics, and advisors from various related informatics projects. The project sprang into existence too big to build.

2. Complete your initial goals.

Projects that are closely tied to a community (the cancer research community in the case of CaBIG™, tend to expand their goals based on the interests of enthusiastic community members. It is very common for project managers to be approached by individuals and small groups of people asking that their pet projects be added to the list of project goals. Requests that come from powerful and influential members of the community cannot be ignored. Somehow project managers must placate their constituents without losing focus on their original goals. It is not sufficient to show that the resource is managing to do a lot of different things; managers must be able to complete their critical goals. Failing to do so was a problem for CaBig™. As a counter-example, consider the amazing success of Google. Today, we enjoy the benefits of Google Earth, Google Maps, Google Books, and so one. But the Google people started with a simple, albeit large and all encompassing, search engine. Projects were added after the search engine had been created and popularized.

3. Do not try to do everything yourself.

There is a tendency today for large projects to seek representation in every ongoing effort that relates in any way to the project. For example, a standards effort in the cancer community might send representatives to every committee and standards project in the general area of health technology interoperability. Likewise, narrowly focused standards efforts (e.g., gene array specifications, microscopy specifications) often attract representatives from large corporations and from other standards committees. The push toward internecine activity is based on the belief that the ultimate goal of software interoperability and data integration can only be achieved by broadening the level of participation. In practice, these interchanges make it difficult for project managers to achieve any kind of focus. Each workday is diluted with de-briefings on other projects, conferences, and committee meetings.

Life is about balance. Managers need to have some sense of what is happening in the world outside of their own project, but they must not digress from their own goals. In many cases, careful attention to the Big Data fundamentals (e.g., specifying data fully, identifying and classifying data objects, achieving introspection), should suffice in creating a functional resource that can operate with other resources. Data is fungible; a well-specified data model can often to ported to other formats, other standards and other specifications, as needed.

4. Do not depend on things that you cannot depend on.

This tautology should never be forgotten or trivialized. It is quite common for Big Data resources to choose hardware, software, standards, and specifications that cannot possibly serve their needs. Oblivious to reality, they will choose a currently popular, but flawed

methodology, hoping some miracle will save them. So strong is this belief that things will somehow "work out" that virtually every type of project proposal (e.g., grant application, business proposal, book deal) contains a hidden deus ex machina; an implied request that the reviewer suspend his disbelief. Allowing for human nature, some grant reviewers extend a "one-miracle per grant" policy. An applicant can ask for one miracle, but no more.

After CaBig™ was terminated, Barry Smith, a big thinker in the rather small field of ontology, wrote an editorial entitled "CaBIG™ has another fundamental problem: it relies on "incoherent" messaging standard" [38]. In his editorial Smith suggested that HL7, a data model specification used by CaBig™ could not possibly work, and that it had proven to be a failure by those people who actually tried to implement the specification and use it for its intended purposes [38]. At about the same time that CaBig was being terminated, the $17 billion interoperability project undertaken by the U.K.'s National Health Service was scuttled. This failed program had been called "the world's biggest civil information technology program" [8]. Back in 2001, a report published by the NHS Information Authority cited fundamental flaws in HL7 [39]. These flaws included intrinsic difficulties in establishing a workable identifier system. The report concluded that despite these problems, choosing HL7 was strategically correct, as it was the only data model with a process of continual review and update [39]. At the time, everyone was hoping for a miracle. The miracle did not come for CaBig™; nor had it come for the UK's interoperability project. No one can say to what degree, if any, HL7 flaws contributed to the downfall of these projects; but flaws in the data model could not have been very helpful.

5. Use existing, thoroughly tested open source technologies wherever possible.

There is a healthy appetite among information technologists for new and improved technologies. Though this preference may serve well for small and short-term projects, it is often counterproductive for Big Data efforts. All Big Data projects are complex, and there is seldom room to compound complexities by tossing innovative software into the mix. Unless there is a compelling reason to use new technology, it is usually much safer to use older technology that it adequate for the tasks at hand. Stable open source solutions, particularly when there is an active community that supports the software, is often the best choice. Aside from cost considerations (most open source software is free), there is the added benefit of longevity. Unlike commercial software, which can be discontinued or replaced by applications that are incompatible with installed versions, popular open source software tends to stay viable. In the case of CaBig™, the working group indicated that the project chose new technologies, when older technologies would suffice.

6. Avoid developing solutions for problems that nobody really cares about.

I have a colleague who works in the field of computer-aided diagnosis, an interesting field that has not yet garnered widespread acceptance in the medical community. Apparently, clinicians still prefer to reach their diagnoses through their own efforts, without the aid of computer software [40]. Perhaps, he thought, the aid of a computer program might be appreciated in areas where physicians were in short supply; such as developing countries.

He thought that it would be useful to find a market for computer aided diagnostic software somewhere in Africa. Of course, healthcare limitations in developing countries are often basic availability issues (e.g., access to hospitals, beds, antibiotics, sterile materials, equipment, and so forth). Access to diagnostic computer programs, developed on clinical data sets collected on U.S. patients, may not be "what the doctor ordered."

In the case of CaBig, the working group found that CaBig™ was developing powerful new technologies for which there was no apparent need. It is only human nature to want to make a difference in the world. For Big Data project managers, it is sometimes best to wait until the world asks you for your input.

7. A Big Data resource should not focus its attention on itself.

Big data projects often involve a great number of people. Those involved in such efforts may come to believe that the resource itself has an intrinsic value that exceeds the value of its rendered services [41]. Experience would indicate that most users, even avid users, are not interested in the details. The couch potato may sit transfixed in front of his television for hours on end, but he is not likely to pursue an interest in the technologies underlying signal transmissions, or high definition image construction. Likewise, the public has no interest in knowing any of the protocols and models that underlie a Big Data resource. As someone who was asked to review manuscripts published by the scientific contributors to CaBig™, it was my impression that publications emanating from this effort were largely self-congratulatory pieces describing various aspects of the project, in details that would have meaning only to the fellow members of the team [42].

Program managers should never forget that a Big Data resource is all about the data, and how the data is analyzed. The resource itself, rightly or wrongly, should not be the focus of public attention.

Section 15.7. Case Study: The Gaussian Copula Function

> *America is the only country where a significant proportion of the population believes that professional wrestling is real but the moon landing was faked.*
>
> *David Letterman*

It is important to remember that mathematics only describes observed relationships. It does not explain how those relationships are achieved. A clever physicist such as James Clerk Maxwell can write a set of equations that describe how electric charges and electric currents create electric and magnetic fields, but equations cannot tell us what the meaning is of magnetism. I would venture to say that there isn't a physicist who truly understands the meaning of magnetism, or electricity, or matter, or time.

What applies to the physicist applies to the economist. Recent experience with the Gaussian copula function provides a cautionary tale [43]. This formerly honored and currently vilified formula, developed for Wall Street, was used to calculate the risk of default correlation (i.e., the likelihood that two investment vehicles would default together) based

$$c_R^{\text{Gauss}}(u) = \frac{1}{\sqrt{\det R}} \exp\left(-\frac{1}{2}\begin{pmatrix}\Phi^{-1}(u_1)\\ \vdots \\ \Phi^{-1}(u_d)\end{pmatrix}^T \cdot \left(R^{-1} - I\right) \cdot \begin{pmatrix}\Phi^{-1}(u_1)\\ \vdots \\ \Phi^{-1}(u_d)\end{pmatrix}\right),$$

FIG. 15.2 For any readers who may be curious, this formula represents the density of the Gaussian copula function [45]. The Gaussian copula is a distribution over the unit multidimensional cube. R is the parameter matrix. I is the identity matrix. Theta is the inverse cumulative distribution function of a standard normal.

on the current market value of the vehicles, and without factoring in historical data (Fig. 15.2). The Gaussian copula function was easy to implement, and became a favorite model for predicting risk in the securitization market. Though the formula had its early detractors, it soon became the driving model on Wall Street. In about 2008, the function simply stopped working. At about the same time, stock markets collapsed everywhere on planet earth. In some circles, the Gaussian copula function is blamed for the global economic disaster [44]. [Glossary Correlation distance, Nongeneralizable predictor]

Glossary

Autocoding When nomenclature coding is done automatically, by a computer program, the process is known as "autocoding" or "autoencoding".

Autoencoding Synonym for autocoding.

BLOB A large assemblage of binary data (e.g., images, movies, multimedia files, even collections of executable binary code) that are associated that have a common group identifier and that can, in theory, be moved (from computer to computer) or searched as a single data object. Traditional databases do not easily handle BLOBs. BLOBs belong to Big Data.

Class-oriented programming A type of object-oriented programming for which all object instances and all object methods must belong to a class. Hence, in a class-oriented programming language, any new methods and instances that do not sensibly fall within an existing class must be accommodated with a newly created subclass. All invocations of methods, even those sent directly to a class instance, are automatically delivered to the class containing the instance. Class-oriented programming languages embody a specified representation of the real world in which all objects reside within defined classes. Important features such as method inheritance (through class lineage), and introspection (through object and class identifiers) can be very simply implemented in class-oriented programming languages. Powerful scripts can be written with just a few short lines of code, using class-oriented programming languages, by invoking the names of methods inherited by data objects assigned to classes. More importantly, class-oriented languages provide an easy way to discover and test relationships among objects.

Cloud computing According to the U.S. National Institute of Standards (NIST) and Technology cloud computing enables "ubiquitous, convenient, on-demand network access to a shared pool of configurable computing resources (e.g., networks, servers, storage, applications, and services) that can be rapidly provisioned and released with minimal management effort or service provider interaction" [46]. As the NIST definition would suggest, cloud computing is similar to Big Data, but there are several features that are expected in one and not the other. Cloud computing typically offers an interface and a collection of in-cloud computational services. Cloud data is typically contributed by a large community, and the contributed data is deposited often for no reason other than to provide convenient storage. These features are not expected in Big Data resources. Perhaps the most important distinction

between a cloud computing and Big Data relates to mutability. Because cloud data is contributed by many different entities, for many purposes, nobody expects much constancy; data can be freely extracted from the cloud, or modified in place. In the cloud, the greatest emphasis is placed on controlling computational access to cloud data; with less emphasis on controlling the content of the cloud. In contrast, Big Data resources are designed to achieve a chosen set of goals using a constructed set of data. In most cases, the data held in a Big Data resource is immutable. Once it is entered into the resource, it cannot be modified or deleted without a very good reason.

Correlation distance Also known as correlation score. The correlation distance provides a measure of similarity between two variables. Two similar variables will rise and fall together [47,48]. The Pearson correlation score is popular, and can be easily implemented [49,50]. It produces a score that varies from −1 to 1. A score of 1 indicates perfect correlation; a score of -1 indicates perfect anti-correlation (i.e., one variable rises while the other falls). A Pearson score of 0 indicates lack of correlation. Other correlation measures can be applied to Big Data sets [47,48].

Fair use Copyright and Patent are legal constructs designed to provide intellectual property holders with the uninfringed power to profit from their creative labors, while still permitting the public to have full access to the holders' property. When Public use of copyrighted material does not limit its profitability to the copyright holder, then the "fair use" of the material is generally permitted, even when those uses exceed customary copyright limits. Most countries have some sort of "fair use" provisions for copyrighted material. In the United States, Fair Use is described in the Copyright Act of 1976, Title 17, U.S. Code, section 107, titled, Limitations on exclusive rights: Fair use. Here is an excerpt of the Act: "Notwithstanding the provisions of sections 106 and 106A, the fair use of a copyrighted work, including such use by reproduction in copies or phonorecords or by any other means specified by that section, for purposes such as criticism, comment, news reporting, teaching (including multiple copies for classroom use), scholarship, or research, is not an infringement of copyright. In determining whether the use made of a work in any particular case is a fair use the factors to be considered shall include (1) the purpose and character of the use, including whether such use is of a commercial nature or is for nonprofit educational purposes; (2) the nature of the copyrighted work; (3) the amount and substantiality of the portion used in relation to the copyrighted work as a whole; and (4) the effect of the use upon the potential market for or value of the copyrighted work. The fact that a work is unpublished shall not itself bar a finding of fair use if such finding is made upon consideration of all the above factors" [51].

Grid A collection of computers and computer resources (typically networked servers) that are coordinated to provide a desired functionality. In the most advanced Grid computing architecture, requests can be broken into computational tasks that are processed in parallel on multiple computers and transparently (from the client's perspective) assembled and returned. The Grid is the intellectual predecessor of Cloud computing. Cloud computing is less physically and administratively restricted than Grid computing.

Linear regression A method for obtaining a straight line through a two-dimensional scatter plot. It is not, as it is commonly a "best fit" technique, but it does minimize the sum of squared errors (in the y-axis values) under the assumption that the x-axis values are correct and exact. This means that you would get a different straight line if you regress x on y; rather than y on x. Linear regression is a popular method that has been extended, modified, and modeled for many different processes, including machine learning. Data analysts who use linear regression should be cautioned that it is a method, much like the venerable P-value, that is commonly misinterpreted [25].

Nongeneralizable predictor Sometimes data analysis can yield results that are true, but nongeneralizable (i.e., irrelevant to everything outside the set of data objects under study). The most useful scientific findings are generalizable (e.g., the laws of physics operate on the planet Jupiter or the star Alpha Centauri much as they do on earth). Many of the most popular analytic methods are not generalizable because they produce predictions that only apply to highly restricted sets of data; or the

predictions are not explainable by any underlying theory that relates input data with the calculated predictions. Data analysis is incomplete until a comprehensible, generalizable and testable theory for the predictive method is developed.

***P* value** The *P* value is the probability of getting a set of results that are as extreme or more extreme as the set of results you observed, assuming that the null hypothesis is true (that there is no statistical difference between the results). The *P*-value has come under great criticism over the decades, with a growing consensus that the *P*-value is often misinterpreted, used incorrectly, or used in situations wherein it does not apply [24]. In the realm of Big Data, repeated samplings of data from large data sets will produce small *P*-values that cannot be directly applied to determining statistical significance. It is best to think of the *P*-value as just another piece of information that tells you something about how sets of observations compare with one another; and not as a test of statistical significance.

Predictive modeling contests Everyone knows that science is competitive, but very few areas of science have been constructed as a competitive game. Predictive analytics is an exception. Kaggle is a Web site that runs predictive-modeling contests. Their motto is "We're making data science a sport." Competitors with the most successful predictive models win prizes. Prizes vary from thousands to millions of dollars, and hundreds of teams may enter the frays [52].

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16

Data Reanalysis: Much More Important Than Analysis

OUTLINE

Section 16.1. First Analysis (Nearly) Always Wrong

A new thing is just an old thing that hasn't had an opportunity to disappoint you.
Anon

As we were celebrating the many scientific breakthroughs attributed to Big Data analyses, a disquieting observation intruded upon the festivities. It seems that many of the fundamental studies in the field had yielded irreproducible results. Expensive studies, on massive volumes of data, were providing conclusions that were no more reliable than coin tosses. When we tried to understand why this was happening, we discovered that just about everything that could go wrong was indeed going wrong. Many of the faulty studies came from the field of medicine, but medical failures are easy to spot when patients do not respond to treatment as hoped. We really have no idea as to how many Big Data conclusions from the fields of business, politics, economics, and marketing have been leading us astray.

Consider these shocking headlines.

– "Unreliable research: Trouble at the lab" [1]. The Economist, in 2013 ran an article examining flawed biomedical research. The magazine article referred to an NIH official who indicated that "researchers would find it hard to reproduce at least three-quarters of all published biomedical findings, the public part of the process seems to have failed." The article described a study conducted at the pharmaceutical company Amgen, wherein 53 landmark studies were repeated. The Amgen scientists were successful at reproducing the results of only 6 of the 53 studies. Another group, at Bayer HealthCare, repeated 63 studies. The Bayer group succeeded in reproducing the results of only one-fourth of the original studies.

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- "A decade of reversal: an analysis of 146 contradicted medical practices" [2]. The authors reviewed 363 journal articles, re-examining established standards of medical care. Among these articles were 146 manuscripts (40.2%) claiming that an existing standard of care had no clinical value.
- "Cancer fight: unclear tests for new drug" [3]. This New York Times article examined whether a common test performed on breast cancer tissue (Her2) was repeatable. It was shown that for patients who tested positive for Her2, a repeat test indicated that 20% of the original positive assays were actually negative (i.e., falsely positive on the initial test) [3].
- "Reproducibility crisis: Blame it on the antibodies" [4]. Biomarker developers are finding that they cannot rely on different batches of a reagent to react in a consistent manner, from test to test. Hence, laboratory analytic methods, developed using a controlled set of reagents, may not have any diagnostic value when applied by other laboratories, using different sets of the same analytes [4].
- "Why most published research findings are false" [5]. Modern scientists often search for small effect sizes, using a wide range of available analytic techniques, and a flexible interpretation of outcome results. The manuscript's author found that research conclusions are more likely to be false than true [5,6].
- "We found only one-third of published psychology research is reliable—now what?" [7]. The manuscript authors suggest that the results of a first study should be considered preliminary.
- "A reasonable doubt, the false promise of DNA testing" [8]. An account published in The Atlantic highlights the errors in the analysis of DNA mixtures.

It is now abundantly clear that many scientific findings, particularly those findings based on analyses of large and complex data sets, are yielding irreproducible results [9]. The economic cost attributed to irreproducibility in preclinical studies (i.e., preliminary medical research that occurs before testing on human subjects can begin), is estimated at $28 billion dollars per year, in the United States alone [10].

Anyone who attempts to stay current in the sciences soon learns that much of the published literature is irreproducible [9]; and that almost anything published today might be retracted tomorrow. This appalling truth applies to some of the most respected and trusted laboratories in the world [11–18]. Those of us who have been involved in assessing the rate of progress in disease research are painfully aware of the numerous reports indicating a general slowdown in medical progress [19–26]. For the optimists, it is tempting to assume that the problems that we may be experiencing today are par for the course, and temporary. It is the nature of science to stall for a while and lurch forwards in sudden fits. Errors and retractions will always be with us so long as humans are involved in the scientific process. For the pessimists among us, there seems to be something going on that is really new and different; a game changer. This game changer is the "complexity barrier", a term credited to Boris Beizer, who used it to describe the impossibility of managing increasingly complex software applications [27]. The complexity barrier applies to every modern Big Data project [28–30].

Some of the mistakes that lead to erroneous conclusions in complex, data-intensive research are well known, and include the following:

– Errors in sample selection, labeling, and measurement

Data errors and data documentation errors are common, and there are many examples, from the scientific literature, where such errors are documented [31–35]. Setting aside sampling errors, data analysts must contend with the problem of insufficient sampling [36]. Experimental acumen cannot compensate for a statistically inadequate number of sample specimens.

– Outright fraud

We do not know the frequency of scientific fraud, but there is no reason to believe that fraud is rare [18,37–39]. When a scientist's career is on the line, the temptations to fabricate or fudge data can be overwhelming. The literature is rich with examples of fraud committed in some of the most respected laboratories on earth [12,39–49]. Considering that Big Data is collected from a multitude of researchers, it should come as no great surprise to learn that some of the data included in Big Data resources is fabricated or fraudulent.

– Misinterpretation of the data

The most common source of scientific error is post-analytic, arising from misinterpretation of results [5,24,50–56]. Virtually every journal article contains, hidden in the introduction and discussion sections, some distortion of fact or misleading assertion. Scientists cannot be objective about their own work. As humans, we tend to interpret observations to reinforce our beliefs and prejudices and to advance our agendas [39].

Large, multi-institutional studies involving many human subjects, many specimens, and large collections of data, analyzed by teams of statisticians and computer scientists, carry the veneer of respectability. Manuscript reviewers may be reluctant to reject a work submitted by a group of 100 scientists. Nonetheless, large studies are just as susceptible to errors of data misinterpretation as are studies performed by a single investigator, on a small set of data. Today, some of the largest experimental studies and clinical trials produce results with very small differences between the experimental group and the control group (e.g., an extension of cancer survival time of two weeks, a 10% difference in biomarker levels). When the stakes are high, as is always the case with expensive multi-institutional studies, scientists will be inclined to exaggerate the benefits of a positive finding, no matter how insignificant the results may be. [Glossary Sponsor bias]

One of the most common strategies whereby scientists distort their own results, to advance a self-serving conclusion, is message framing [57]. In message framing, scientists omit from discussion any pertinent findings that might diminish or discredit their own conclusions. The common practice of message framing is often conducted on a subconscious, or at least a sub-rational, level. A scientist is not apt to read articles whose conclusions contradict his own hypotheses and will not cite disputatious works in his manuscripts. Furthermore, if a paradigm is held in high esteem by a majority of the

scientists in a field, then works that contradict the paradigm are not likely to pass peer review. Hence, it is difficult for contrary articles to be published in scientific journals. In any case the message delivered in a journal article is almost always framed in a manner that promotes the author's interpretation.

It must be noted that throughout human history, no scientist has ever gotten into any serious trouble for misinterpreting results. Scientific misconduct comes, as a rule, from the purposeful production of bad data, either through falsification, fabrication, or through the refusal to remove and retract data that is known to be false, plagiarized, or otherwise invalid. In the United States, allegations of research misconduct are investigated by the Office of Research Integrity. Funding agencies in other countries have similar watchdog institutions. The Office of Research Integrity makes its findings a matter of public record [58]. Of 150 cases investigated between 1993 and 1997, all but one case had an alleged component of data falsification, fabrication or plagiarism [59]. In 2007, of the 28 investigated cases, 100% involved allegations of falsification, fabrication, or both [60]. No cases of misconduct based on data misinterpretation were prosecuted. Perhaps the Office of Research Integrity understands that the self-serving interpretation of data in entrenched deep within the human psyche.

Big Data analysis is difficult, and there is no way to work with complex information without making mistakes. This being the case, it seems prudent to assume that every scientific publication, based on the analysis of a single set of data, Big or small, should be considered tentative, until other laboratories confirm the findings.

Section 16.2. Why Reanalysis Is More Important Than Analysis

Prediction is very difficult, especially if it's about the future.

Niels Bohr

One of the nicest things about Big Data, aside from its ample size, is its permanence. We know that if we commit some error on the first analysis of a Big Data collection, we can always get a second bite at the apple; another chance to go back and correct our error, and to possibly produce a conclusion that is more important than anything we originally anticipated. Considering that many of the published studies coming out today are based on the analysis of massive sets of data, the importance of reanalysis cannot be overestimated.

Let us look at some of the specific roles filled by data reanalysis.

– **Verification of data and validation of conclusions**

Verification involves checking to determine whether the data was obtained properly (i.e., according to approved protocols), and that the data accurately measured what it was intended to measure, on the correct specimens, and that all steps in data processing were done using well-documented and approved protocols. Verification often requires a level of expertise that is at least as high as the expertise of the individuals who produced the data [61]. Data verification requires a full understanding of the many steps involved in data

collection and can be a time-consuming task. In one celebrated case, in which two statisticians reviewed a microarray study performed at Duke University, the time devoted to the verification effort was reported to be 2000 hours [62]. To put this in perspective, the official work-year, according to the U.S. Office of Personnel Management, is 2087 hours. Because data verification requires deep knowledge of the data being studied, it stands to reason that data verification is greatly facilitated by preparing well-annotated data that supports introspection.

Validation is a different process than verification. Whereas verification checks the data upon which conclusions are drawn, validation checks to see if the conclusions drawn from the data are correct. Validation usually begins by repeating the same analysis of the same data, using the methods that were originally recommended. Obviously, if a different set of conclusions is reached, using the same data and methods, then the original conclusions failed validation. Validation may also involve applying a different set of analytic methods to the same data, to determine if the conclusions are consistent. Data can be legitimately analyzed by multiple different methods. The ability to draw the same conclusion from a data set, consistently, from multiple methods of analysis, is a type of validation.

Another type of validation involves testing new hypotheses, based on the assumed validity of the original conclusions. For example, if you were to accept Darwin's theory of evolution, then you would expect to find a chronologic archive of fossils in ascending strata of shale. This being the case, paleontologists provided independent validation to Darwin's conclusions.

Scientists rankle at the idea that their data must be inspected, reanalyzed, and sometimes repeated, by other scientists, including competitors. Scientists should understand that data validation requires a great deal of effort, and that the scientists who devote themselves to this task are often interrupting their own careers because they believe that the results under review are of sufficient importance to justify their sacrifice. **Also, the primary purpose of every validation effort is to legitimize the original work, not to discredit the work**. It is better to have a genuine scientific advancement than to have a huge waste of everyone's time and money. [Glossary Primary data, Secondary data]

There is an old saying that "God did not make us perfect, so he compensated by making us blind to our own faults." Verification and validation help us to compensate for our blindness, but we cannot attain definitive conclusions in every case. Realistically, the most we can expect is to verify that the data was obtained properly and to validate that the conclusions fit the results [52,62–66]. To help us, there is a rich literature containing guidelines for achieving validation, including a suite of helpful algorithms, software, devices, statistical methods, and mathematical models [61,67–70].

– **Clarifications and improvements upon earlier studies**

Original data sets can be reanalyzed using alternate or improved methods to attain outcomes of greater precision or reliability than the outcomes produced in the original analysis. Nowhere has this been more successful than in the field of forensics, where newer studies based on experience with large sets of data have led to fundamental changes in the way that forensic evidence is interpreted [8,71–74].

– **Performing additional analyses and updating results from earlier studies**

It is impossible to fully analyze a complex study on the first attempt. There will always be some analytic opportunity that was overlooked [75]. Furthermore, as new data arrives, the original data needs to be reanalyzed, with the newer data. In some cases, the newer data permits the data curator to fill in missing data points, to enter corrections in the original data, and to achieve a more accurate assessment of outlier data points in the original data set. It is a terrible waste to simply abandon an old project, when a reanalysis at some future time, would help tie loose ends and clarify unanswered questions remaining from the first analysis of the original data [76].

– **Extending the scope of the original study**

Sometimes, data collected for one project can be usefully merged with data collected in other projects. Such projects may pertain to previous, concurrent, or future works, just so long as they contain related data. In Chapter 17, we will be discussing data repurposing, which involves using Big Data to answer questions and to achieve results that were not anticipated by the designers of the Big Data resource.

Section 16.3. Case Study: Reanalysis of Old JADE Collider Data

Life can only be understood backwards; but it must be lived forwards.

Soren Kierkegaard

In the 1980s, the PETRA collider conducted a number of so-called atom smashing experiments designed to measure the force required to bind together quarks and gluons, the fundamental components of protons and neutrons. In 1986, the PETRA collider was decommissioned and replaced with colliders that operated at higher energy levels. Several decades passed, and advances in physics raised a new set of questions that could only be answered with observations on low-energy collisions; the kind of observations collected by PETRA and omitted by present-day colliders [77].

An effort to retrieve the 1980s data was spearheaded by Siegfried Bethke, one of the original scientists in PETRA's JADE project [78]. In the period following the decommissioning of PETRA, the original data had been dispersed to various laboratories. Some of the JADE data was simply lost, and none of the data was collected in a format or a medium that was directly accessible.

The project was divided into three missions, involving three teams of scientists. One team rescued the data for archived tapes and transferred the data into a modern medium and format. The second team improved the original JADE software, fitting it to modern computer platforms. By applying software that used updated Monte Carlo simulations, the second team generated a new set of data files. The third team reanalyzed the regenerated data using modern methods and improved calculations.

The project culminated in the production of numerous scientific contributions that could not have been achieved without the old JADE data. Success was credited, at least in part, to the participation of some of the same individuals who collected the original data.

Section 16.4. Case Study: Vindication Through Reanalysis

> *That which can be asserted without evidence, can be dismissed without evidence.*
>
> *Christopher Hitchens*

In 1978, Joseph Strauch published a phylogenetic taxonomy of Charadriiformes birds (i.e., a subclassification based on evolutionary descent), by studying their bones (i.e., via osteology) [79]. When he was finished his project, he left his osteologic data for others to reanalyze. As it happened, his conclusions stirred a controversy that persisted over several decades. Nearly 20 years later, Phillip Chu took a hard look at Strauch's measurements [80]. Chu re-coded Strauch's data to eliminate objectionable feature assignments. Chu conducted a parsimony analysis of the data rather than using Strauch's compatibility analysis; both being methods that establish phylogenetic order. In the end, Chu's study confirmed Strauch's findings.

It is not particularly easy to publish journal manuscripts that vindicate earlier works. Journal editors, traditionally, are interested in publishing new science; not in revisiting previously published studies. It is plausible that Chu's paper, reanalyzing Strauch's work, was worthy of publication only because Strauch's early work had been publicly challenged by his colleagues [81]. Journal editors should be receptive to reanalysis manuscripts as they often provide new insights that advance their fields [82]. In many cases, reanalysis is the most effect way by which scientific truth can be established.

Reanalysis can only be performed on studies for which data is available. Scientists can avoid having their studies reanalyzed by simply withholding their data from their colleagues.

Section 16.5. Case Study: Finding New Planets From Old Data

> *Many an object is not seen, though it falls within the range of our visual ray, because it does not come within the range of our intellectual ray, i.e. we are not looking for it. So, in the largest sense, we find only the world we look for.*
>
> *Henry David Thoreau in Journal, 2 July 1857*

Astronomers gather enormous amounts of information on stars. Such data includes direct photographic images of stars, using improved telescopes (e.g., Hubble Space Telescope), high-resolution spectroscopy data, X-ray data (e.g., from NASA's Chandra X-ray

observatory). As it happens, if a star is orbited by planets, those planets will have some effect, over the course of time, on the measurements collected on the star [83].

Over the past decade, using preexisting star data, astronomers have found evidence for thousands of extrasolar planets (exoplanets). Some of the planet-hunting techniques include [83]:

- Transit method. Exoplanets dim the light received from a star during their transit.
- Radial velocity or Doppler method. Exoplanets can cause the star's speed to vary with respect to the speed at which the star moves toward or away from the earth, and this variation in speed causes a Doppler shift in the star's emitted spectral lines.
- Transit timing variation. If a star is orbited by multiple planets then the time when an exopolanet begins its transit across the star and the duration of its transit will vary depending on the other planets in the vicinity at the time of transit.
- Gravitational microlensing. Exoplanets orbiting a lensing star can produce perturbations in the measured magnification of the lensing phenomenon.
- Astrometry. Orbiting exoplanets can change the star's position in the sky.
- Pulsar timing. Orbiting exoplanets may cause small perturbations in the timing of radio wave pulsations. This method, which applies only to planets orbiting pulsars, was employed to find the first confirmed exoplanet in 1992.
- Direct imaging. When the exoplanets are large and the star is relatively close to the earth the exoplanets can be imaged directly by blocking the light produced by their star (Fig. 16.1).

Today, new methods of finding exoplanets are being developed. Existing data is being reanalyzed to accommodate new techniques as they arrive. Data that has already been

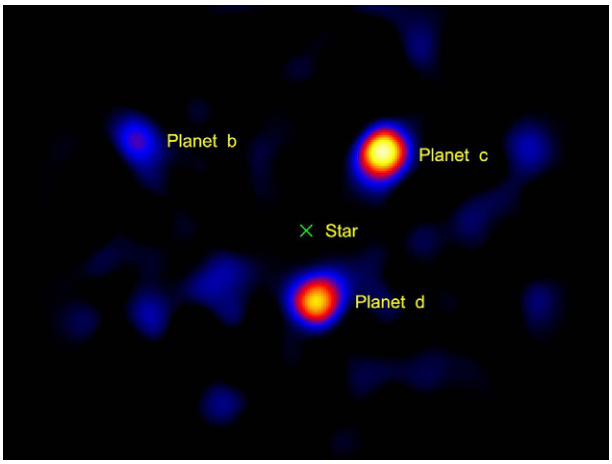

FIG. 16.1 Actual image of three exoplanets orbiting HR8799, 120 light years from earth, was obtained. The orbiting exoplanets were made visible in the image, by blocking out the image of their star. *From NASA, obtained with the Palomar Observatory's Hale Telescope, public domain.*

used to find exoplanets is being reanalyzed to validate the original conclusions, and to help find additional planets missed in the first analysis, and to uncover new information about exoplanets that have been discovered [84].

Glossary

Primary data The original set of data collected to serve a particular purpose or to answer a particular set of questions, and intended for use by the same individuals who collected the data.

Secondary data Data collected by someone else. Much of the data analyses performed today are done on secondary data [85]. Most verification and validation studies depend upon access to high-quality secondary data. Because secondary data is prepared by someone else, who cannot anticipate how you will use the data, it is important to provide secondary data that is simple and introspective.

Sponsor bias Are the results of big data analytics skewed in favor of the corporate sponsors of the resource? In a fascinating meta-analysis, Yank and coworkers asked whether the results of clinical trials, conducted with financial ties to a drug company, were biased to produce results favorable to the sponsors [86]. They reviewed the literature on clinical trials for anti-hypertensive agents, and found that ties to a drug company did not bias the results (i.e., the experimental data), but they did bias the conclusions (i.e., the interpretations drawn from the results). This suggests that regardless of the results of a trial, the conclusions published by the investigators were more likely to be favorable, if the trial were financed by a drug company. This should come as no surprise. Two scientists can look at the same results and draw entirely different conclusions.

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17

Repurposing Big Data

OUTLINE

Section 17.1. What Is Data Repurposing?

If you want to make an apple pie from scratch, you must first create the universe.
Carl Sagan

Big Data resources are so very difficult to create and maintain that they really should not be devoted to any single use. We might as well get the most for our investments, and this means that we should repurpose our data. Data repurposing involves taking pre-existing data and performing any of the following [1]:

– **Finding new uses for data**

Fingerprints have been used, since antiquity, as a method for establishing the identity of individuals. Fingerprints were pressed onto clay tablets, seals, and even pottery left by ancient civilizations that included Minoan, Greek, Japanese, and Chinese. As early as the second millennium BCE, fingerprints were used as a type of signature in Babylon, and ancient Babylonian policemen recorded the fingerprints of criminals.

Toward the close of the 19th century, Francis Galton repurposed fingerprint data to pursue his own particular interests. Galton was primarily interested in the heritability and racial characteristics of fingerprints, a field of study that can be described as a scientific dead-end. Nonetheless, in pursuit of his interests, he devised a way of classifying fingerprints by patterns (e.g., plain arch, tented arch, simple loop, central pocket loop, double loop, lateral pocket loop, and plain whorl). This classification launched the new science of fingerprint identification, an area of research that has been actively pursued and improved over the past 120 years (Fig. 17.1).

Principles and Practice of Big Data. https://doi.org/10.1016/B978-0-12-815609-4.00017-0

FIG. 17.1 U.S. Federal Bureau of Investigation Fingerprint Division, World War II. *From FBI, public domain.*

In addition to Galton's novel classification methods, two closely related technological enhancements vastly increased the importance of fingerprints. The first was the incredibly simple procedure of recording sets of fingerprints, on paper, with indelible ink. With the simple fingerprint card, the quality of fingerprints improved, and the process of sharing and comparing recorded fingerprints became more practical. The second enhancement was the decision to collect fingerprint cards in permanent population databases (literally, digital data). Fingerprint databases enabled forensic scientists to match fingerprints found at the scene of a crime, with fingerprints stored in the database. The task of fingerprint matching was greatly simplified by confining comparisons to prints that shared the same class-based profiles, as described by Galton.

Repurposing efforts have expanded the use of fingerprints to include authentication (i.e., proving you are who you claim to be), keying (e.g., opening locked devices based on an authenticated fingerprint or some other identifying biometric), tracking (e.g., establishing the path and whereabouts of an individual by following a trail of fingerprints or other identifiers), and body part identification (i.e., identifying the remains of individuals recovered from mass graves or from the sites of catastrophic events). In the past decade, flaws in the vaunted process of fingerprint identification have been documented, and the improvement of the science of identification is an active area of investigation [2].

Today, most of what we think of as the forensic sciences is based on object identification (e.g., biometrics, pollen identification, trace chemical investigation, tire mark investigation, and so on). When a data object is uniquely identified, its association with additional data can be collected, aggregated, and retrieved, as needed.

– **Performing original research that could not have been performed when the data was collected**

History is replete with examples of old data driving new discoveries. A recent headline story explains how century old tidal data plausibly explained the appearance of the

iceberg that sank the titanic, on April 15, 1912 [3]. Records show that several months earlier, in 1912, the moon, Earth, and sun aligned to produce a strong tidal pull, and this happened when the moon was the closest to the earth in 1400 years. The resulting tidal surge was sufficient to break the January Labrador ice sheet, sending an unusual number of icebergs toward the open North Atlantic waters. The Labrador icebergs arrived in the commercial shipping lanes four months later, in time for a fateful rendezvous with the Titanic. Back in January 1912, when tidal measurements were being collected, nobody foresaw that the data would be examined a century later.

Clever scientists are finding that old data can be reanalyzed to answer questions that were not anticipated by the scientists who performed the original study. Getting new uses from old data is the most cost-effective means of conducting research, and should be encouraged [1]. [Glossary Data archeology]

– **Creating novel data sets through data file linkages**

Introspective data, data triples, and data schemas are concepts that had little resonance before the days of Big Data. Using techniques that link heterogeneous forms of data to Web Locations is the basis for the so-called Semantic Web, the largest Big Data resource available to everyone [4]. The Semantic Web can be imagined as one enormous data re-purposing project in which everyone pursues their own purposes. [Glossary Heterogeneous data]

For data professionals, repurposing will often involve one or more of the following efforts:

– Finding subsets in a population once thought to be homogeneous
– Seeking new relationships among data objects
– Creating new concepts or ways of thinking about old concepts based on a re-examination of data
– Fine-tuning existing data models
– Starting over and remodeling systems

Section 17.2. Dark Data, Abandoned Data, and Legacy Data

> *We need above all to know about changes; no one wants or needs to be reminded 16 hours a day that his shoes are on.*
>
> *David Hubel*

Every child believes, for a time, that the universe began with his own birth. Anything preceding his birth is unreal, and of no consequence. Many Big Data resources have a similar disregard for events that preceded their birth. If events occurred prior to the creation of the Big Data resource, then those events have no consequence and can be safely ignored. Of course, this is absurd. It is accurate to think of new data as the result of events that involved old data; nothing in the universe occurs in the absence of preceding events.

Today, a large part of data science is devoted to finding trends in data; determining the simple functions that model the variation of data over time, and predicting how data will change in the future. These analytic activities require prior data that is annotated with a time measurement. Analysis of such data often reveals long-term trends, short-term trends, and periodic trends, often with characteristic forms (e.g., linear, exponential, power series). Hence, new data has very little meaning when it is not interpreted along with old data.

It is a shame that legacy data gets such shabby treatment by Big Data creators. Old data often resides in obsolete formats, on obsolete media, without proper annotation, and is collected under dubious circumstances. The incorporation of legacy data into modern Big Data resources is a tall order, but we need to make an effort to save legacy data whenever possible. Managers of Big Data resources are often expected to absorb smaller, older data sets. We cannot just pretend that such data has a lesser role than new data.

The healthcare industry is a prime example of Big Data in search of a legacy. President Barack Obama had set a goal for every American to have a secure medical record. What might such records include? Let us consider the medical record for a hypothetical patient named Lily Livesy, age 92. Not only has Lily outlived her doctors; she has outlived most of her hospitals. Though she lived in one city all her life, several of the hospitals that administered her medical care have been closed, and the records destroyed. In the past thirty years, she has received medical care at various doctor's offices, and in various departments in various hospitals. Some of these hospitals kept paper records; some had electronic records. Only one of the hospitals had anything that might be likened to an integrated hospital information system that aggregated transaction records produced by the various hospital departments (pharmacy, pathology, radiology, surgery, medicine, and so on). This hospital initiated a new Electronic Health Record system in the year 2013. Unfortunately, the new system is not compatible with the same hospital's prior information system, and the old records did not transfer to the new system. Consequently, in the year 2019, Lily Livesy, age 92, has one Electronic Health Record, residing in one hospital's information system, with no contribution from any other medical facility, and this Electronic Health Record contains a secure identifier, but no actual medical information. Her 92 year-long medical history is virtually blank. The same data deficits would apply to millions of other Americans. This is why, despite our best intentions, complete medical records, extending from birth to death, for all American citizens, will not be attainable anytime this century.

Often, the utility of legacy data comes as an afterthought inspired by a preliminary analysis of contemporary data. If a cancer researcher notices that the incidence of a certain tumor is high, he or she would naturally want to know whether the incidence of the tumor has been increasing over the past five years, ten years, 15 years and so on. A forensic criminologist who collects a CODIS signature on a sample of DNA might desperately need to check his sample against CODIS signatures collected over the past five decades. The most useful Big Data resources reach back through time. [Glossary CODIS]

Legacy data plays a crucial role in correcting the current record. It is not unusual for people to rely on flawed data. If we knew the full history of the data, including how it

was originally collected, and how it was modified over time, we might avoid reaching erroneous conclusions. Several years ago, newspaper headlines drew attention to a modern manual for prisoner interrogation, used by U.S. forces stationed in Guantanamo. It turned out that the manual was a republication of a discredited Chinese operations manual used during the Korean War. The chain of documentation linking the current manual back to the original source had been broken [5]. In another example of lost legacy data, a Supreme Court decision was based, in part, on flawed information; an earlier statute had been overlooked [6]. Had the legacy data been raised during deliberations, an alternate Supreme Court verdict may have prevailed. To know the history of a data source, we need access to the legacy data that documents the original sources of our data, and permits us to trace the modifications of the data, over time.

It is human nature to evaluate the world through direct observations. If we want to know the length of an object, we measure its length with a ruler. If we want to know the number of eggs in a basket, we count the eggs. There are times when direct observations are not the best way to understand our world. If we are clever, we can determine the height of an object by comparing the length of its shadow, with the length of the shadow of an object of known height. We can estimate the number of eggs in a basket by weighing the basket, with and without the eggs, and dividing the total weight of the eggs by the predetermined average weight of a single egg. When we have a wealth of descriptive data about many different objects in our environment, we can derive new meaning from old measurements. The remainder of this chapter is devoted to five cases in point.

Section 17.3. Case Study: From Postal Code to Demographic Keystone

When you get to a fork in the road, take it.

Yogi Berra

There are three ways to assign integers to objects: cardinals, ordinal, and nominals. Cardinals tell us the number of objects (e.g., 2, 5, or ten items). Ordinals give us a rank (e.g., 1st, or 5th, or 8th place in a list). Nominal means "in name only", and nominals are arbitrary numbers that help identify an object. Telephone numbers, social security numbers, and zip codes are nominals. Nominals can be added together or multiplied, and divided, but it would be pointless to do so. Despite its self-effacing definition and its limited mathematical utility, nominal data sets are among the most useful of legacy data resources [1].

Zip codes were contrived by the U.S. Postal service to speed the distribution of mail. The original 5-digit zip codes were introduced in the early 1960s, with each zip code representing a geographic area containing a roughly equivalent segment of the population. The first three digits of the zip code identify mail distribution centers, from which mail sorted by the remaining two digits is distributed to the proper post offices. In the 1980s, an

additional 4 digits was appended to the zip code, identifying individual buildings within the boundary of the 5-digit code.

Because zip codes describe geographic and demographic areas, they can be assigned a longitude, latitude, and elevation, typically measured at the geographic center of its boundaries. All data to which a zip code is attached (e.g., addresses, charge card transactions, crime reports, occurrences of reportable diseases, deaths, electricity consumption, water resources, homes receiving cable television, broadband usage) can be organized with the zip code serving as its primary record key. The lowly zip code, intended as an aid to mailmen, has been repurposed to serve entrepreneurs, epidemiologists, resource managers, and many others.

Section 17.4. Case Study: Scientific Inferencing From a Database of Genetic Sequences

> *It [natural selection] is all about the survival of self-replicating instructions for self-replication.*
>
> *Richard Dawkins [7]*

With the exception of identical twins, parthenogenetic offspring, and clones, every organism on earth has a unique sequence of DNA-forming nucleotides that distinguishes its genetic material (i.e., it's genome) from the genome of every other organism. If we were to have a record of the complete sequence of nucleotides in an individual's genome, we could distinguish that individual from every other organism on earth, by comparing genome sequences. This would require a lot of digital storage for every organism. In the case of humans, the genome is 3 billion nucleotides in length. As luck would have it, because there is enormous variation in genome sequence, from individual to individual, the identity of human individuals can be established by sampling short segments of DNA [1].

CODIS (Combined DNA Index System) collects the unique nucleotide sequences of the equivalent 13 segments of DNA, for every individual included in the database [8]. Using CODIS, DNA sampled at a crime scene can be matched against DNA samples contained in the database. Hence, the identity of individuals whose DNA is found at a crime scene can often be established. In the absence of a match it is sometimes possible to establish the genetic relationship (i.e., paternal or maternal relatives) between crime scene samples and individuals included in the database.

CODIS serves as an example of a database with narrow scope (i.e., names of people and associated DNA sequences), and broad societal value. The basic design of the CODIS database can be extended to any organism. For example, a database of DNA samples collected from individual trees in a geographic location can establish the source of seeds or pollen grains sticking to an article of clothing, and this information might lead to the location where a criminal event transpired. A population database containing full

genome DNA sequences could be used to determine the presence or absence of disease-causing genes in individuals or to predict the response of an individual to a particular drug [9–12].

Section 17.5. Case Study: Linking Global Warming to High-Intensity Hurricanes

> *You can observe a lot by watching.*
>
> *Yogi Berra*

The UK Hadley Centre maintains a database of sea surface temperatures, over a 5-degree latitude-longitude global grid, from the year 1850, to the present, and updated monthly [13]. This data tells us how the ocean temperature changes seasonally and geographically, over time. Kerry Emanuel found a new use for the Hadley data when he noticed an association between regionally increased ocean temperatures and particularly strong hurricanes spawned in these same regions. Reviewing 50 years of data, Emanuel confirmed that the intensity of hurricanes increased in step with the warming of the North Atlantic and Pacific oceans [14]. A data set, intended primarily for charting trends in water temperature and correlating those trends with the oceanic reach of sea ice, found a new use: forecasting the intensity of hurricanes [1].

Section 17.6. Case Study: Inferring Climate Trends With Geologic Data

> *We waste a lot of time waiting for spectacular new material. We haven't sat down and taken a very close look at the material we have.*
>
> *Bettina Stangneth, historian and author of "Eichmann Before Jerusalem: The Unexamined Life of a Mass Murderer" [15]*

Mountains are like icebergs made of rock. The bulk of a mountain is buried underground. When the top of the mountain is eroded, the weight of the mountain is reduced, and the mountain bobs upwards, a little bit. The natural process through which mountains are flattened, over eons, requires the erosion of its surface plus its ever-rising subsurface.

When water is sucked from a mountain, the mountain lightens and rises. Likewise, if the water is sucked out of a tectonic plate, the entire plate (i.e., the surface of the planet overlying the plate) will rise. The National Science Foundation's Plate Boundary Observatory provides precise measurements of ground positions from data generated by GPS (Global Positioning System) satellites. A group of scientists working at the Scripps Institution of Oceanography found that all of the ground stations in the western United States exhibited measurable uplift. In the period 2003–04, the western states rose an average of 0.15 inches, and the western mountains rose more than half an inch in the same period.

This wide rise coincides with a long drought in the west. It would seem that the only explanation for the uplift of the tectonic plate, and the greater uplift of the western mountains, is the loss of water, via evaporation, without replacement. So strong is the relationship between water loss and mountain rise that water resources in the west can now be tracked with GPS ground measurements [16,1].

Section 17.7. Case Study: Lunar Orbiter Image Recovery Project

> *The world is the totality of facts, not things. (Die Welt ist die Gesamtheit der Tatsachen, nicht der Dinge)*
>
> *Ludwig Wittgenstein*

Following the first Apollo mission to the moon (Apollo 11, July 20, 1969), the five subsequent Apollo missions left behind recording instruments on the lunar surface. The collective set of downlinked data received from these instruments in known as the Apollo Lunar Surface Experiments Package (ALSEP). More than 11,000 data tapes were recorded [1].

During the Apollo program, control and use of the tapes, as well as the responsibility to safely archive the tapes, was transferred among various agencies and institutions. When the Apollo mission ended, funds were low, and a portion of the data that had been distributed to various investigators and agencies was never sent to the official archives [17]. It should come as no surprise that, at the present time, about half of the ALSEP tapes are missing; their whereabouts uncertain. Of the available tapes, much of the data is difficult to access, due to the use of abandoned data media (i.e., 7 and 9 track tapes) and obsolete data formats [17].

Available ALSEP data, when converted into a modern data format, has proven to be a valuable asset, when reanalyzed with modern analytic tools (Figs. 17.2 and 17.3). For example, the first analyses of ALSEP's seismic data, conducted 35 years ago, indicated that about 1300 deep moonquakes had occurred during the period when the data was being downlinked. The field of seismic analysis has advanced in the interim. A reanalysis of the

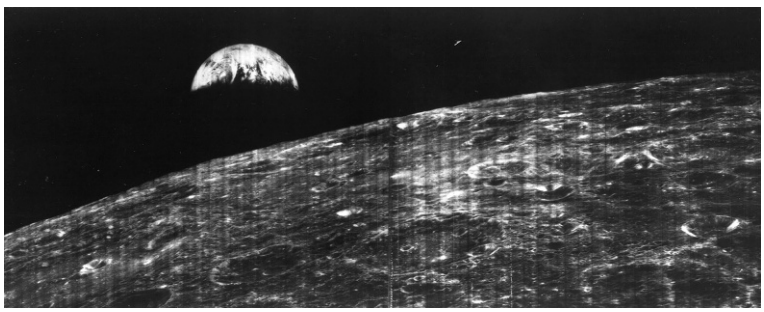

FIG. 17.2 Earth's first view of itself, from a location near the moon, by the United States Lunar Orbiter I, on August 23, 1966. *From U.S. National Aeronautics and Space Administration (NASA), public domain.*

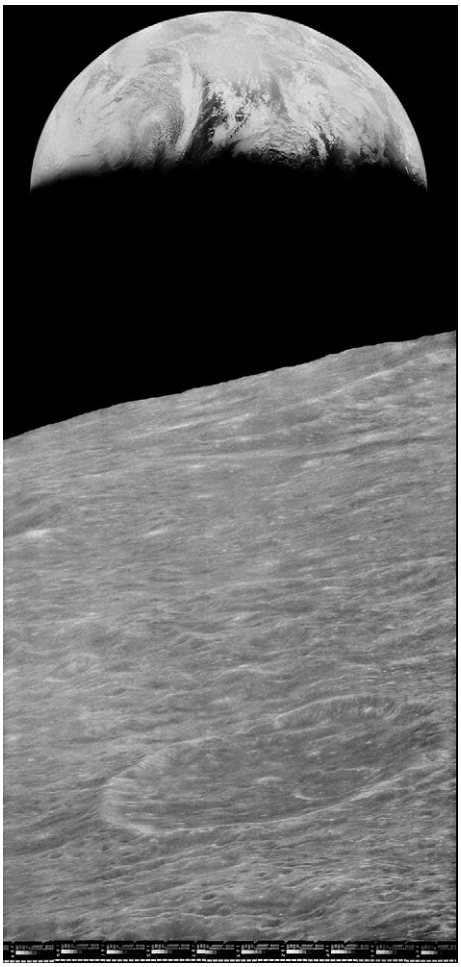

FIG. 17.3 Same image, but processed and enhanced by NASA. *From NASA, public domain.*

same data, using modern techniques, has produced an upward revision of the first estimate; to about 7000 deep moonquakes [17].

Today, there is a renewed push to find, collect and archive the missing ALSEP data. Why is there a sudden urgency to finish a chore that should have been completed decades ago? Simply put, the tapes must be restored before the last of the original investigators, who alone understand the scope and organization of the data, vanish into retirement or death.

Glossary

CODIS Abbreviation for Combined DNA Index System. CODIS is a collection of the unique nucleotide sequences of the equivalent 13 segments of DNA, for every individual included in the database [8]. The CODIS database is used by law enforcement personnel and contains identifying DNA sequences

for individuals who have been processed within the criminal justice system. DNA obtained at a crime scene can be matched against DNA samples contained in the database. Hence, the identity of individuals whose DNA is found at a crime scene can often be established. In the absence of a match, it is sometimes possible to establish the genetic relationship (i.e., paternal or maternal relatives) between crime scene samples and individuals included in the database.

Data archeology The process of recovering information held in abandoned or unpopular physical storage devices, or packaged in formats that are no longer widely recognized, and hence unsupported by most software applications. The definition encompasses truly ancient data, such as cuneiform inscriptions stored on clay tablets circa 3300 BCE, and digital data stored on 5.25-inch floppy disks in Xyrite word-processor format, circa 1994.

Heterogeneous data Sets of data that are dissimilar with regard to content, purpose, format, organization, and annotations. One of the purposes of Big Data is to discover relationships among heterogeneous data sources. For example, epidemiologic data sets may be of service to molecular biologists who have gene sequence data on diverse human populations. The epidemiologic data is likely to contain different types of data values, annotated and formatted in a manner that is completely different from the data and annotations in a gene sequence database. The two types of related data, epidemiologic and genetic, have dissimilar content; hence they are heterogeneous to one another.

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18

Data Sharing and Data Security

OUTLINE

Section 18.1. What Is Data Sharing, and Why Don't We Do More of It?

> *It's antithetical to the basic norms of science to make claims that cannot be validated because the necessary data are proprietary.*
>
> *Michael Eisen [1]*

Without data sharing, there can be very little progress in the field of Big Data. The reasons for this are simple:

- Research findings have limited value unless they are correlated with data contained in other databases.
- All findings, even those based on verified data, are tentative and must be validated against data contained in multiple datasets.
- Unless data is shared, scientists cannot build upon the work of others, and science devolves into a collection of research laboratories working in isolation from one another, leading to intellectual stagnation [1,2].
- Scientific conclusions have no credibility when the research community, oversight agencies, and the interested public cannot review the data upon which the findings were based and the details of how that data was measured.

Without data sharing, we do not have science. We just have people with their own agendas asking us to believe their conclusions. A long list of anguished position papers, urging researchers to share their data, has been published [3–8]. To be sure, there are technical obstacles to data sharing, but for every technical obstacle, there is a wealth of literature offering solutions [9–20].

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Despite the imperatives of data sharing, scientists have been slow to adopt data sharing policies [6]. Because the issue of data sharing is so important to the field of Big Data, it is worth reviewing the impediments to its successful implementation.

Section 18.2. Common Complaints

Science advances funeral by funeral.

Folk wisdom

Here is a listing of the commonly heard reasons for withholding data from the public, along with suggested remedies.

– **To protect scientists from "research parasites"**

A recent opinion expressed by two editors of the New England Journal of Medicine, in an essay entitled "Data Sharing," expressed concern that a new brand of researcher uses data generated by others, for his or her own ends. The editors indicated that some front-line researchers characterize such individuals as "research parasites" [21]. The essayists suggested that researchers who want to use the data produced by others should do so by forming collaborative partnerships with the group that produced the original data [21].

The idea of collaborative partnerships may have been a reasonable strategy 30 years ago, before the emergence of enormous datasets, built from the work of hundreds of data contributors. Negotiating for data, with the promise of developing a mutually beneficial collaboration, is not a feasible option. Today, scientific projects may involve dozens or hundreds of scientists, with no single individual claiming ownership or responsibility for the aggregate data set. The individual contributors may have only the dimmest awareness of their own role in the effort. Under these circumstances, an outside investigator is unlikely to find an identifiable individual or group of individuals with the technical expertise, the scientific judgment, the legal standing, the ethical authority, and the strength of will, to negotiate a new collaboration and to surrender a large set of data.

Today, well-designed data sets can be merged with other sources of data, and repurposed for studies that were never contemplated by the original data contributors [22]. The goal of Big Data is to create data sets that can be utilized by the entire scientific community, with minimal barriers to access. **Characterizing data users as "research parasites," as witnessed in the New England Journal of Medicine article, misses the whole point of Big Data science** [21].

– **To avoid data misinterpretation**

Every scientist who releases data to the public must contend with the fear that a member of the public will misinterpret the data, reach an opposite conclusion, publish their false interpretation, and destroy the career of the trusting soul who was kind enough to provide the ammunition for his own execution. Teams of scientists developing a new drug or treatment protocol, may fear that if their data is released to the public, their

competitors may seize the opportunity to unjustly critique their work and thus jeopardize their project.

Examples of such injustices have been sought, but not found [6]. There is no evidence that would lead anyone to believe that a misinterpretation of data has ever overshadowed a correct interpretation of data. Scientists have endured the withering criticisms of their colleagues since time immemorial. As they say, it comes with the territory. Hiding data for the purpose of avoiding criticism is unprofessional.

– **To limit access to responsible professionals**

Some researchers believe that data sharing must be a conditional process wherein investigators submit their data requests to a committee of scientists who decide whether the request is justified [23]. In some cases, the committee retains the right to review any results predicated on the shared data, with the intention of disallowing publication of results that they consider to be objectionable.

There are serious drawbacks to subjecting scientists to a committee approval process. The public needs unfettered access to the original data upon which published research results are based. Anything less makes it impossible to validate the conclusions drawn from the data, and invites all manner of scientific fraud. In the United States, this opinion is codified by law. The Data Quality Act of 2002 restrains government agencies from developing policies based on data that is unavailable for public review [24–27]. [Glossary Data Quality Act]

– **To sustain the traditional role of data protector**

Lawyers, bankers, healthcare workers, and civil servants are trained to preserve confidentiality; much like priests protect the confessional. It is understandable that many professionals are reluctant to share their data with the world-at-large. Nonetheless, it is unreasonable to hide data that has scientific value.

Before confidential information is released, data holders must be convinced that data sharing can be accomplished without breaching confidentiality, and that the effort spent in the process will yield some benefit to the individuals whose data is being appropriated. A large literature on the subject of safely sharing confidential data is readily available [28–33].

– **To await forthcoming universal data standards**

Trying to merge data sets that are disorganized is impossible, as is merging data sets wherein equivalent types of data are discordantly annotated. Because researchers and other data collectors use a variety of different types of software to collect and organize their data, obstacles raised by data incompatibility have been a major impediment to data sharing. The knee-jerk solution to the problem has always been to create new data standards.

In the past few decades, the standards-making process has evolved into a major industry [34]. There are standards for describing, organizing, and transmitting data. There are

dozens, maybe hundreds, of standards, nomenclatures, classifications, and ontologies for the various domains of Big Data information, and all of these intellectual products are subject to multiple revisions. [Glossary Classification versus ontology]

The hunger for standards is insatiable [35]. The calls for new standards and new ontologies never seems to end. The many shortcomings of standards were discussed at length in Chapter 7, "Standards and Data Integration." It must be noted that the proliferation of standards, many of which are abandoned soon after they are created, has served to increase the complexity and decrease the permanence of Big Data resources [28,36].

Despite all the effort devoted to data standards, there is no widely adopted system for organizing and sharing all the different types of data encountered in Big Data resources. Perhaps the "standard" answer is not the correct answer, in this instance. Specifications, discussed in detail in Section 7.2, are a possible alternative to standards, and should be considered an option for those who are open to suggestion in this matter.

– **To protect legal ownership**

Ownership is a mercantile concept conferring the right to sell. If someone owns a cow, that means that they have the right to sell the cow. If you own a house, even a mortgaged house, then you have the right to sell the house. Let's focus on one particular type of confidential record that pertains to virtually everyone: the medical record. Who owns your confidential medical record? Is it owned by the patient? Is it owned by the medical center? Is it owned by anyone?

In law, there does not seem to be anyone who has the right to sell medical records; hence, it is likely that nobody can claim ownership. Still, medical institutions have a fiduciary responsibility to maintain medical records for their patients, and this entitles both patients and healthcare providers to use the records, as needed. Patients have the right to ask hospitals to send their medical records to other medical centers or to themselves. Hospitals are expected to archive tissues, medical reports and patient charts to serve the patient and society. In the United States, State health departments, the Centers for Disease Control and Prevention (CDC), and cancer registries all expect medical centers to deliver medical reports on request.

In all the aforementioned examples, data sharing is conducted without jeopardizing, or otherwise influencing, the data holder's claim of ownership.

– **To comply with rules issued from above**

It is not uncommon for researchers to claim that they would love to share their data, but they are forbidden from doing so by the lawyers and administrators at their institutions. Two issues tend to dissuade administrators from data sharing. The first is legal liability. Institutions have a responsibility to avoid punitive tort claims, such as those that may arise if human subjects complain that their privacy has been violated when their confidential information is shared. From the viewpoint of the institution, the simplest remedy is to forbid scientists from sharing their data. Secondly, institutions want to protect their own intellectual property, and this would include patents, drug discoveries, manufacturing

processes, and even data generated by their staff scientists. Institutions may sometimes equate data sharing with poor stewardship of intellectual property. [Glossary Intellectual property]

When an institution forbids data sharing, as a matter of policy, scientists should argue that the institution cannot facilitate or promote its own research. Simply put, if Institution A does not share its data with Institution B, then Institution B will not share its data with Institution A. In addition, when Institution A publishes a scientific breakthrough, then Institution B will not find those claims credible, until their own researchers can review the primary data.

It is easy to forget that society, as a whole, benefits when scientific projects lead to discoveries. Without data sharing, those benefits will come at a glacial pace, and at great expense. Institutions have a societal obligation to advance science through data sharing.

– **To demand reimbursement**

Professionals are, by definition, people who are paid for their services. Professionals who go to the trouble of providing data to the public will want to be reimbursed. Data holders can be reassured that if they have created data at their own expense, for their own private use, then that data is theirs to keep. Nobody will take that data from them. But if the data holders have made public assertions based on their data, then they should understand that the scientific community will not give those assertions any credence, without having the data available for review.

The price that researchers pay for withholding their data (i.e., lack of validation of conclusions and professional obscurity) far exceeds the negligible costs of data sharing. Contrariwise, if the data is shared, and their results are validated, then their payment may come in the form of future grants, patents, prestige, and successful collaborations.

– **To avoid distributing flawed data**

Scientists are reluctant to release data that is full of errors. In particular, data curators may fear that if such data is released to the public, they will be inundated with complaints from angry data analysts, demanding that every error be corrected.

A 2011 study has shown that researchers with high quality data were, generally, willing to share their data [37]. Researchers who had weak data, that might support various interpretations and contrasting conclusions, were less willing to share their data. It is important to convince the scientists who create and hold data that the researchers who use their data, without asking permission and without forming collaborations, are not "research parasites"; they are the people who will validate good work, improve upon imperfect work, and create new work from otherwise abandoned data. The societal push toward data sharing should provide a strong impetus for scientists to improve the value of their data, so that they will something worth sharing.

Aside from corrections, all data sets need constant updating, and there are proper and improper ways of revising data (discussed in Section 8.1, "The Importance of Data that

Cannot Change"). Dealing with change, in the form of revised systems of annotations, and revised data elements, is part of the job of the data curator.

Institutions cannot refuse to share their data simply because their data contains errors or is awaiting revisions. Flawed data is common, and it's a safe bet that every large data set contains errors [38]. Institutions and scientific teams should hire professionals with the requisite skills to properly prepare, correct, and improve upon their data collections.

– **To protect against data hackers**

Properly deidentified, Big Data records may contain information that, when combined with data held in other databases, may uniquely identify patients [39]. As an obvious example, if a medical record contains an un-named patient's birth date, gender and zip-code, and a public database lists names of people in a zip-code, along with their birth dates and gender, it is a simple step to ascertain the identity of "deidentified" patients.

A specific instance, making national news headlines, may serve to clarify just how this may happen [40]. A 15-year-old boy was fathered using anonymously donated sperm. The boy wanted to know the identity of his biological father. A private company, had created a DNA Database from 45,000 DNA samples. The purpose of the database was to allow clients to discover kin by having their DNA compared with all the DNA samples in the database. The boy sent his DNA sample to the company, along with a fee. A comparison of the boy's Y chromosome DNA (inherited exclusively from the father) was compared with Y chromosome DNA in the database. The names of two men with close matches to the boy's Y chromosome were found.

The boy's mother had been provided (from the sperm bank) with the sperm donor's date of birth and birthplace. The boy used an online service to obtain the name of every man born in the sperm donor's place of birth on the sperm donor's date of birth. Among those names, one name matched one of the two Y-chromosome matches from the DNA database search. This name, according to newspaper reports, identified the child's father. [Glossary Y-chromosome]

In this case, the boy had access to his own uniquely identifying information (i.e., his DNA and specifically his Y chromosome DNA), and he was lucky to be provided with the date of birth and birthplace of his biological father. He was also extremely lucky that the biological father had registered his DNA in a database of 45,000 samples. And he was lucky that the DNA database revealed the names of its human subjects. The boy's success in identifying his father required a string of unlikely events, and a lax attitude toward subject privacy on the part of the personnel at the sperm bank and the personnel at the DNA database.

Regardless of theoretical security flaws, the criminal or malicious identification of human subjects included in deidentified research data sets is extremely rare. More commonly, confidential records (e.g., personnel records, credit records, fully identified medical records) are stolen wholesale, relieving thieves from the intellectually challenging task of finding obscure information that may link a deidentified record to the identity of its subject.

– **To preserve compartmentalization of data**

Most data created by modern laboratories has not been prepared in a manner that permits its meaningful use in other laboratories. In many cases the data has been compartmentalized, so that the data is disbursed in different laboratories. It is par for the course that a no single individual has taken the responsibility of collecting and reviewing all of the data that has been used to support the published conclusions of a multi-institutional project.

In the late 1990s, Dr. Wu Suk Hwang was a world-famous cloning researcher. The government of South Korea was so proud of Dr. Hwang that they issued a commemorative stamp to celebrate his laboratory's achievements. Dr. Hwang's status drastically changed when fabrications were discovered in a number of the manuscripts produced by his laboratory. Dr. Hwang had a habit of placing respected scientists as co-authors on his papers [41]. When the news broke, Hwang pointed a finger at several of his collaborators.

A remarkable aspect of Dr. Hwang's publications was his ability to deceive the coworkers in his own laboratory, and the co-authors located in laboratories around the world, for a very long time. Dr. Hwang used a technique known as compartmentalization; dividing his projects into tasks distributed to small groups of scientists who specialized in one step of the research process. By so doing, his coworkers never had access to the entire project's data. The data required to validate the final achievement of the research was not examined by his co-workers [42,41].

For several years, South Korean politicians defended the scientist, to the extent of questioning the patriotism of his critics. Over time, additional violations committed by Dr. Hwang were brought to light. In 2009, Hwang was sentenced in Seoul, S. Korea, to a two-year suspended prison sentence for embezzlement and bioethical violations; but he was never found guilty of fabrication [43].

Large data projects are almost always compartmentalized. When you have dozens or even hundreds of individuals contributing to a project, compartmentalization occurs quite naturally. In fact, what would you do without compartmentalization? Wait for every scientist involved in the project to review and approve one another's data? Today, large scientific projects may involve hundreds of scientists. Without compartmentalization, nothing would ever get published. The lesson here is that at the end of every research project, all of the data that contributed to the results must be gathered together as an organized and well-annotated dataset for public review.

– **To guard research protocols**

In every scientific study, the measurements included in the data must be linked to the study protocols (e.g., laboratory procedures) that produced the data. In some cases, the protocols are not well documented. In other cases, the protocols are well documented, but the researchers may have failed to follow the recommended protocols; thus rendering the data irreproducible. Occasionally, the protocols are the intellectual property of an

entity other than the persons who created the data. In all these instances, the data holders may be reluctant to share their protocols with the public.

– **To conceal instances of missing data**

It is almost inevitable, when data sets are large and complex, that there will be some missing data points. In this case, data may be added "by imputation." This involves computing a statistical best bet on what the missing data element value might have been, and inserting the calculated number into the data set. A data manager may be reluctant to release to the public a database with "fudged" data.

It is perfectly legitimate to include imputed data points, on the condition that all the data is properly annotated, so that reviewers are aware of imputed values, and of the methods used to generate such values.

– **To avoid bureaucratic hurdles**

As discussed in Section 9.3, "Data that Comes with Conditions," institutions may resort to Kafkaesque measures to insure that only qualified and trusted individuals gain access to research data. It should come as no surprise that formal requests for data may take two years or longer to review and approve [44]. The approval process is so cumbersome, that it simply cannot be implemented without creating major inconveniences and delays, for everyone involved (i.e., data manager and data supplicant).

In the United States, federal agencies often seek to share data with one another. Such transactions require Memoranda of Understanding between agencies, and these memoranda can take months to negotiate and finalize [44]. In some cases, try as they might, data is not shared among federal agencies due to a lack of regulatory authorization that cannot be resolved to anyone's favor [44].

Hyper vigilance, on the part of U.S. Federal agencies, may stem from unfortunate incidents from the past that cannot be easily forgotten. One such incident, which attracted international attention, occurred when the United States accidentally released details of hundreds of the nuclear sites and programs, including the exact locations of nuclear stockpiles [45]. Despite their reluctance to share some forms of data, U.S. agencies have been remarkably generous with bioinformatics data, and the National Institutes of Health commonly attaches data sharing requirements to grants, and other awards.

In the U.S., Federal regulations impose strict controls on sharing identified medical data. Those same regulations specify that deidentified human subject data is exempted from those controls, and can be freely shared [32,33]. Data holders must learn the proper methods for deidentifying or anonymizing private and confidential medical data.

Whew! Where does this leave us? Data sharing is not easy. Nonetheless, published claims cannot be validated unless the data is made available to the public for review, and science cannot advance if scientists cannot build upon the data produced by their colleagues. Research institutions, both public and private, must find ways to deal with the problem, despite the difficulties. They might start by hiring scientists who are steeped in the craft of data sharing.

Section 18.3. Data Security and Cryptographic Protocols

No matter how cynical you become, it's never enough to keep up.

Lily Tomlin

Let us be practical. Nearly everyone has confidential information on their computers. Often, this information resides in a few very private files. If those files fell into the hands of the wrong people, the results would be calamitous. For myself, I encrypt my sensitive files. When I need to work with those files, I decrypt them. When I'm finished working with them, I encrypt them again. These files are important to me, so I keep copies of the encrypted files on thumb drives and on an external server. I don't care if my thumb drives are lost or stolen. I don't care if a hacker gets access to the server that stores my files. The files are encrypted, and only I know how to decrypt them.

Anyone in the data sciences will tell you that it is important to encrypt your data files, particularly when you are transferring files via the internet. Very few data scientists follow their own advice. Scientists, despite what you may believe, are not a particularly disciplined group of individuals. Few scientists get into the habit of encrypting their files. Perhaps they perceive the process as being too complex.

For serious encryption, you will want to step up to OpenSSL. OpenSSL is an open source collection of message digest protocols (i.e., protocols that yield one-way hashes) and encryption protocols. This useful set of utilities, with implementations for various operating systems, is available at no cost from:

https://www.openssl.org/related/binaries.html

Encryption algorithms and suites of cipher strategies available through OpenSLL include: RSA, DH (numerous protocols), DSS, ECDH, TLS, AES (including 128 and 256 bit keys), CAMELLIA, DES (including triple DES), RC4, IDEA, SEED, PSK, and numerous GOST protocols. In addition, implementations of popular one-way hash algorithms are provided (i.e., MD5 and SHA, including SHA384). OpenSSL comes with an Apache-style open source license. [Glossary AES]

For Windows users, the OpenSSL download contains three files that are necessary for file encryption: openssl.exe, ssleay32.dll, and libeay32.dll. If these three files are located in your current directory, you can encrypt any file, directly from the command prompt, as shown:

```
openssl aes128 -in public.txt -out secret.aes -pass pass:abcdefgh
```

The command line provides your chosen password, "abcdefgh" to the aes128 encryption algorithm, which takes the file public.txt and produces an AES-encrypted output file, secret.aes. Of course, once you've encrypted a file, you will need a decryption method. Here's a short command line that decrypts the encrypted file created by the preceding command line:

```
openssl aes128 -d -in secret.aes -out decrypted.txt -pass pass:
abcdefgh
```

We see that decryption involves inserting the "-d" option into the command line. AES is an example of a symmetric encryption algorithm, which means that the encryption password also serves as the decryption password.

Encrypting and decrypting individual strings, files, groups of files, and directory contents is extremely simple and can provide a level of security that is likely to be commensurate with your personal needs.

Here is a short Python script, aes.py, that encrypts all the files included in a list, and deposits the encrypted files in a thumb drive sitting in the "f:" drive.

```
import sys, os, re
filelist = ['diener.txt','simplify.txt','re-ana.txt', 'phenocop.
txt', 'mystery.txt','disaster.txt', 'factnote.txt', 'perlbig.txt',
'referen.txt', 'create.txt', 'exploreo.txt']
pattern = re.compile("txt")
for filename in filelist:
  out_filename = pattern.sub('enc', filename)
  out_filename = "f:\\" + out_filename
  print(out_filename)
  cmdstring = "openssl aes128 -in " + filename + " -out " + out_filename +
  " -pass pass:abcdefgh"
  os.system(cmdstring)
```

– **Public and private key cryptographic protocols**

Many cryptographic algorithms are symmetric; the password used to encrypt a file is the same as the password used to decrypt the file. In an asymmetric cryptographic algorithm, the password that is used to encrypt a file is different from the password that is used to decrypt the file. The encrypting password is referred to as the public key, by convention. The public key can be distributed to friends or posted on a public web site. The decrypting password is referred to as the private key, and it must never be shared.

How is a public/private key system used? If Alice were to encrypt a file with Bob's public key, only Bob's private key could decrypt the file. If Bob does not lose his private key, and if Bob does not allow his private key t o be shared or stolen, then only Bob can decrypt files encrypted with his public key. Alice can send the encrypted file, without worrying that the encrypted file could be intercepted and opened by someone other than Bob.

As discussed, openssl can be run via command lines, from the system prompt (e.g., c:\> in Windows systems). Let's generate a public/private key pair that we'll use for RSA encryption.

```
openssl genpkey -algorithm RSA -out private_key.pem -pkeyopt
rsa_keygen_bits:2048
openssl rsa -pubout -in private_key.pem -out public_key.pem
```

These two commands produced two files, each containing a cryptographic key. The private key file is private_key.pm. The public key file is public_key.pem. Let's encrypt a file (sample.txt) using RSA encryption and the public key we just created (public_key.pem)

```
openssl rsautl -encrypt -inkey public_key.pem -pubin -in sample.txt -
out sample.ssl
```

This produces an encrypted file, sample.ssl. Let's decrypt the encrypted file (sample.ssl) using the private key that we have created (private_key.pem)

```
openssl rsautl -decrypt -inkey private_key.pem -in sample.ssl -out
decrypted.txt
```

In common usage, this protocol only transmits small message files, such as passwords. Alice could send a large file, strongly encrypted with AES. In a separate exchange, Alice and Bob would use public and private keys to transmit the password. First, Alice would encrypt the password with Bob's public key. The encrypted message would be sent to Bob. Bob would decrypt the message with his private key, thus producing the password. Bob would use the password to decrypt the large AES-encrypted file. A large variety of security protocols have been devised, utilizing public/private key pairs, suiting a variety of purposes.

The public/private keys can also be used to provide the so-called digital signature of the individual holding the private key.

To sign and authenticate a transferred data file (e.g., mydata.txt), the following three steps must be taken:

1. Alice creates a one-way hash of her data file, mydata.txt, and creates a new file, called hashfile, to hold the one-way hash value.
   ```
   openssl dgst -sha256 mydata.txt > hashfile
   ```
2. Alice signs the hashfile with her private key, to produce a digital signature in the file "signaturefile":
   ```
   openssl rsautl -sign -inkey private_key.pem -keyform PEM -in
   hashfile >signaturefile
   ```
3. Alice sends mydata.txt and the signature file("signature") to Bob
4. Bob verifies the signature, with his public key.
   ```
   openssl rsautl -verify -inkey public_key.pem -pubin -keyform PEM -in
   signaturefile
   ```
   The verified contents of the signature file is the original hash created by Alice, of mydata.txt
   ```
   SHA256(mydata.txt)= 6e2a1dbf9ea8cbf2accb64f33ff83c7040413963e
   69c736accdf47de0bc16b1a
   ```
   This verifies Alice's signature and yields Alice's hash of her mydata.txt file
5. Bob conducts his own one-way hash on his received file, mydata.txt.
   ```
   openssl dgst -sha256 mydata.txt
   ```

This produces the following hash value, which is the same value that was decrypted from Alice's signature

```
SHA256(mydata.txt)= 6e2a1dbf9ea8cbf2accb64f33ff83c7040413963e69c
736accdf47de0bc16b1a
```

Because the received mydata.txt file has the same one-way hash value as the sent mydata.txt file, and because Bob has verified that the sent mydata.txt file was signed by Alice, then Bob has taken all steps necessary to authenticate the file (i.e., to show that the received file is the file that Alice sent).

There are some limitations to this protocol. Anyone in possession of Alice's private key can "sign" for Alice. Hence the signature is not equivalent to a hand-written signature or to a biometric that uniquely identifies Alice (e.g., iris image, CODIS gene sequences, full set of fingerprints). Really, all the process tells us is that a document was sent by someone in possession of Alice's private key. We never really know who sent the document.

The signature does not attest to anything, other than that a person with Alice's key actually sent the document. There is nothing about the process that would indicate that she personally verifies that the content of the transmitted material is accurate or that the content was created by Alice or that she agrees with the contents.

Cryptography is fascinating, but experts who work in the field of data security will tell you that cryptographic algorithms and protocols can never substitute for a thoughtful data security plan that is implemented with the participation and cooperation of the staff of an organization [46,47]. In many instances, security breaches occur when individuals, often trusted employees, violate protocol and/or behave recklessly. Hence, data security is more often a "people thing" than a "computer thing". Nonetheless, if you are not a multi-million dollar institution, and simply want to keep some of your data private, here are a few tips that you might find helpful. If you have really important data, the kind that could hurt yourself or others if the data were to fall into the wrong hands, then you should totally disregard the advice that follows and seek the help of a professional security agent.

– Save yourself a lot of grief by settling for a level of security that is appropriate and reasonable for your own needs.

Don't use a bank vault when a padlock will suffice.

– Avail yourself of no-cost solutions.

Some of the finest encryption algorithms, and their implementations, are publicly available in OpenSSL and other sources.

– The likelihood that you will lose your passwords is much higher than the likelihood that someone will steal your passwords.

Develop a good system for passkey management that is suited to your own needs.

– The security of the system should not be based on hiding your encrypted files or keeping the encryption algorithm secret.

The greatest value of modern encryption protocols is that it makes no difference whether anyone steals or copies your encrypted files, or learns your encryption algorithm.

– File encryption and decryption should be computationally fast.

Fast, open source protocols are readily available.

– File encryption should be done automatically, as part of some computer routine (e.g., a backup routine), or as a chron job (i.e., a process that occurs at predetermined time).

You should be able to batch-encrypt and batch-decrypt any number of files all at once (i.e., from a command loop within a script), and you should be able to combine encryption with other file maintenance activities. For example, you should be able to implement a simple script that loops through every file in a directory, or a directory tree (i.e., all the files in all of the subdirectories under the directory), all at once, adding file header and metadata information into the file, scrubbing data as appropriate, calculating a one-way hash (i.e., message digest) of the finished file, and producing an encrypted file output.

– You should never implement an encryption system that is more complex than you can understand [48].

Your data may be important to you, and to a few of your colleagues, but the remainder of the world looks upon your output with glazed eyes. If you are the type of person who would protect your valuables with a padlock, rather than a safety deposit box, then you should probably be thinking less about encryption strength and more about encryption operability. Ask yourself whether the encryption protocols that you use today shall be widely available, platform-independent and vendor independent, 5, 10 or 50 years from now. Will you always be able to decrypt your own encrypted files?

– Don't depend on redundancy

At first blush, it would be hard to argue that redundancy, in the context of information systems, is a bad thing. With redundancy, when one server fails, another picks up the slack; if a software system crashes, its duplicate takes over; when one file is lost, it is replaced by its back-up copy. It all seems good.

The problem with redundancy is that it makes the system more complex. The operators of a Big Data resource with built-in redundancies must maintain the operability of the redundant systems in addition to the primary systems. More importantly, the introduction of redundancies introduces a new set of interdependencies (i.e., how the parts of the system interact), and the consequences of those interdependencies may be difficult to anticipate.

In recent memory, the most dramatic example of a failed redundant system involved the Japanese nuclear power plant at Fukushima. The plant was designed with redundant systems. If the power failed, a secondary power generator would kick in. On March 11, 2011, a powerful earthquake off the shore of Japan produced a tidal wave that cut the nuclear reactor's access to the electric power grid. The back-up generators were flooded

by the same tidal wave. The nuclear facilities were cut off from emergency assistance; also due to the tidal wave. Subsequent meltdowns and radiation leaks produced the worst nuclear disaster since Chernobyl.

As discussed previously in this chapter, on June 4, 1996, the first flight of the Ariane 5 rocket self-destructed, 37 seconds after launch. There was a bug in the software, but the Ariane had been fitted with a back-up computer. The back-up was no help; the same bug that crippled the primary computer put the back-up computer out of business [49]. The lesson here, and from the Fukushima nuclear disaster, is that redundant systems are often ineffective if they are susceptible to the same destructive events that caused failure in the primary systems.

Computer software and hardware problems may occur due to unanticipated interactions among software and hardware components. Redundancy, by contributing to system complexity, and by providing an additional opportunity for components to interact in an unpredictable manner, may actually increase the likelihood of a system-wide crash. Cases have been documented wherein system-wide software problems arose due to bugs in the systems that controlled the redundant subsystems [49].

A common security measure involves backing up files and storing the back-up files off-site. If there is a fire, flood, or natural catastrophe at the computer center, or if the computer center is sabotaged, then the back-up files can be withdrawn from the external site and eventually restored. The drawback of this approach is that the back-up files create a security risk. In Portland Oregon, in 2006, 365,000 medical records were stolen from Providence Home Services, a division of Seattle-based Providence Health Systems [50]. The thief was an employee who was handed the back-up files and instructed to store them in his home, as a security measure. In this case, the theft of identified medical records was a command performance. The thief complied with the victim's request to be robbed, as a condition of his employment. At the very least, the employer should have encrypted the back-up files before handing them over to an employee.

Nature takes a middle-of-the-road approach on redundancy. Humans evolved to have two eyes, two arms, two legs, two kidneys, and so on. Not every organ comes in duplicate. We have one heart, one brain, one liver, one spleen. There are no organs that come in triplicate. Human redundancy is subject to some of the same vulnerabilities as computer redundancy. A systemic poison that causes toxicity in one organ will cause equivalent toxicity in its contra-lateral twin.

– Save Time and Money; Don't Protect Data that Does not Need Protection

Big Data managers tend to be overprotective of the data held in their resources, a professional habit that can work in their favor. In many cases, though, when data is of a purely academic nature, containing no private information, and is generally accessible from alternate sources, there really is no reason to erect elaborate security barriers.

Security planning always depends on the perception of the value of the data held in the resource (i.e., Is the data in the Big Data resource worth anything?), and the risks that the data might be used to harm individuals (e.g., through identity theft). In many cases, the data held

in Big Data resources has no intrinsic monetary value and poses no risks to individuals. The value of most Big Data resource is closely tied to its popularity. A resource used by millions of people provides opportunities for advertising and attracts funders and investors.

Regarding the release of potentially harmful data, it seems prudent to assess, from the outset, whether there is a simple method by which the data can be rendered harmless. In many cases, deidentification can be achieved through a combination of data scrubbing, and expunging data fields that might conceivably tie a record to an individual. If your data set contains no unique records (i.e., if every record in the system can be matched with another record, from another individual, for which every data field is identical), then it is impossible to link any given record to an individual, with certainty. In many cases, it is a simple matter to create an enormous data set wherein every record is matched by many other records that contain the same informational fields. This process is sometimes referred to as record ambiguation [51].

Sometimes a Big Data team is compelled to yield to the demands of their data contributors, even when those demands are unreasonable. An individual who contributes data to a resource may insist upon assurances that a portion of any profit resulting from the use of their contributed data will be returned as royalties, shares in the company, or some other form of remuneration. In this case, the onus of security shifts from protecting the data to protecting the financial interests of the data providers. When every piece of data is a source of profit, measures must be put into place to track how each piece of data is used, and by whom. Such measures are often impractical, and have great nuisance value for data managers and data users. The custom of capitalizing on every conceivable opportunity for profit is a cultural phenomenon, not a scientific imperative.

Section 18.4. Case Study: Life on Mars

> *You must accept one of two basic premises: Either we are alone in the universe, or we are not alone in the universe. And either way, the implications are staggering.*
>
> *Wernher von Braun*

On September 3, 1976, the Viking Lander 2 touched down upon the planet mars, where it remained operational for the next 3 years, 7 months and 8 days. Soon after landing, it performed an interesting remote-controlled experiment. Using samples of martian dirt, astrobiologists measured the conversion of radioactively-labeled precursors into more complex carbon-based molecules; the so-called Labeled-Release study. For this study, control samples of dirt were heated to a high temperature (i.e., sterilized), and likewise exposed to radioactively-labeled precursors, without producing complex carbon-containing molecules. The tentative conclusion, published soon thereafter, was that Martian organisms in the samples of dirt had built carbon-based molecules through a metabolic pathway [52]. As you might expect, the conclusion was immediately challenged, and remains controversial, to this day, nearly 32 years later [22].

In the years since 1976, long after the initial paper was published, the data from the Labeled-Release study has been available to scientists, for re-analysis. New analytic techniques have been applied to the data, and new interpretations have been published [52]. As additional missions have reached mars, more data has emerged (i.e., the detection of water and methane), also supporting the conclusion that there is life on mars. None of the data is conclusive; Martian organisms have not been isolated. The point made here is that the shared Labeled-Release data is accessible and permanent, and can be studied again and again, compared or combined with new data, and argued ad nauseum [22].

Section 18.5. Case Study: Personal Identifiers

Secret agent man, secret agent man
They've given you a number and taken away your name
Theme from the television show "Secret Agent", airing in the United States from 1964–66; song written by P. F. Sloan and Steve Barriby

We came to a conclusion in 2002. I don't think you can do it (create an electronic health record) without a national identifier.

Peter Drury [53]

An awful lot of the data collected by scientists concerns people (e.g., financial data, marketing data, medical data). Given everything discussed so far in this book regarding the importance of providing data object uniqueness, you would think that we would all be assigned our own personal identifiers by now.

Of course, nothing could be further from the truth. Each of us are associated with dozens, if not hundreds of irreconcilable identifiers intended to serve a particular need at a particular moment in time. These include bank accounts, credit cards, loan applications, brokerage and other investment accounts, library cards, and voter IDs. In the United States, a patient may be assigned separate identifiers for the various doctors' offices, clinics and hospitals that she visits over the course of her life. As mentioned, a single hospital may assign a patient many different "unique" identifiers, for each department visited, for each newly installed hospital information system, and whenever the admission clerk forgets to ask the patient if he or she had been previously registered. U.S. Hospitals try to reconcile the different identifiers for a patient under a so-called Enterprise Master Patient Index, but experience has shown the problems encountered are insurmountable. As one example, in Houston's patient index system, which includes 3.5 million patients, there are about 250,000 patients that have a first and last name in common with at least one other registrant, and there are 70,000 instances wherein two people share the same first name, last name, and birthdate [54]. There is a growing awareness that efforts at reconciling systems wherein individual patients are registered multiple times, are never entirely satisfactory [53].

The subject of data security cannot be closed without mention of the National Patient Identifier. Some countries employ a National Patient Identifier (NPI) system. In these cases, when a citizen receives treatment at any medical facility in the country, the transaction is recorded under the same permanent and unique identifier. Doing so enables the data collected on individuals, from multiple hospitals, to be merged. Hence, physicians can retrieve patient data that was collected anywhere in the nation. In countries with NPIs, data scientists have access to complete patient records and can perform healthcare studies that would be impossible to perform in countries that lack NPI systems. In the United States, where a system of NPIs has not been adopted, there is a perception that such a system would constitute an invasion of privacy. Readers from outside the United States are probably wondering why the United States is so insecure on this issue.

In the United States, the call for a national patient identification system is raised, from time to time. The benefits to patients and to society are many. Aside from its absolutely necessary role in creating data that can be sensibly aggregated and meaningfully analyzed, it also serves to protect the privacy of individuals by eliminating the need for less secure forms of identification (e.g., credit cards, drivers licenses).

Regardless, U.S. citizens are reluctant to have an identifying number that is associated with a federally controlled electronic record of their private medical information. To show its disdain for personal identifiers, the U.S. Congress passed Public Law 105-277, in 1999, prohibiting the Department of Health and Human Services from using its funds to develop personal health identifiers, without first obtaining congressional approval [55].

In part, this distrust results from the lack of any national insurance system in the United States. Most health insurance in the United States is private, and private insurers have wide discretion over the fees and services provided to enrollees. There is a fear that if there were a national patient identifier with centralized electronic medical records, insurers may withhold reimbursements or raise premiums or otherwise endanger the health of patients. Because the cost of U.S. medical care is the highest in the world, medical bills for uninsured patients can quickly mount, impoverishing individuals and families [56].

Realistically, no data is totally safe. Data breaches today may involve hundreds of millions of confidential records. The majority of Americans have had social security numbers, credit card information, and private identifiers (e.g., birth dates, city of birth, names of relatives) misappropriated or stolen. Medical records have been stolen in large number. Furthermore, governments demand and receive access to our confidential medical records, when they deem it necessary [57]. Forbidding National Patient Identifiers has not made us safe. [Glossary Social Security Number]

Maybe we should ask ourselves the following: “Is it rational to forfeit the very real opportunity of developing new safe and effective treatments for serious diseases, for the very small likelihood that someone will crack my deidentified research record and somehow leverage this information to my disadvantage?”

Suppose everyone in the United States were given a choice: you can be included in a national patient identifier system, or you can opt out. Most likely, there would be many

millions of citizens who would opt out of the offer, seeing no particular advantage in having a national patient identifier, and sensing some potential harm. Now, suppose you were told that if you chose to opt out, you would not be permitted to enjoy any of the health benefits coming from studies performed with data collected through the national patient identifier system. New safe and effective drugs, warnings of emerging epidemics, information on side effects associated with your medications, biomarker tests for preventable illnesses, and so on, would be reserved for individuals with national patient identifiers. Those who made no effort to help the system would be barred from any of the benefits that the system provided. Would you reconsider your refusal to accept a national patient identifier, if you knew the consequences? Of course, this is a fanciful scenario, but it makes a point.

Glossary

AES The Advanced Encryption Standard (AES) is the cryptographic standard endorsed by the U.S. government as a replacement for the old government standard, DES (Data Encryption Standard). AES was chosen from among many different encryption protocols submitted in a cryptographic contest conducted by the U.S. National Institute of Standards and Technology, in 2001. AES is also known as Rijndael, after its developer. It is a symmetric encryption standard, meaning that the same password used for encryption is also used for decryption.

Classification versus ontology A classification is a system in which every object in a knowledge domain is assigned to a class within a hierarchy of classes. The properties of superclasses are inherited by the subclasses. Every class has one immediate superclass (i.e., parent class), although a parent class may have more than one immediate subclass (i.e., child class). Objects do not change their class assignment in a classification, unless there was a mistake in the assignment. For example, a rabbit is always a rabbit, and does not change into a tiger. Classifications can be thought of as the simplest and most restrictive type of ontology, and serve to reduce the complexity of a knowledge domain [58]. Classifications can be easily modeled in an object-oriented programming language and are non-chaotic (i.e., calculations performed on the members and classes of a classification should yield the same output, each time the calculation is performed). A classification should be distinguished from an ontology. In an ontology, a class may have more than one parent class and an object may be a member of more than one class. A classification can be considered a special type of ontology wherein each class is limited to a single parent class and each object has membership in one and only one class.

Data Quality Act In the United States the data upon which public policy is based must have quality and must be available for review by the public. Simply put, public policy must be based on verifiable data. The Data Quality Act of 2002, requires the Office of Management and Budget to develop government-wide standards for data quality [24].

Intellectual property Data, software, algorithms, and applications that are created by an entity capable of ownership (e.g., humans, corporations, universities). The entity holds rights over the manner in which the intellectual property can be used and distributed. Protections for intellectual property may come in the form of copyrights and patent. Copyright applies to published information. Patents apply to novel processes and inventions. Certain types of intellectual property can only be protected by being secretive. For example, magic tricks cannot be copyrighted or patented; this is why magicians guard their intellectual property so closely. Intellectual property can be sold outright, essentially transferring ownership to another entity; but this would be a rare event. In other cases, intellectual property is retained by the creator who permits its limited use to others via a legal contrivance (e.g., license, contract, transfer agreement, royalty, usage fee, and so on). In some cases, ownership of the intellectual

property is retained, but the property is freely shared with the world (e.g., open source license, GNU license, FOSS license, Creative Commons license).

Social Security Number The common strategy, in the United States, of employing social security numbers as identifiers is often counterproductive, owing to entry error, mistaken memory, or the intention to deceive. Efforts to reduce errors by requiring individuals to produce their original social security cards puts an unreasonable burden on honest individuals, who rarely carry their cards, and provides an advantage to dishonest individuals, who can easily forge social security cards. Institutions that compel patients to provide a social security number have dubious legal standing. The social security number was originally intended as a device for validating a person's standing in the social security system. More recently, the purpose of the social security number has been expanded to track taxable transactions (i.e., bank accounts, salaries). Other uses of the social security number are not protected by law. The Social Security Act (Section 208 of Title 42 U.S. Code 408) prohibits most entities from compelling anyone to divulge his/her social security number. Legislation or judicial action may one day stop healthcare institutions from compelling patients to divulge their social security numbers as a condition for providing medical care. Prudent and forward-thinking institutions will limit their reliance on social security numbers as personal identifiers.

Y-chromosome A small chromosome present in males and inherited from the father. The normal complement of chromosomes in male cells has one Y chromosome and one X chromosome. The normal complement of chromosomes in female cells has two X chromosomes and no Y chromosomes. Analysis of the Y chromosome is useful for determining paternal lineage.

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19

Legalities

OUTLINE

Section 19.1. Responsibility for the Accuracy and Legitimacy of Data

> *At this very moment, there's an odds-on chance that someone in your organization is making a poor decision on the basis of information that was enormously expensive to collect.*
>
> *Shvetank Shah, Andrew Horne, and Jaime Capella [1]*

> *In 2031, lawyers will be commonly a part of most development teams.*
>
> *Grady Booch*

I am not a lawyer, and this chapter is not intended to provide legal advice to the readers. It is best to think of this chapter as an essay that covers the issues that responsible managers of Big Data resources worry about, all of the time. When I was a program director at the National Institutes of Health, I worked on resources that collected and analyzed medical data. My colleagues and I worked through the perceived legal risks that encumbered all of our projects. For the most part, our discussions focused on four issues: (1) responsibility for the accuracy of the contained data; (2) rights to create, use, and share the data held in the resource; (3) intellectual property encumbrances incurred from the use of standards required for data representation and data exchange; and (4) protections for individuals whose personal information is used in the resource. Big Data managers contend with a

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wide assortment of legal issues, but these four problems, that never seem to go away, will be described in this chapter.

The contents of small data resources can be closely inspected and verified. This is not the case for Big Data. Because Big Data resources are constantly growing, and because the sources of the data are often numerous and not strictly controlled, it is a safe bet that some of the data is incorrect. The reflexive position taken by some data managers can be succinctly stated as: "It is not my problem!"

To a small extent, measures taken to improve the quality of data contained in a Big Data resource will depend on how the data will be used. Will the data be used for mission-critical endeavors? In the medical realm, will the data be used to make diagnostic or treatment decisions? These contingencies raise the stakes for Big Data resources, but the data manager's responsibility is largely the same, regardless of the intended use of the resource. Every Big Data resource must have in place a system whereby data quality is constantly checked, errors are documented, corrective actions are taken, and improvement is documented. Without a quality assurance plan, the resource puts itself in great legal jeopardy. In addition to retaining legal counsel, data managers would be wise to follow a few simple measures:

– **Make no unjustified claims.**

It is important that statements issuing from the Big Data resource, including claims made in advertisements and informational brochures, and verbal or written communications with clients, should never promise data accuracy. People who insist on accuracy should confine their attention to small data resources. If your Big Data resource has made no effort to ensure that the data is true and accurate, then you owe it to your users to indicate as much.

– **Require your sources to take necessary measures to provide accurate data.**

Sources that contribute to Big Data resources should have their own operation protocols, and these protocols must be made available to the manager of the Big Data resource. In addition, sources should certify that that their contributed data conforms, as best as they can ascertain, to their data policies.

– **Have procedures in place ensuring that the data provided by outside sources is accurately represented within the resource.**

Big Data managers should exercise reasonable diligence to ensure that the received data is legitimate, and to verify such data when it is received.

– **Warn your data users that their analytic results, based on the resource's data, must be validated against external data sources.**

It may seem obvious to you that conclusions drawn from the analyses of Big Data are always tentative, and must be validated against data from other sources. Sometimes

data analysts need to be protected from their own naiveté, necessitating an explicit warning.

– **Open your verification procedures to review (preferably public review).**

Users find it unsettling to read exculpatory verbiage in user licenses, expressing that the data provider cannot guarantee the accuracy of the data and cannot be held liable for any negative consequences that might arise from the use of the data. At the very least, data managers should re-assure their users that reasonable measures have been taken to verify the data contained in the resource. Furthermore, those measures should be available for review by any and all potential data users.

– **Provide a method by which complainants can be heard.**

This may actually be one of those rare instances when the immutability of a Big Data resource is broken. If material is known to be illegal or if the material is a potential danger to individuals, then it may be necessary to expunge the data (i.e., violate data immutability).

– **Be prepared to defend your data and your procedures**

Big Data managers must understand their data. The conclusions drawn from their data may someday serve as evidence in legal proceedings, including all manner of arbitration and litigations, both civil and criminal. In the case of Daubert v Merrell Dow Pharmaceuticals, Inc., the U.S. Supreme Court ruled that trial judges must determine the relevance and adequacy of data-based evidence presented by expert witnesses. Judicial oversight is conducted through a pre-trial review that "entails a preliminary assessment of whether the reasoning or methodology underlying the testimony is scientifically valid and of whether that reasoning or methodology properly can be applied to the facts in issue" [2]. Hence, Big Data managers must constantly strive to assure that the data contained in their resources are fully described and linked to the protocols through which the data was obtained. Any verification processes, through which data is entered and checked into the resource, may be reviewed by government committees and courts.

When Big Data resources are used to influence the governmental process, special regulatory conditions may apply. The U.S. government passed the Data Quality Act in 2001, as part of the FY 2001 Consolidated Appropriations Act (Pub. L. No. 106-554) [3,4]. The Act requires Federal Agencies to base their policies on high quality data and to permit the public to challenge and correct inaccurate data [5]. The drawback to this legislation, is that science is a messy process, and data may not always attain a high quality. Data that fails to meet standards of quality may be rejected by government committees or may be seized upon by lobbyists to abrogate good policies that were based on the imperfect data [6–8]. [Glossary Data Quality Act]

Data managers chant a common lament: "I cannot be held responsible for everything!" They have a point, but their inability to control everything does not relieve them of their responsibility to exercise a high degree of data diligence.

Section 19.2. Rights to Create, Use, and Share the Resource

Free software is a matter of liberty, not price.

Richard Stallman

As mentioned earlier, ownership is a mercantile concept; the owner of an item is the person who can sell the item. If you own a cow, then you can sell the cow. Once the cow is sold, you no longer own the cow; the cow has a new owner. This simple ownership arrangement does not work well for Big Data. Data can be copied ad infinitum. In virtually all cases financial transactions that involve the transfer of data do not actually result in the loss of the data by the provider. The data provider continues to hold the data after the transaction has transpired. In the Big Data universe, Big Data is not "owned" in the usual sense of the word; data is intangible. This explains why the term "service" pops up so often in the information field (e.g., Internet Service Providers, Web Services, List Servers). Data is more often a service than an owned commodity. [Glossary Web service]

Because Big Data comes from many sources, different uses, and can be retrieved via federated queries across multiple resources (Big and small), the customary laws pertaining to property rights can be difficult to apply. Big Data managers need to know whether they have the right to acquire and distribute the data held in their resources. It may be easiest to think in terms of two separable issues: laws dealing with data acquisition, and laws dealing with data distribution.

Information produced through a creative effort (e.g., books, newspapers, journal articles) usually falls under copyright law. This means that you cannot freely obtain and distribute these materials. Exceptions would include books that fall into the public domain (e.g., books produced by the federal government, and books whose copyright term has expired). Other exceptions might include copyrighted material that fall under Fair Use provisions [9]. Fair Use provisions permit the distribution of copyrighted material if it is done solely for the public good, with no profit motive, and if it can be done in a way that does not financially harm the copyright holder (e.g., does not result in the loss of sales and royalties).

Most Big Data resources are primarily composed of raw data, along with annotations to the data. The data may consist of measurements of physical objects and events, and short informational attributes appended to abstract data objects. These types of data are generally not produced through a creative effort, and would not fall under copyright law. In the United States, the most cited precedent relevant to data acquisition is Feist Publishing, Inc. v. Rural Telephone Service Co. When Rural Telephone Co. refused to license their alphabetized listing of names and telephone numbers to Feist Publishing, Inc., Feist proceeded to copy and use the data. Rural Telephone Co. claimed copyright infringement. The court ruled that merely collecting data into a list does not constitute a creative work and was not protected by copyright.

European courts differ somewhat from American courts with regard to copyright protections. Like their American counterparts, Europeans interpret copyright to cover

creative works, not data collections. However, the 1996 European Database Directive instructs courts to extend sui generis (i.e., one of a kind or exceptional) protection to databases. In Europe, databases created with a significant investment of time, effort and money cannot be freely copied for commercial use. The idea behind such a directive is to protect the investments made by database builders. By protecting the database owner the European law attempts to promote the creation of new Big Data resources along with the commercial activities that follow.

Insofar as Big Data resources have international audiences, differences in database laws across different countries can be very frustrating for data managers who strive for legal clarity. Consequently, providers and users often develop their own solutions, as needed. Acquisition of commercial data (i.e., data that does not belong to the public domain), much like access to commercial software, is often achieved through legal agreements (e.g., licenses or contracts) between the data providers and the data users.

Regarding laws dealing with holding and distributing data, the Digital Millennium Copyright Act of 1998 (DMCA) applies in the United States. This law deals primarily with anti-piracy security measures built into commercial digital products [10]. The law also contains a section (Title II) dealing with the obligations of online service providers who inadvertently distribute copyrighted material. Service providers may be protected from copyright infringement liability if they block access to the copyrighted material when the copyright holder or the holder's agent claims infringement. To qualify for liability protection, service providers must comply with various guidelines (i.e., the so-called safe harbor guidelines) included in the Act. In most instances, compliant service providers would also be protected from infringement claims when their sites link to other sites that contain infringing materials. [Glossary DMCA]

Whereas the DMCA provides some liability relief for inadvertent copyright infringers, the United States No Electronic Theft Act of 1997 (NET Act) makes possible the criminal prosecution of infringers who distribute copyrighted material for non-commercial purposes (i.e., for free) [11]. In the early days of the Internet, there was a commonly held, but unfounded, belief that copyrighted material could be held and distributed without fear of legal retribution, if no profit was involved. This belief, perhaps based on an overly liberal interpretation of the Fair Use provisions, came to an end with the NET Act.

Without delving into legal minutiae, here are a few general suggestions for data managers:

1. Require your sources to substantiate their claim that the data is theirs to contribute. Nobody should be submitting data that they do not own or that they do not have the right to distribute.
2. Require your sources to indicate that the data was collected in a manner that did not harm individuals and that the data can be distributed without harming individuals.
3. Use government data whenever feasible. Much of the best data available to Big Data resources comes absolutely free from the U.S. government and other governments that have a policy of contributing their official data to the public domain. Big Data resources

can freely copy and redistribute public domain government data. Links to the major sources of prepared U.S. government data are found at: http://www.data.gov/. In addition, virtually all data collected by the government, including data collected through federal grants, and data used to determine public actions, policies, or regulations, can be requested through the Freedom of Information Act [12]. Many countries provide their citizens with the right to acquire data that was generated with government (i.e., taxpayer) funds.

4. Pay for legitimate data when feasible. It seldom makes good sense to copy a data set into a Big Data resource, if that data requires constant updating and curation. For example, a comprehensive list of restaurants, with their addresses and phone numbers, is always a work in progress. Restaurants open, close, move their locations, acquire new phones numbers, revise their menus, and modify their hours of operation. If there is a database resource that collects and updates this information, there may be little reason to replicate these activities within another data resource. It may make much more sense to license the database or to license access to the database. A federated data service, wherein queries to your Big Data resource are automatically outsourced to other databases, depending on the query subject, may be much more feasible than expanding your resource to include every type of information. In many circumstances the best and the safest method of using and distributing data may come from negotiating payments for external data.

Section 19.3. Copyright and Patent Infringements Incurred by Using Standards

She was incapable of saying please, incapable of saying thank you and incapable of saying sorry, all the while creating a surge in the demand for these expressions.

Edward St. Aubyn, in his book, "At Last"

As described in Chapter 7, the standards that you have been using in your Big Data resource may actually belong to somebody else. Strange as it may seem, standards are intellectual property and can be copyrighted, patented, or licensed. Not only may a standard be patented, but specific uses of the standard may also be patented, and the patents on uses of the copyright may be held by entities who were not at all involved in the creation of the standard.

If you choose to pay a license fee for the use of a proprietary standard, you might find that the costs exceed the sticker price [13]. The license agreement for the standard may impose unwanted restrictions on the use of the standard. For example, a standard may be distributed under a license that prohibits you from freely distributing the intellectual product of the standard (i.e., materials created through the use of the standard). This may mean that your users will not be able to extract and download data that has been formatted in conformance with the standard, or annotated with codes, numbers, terms or other

information that could not have been created without the use of the standard. The same restrictions might apply to licensed software.

The building blocks of Big Data resources may hide intellectual property [14,13]. This is particularly true for software, which may inadvertently contain subroutines or lines of code that fall under a claim within an issued patent. One day, you might receive a letter from a lawyer who represents a patent holder, asserting that a fragment of code included in a piece of your software infringes his client's patent. The letter may assert the patent and demand that you cease using the patent holder's intellectual property. More commonly, the letter will simply indicate that a conflict has arisen and will suggest that both parties (your Big Data resource and the patent holder) should seek a negotiated remedy. In either case, most Big Data resources will keep a law firm on retainer for such occasions. Do not despair; the ultimate goal of the patent holder is to acquire royalty payments; not to initiate a lawsuit.

Big Data resources are complex and contain many different types of data objects that may have been transformed, annotated, or formatted by many different methods. The uses of these methods may be restricted under licenses, contracts and other legal contrivances. A few precautionary steps may help reduce your risks:

- Whenever possible, use free and open source standards, software, nomenclatures, and ontologies for all of your data annotations. Do not disparage free and open source products. In the world of Big Data, many of the best standards, data formats, nomenclatures, classifications, software, and programming languages are free and open source [15].
- Inventory your standards, software, nomenclatures, and ontologies. For each item, write a description of any restrictions that might apply to your resource.
- Investigate on the Web. See if there are any legal actions, active or settled, involving any of the materials you might use. Visit the U.S. Patent Office to determine whether there are patent claims on the uses of the standards, software, nomenclatures and ontologies held in your resource. Most likely, your Big Data resource will send and receive data beyond the U.S. Consult the World Intellectual Property Organization (WIPO). Do not restrict your search to proprietary materials. Free and open source materials may contain embedded intellectual property and other encumbrances.
- Talk to your legal staff before you commit to using any proprietary product. Your law firm will need to be involved in virtually every aspect of the design and operation of your Big Data resource.
- If you must use licensed materials, carefully read the "Terms of Use" in the agreement. Licenses are written by lawyers who are paid to represent their client (the Licensor). In most cases, the lawyer will be unaware of the special use requirements of Big Data resources. The Terms of Use may preclude the customary activities of a Big Data resource (e.g., sharing data across networks, responding to large numbers of queries with annotated data, storing data on multiple servers in widely distributed geographic locations). As noted previously, it is important to have a lawyer review license

agreements before they are signed, but the data manager is in the best position to anticipate provisions that might reduce the value of a Big Data resource.

Big Data would greatly benefit from a universal framework supporting resource interoperability [16]. At present, every data manager must fend for herself.

Section 19.4. Protections for Individuals

Everything is gone;
Your life's work has been destroyed.
Squeeze trigger (yes/no)?

Computer-inspired haiku by David Carlson

Data managers must be familiar with the concept of tort. Tort relates to acts that result in harm. Tort does not require an illegal act; it only requires a harm and a person or entity who contributes to the harm and who is liable for the damages. Tort works like this; if you are held liable for harm to another entity, then you must compensate the victim to an extent that makes the victim whole (i.e., brings the victim back to where he was before suffering harm). If the victim makes a case that the harm resulted from negligence or due to conditions that could have been corrected through customary caution, then punitive fees can be added to the victim's award. The punitive fees can greatly exceed the restorative fees. Consequently, it behooves every data manager to constantly ask themselves whether their Big Data resource can result in harm to individuals (i.e., the users of the data, or the subjects of the data). Needless to say, Big Data managers must seek specialized legal advice to minimize tort-related risks.

In the Big Data universe, tort often involves the harms that befall individuals when their confidential data files have been breached. I was raised in Baltimore, not far from the community of Catonsville. Catonsville was the site of a 1968 protest against United States involvement the Vietnam War. Nine anti-war activists stormed into a draft office, stole files, and publicly burned the files. The Catonsville 9 attained instant international notoriety. The number of files destroyed: 379. In the Big Data era the ante has been upped by many orders of magnitude. Today, when records are stolen or destroyed, you can expect the numbers to be in the millions, or even hundreds of millions [17].

In May, 2006, 26.5 million records on military veterans were stolen, including Social Security numbers and birth dates. The records had been taken home by a data analyst employed by the Department of Veterans Affairs. His laptop, containing all this information, was stolen. A class action lawsuit was brought on behalf of the 26.5 million aggrieved veterans. Three years later, the Department of Veterans Affairs paid $20 million to settle the matter [18]. In the United Kingdom, a copy of medical and banking records on 25 million Britons were lost in the mail [19]. The error led to the sudden resignation of the chairman of Her Majesty's Revenue and Customs [19].

There are occasions when security is broken, but no theft occurs. In these instances, resource managers may be unaware of the privacy breach for a surprisingly long period

of time. Medical data collected on about 20,000 patients was posted on a public Web site in 2010. The data included patient names, diagnosis codes, and administrative information on admissions and discharges occurring in a six month period in 2009. The data stayed posted on the public Web site for about a year before a patient happened to see the data and reported the breach to the hospital [20]. Accidental breaches are common in many different fields [21].

Today, healthcare organizations must report data breaches that affect more than 500 people. Hundreds of such breaches have been reported. These breaches cost the healthcare industry in excess of $6 billion annually, and the costs are increasing, not decreasing [17]. Other industries have data breaches but are not required to report incidents.

Industry costs do not reflect the personal costs in time, emotional distress, and money suffered by individuals coping with identity theft. In the Big Data field, everyone's deepest fear is identity theft. None of us wants to contemplate what may happen when another person has access to their financial accounts or gains the opportunity to create new accounts under the stolen identity.

Security issues are inseparable from issues related to privacy and confidentiality. We have dealt with some of the more technical issues of data security in Section 18.3, "Data Security and Cryptographic Protocols". In this chapter, we can review a few of the commonsense measures that will reduce the likelihood of identification theft.

1. Do not collect or provide information that will link an individual to his or her data record unless you really need the information. If you do not have information that links a record to a named individual, then you cannot inadvertently expose the information. Names, social security numbers, credit card numbers, and birth dates constitute the core information sought by identity thieves. Big Data resources should seriously consider whether such information needs to be stored within the resource. Does your resource really need to collect social security numbers and credit card numbers? Can the person's name be adequately replaced with an internal identifier? Do you need a birth date when a birth year might suffice? When these data items are necessary, do they need to be included in data records that are accessible to employees?
2. Work with deidentified records whenever possible. Deidentification may not be a perfect way to render records harmless; but it takes you very close to your goal. A thoughtfully deidentified data set has quite limited value to identity thieves.
3. All files should be encrypted whenever possible. Most breaches involve the theft of unencrypted records. Breaking an encrypted record is quite difficult and far beyond the technical expertise of most thieves.
4. Back-up data should be encrypted, inventoried, and closely monitored. Back-up data is a vulnerability. Thieves would be just as happy to steal your back-up data as your original data. Because theft of back-up data does not result in a system crash, such thefts can go undetected. It is very important to secure your back-up data and to deploy a system that monitors when back-up data is removed, copied, misplaced, destroyed, or otherwise modified.

Section 19.5. Consent

> *MRECs [Medical Research Ethics Committees] sometimes place extreme demands on researchers. These demands have included gaining consent for each step of the research and ensuring data are destroyed on completion of a project...*
>
> *Louise Corti, Annette Day, and Gill Backhouse [22]*

For data managers who deal with medical data, or with any data whose use puts human subjects at risk, consent issues will loom as a dominant legal issue. The reason why consent is a consuming issue for data managers has very little to do with its risks; the risks associated with obtaining improper consent are very small. Consent issues are important because consenting data can be incredibly expensive to implement. The consent process can easily consume the major portion of the data manager's time, and cost-effective implementations are difficult to achieve.

In the context of Big Data, informed consent occurs when a human agrees to accept the risk of harm resulting from the collection and use of their personal data. In principle, every consent transaction is simple. Someone involved with the Big Data resource approaches a person and indicates the data that he would like to collect for the data project. He indicates the potential harms that may occur if consent is granted. If relevant, he indicates the measures that will be taken to minimize the risk of harm. The human subject either signs, or does not sign, the consent form. If the subject signs the form, then his data can be included in the Big Data resource. [Glossary Informed consent, Bayh-Dole Act]

It is important that data managers understand the purpose of the consent form, so that it is not confused with other types of legal agreements between data owners and data contributors. The consent form is exclusively devoted to issues of risk to human subjects. It should not be confused with a commercial agreement (i.e., financial incentives for data use), or with an intellectual property agreement (i.e., specifying who controls the uses of the data); or with scientific descriptions of the project (i.e., determining how the data is to be used and for which specific purposes).

The term "informed consent" is often misinterpreted to mean that the patient must be fully informed of the details of the Big Data project with an exhaustive list of all the possible uses of their personal data. Not so. The "informed" in "informed consent" refers to knowledge of the risks involved in the study, not the details of the study itself. It is reasonable to stipulate that the data in Big Data resources is held permanently, and can be used by many individuals, for a wide variety of purposes that cannot be predetermined. Filling the consent form with detailed information about the uses of the resource is counterproductive, if it distracts from the primary purpose of the form; to explain the risks.

What are the risks to human subjects in a Big Data project? With few exceptions, Big Data risks are confined to two related consequences: loss of confidentiality and loss of privacy.

The concepts of confidentiality and of privacy are often confused, and it is useful to clarify their separate meanings. Confidentiality is the process of keeping a person's secret.

Privacy is the process of ensuring that the person will not be annoyed, betrayed, or harmed as a result of his decision to give you his secret. For example, if you give me your unlisted telephone number in confidence, then I am expected to protect this confidentiality by never revealing the number to other persons. I may also be expected to protect your privacy by never using the telephone number to call you unnecessarily, at all hours of the day and night (i.e., annoying you with your private information). In this case the same information object (i.e., your unlisted telephone number) is encumbered by confidentiality (i.e., keeping the unlisted number secret) and privacy (i.e., not using the unlisted number to annoy you).

To cover confidentiality risks the consent form could indicate that personal information will be collected, but that measures will be taken to ensure that the data will not be linked to your name. In many circumstances, that may be all that is needed. Few patients really care if anyone discovers that their gall bladder was removed in 1995. When the personal information is of a highly sensitive nature, the consent form may elaborate on the security measures that ensure confidentiality.

The risk of losing privacy is a somewhat more subtle risk than the loss of confidentiality. In practical terms, for Big Data projects, loss of privacy occurs when the members of the Big Data resource come back to the human subject with a request for additional information, or with information regarding the results of the study. The consent form should indicate any constraints that the Big Data resource has put into place to ensure that subjects are not annoyed with unwelcome future contacts by members of the project. In some cases the Big Data project will anticipate the need to recontact human subjects (i.e., to invade their privacy). In this case the consent form must contain language informing the subjects that privacy will not be fully protected. In many cases subjects do not particularly care, one way or the other. They are happy to participate in projects that will benefit society, and they do not mind answering a phone call at some future time. The problem for the Big Data resource will come if and when subjects have a change of heart, and they decide to withdraw consent.

Obtaining consent from human subjects carries its own administrative and computational challenges; many of which are unanticipated by Big Data managers. Consent-related tasks include the following:

1. Creating a legally valid consent form.

There are many ways to write a bad consent form. The most common mistake is inserting consent clauses among the fine-print verbiage of broader legal documents (e.g., contracts, agreements, licenses). This is a bad mistake for several reasons. The validity of informed consent can be challenged if an individual can claim that he or she was not adequately informed. The consent form should be devoted to a single topic, consent, and should not be inserted into other legal forms that require the subject's signature.

The consent form should be written in language that the average person can understand. In many cases, particularly in medical settings, informed consent should be read aloud by an individual who is capable of explaining difficult passages in the consent document.

Consent forms should not contain exculpatory clauses. For example, the consent form should not contain language expressing that the Big Data resource cannot be held liable for harm resulting from the use of the consenter's data. Neither should the form ask signers to waive any of their normal rights.

The consent form should have a signature section, indicating an affirmative consent. Certain types of informed consent may require the signature of a witness, and consent protocols should have provisions for surrogate signatures (e.g., of a parent or legal guardian). It is common for consent forms to provide an opportunity for subjects to respond in the negative (i.e., to sign a statement indicating that consent is denied). Doing so is seldom a good idea, for several reasons. First, the negative (non-affirmative) statement is not legally required and there are no circumstances for which a non-affirmative statement has any practical value. Secondly, individuals should not feel compelled to respond in any way to the consent form. If they freely choose to give consent, they can sign the form. If they do not wish to give consent, they should not be coerced to sign their names to a statement of denial. Thirdly, a non-affirmative statement can produce great confusion in the future, when an individual consents to having the same record used for another research project, or when the individual has a change of heart, and decides to provide consent for the same project.

The consent form should reveal circumstances that might influence a person's decision to provide consent. For example, if the investigators have a commercial interest in the outcome of the study, then that information should be included in the consent form. It is reasonable for individuals to fear that they might suffer harm if the investigators have something to gain by a particular outcome of an experiment or analysis.

Traditionally, consent is not open-ended. Consent generally applies to a particular project that is conducted over a specified period of time. Consent ends when the project ends. There has been a trend to lengthen the window of time to which consent applies, to accommodate projects that might reasonably be expected to extend over many years. For example, the Framingham study on heart disease has been in progress for more than 60 years [23]. If the Big Data project intends to use consented data for an indefinite period, as it almost always does, then the consent form must clarify this condition.

Most importantly, the consent form should carefully describe the risks of participation. In the case of Big Data analyses, the risks are typically confined to loss of confidentiality or loss of privacy.

2. Obtaining informed consent.

The U.S. Census is an established project that occurs every decade. The methods and the goals of the census have been developed over many decades. About 600,000 census workers are involved; their jobs are to obtain signed census forms from about 250 million individuals. The cost of each census is about $14 billion. Keeping these numbers in your mind, imagine that you are a Big Data manager. You maintain and operate a global Big Data resource, with data on over 2 billion individuals (8 times the population of the United States). You are informed by your supervisor that a new project for the resource will require

you to obtain informed consent on the resource's catchment population. You are told that you will be assigned ten additional part-time workers to help you. You are given a budget of $100,000 for the project. When you complain that you need more help and a larger budget, you are told that you should use the computational power of the Big Data resource to facilitate the effort. You start looking for another job.

There are no easy ways to obtain informed consent. Popular marketing techniques that use automated or passive affirmations cannot be used to obtain informed consent. For example, opt out forms in which human subjects must take an action to be excluded from participating in a potentially harmful data collection effort are unacceptable. Informed consent must be affirmative. Forms should not be promissory (i.e., should not promise a reward for participation). Informed consent must be voluntary and uncompensated.

Consent must be obtained without coercion. Individuals cannot be denied customary treatment or access to goods and services if they refuse to grant consent. There are circumstances for which the choice of person who seeks informed consent may be considered coercive. A patient might feel threatened by a surgeon who waves a research-related consent form in their face minutes before a scheduled procedure. Big Data managers must be careful to obtain consent without intimidation.

The consent form must be signed if it is to have any legal value. This means that a Web page submission is unacceptable unless it can be reasonably determined that the person providing the consent is the same person who is listed in the submitted Web page. This would usually necessitate an authenticated password, at minimum. Issues of identity theft, password insecurity, and the general difficulty of managing electronic signatures make Web-based consent a difficult process.

The process of obtaining consent has never been easy. It cannot be fully automated because there will always be people whose contact information (e.g., email accounts) are invalid or who ignore all attempts at contact. To this date, nobody has found an inexpensive or labor-free method for obtaining informed consent from large numbers of individuals.

3. Preserving consent.

After consent has been obtained, it must be preserved. This means that the original paper document or a well-authenticated electronic document, with a verified signature, must be preserved. The consent form must be linked to the particular record for which it applies and to the protocol or protocols for which the consent applies. An individual may sign many different consent forms, for different data uses. The data manager must keep all of these forms safe and organized. If these documents are lost or stolen, then the entire resource can be jeopardized.

4. Ensuring that the consent status is kept confidential.

The consent forms themselves are potential sources of harm to patients. They contain information related to special studies or experiments or subsets of the population that include the individual. The consent form also contains the individual's name. If an

unauthorized person comes into possession of consent forms, then the confidentiality of the individuality would be lost.

5. Determining whether biases are introduced by the consent process.

After all the consents have been collected, someone must determine whether the consented population introduces bias. The data analyst would ask: "Is the group of people who provide consent in any way different from the group of people who refuse to provide consent?" and, if so, "Will differences between the consenters and the non-consenters bias analytic outcomes?" A data analyst might look for specific differences among the consented and unconsented group in features that are relevant to the question under study. For example, for a medical disease study, are there differences in the incidence of the disease between the consenting group and the non-consenting group? Are there differences in the ages at which the disease occurs in consenters and non-consenters?

6. Creating a process whereby reversals and modifications of consent can be recorded and flagged.

In most cases, consent can be retracted. Retraction is particularly important in long or indefinite studies. The data manager must have a way of tracking consents and documenting a new consent status. For any future use of the data, occurring after the consent status has changed, the subject's data records must not be available to the data analyst.

7. Maintaining records of consent actions.

Tracking consent data is extremely difficult. Here are a few consent-related activities that Big Data managers must record and curate: "Does each consent form have an identifier?" "Does each consent form link to a document that describes the process by which the consent form was approved?" "If paper consent forms were used, can the data manager find and produce the physical consent document?", "Was the consent restricted, permitting certain uses of the data and forbidding other types of data uses?" "Is each consent restriction tagged for tracking?", "If the consent form was signed, is there a protocol in place by which the signature is checked to determine authenticity?", "Does the data manager have a recorded policy that covers situations wherein subjects cannot provide an informed consent (e.g., infants, patients with dementia)?", "Does the resource have protocols for using surrogate signatures for children and subjects who have guardians or assignees with power-of-attorney?", "Does the Big Data resource have policies that exclude classes of individuals from providing informed consent?", "Is there a protocol to deal with subjects who withdraw consent or modify their original consent?" "Does the resource track data related to consent withdrawals and modifications?"

8. Educating staff on the liberties and limitations of consented research.

Many Big Data managers neglect to train their staff on legal matters, including consent-related issues. Information technologists may erect strong mental barriers to exclude the kinds of legal issues that obfuscate the field of data law. Data managers have no choice

but to persevere. It is unlikely that factors such as staff indifference and workplace incompetence will serve as mitigating factors when tort claims are adjudicated.

Section 19.6. Unconsented Data

> *The main point in our favor is that there is little or no case law, at least in the UK, which has unearthed any complaints by research participants about misuse of their contributions.*
>
> *Louise Corti, Annette Day, and Gill Backhouse [22]*

There are enormous technical difficulties and legal perils in the consent process. Is there some way of avoiding the whole mess?

I have worked for decades in an information-centric culture that has elevated the consent process to an ethical imperative. It is commonly held that the consent process protects individuals from harm, and data managers from liability. In the opinion of many of my colleagues, all confidential data on individuals should be consented into the database, unless there is a very good reason to the contrary.

After many years of dealing with the consent issue, I have reached a very different conclusion. To my way of thinking, consent should be avoided, if feasible; it should only be used as a last resort. In most circumstances, it is far preferable for all concerned to simply render data records harmless, and to use them without obtaining consent. As the dependence on consent has grown over the past few decades, several new issues, all having deleterious societal effects, have arisen:

1. Consent can be an unmerited revenue source for data managers.

When consent must be obtained on thousands or millions of individuals, the consenting costs can actually exceed the costs of preparing and using the data. When these costs are passed on to investors, or to taxpayers (in the case of public Big Data resources), it raises the perceived importance and the general cash flow for the resource. Though data managers are earnest and humble, as a rule, there are some managers who feel comfortable working on projects of dubious scientific value, and a low likelihood of success, if there is ample funding. Tasks related to the consent process cost money, without materially contributing to the research output. Because funding institutions must support consenting efforts, grant writers for Big Data projects can request and receive obscenely large awards, when consent is required.

2. The act of obtaining consent is itself a confidentiality risk.

The moment you ask for consent, you're creating a new security weakness, because the consent form contains sensitive information about the subject and the research project. The consent form must be stored, and retrieved as needed. As more and more people have access to copies of the consent forms, the risk of a confidentiality breach increases.

An irony of Big Data research is that the potential harm associated with soliciting consent may easily exceed the potential harms of participating as a subject in a Big Data project.

3. Consent issues may preoccupy data managers, diverting attention from other responsibilities.

There is a limit to the number of problems anyone can worry about. If half of your research effort is devoted to obtaining, storing, flagging, and retrieving consent forms, then you are less likely to pay attention to other aspects of the project. One of the chief lessons of this book is that, at the current time, most of our Big Data resources teeter on the brink of failure. The consent process can easily push a resource over the brink.

4. Consented research has been used for unintended purposes.

Once you have received permission to use personal data in a consented study, the data remains forever. Scientists can use this data freely, for any purpose, if they deidentify the data or if the original consent form indicates that the data might be used for future unspecified purposes. The latter option fueled the Havasupai lawsuit, to be discussed in the final section of this chapter.

As it happens, consent can be avoided altogether if the data in the resource has been rendered harmless through deidentification. Let's remember that the purpose of the consent form is to provide individuals with the choice to decline the risks associated with the use of their data in the Big Data resource. If there are no risks, there is no need to obtain consent. Data managers taking the unconsented path to data use need to ask themselves the following question. "Can I devise a way by which the data can be used, without risk to the individual?"

Exceptions exist. Regulations that restrict the use of data for designated groups of individuals may apply, even when no risk of harm is ascertained. Data confidentiality and privacy concerns are among the most difficult issues facing Big Data resources. Obtaining the advice of legal counsel is always wise.

The widespread use and public distribution of fully deidentified data records is a sort of holy grail for data miners. Medical records, financial transactions, collections of private electronic communications conducted over air and wire all contribute to the dark matter of the information universe. Everyone knows that this hidden data exists (we each contribute to these data collections), that this hidden data is much bigger than the data that we actually see, and that this data is the basic glue that binds the information universe. Nonetheless, most of the data created for the information universe is considered private. Private data is controlled by a small number of corporations who guard their data against prying eyes, while they use the data, to the extent allowed by law, to suit their own agendas. Why isn't Big Data routinely deidentified using methods discussed earlier, as discussed in Sections 3.6 and 3.7, and distributed for public review and analysis? Here are some of the reasons:

– Commercially available deidentification/scrubbing software is slow. It cannot cope with the exabytes of information being produced each year.

- None of the commercially available deidentification/scrubbing software does a perfect job. These software applications merely reduce the number of identifiers in records; they leave behind an irreducible amount of identifying information.
- Even if deidentification/scrubbing software actually were to perform as claimed, removing every identifier and every byte of unwanted data from electronic records, some records might be identified through the use of external database resources that establish identities through non-identifying details contained in records.
- Big Data managers are highly risk averse and would rather hoard their data than face the risk, no matter how unlikely, of a possible tort suit from an aggrieved individual.
- Big Data managers are comfortable with restricted data sharing, through legal instruments such as Data Use Agreements. Through such agreements, selected sets of data extracted from a Big Data resource are provided to one or a few entities who use the data for their own projects and who do not distribute the data to other entities. [Glossary Data sharing]
- Data deidentification methods, like many of the useful methods in the information field, can be patented. Some of the methods for deidentification have fallen under patent restriction, or have been incorporated into commercial software that is not freely available to data managers [24]. For some data managers, royalty and license costs are additional reasons for abandoning the deidentification process.
- Big Data managers are not fully convinced that deidentification is possible, even under ideal circumstances.

It may seem impossible, but information that is not considered identifying may actually be used to discover the name of the person linked to deidentified records. Basically, deidentification is easy to break when deidentified data can be linked to a name in an identified database containing fields that are included in both databases. This is the common trick underlying virtually every method designed to associate a name with a deidentified record.

Data managers who provide deidentified data sets to the public must worry whether there is, or ever will be, an available identified database that can be used to link fields, or combinations of fields, to their deidentified data, and thus link their records to the names of individuals. This worry weighs so heavily on data managers and on legal consultants for Big Data resources that there are very few examples of publicly available deidentified databases. Everyone in the field of Big Data is afraid of the legal repercussions that will follow when the confidentiality of their data records is broken.

Section 19.7. Privacy Policies

No keyboard present
Hit F1 to continue
Zen engineering?

Computer-inspired haiku by Jim Griffith

Discussions of privacy and confidentiality seem to always focus on the tension that results when the interests of the data holders conflict with the interests of the data subjects. These issues can be intractable when each side has a legitimate claim to their own preferences (businesses need to make profit, and individuals need some level of privacy).

At some point, every Big Data manager must create a Privacy Policy, and abide by their own rules. It has been my experience that legal problems arise when companies have no privacy policy, or have a privacy policy that is not well-documented, or have a privacy policy that is closed to scrutiny, or have a fragmented privacy policy, or fail to follow their own policy. If the company is open with its policy (i.e., permits the policy to be scrutinized by the public), and willing to change the policy if it fails to adequately protect individuals from harm, then the company is not likely to encounter any major problems.

Privacy protection protocols do not need to be perfect. They do, however, need to be followed. Companies are much more likely to get into trouble for ignoring their own policies than for following an imperfect policy. For a policy to be followed, the policy must be simple. Otherwise, the employees will be incapable of leaning the policies. Unknowable policies tend to be ignored by the unknowing staff.

Every Big Data project should make the effort to produce a thoughtful set of policies to protect the confidentiality of their records and the privacy of data subjects. These policies should be studied by every member of a Big Data project, and should be modified as needed, and reviewed at regular intervals. Every modification and review should be thoroughly documented. Every breach or failure of every policy must be investigated, promptly, and the results of the investigation, including any and all actions taken, must be documented. Competent data managers will make it their priority to see that the protocols are followed and that their review process is fully documented.

If you are a Big Data manager endowed with a overactive imagination, it is possible to envision all types of unlikely scenarios in which confidentiality can be breached. Nobody is perfect, and nobody expects perfection from any human endeavor. Much of law is based on a standard of "reasonableness." Humans are not held to an unreasonable standard. As an example, the privacy law that applies to hospitals and healthcare organizations contains 390 occurrences of the word "reasonable" [25]. A reasonable approach to confidentiality and privacy is all that can be expected from a complex human endeavor.

Section 19.8. Case Study: Timely Access to Big Data

Don't accept your dog's admiration as conclusive evidence that you are wonderful.
Ann Landers

In the clinical bioinformatics world, testing laboratories must have access to detailed population data, on millions of gene variants, with which to correlate their findings [26–31]. Specifically, genetics laboratories need to know whether a gene variant is present in the normal population that has no clinical significance; or whether variants are associated

with disease. The lives of patients are put at risk when we are deprived of timely and open access to data relating genetic findings to clinical phenotypes.

In 2008, a 2-year-old child had a severe seizure, and died. In the prior year, the child had undergone genetic testing. The child's doctors were concerned that the patient might have Dravet's syndrome, a seizure disorder in which about 80% of patients have a mutation in the SCN1A gene. The laboratory discovered a mutation in the child's SCN1A gene, but remarked in their report that the mutation was a variant of unknown significance. That is to say that the reference database of sequence variants, used by the laboratory, did not contain information that specifically linked the child's SCN1A mutation to Dravet syndrome. In this circumstance, the laboratory report indicated that the gene test was "inconclusive"; they could neither rule in or rule out the possibility that the found mutation was diagnostic of Dravet syndrome.

Some time later, the child died.

In a wrongful death lawsuit filed by the child's mother, the complaint was made that two published reports, appearing in 2006 and 2007, had linked the specific SCN1A gene mutation, that was subsequently found in her child's DNA, with an epileptic encephalopathy [32]. According to the mother, the reporting laboratory should have known the significance of her child's mutation [32,33]. Regardless of the verdict rendered at this trial, the circumstances serve as fair warning. In the era of Big Data, testing laboratories need access to the most current data available, including the data generated by competing laboratories.

Section 19.9. Case Study: The Havasupai Story

Freeing yourself was one thing; claiming ownership of that freed self was another.
Toni Morrison

For those who seek consent for research, the case of the Havasupai Tribe v. Arizona Board of Regents holds us in thrall. The facts of the case play out over a 21-year period, from 1989 to 2010. In 1989 Arizona University obtained genetic samples from several hundred members of the Havasupai Tribe, a community with a high prevalence of Type II diabetes. In addition to their use in diabetes research, the informed consent indicated the samples might be used for research on "behavioral and medical disorders," not otherwise specified. The researchers tried but failed to make headway linking genes sampled from the Havasupai tribe with cases of diabetes. The gene samples were subsequently used for ancillary studies that included schizophrenia and for studies on the demographic trends among the Havasupai. These ancillary studies were performed without the knowledge of the Havasupai. In 2003 a member of the Havasupai tribe happened to attend a lecture, at Arizona State University, on the various studies performed with the Havasupai DNA samples.

The Havasupai tribe was enraged. They were opposed to the use of their DNA samples for studies of schizophrenia or for the studies of demographic trends. In their opinions,

these studies did not benefit the Havasupai and touched upon questions that were considered embarrassing and taboo, including the topic of consanguineous matings, and the prevalence rates of mental illnesses within the tribe.

In 2004, the Havasupai Tribe filed a lawsuit indicating lapses in the informed consent process, violation of civil rights, violation of confidentiality, and unapproved use of the samples. The case was dismissed on procedural grounds, but was reinstated by the Arizona Court of Appeals, in 2008 [34].

Reinstatement of the case led to lengthy and costly legal maneuvers. Eventually, the case was settled out of court. Arizona State University agreed to pay individuals in the Havasupai tribe a total of $700,000. This award is considerably less than the legal costs already incurred by the University. Arizona State University also agreed to return the disputed DNA samples to the Havasupai tribe.

If the Havasupai tribe had won anything in this dispute, it must have been a Pyrrhic victory. Because the case was settled out of court, no legal decision was rendered, and no clarifying precedent was established.

Though I am not qualified to comment on the legal fine-points, several of the principles related to the acquisition and use of data are relevant and can be discussed as topics of general interest.

First, the purpose of an informed consent document is to list the harm that might befall the individual who gives consent, as a consequence of his or her participation as a human subject. Consent relates only to harm; consent does not relate to approval for research. Laypersons should not be put into a situation wherein they must judge the value of research goals. By signing consent, the signator indicates that he or she is aware of the potential harm from the research, and agrees to accept the risk. In the case of samples or data records contributed to a Big Data resource, consenters must be warned, in writing, that the data will be used for purposes that cannot be specified in the consent form.

Secondly, most consent is obtained to achieve one primary purpose, and this purpose is customarily described briefly in the consent form. The person who consents often wants to know that the risks that he or she is accepting will be compensated by some potential benefit to society. In the case of the Havasupai Tribe v. Arizona State University, the tribe sought to exert control over how their DNA would be used [35]. It would seem that the Havasupai Tribe members believed that their DNA should be used exclusively for scientific efforts that would benefit the tribe. There is no ethical requirement that binds scientists to conduct their research for the sole benefit of one group of individuals. A good consent form will clearly state that research conducted cannot be expected to be of any direct value to the consenter.

Finally, the consent form should include all of the potential harms that might befall the consenter as a consequence of his or her participation. It may be impossible to anticipate every possible adverse consequence to a research participant. In this case, the scientists at Arizona State University did not anticipate that the members of the Havasuapai Tribe would be harmed if their gene data was used for ancillary research purposes. I would expect that the researchers at Arizona State University do not believe that their research

produced any real harm. The Havasupai tribal members believe otherwise. It would seem that the Havasupai believed that their DNA samples were abused, and that their trust had been violated.

Had the original consent form listed all of the potential harms, as perceived by the Havasupai, then the incident could have been avoided. The Havasupai could have reached an informed decision weighing the potential benefits of diabetes research against the uncertain consequences of using their DNA samples for future research projects that might be considered taboo.

Why had the Havasupai signed their consent forms? Had any members of the Havasupai tribe voiced concerns over the unspecified medical and behavioral disorders mentioned in the consent form, then the incident could have been avoided.

In a sense, the Havasupai v. Arizona Board of Regents lawsuit hinged on a misunderstanding. The Havasupai did not understand how scientists use information to pursue new questions. The Board of Regents did not understand the harms that occur when data is used for legitimate scientific purposes. The take home lesson for data managers is the following: to the extent humanly possible, ensure that consent documents contain a complete listing of relevant adverse consequences. In some cases, this may involve writing the consent form with the assistance of members of the group whose consent is sought.

Glossary

Bayh-Dole Act The Patent and Trademark Amendments of 1980, P.L. 96-517. Adopted in 1980, the U.S. Bayh-Dole legislation and subsequent extensions gave universities and corporations the right to keep and control any intellectual property (including data sets) developed under federal grants. The Bayh-Dole Act has provided entrepreneurial opportunities for researchers who work under federal grants, but has created conflicts of interest that should be disclosed to human subjects during the informed consent process. It is within the realm of possibility that a researcher who stands to gain considerable wealth, depending on the outcome of the project, may behave recklessly or dishonestly to achieve his or her ends.

DMCA Digital Millennium Copyright Act, signed into law in 1998. This law deals with many different areas of copyright protection, most of which are only peripherally relevant to Big Data. In particular, the law focuses on copyright protections for recorded works, particularly works that have been theft-protected by the copyright holders [10]. The law also contains a section (Title II) dealing with the obligations of online service providers who inadvertently distribute copyrighted material. Service providers may be protected from copyright infringement liability if they block access to the copyrighted material when the copyright holder or the holder's agent claims infringement. To qualify for liability protection, service providers must comply with various guidelines (i.e., the so-called safe harbor guidelines) included in the Act.

Data Quality Act In the United States the data upon which public policy is based must have quality and must be available for review by the public. Simply put, public policy must be based on verifiable data. The Data Quality Act of 2002, requires the Office of Management and Budget to develop government-wide standards for data quality [3].

Data sharing Providing one's own data to another person or entity. This process may involve free or purchased data, and it may be done willingly, or under coercion, as in compliance with regulations, laws, or court orders.

Informed consent Human subjects who are put at risk must provide affirmative consent, if they are to be included in a government-sponsored study. This legally applies in the United States and most other nations, and ethically applies to any study that involves putting humans at risk. To this end, researchers provide prospective human subjects with an "informed consent" document that informs the subject of the risks of the study, and discloses foreseen financial conflicts among the researchers. The informed consent must be clear to laymen, must be revocable (i.e., subjects can change their mind and withdraw from the study, if feasible to do so), must not contain exculpatory language (e.g., no waivers of responsibility for the researchers), must not promise any benefit or monetary compensation as a reward for participation, and must not be coercive (i.e., must not suggest a negative consequence as a result of non-participation).

Web service Server-based collections of data, plus a collection of software routines operating on the data, that can be accessed by remote clients. One of the features of Web services is that they permit client users (e.g., humans or software agents) to discover the kinds of data and methods offered by the Web Service and the rules for submitting server requests. To access Web services, clients must compose their requests as messages conveyed in a language that the server is configured to accept, a so-called Web services language.

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20

Societal Issues

OUTLINE

Section 20.1. How Big Data Is Perceived by the Public

The greatest enemy of knowledge is not ignorance, it is the illusion of knowledge.
Stephen Hawking

Big Data, even the Big Data that we use in scientific pursuits, is a social endeavor. The future directions of Big Data will be strongly influenced by social, political, and economic forces. Will scientists archive their experimental data in publicly accessible Big Data resources? Will scientists adopt useful standards for their operational policies and their data? The answers depend on a host of issues related to funding source (e.g., private or public), cost, and perceived risks. How scientists use Big Data may provide the strongest argument for or against the public's support for Big Data resources.

The purposes of Big Data can be imagined as one of the following dramatic settings:

– **The Big Snoop (hoarding information about individuals, for investigative purposes)**

In this hypothesis, Big Data exists for private investigators, police departments, and snoopy individuals who want to screen, scrutinize, and invade the privacy of individuals, for their own purposes. There is basis in reality to support this hypothesis. Investigators, including the FBI, use Big Data resources, such as: fingerprint databases, DNA databases, legal records, air travel records, arrest and conviction records, school records, home ownership records, geneology trees, credit card transactions, financial transactions, tax records, census records, Facebook pages, tweets, emails, and sundry electronic residua. The modern private eye has profited from Big Data, as have law enforcement officers. It is unsettling that savvy individuals have

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used Big Data to harass, stalk, and breach the privacy of other individuals. These activities have left some individuals dreading future sanctioned or unsanctioned uses of big Data. On the up side, there is a real possibility that Big Data will serve to prevent crime, bring criminals to justice, and enhance the security of law-abiding citizens. The value of Big Data, as a method to reduce crime, has not fully engaged the public consciousness.

– **Big Brother (collecting information on individuals to control the general population)**

Modern governments obtain data from surveillance cameras and sophisticated eavesdropping techniques, and from a wide variety of information collected in the course of official operations. Much of the data collected by governments is mandated by law (e.g., census data, income tax data, birth certificates), and cannot be avoided. When a government sponsors Big Data collections, there will always be some anxiety that the Big Data resource will be used to control the public, reducing our freedoms of movement, expression, and thought. On the plus side, such population-wide studies may eventually reduce the incidence of terrorist attacks, confine the spread of epidemics and emerging diseases, increase highway safety, and improve the public welfare.

– **Borg invasion (collecting information to absorb information on a population)**

I assume that if you are reading this book on Big Data, you most likely are a Star Trek devotee, and understand fully that the Borg are a race of collectivist aliens who travel through galaxies, absorbing knowledge from civilizations encountered along the way. The conquered worlds are absorbed into the Borg "collective" while their scientific and cultural achievements are added to a Big Data resource. According to the Borg hypothesis, Big Data is the download of a civilization. Big Data analysts predict and control the activities of populations: how crowds move through an airport; when and where traffic jams are likely to occur; when political uprisings will occur; how many people will buy tickets for the next 3-D movie production. Resistance is futile.

– **Junkyard (a place to put our stuff)**

The late great comedian, George Carlin, famously chided us for wasting our time, money, and consciousness on one intractable problem: "Where do we put all our stuff?" Before the advent of Big Data, electronic information was ephemeral; created and then lost. With cloud computing, and with search engines that encompass the Web, and with depositories for our personal data, Big Data becomes an infinite storage attic. Your stuff is safe, forever, and it is available to you when you need it.

When the ancient Sumerians recorded buy-sell transactions, they used clay tablets. They used the same medium for recording novels, such as the Gilgamesh epic. These tablets have endured well over 4000 years. To this day, scholars of antiquity study and translate the Sumerian data sets. The safety, availability and permanence of electronic "cloud" data is a claim that will be tested, over time. When we are all dead and gone, will our data persist for even a fraction of the time that the Sumerian tablets have endured?

– **Scavenger hunt (searching for treasure)**

Big Data is a collection of everything, created for the purpose of searching for individual items and facts. According to the Scavenger hunt hypothesis, Big Data is everything you ever wanted to know about everything. A new class of professionals will emerge, trained to find any information their clients may need, by mining Big Data resources. It remains to be seen whether the most important things in life will ever be found in Big Data resources.

– **Egghead heaven (collecting information to draw generalized scientific conclusions)**

The National Science Foundation has issued a program solicitation entitled Core Techniques and Technologies for Advancing Big Data Science & Engineering [1]. This document encapsulates the Egghead hypothesis of Big Data.

"The Core Techniques and Technologies for Advancing Big Data Science and Engineering (BIGDATA) solicitation aims to advance the core scientific and technological means of managing, analyzing, visualizing, and extracting useful information from large, diverse, distributed, and heterogeneous data sets so as to: accelerate the progress of scientific discovery and innovation; lead to new fields of inquiry that would not otherwise be possible; encourage the development of new data analytic tools and algorithms; facilitate scalable, accessible, and sustainable data infrastructure; increase understanding of human and social processes and interactions; and promote economic growth, improved health, and quality of life. The new knowledge, tools, practices, and infrastructures produced will enable breakthrough discoveries and innovation in science, engineering, medicine, commerce, education, and national security-laying the foundations for US competitiveness for many decades to come [1]."

– **In your Facebook (a social archive that generates money)**

The underlying assumption here is that people want to use their computers to interact with other people (i.e., make friends and contacts, share thoughts, arrange social engagements, give and receive emotional support, and memorialize their lives). Some might dismiss social networks as a ruse whereby humans connect with their computers, while disconnecting themselves from committed human relationships that demand self-sacrifice and compassion. Still, a billion members cannot all be wrong, and the data collected by social networks must tell us something about what humans want, need, dislike, avoid, love, and, most importantly, buy. The Facebook hypothesis is the antithesis of the Egghead hypothesis in that participants purposefully add their most private thoughts and desires to the Big Data collection so that others will recognize them as unique individuals.

– **Much ado about nothing (Big Data does not qualify as anything new)**

According to some detractors, Big Data represents what we have always done, but with more data. This last statement, which is somewhat of an anti-hypothesis, is actually prevalent among quite a few computer scientists. They would like to think that everything

they learned in the final decades of the 20th century will carry them smoothly through their careers in the 21st century. Many such computer scientists hold positions of leadership and responsibility in the realm of information management. They may be correct; time will either vindicate or condemn them.

Discourse on Big Data is hindered by the divergence of opinions on the nature of the subject. A proponent of the Nihilist hypothesis will not be interested in introspection, identifiers, semantics, or any of the Big Data issues that do not apply to traditional data sets. Proponents of the George Carlin hypothesis will not dwell on the fine points of Big Data analysis if their goal is limited to archiving files in the Big Data cloud. If you read blogs and magazine articles on Big Data, from diverse sources (e.g., science magazines, popular culture magazines, news syndicates, financial bulletins), you will find that the authors are all talking about fundamentally different subjects called by the same name; Big Data. [Glossary Semantics]

To paraphrase James Joyce, there are many sides to an issue; unfortunately, I am only able to occupy one of them. I closely follow the National Science Foundation's lead (vida supra). The focus for this chapter is the Egghead hypothesis; using Big Data to advance science.

Section 20.2. Reducing Costs and Increasing Productivity With Big Data

Every randomized clinical trial is an observational study on day two.

Ralph Horwitz

We tend to think of Big Data exclusively as an enormous source of data; for analysis and for fact-finding. Perhaps we should think of Big Data as a time-saver; something that helps us do our jobs more efficiently, and at reduced cost. It is easy to see how instant access to industry catalogs, inventory data, transaction logs, and communication records can improve the efficiency of businesses. It is less easy to see how Big Data can speed up scientific research, an endeavor customarily based on labor-intensive, and tedious experiments conducted by scientists and technicians in research laboratories. For many fields of science, the traditional approach to experimentation has reached its fiscal and temporal limits; the world lacks the money and the time to do research the old-fashioned way. Everyone is hoping for something to spark the next wave of scientific progress, and that spark may be Big Data.

Here is the problem facing scientists today. Scientific experiments have increased in scale, cost, and time, but the incremental progress resulting from each experiment is no greater today than it was fifty years ago. In the field of medicine, 50-year progress between 1910 and 1960 greatly outpaced progress between 1960 and 2010. Has society reached a state of diminishing returns on its investment in science?

By 1960, industrial science reached the level that we see today. In 1960, we had home television (1947), transistors (1948), commercial jets (1949), nuclear bombs (fission,

fusion in 1952), solar cells (1954), fission reactors (1954), satellites orbiting the earth (Sputnik I, 1957), integrated circuits (1958), photocopying (1958), probes on the moon (Lunik II, 1959), practical business computers (1959), and lasers (1960). Nearly all the engineering and scientific advances that shape our world today were discovered prior to 1960.

These engineering and scientific advancements pale in comparison to the advances in medicine that occurred between 1920 and 1960. In 1921, we had insulin. Over the next four decades, we developed antibiotics effective against an enormous range of infectious diseases, including tuberculosis. Civil engineers prevented a wide range of common diseases using a clean water supply and improved waste management. Safe methods to preserve food, such as canning, refrigeration, and freezing saved countless lives. In 1941, Papanicolaou introduced the Pap smear technique to screen for precancerous cervical lesions, resulting in a 70% drop in the death rate from uterine cervical cancer, one of the leading causes of cancer deaths in women. By 1947, we had overwhelming epidemiologic evidence that cigarettes caused lung cancer. No subsequent advances in cancer research have yielded reductions in cancer death rates that are comparable to the benefits achieved with Pap smear screening and cigarette avoidance. The first polio vaccine and the invention of oral contraceptives came in 1954. By the mid 1950s, sterile surgical technique was widely practiced, bringing a precipitous drop in post-surgical and post-partum deaths. The great achievements in molecular biology, from Linus Pauling, James D. Watson, and Francis Crick, came in the 1950s.

If the rate of scientific accomplishment were dependent upon the number of scientists on the job, you would expect that progress would be accelerating, not decelerating. According to the National Science Foundation, 18,052 science and engineering doctoral degrees were awarded in the United States, in 1970. By 1997, that number had risen to 26,847, nearly a 50% increase in the annual production of the highest level scientists [2]. The growing work force of scientists failed to advance science at rates achieved in an earlier era; but not for lack of funding. In 1953, according to the National Science Foundation, the total United States expenditures on research and development was $5.16 billion, expressed in current dollar values. In 1998, that number has risen to $227 billion, greater than a 40-fold increase in research spending [2]. Most would agree that, over this same period, we have not seen a 40-fold increase in the rate of scientific progress.

Big Data provides a way to accelerate scientific progress by providing a large, permanent, and growing collection of data obtained from many different sources; thus sparing researchers the time and expense of collecting all of the data that they use, for very limited purposes, for a short span of time.

In the field of experimental medicine, Big Data provides researchers with an opportunity to bypass the expensive and time-consuming clinical trial process. With access to millions of medical records and billions of medical tests, researchers can find subpopulations of patients with a key set of clinical features that would qualify them for inclusion in narrowly focused, small trials [3]. The biological effects of drugs, and the long-term clinical outcomes, can sometimes be assessed retrospectively on medical records held

in Big Data resources. The effects of drugs, at different doses, or in combination with other drugs, can be evaluated by analyzing large numbers of treated patients. Evaluations of drugs for optimal doses, and optical treatment schedule, in combination with other drugs, is something that simply cannot be answered by clinical trials (there are too many variables to control).

Perhaps the most important scientific application of Big Data will be as a validation tool for small data experiments. All experiments, including the most expensive prospective clinical trials, are human endeavors and are subject to all of the weaknesses and flaws that characterize the human behavior [4–6]. Like any human endeavor, experiments must be validated, and the validation of an experiment, if repeated in several labs, will cost more than the original study. Using Big Data, it may be feasible to confirm experimental findings based on a small, prospective studies, if the small-scale data is consistent with observations made on very large populations [7]. In some cases, confirmatory Big Data observations, though not conclusive in themselves, may enhance our ability to select the most promising experimental studies for further analysis. Moreover, in the case of drug trials, observations of potential side effects, non-responsive subpopulations, and serendipitous beneficial drug activities may be uncovered in a Big Data resource.

In the past, statisticians have criticized the use of retrospective data in drug evaluations. There are just too many biases and too many opportunities to reach valueless or misleading conclusions. Today, there is a growing feeling that we just do not have the luxury of abandoning Big Data. Using these large resources may be worth a try, if we are provided access to the best available data, and if our results are interpreted by competent analysts, and sensibly validated. Today, statisticians are finding opportunities afforded by retrospective studies for establishing causality, once considered the exclusive domain of prospective experiments [8–10]. One of the most promising areas of Big Data studies, over the next decade or longer, will be in the area of retrospective experimental design. The incentives are high. Funding agencies, and corporations should ask themselves, before financing any new and expensive research initiative, whether the study can be performed using existing data held in Big Data resources [11].

Section 20.3. Public Mistrust

Never attribute to malice that which is adequately explained by stupidity
Commonly attributed to Robert J. Hanlon, but echoed by countless others over the ages

Much of the reluctance to share data is based on mistrust. Corporations, medical centers, and other entities that collect data on individuals will argue, quite reasonably, that they have a fiduciary responsibility to the individuals whose data is held in their repositories. Sharing such data with the public would violate the privacy of their clients. Individuals agree. Few of us would choose to have our medical records, financial transactions, and the details of our personal lives examined by the public.

Recent campaigns have been launched against the "database state." One such example is NO2ID, a British campaign against ID cards and a National Identify Register. Other anti-database campaigns include TheBigOptOut.org which campaigns against involuntary participation in the United Kingdom medical record database and LeaveThemKidsAlone, protesting fingerprinting in schools.

When the identifying information that links a personal record to a named individual is removed, then the residual data becomes disembodied values and descriptors. Properly deidentified data poses little or no threat to humans, but it has great value for scientific research. The public receives the benefits of deidentified medical data every day. This data is used to monitor the incidence and the distribution of cancer, detect emerging infectious diseases, plan public health initiatives, rationally appropriate public assistance funds, manage public resources, and monitor industrial hazards. Deidentified data collected from individuals provides objective data that describes us to ourselves. Without this data, society is less safe, less healthy, less smart, and less civilized.

Those of us who value our privacy and our personal freedom have a legitimate interest in restraining Big Data. Yet, we must admit that nothing comes free in this world. Individuals who receive the benefits of Big Data, should expect to pay something back. In return for contributing private records to Big Data resources, the public should expect resources to apply the strictest privacy protocols to their data. Leaks should be monitored, and resources that leak private data should be disciplined and rehabilitated. Non-compliant resources should be closed.

There are about a billion people who have Facebook accounts wherein they describe the intimate details of their lives. This private information is hanging in the cloud, to be aggregated, analyzed and put to all manner of trivial, commercial purposes. Yet, many of these same Facebook users would not permit their deidentified medical records to be used to save lives. It would be ideal if there were no privacy or confidentiality risks associated with Big Data. Unfortunately, zero-risk is not obtainable. However, it is technically possible to reduce the imagined risks of Big Data to something far below the known risks that we take with every electronic monetary transaction, every transfer of information, every move we make in public places, every click on our keyboards, and every tap on our smartphones. Brave new world!

Section 20.4. Saving Us From Ourselves

Man needs more to be reminded than instructed.

Samuel Johnson

Ever since computers were invented, there has been a push toward developing decision-making algorithms. The idea has been that computers can calculate better and faster than humans and can process more data than humans. Given the proper data and algorithms, computers can make better decisions than humans. In some areas, this is true. Computers can beat us at chess, they can calculate missile trajectories, and they can crack encryption

codes. They can do many things better and faster than humans. In general the things that computers do best are the things that humans cannot do at all.

If you look over the past half century of computer history, computers have not made much headway in the general area of decision-making. Humans continue to muddle through their days, making their own decisions. We do not appoint computers to sit in juries, doctors seldom ask a computer for their diagnostic opinions, computers do not decide which grant applications receive funding, and computers do not design our clothing. Despite billions of dollars spent on research on artificial intelligence, the field of computer-aided decision-making has fallen short of early expectations [12–15]. It seems we humans still prefer to make our own mistakes, unassisted. [Glossary Artificial intelligence, Machine learning]

Although computers play a minor role in helping us make correct decisions, they can play a crucial role in helping us avoid incorrect decisions. In the medical realm, medical errors account for about 100,000 deaths and about a million injuries each year, in the United States [16]. Can we use Big Data to avoid such errors? The same question applies to driving errors, manufacturing errors, construction errors, and any realm where human errors have awful consequences.

It really does not make much sense, at this early moment in the evolution of computational machines, to use computers to perform tasks that we humans can do very well. It makes much more sense to use computers to prevent the kinds of errors that humans commit because we lack the qualities found in computers.

Here are a few examples wherein Big Data resources may reduce human errors:

– **Identification errors.**

As discussed at length in Section 3.4, "Really Bad Identifier Methods," identification is a complex process that should involve highly trained staff, particularly during the registration process. Biometrics may help establish uniqueness (i.e., determining that an individual is not registered under another identifier) and authenticity (i.e., determining that an individual is who he claims to be). Computer evaluation of biometric data (e.g., fingerprints, iris imaging, retinal scan, signature, etc.) may serve as an added check against identification errors.

– **Data entry errors.**

Data entry error rates are exceedingly common and range from about 2% of entries up to about 30% of entries, depending on various factors including the data type (e.g., numeric or textual) and length of the entry [17,18].

As society becomes more and more complex, humans become less and less capable of avoiding errors. Errors that have been entered into a data resource can be very difficult to detect and correct. A warning from a computer may help humans avoid making some highly regrettable entry errors. Probably the simplest, but most successful, example of a computational method to find entry errors is the check-digit. The check-digit (which can actually be several digits in length) is a number that is computed from a sequence

(e.g., charge card number) and appended to the end of the sequence. If the sequence is entered incorrectly, the computed check digit will be different from the check-digit that had been embedded as a part of the original (correct) sequence. The check-digit has proven to be a very effective method for reducing data entry errors for identifiers and other important short sequences; and a wide variety of check-digit algorithms are available. [Glossary Checksum]

Spell-checkers are another example of software that finds data errors at the moment of entry. In fact, there are many opportunities for data scientists to develop methods that check for inconsistencies in human-entered data. If we think of an inconsistency as anything that differs from what we would expect to see, based on past experience, than Big Data resources may be the proper repository of "consistent" values with which inconsistencies can be detected.

– **Medical errors.**

Computer systems can suspend prescriptions for which doses exceed expected values, or for which known drug interactions contraindicate use, or for which abuse is suspected (e.g., multiple orders of narcotics from multiple physicians for a single patient). With access to every patient's complete electronic medical record, computers can warn us of idiosyncratic reactions that may occur, and the limits of safe dosages, for any particular patient. With access to biometric identifying information, computers can warn us when a treatment is about to be provided to the wrong patient. As an example, in operating rooms, computers can check that the screened blood components are compatible with the screened blood of the patient; and that the decision to perform the transfusion meets standard guidelines established by the hospital.

– **Rocket launch errors.**

Computers can determine when all sensors report normally (e.g., no frozen o-rings), when all viewed subsystems appear normal (e.g., no torn heat shield tiles hanging from the hull), and when all systems are go (e.g., no abnormalities in the function of individual systems), and when the aggregate system is behaving normally (e.g., no conflicts between subsystems). Rockets are complex, and the job of monitoring every system for errors is a Big Data task.

– **Motor vehicle accidents.**

It is thrilling to know that computers may soon be driving our cars, but most motor vehicle collisions could be prevented if we would simply eliminate from our roads those human drivers who are impaired, distracted, reckless, or otherwise indisposed to obeying the legal rules of driving. With everything we know about electronic surveillance, geopositioning technology, traffic monitoring, vehicle identification, and drug testing, you might think that we would have a method to rid the roads of poor drivers and thereby reduce motor vehicle fatalities. More than 32,000 people die each year from traffic accidents in the United States, and many more individuals are permanently disabled. Big Data technology

could collect, analyze, and instantly react to data collected from highways; and it is easy to see how this information could greatly reduce the rate of motor vehicle deaths. What are we waiting for?

Section 20.5. Who Is Big Data?

> *The horizons of physics, philosophy, and art have of late been too widely separated, and, as a consequence, the language, the methods, and the aims of any one of these studies present a certain amount of difficulty for the student of any other of them.*
>
> *Hermann L. F. Helmholtz, 1885 [19]*

To get the most value from Big Data resources, will we need armies of computer scientists trained with the most advanced techniques in supercomputing? According to an industry report prepared by McKinsey Global Institute, the United States faces a current shortage of 140,000–190,000 professionals adept in the analytic methods required for Big Data [20]. The same group estimates that the United States needs an additional 1.5 million data-savvy managers [20].

Analysis is important; it would be good to have an adequate workforce of professionals trained in a variety of computationally-intensive techniques that can be applied to Big Data resources. Nevertheless, there is little value in applying advanced computational methods to poorly designed resources that lack introspection and data identification. A high-powered computer operated by a highly trained analyst cannot compensate for opaque or corrupted data. Conversely, when the Big Data resource is well designed, the task of data analysis becomes relatively straightforward.

At this time, we have a great many analytic techniques at our disposal, and we have open source software programs that implement these techniques. Every university offers computer science courses and statistics courses that teach these techniques. We will soon reach a time when there will be an oversupply of analysts, and an under-supply of well-prepared data. When this time arrives, there will be a switch in emphasis from data analysis to data preparation. The greatest number of Big Data professionals will be those people who prepare data for analysis.

Will Big Data create new categories of data professionals, for which there are currently no training programs? In the near future, millions of people will devote large portions of their careers toward the design, construction, operation, and curation of Big Data resources. Who are the people best equipped for these tasks?

– **Resource Builders:**

– Big Data Designers

Big Data does not self-assemble into a useful form. It must be designed before any data is collected. The job of designing a Big Data resource cannot be held by any single person, but a data manager (i.e., the person who supervises the project team) is often saddled with

the primary responsibility of proffering a design or model of the resource. Issues such as what data will be included, where the data comes from, how to verify the data, how to annotate and classify the data, how to store and retrieve data, how to access the system, and a thousand other important concerns must be anticipated by the designers. If the design is bad, the Big Data resource will likely fail.

– Big Data Indexers

As discussed in Section 2.4, indexes help us find the data we need, quickly. The Google search engine is, at its heart, an index, built by the PageRank algorithm. Without indexers and the algorithms that organize data in a way that facilitates the kinds of searches that users are likely to conduct, Big Data would have very little appeal. The science of indexing is vastly underrated in universities, and talented indexers are hard to find. Indexers should be actively recruited into most Big Data projects.

– Domain experts

It is impossible to sensibly collect and organize Big Data without having a deep understanding of the data domain. An effective data domain expert has an understanding of the kinds of problems that the data c an help solve, and can communicate her knowledge to the other members of the Big Data project, without resorting to opaque jargon. The domain expert must stay current in her field and should regularly share information with other domain experts in her field and in fields that might be relatable to the project.

– Metadata experts

The most common mistake made by beginners to the metadata field is to create their own metadata tags to describe their data. Metadata experts understand that individualized metadata solutions produce Big Data than cannot be usefully merged with other data sets. Experts need to know the metadata resources that are available on the web, and they must choose metadata descriptors that are defined in permanent, accessible, and popular schemas. Such knowledge is an acquired skill that should be valued by Big Data managers.

– Ontologists and classification experts

As noted in Sections 5.6–5.8, it is almost impossible to create a good classification. Creating, maintaining, and improving a classification is a highly demanding skill, and classification errors can lead to disastrous results for a Big Data resource and its many users. Hence, highly skill taxonomists and ontologists are essential to any Big Data project.

– Software programmers

Software programmers are nice to have around, but they have a tendency to get carried away with large applications and complex graphic user interfaces. Numerous examples shown throughout this book would suggest that most of the useful algorithms in Big Data are actually quite simple. Programmers who have a good working knowledge of many

different algorithms, and who can integrate short implementations of these algorithms, as needed, within the framework of a Big Data Resource, are highly useful.

In many cases, Big Data projects can operate quite well using free and open source database applications. The primary purpose of programmers, in this case, often falls to making incremental additions and adjustments to the bare-bones system. As a general rule, the fewer the additions, the better the results. Programmers who employ good practices (e.g., commenting code, documenting changes, avoiding catastrophic interactions between the different modules of an application) can be more effective than genious-grade programmers who make numerous inscrutable system modifications before moving to a higher-paying job with your competitor.

– Data curators, including legacy experts

Who is responsible for all this immutability that haunts every Big Data resource? Most of the burden falls upon the data curator. The word "curator" derives from the Latin, "curatus," the same root for "curative" and conveys that curators fix things. In a Big Data resource the curator must oversee the accrual of sufficiently annotated legacy and prospective data into the resource; must choose appropriate nomenclatures for annotating the data; must annotate the data; and must supplement records with updated annotations as appropriate, when new versions of nomenclatures, specifications, and standards are applied. The curator is saddled with the almost impossible task of keeping current the annotative scaffold of the Big Data resource, without actually changing any of the existing content of records. In the absence of curation, all resources will eventually fail.

It all seems so tedious! Is it really necessary? Sadly, yes. Over time, data tends to degenerate: records are lost or duplicated, links become defunct, unique identifiers lose their uniqueness, the number of missing values increases, nomenclature terms become obsolete, mappings between terms coded to different standards become decreasingly reliable. As personnel transfer, quit, retire, or die, the institutional memory for the Big Data resource weakens. As the number of contributors to a Big Data resource increases, controlling the quality of the incoming data becomes increasingly difficult. Data, like nature, regresses from order to disorder; unless energy is applied to reverse the process. There is no escape; every reliable Big Data resource is obsessed with self-surveillance and curation.

– Data managers

In most instances the data manager is also the data project manager in charge of a team of workers. Her biggest contribution will involve creating a collegial, productive, and supportive working environment for their team members. The database manager must understand why components of Big Data resources, that are not found in smaller data projects (e.g., metadata, namespaces, ontologies, identifier systems, timestamps) are vital, and why the professionals absorbed in these exclusively Big Data chores are integral to the success of the projects. Team training is crucial in Big Data efforts, and the data manager must help each member of her team understand the roles played by the other members.

The data manager must also understand the importance of old data and data permanence and data immutability.

– Network specialists

Big Data seldom exists in a silo. Throughout this book, and only as a convenience, data is described as something that is conveyed in a document. In reality, data is something that streams between clouds. Network specialists, not discussed in any detail in this book, are individuals who know how to access and link data, wherever it may reside.

– Security experts

Security issues were briefly discussed in Section 18.3, "Data Security and Cryptographic Protocols." Obviously, this import ant subject cannot be treated in any great depth in this book. Suffice it to say, Big Data requires the services of security experts whose knowledge is not confined to the type of encryption protocols described earlier. Data security is more often a personnel problem than a cryptographic puzzle. Breaches are likely to arise due to human carelessness (i.e., failure to comply with security protocols) or from misuse of confid ential information (i.e., carrying around gigabytes of private information on a personal laptop, or storing classified documents at home). Security experts, skilled in the technical and social aspects of their work, fulfill an important role.

– **Resource Users**

– Data validators

What do we really know about the measurements contained in Big Data resources? How can we know what these measurements mean, and whether they are correct? Data managers approach these questions with three closely related activities: data verification, data reproducibility, and validation. As previously mentioned, verification is the process that ensures that data conforms to a set of specifications. As such, it is a pre-analytic process (i.e., done on the data, before it is analyzed). Data reproducibility involves getting the same measurement over and over when you perform the test properly. Validation involves showing that correct conclusions were obtained from a competent analysis of the data. The primary purpose of data validators is to show that the scientific conclusions drawn from a Big Data resource are trustworthy and can be used as the foundation for other studies. The secondary purpose of data validators is to determine when the conclusions drawn from the data are not trustworthy, and to make recommendations that might rectify the situation.

– Data analysts

Most data analysts carry a set of methods that they have used successfully, on small data problems. No doubt, they will apply the same methods to Big Data, with varying results. The data analysts will be the ones who learn, from trial and error, which methods are

computationally impractical on large sets of data, which methods provide results that have no practical value, which methods are unrepeatable, and which methods cannot be validated. The data analysts will also be the ones who try new methods and report on their utility. Because so many of the analytic methods on Big Data are over-hyped, it will be very important to hire data analysts who are objective, honest, and resistant to bouts of hubris.

– Generalist problem solvers

Arguably the most essential new professional is the "generalist problem solver," a term that describes people who have a genuine interest in many different fields, a naturally inquisitive personality, and who have a talent for seeing relationships where others do not. The data held in Big Data resources becomes much more valuable when information from different knowledge domains lead to unexpected associations that enlighten both fields (e.g., veterinary medicine and human medicine, bird migration and global weather patterns, ecologic catastrophes and epidemics of emerging diseases, political upheaval and economic cycles, social media activity and wages in African nations). For these kinds of efforts, someone needs to create a new set of cross-disciplinary questions that could not have been asked prior to the creation of Big Data resources.

Historically, academic training narrows the interests of students and professionals. Students begin their academic careers in college, where they are encouraged to select a major field of study as early as their freshman year. In graduate school, they labor in a sub-discipline, within a rigidly circumscribed department. As postdoctoral trainees, they narrow their interests even further. By the time they become tenured professors, their expertise is so limited that they cannot see how other fields relate to their own studies. The world will always need people who devote their professional careers to a single sub-discipline, to the exclusion of everything else, but the future will need fewer and fewer of these specialists [21]. My experience has been that cross-disciplinary approaches to scientific problems are very difficult to publish in scientific journals that are, with few exceptions, devoted to one exclusive area of research. When a journal editor receives a manuscript that employs methods from another discipline, the editor usually rejects the paper, indicating that it belongs in some other journal. Even when the editor recognizes that the study applies to a problem within the scope of the journal, the editor would have a very difficult time finding reviewers who can evaluate a set of methods from another field. To get the greatest value from Big Data resources, it is important to understand when a problem in one field has an equivalence to a problem from another field. The baseball analyst may have the same problem as the day trader; the astrophysicist may have the same problem as the chemist. We need to have general problem solvers who understand how data from one resource can be integrated with the data from other resources, and how problems from one field can be generalized to other fields, and can be answered with an approach that combines data and methods from several different disciplines. It is important that universities begin to train students as problem solvers, without forcing them into restrictive academic departments.

– Scientists with some minimal programming skills (not usually full-time programmers)

In the 1980s, as the cost of computers plummeted, and desktop units were suddenly affordable to individuals, it was largely assumed that all computer owners would become computer programmers. At the time, there was nothing much worth doing with a computer other than programming and word processing. By the mid-1990s, the Internet grabbed the attention of virtually every computer owner. Interest in programming languages waned, as our interest in social media and recreational uses of the computer grew. It is ironic that we find ourselves inundated with an avalanche of Big Data, just at the time that society, content with online services provided by commercial enterprises, have traded their computers for smartphones. Scientists and other data users will find that they cannot do truly creative work using proprietary software applications. They will always encounter situations wherein software applications fail to meet their exact needs. In these cases it is impractical to seek the services of a full-time programmer.

Today, programming is quite easy. Within a few hours, motivated students can pick up the rudiments of popular scripting languages such as Python, Perl, Ruby and R. With few exceptions, the scripts needed for Big Data analysis are simple and most can be written in under 10 lines of code [22–25]. It is not necessary for Big Data users to reach the level of programming proficiency held by professional programmers. For most scientists, programming is one of those subjects for which a small amount of training preparation will usually suffice. I would strongly urge scientists to return to their computational roots and to develop the requisite skills for analyzing Big Data.

– Data reduction specialists

There will be a need for professionals to develop strategies for reducing the computational requirements of Big Data and for simplifying the way that Big Data is examined. For example, the individuals who developed the CODIS DNA identification system (discussed in Section 17.4, "Case Study: Scientific Inferencing from a Database of Genetic Sequences") relieved forensic analysts from the prodigious task of comparing and storing, for each sampled individual, the 3 billion base pairs that span the length of the human genome. Instead, a selection of 13 short sequences can suffice to identify individual humans. Likewise, classification experts drive down the complexity of their analyses by focusing on data objects that belong to related classes with shared and inherited properties. Similarly, data modelers attempt to describe complex systems with mathematical expressions, with which the behavior of the system can be predicted when a set of parameters are obtained. Experts who can extract, reduce, and simplify Big Data will be in high demand and will be employed in academic centers, federal agencies and corporations.

– Data visualizers

Often, all that is needed to make an important observation is a visualized summary of data. Luckily, there are many data visualization tools that are readily available to today's scientists. Examples of simple data plots using matplotlib (a Python module) or Gnuplot

(an open source application that can be called from the command line) have been shown. Of course, Excel afficionados have, at their disposal, a dazzling number of ways with which they can display their spreadsheet data. Regardless of your chosen tools, anyone working with data should become adept at transforming raw data into pictures.

– Free-lance Big Data consultants

Big Data freelancers are self-employed professionals who have the skills to unlock the secrets that lie within Big Data resources. When they work under contract for large institutions and corporations, they may be called consultants, or freelance analysts. When they sell their data discoveries on the open market, they may be called entrepreneurial analysts. They will be the masters of data introspection, capable of quickly determining whether the data in a resource can yield the answers sought by their clients. Some of these Big Data freelancers will have expertise limited to one or several Big Data resources; expertise that may have been acquired as a regular employee of an institution or corporation, in the years preceding his or her launch into self-employment. Freelancers will have dozens, perhaps hundreds, of small utilities for data visualization and data analysis. When they need assistance with a problem, the freelancer might enlist the help of fellow freelancers. Subcontracted alliances can be arranged quickly, through Internet-based services. The need for bricks-and-mortar facilities, or for institutional support, or for employers and supervisors, will diminish. The freelancer will need to understand the needs of his clients and will be prepared to help the client redefine their specific goals, within the practical constraints imposed by the available data. When the data within a resource is insufficient, the freelancer would be the best person to scout alternate resources. Basically, freelance analysts will live by their wits, exploiting the Big Data resources for the benefit of themselves and their clients.

– Everyone else

As public data becomes increasingly available, there will be an opportunity for everyone to participate in the bounty. See Section 20.7, "Case Study: The Citizen Scientists".

Section 20.6. Hubris and Hyperbole

> *Intellectuals can tell themselves anything, sell themselves any bill of goods, which is why they were so often patsies for the ruling classes in nineteenth-century France and England, or twentieth-century Russia and America.*
>
> *Lillian Hellman*

A Forbes magazine article, published in 2015, running under the title, "Big Data: 20 Mind-Boggling Facts Everyone Must Read," listed some very impressive "facts," including that claim that more data has been created in the past two years than in all of prior history [26]. Included in the article was the claim that by the year 2020, the accumulated data collected worldwide will be about 44 zettabytes (44 trillion gigabytes). The author

wrote, as one of his favorite facts, "At the moment less than 0.5% of all data is ever analyzed and used, just imagine the potential here" [26].

Of course, it is impossible to either verify or to discredit such claims, but experience would suggest that only a small percentage of the data that is collected today is worth the serious attention of data analysts. It is quite rare to find data that has been annotated with even the most minimal information required to conduct credible scientific research. These minimal annotations, as discussed previously, would be the name of the data creator, the owner of the data, the legal restraints on the usage of the data, the date that the data was created, the protocols by which the data was measured and collected, identifiers for data objects, class information on data objects, and metadata describing data within data objects. If you have read the prior chapters, you know the drill.

Make no mistake, despite the obstacles and the risks, the potential value of Big Data is inestimable. A hint at future gains from Big Data comes from the National Science Foundation's (NSF) 2012 solicitation for grants in core techniques for Big Data. The NSF envisions a Big Data future with the following pay-offs [1]:

- "Responses to disaster recovery empower rescue workers and individuals to make timely and effective decisions and provide resources where they are most needed;
- Complete health/disease/genome/environmental knowledge bases enable biomedical discovery and patient-centered therapy; The full complement of health and medical information is available at the point of care for clinical decision-making;
- Accurate high-resolution models support forecasting and management of increasingly stressed watersheds and ecosystems;
- Access to data and software in an easy-to-use format are available to everyone around the globe;
- Consumers can purchase wearable products using materials with novel and unique properties that prevent injuries;
- The transition to use of sustainable chemistry and manufacturing materials has been accelerated to the point that the US leads in advanced manufacturing;
- Consumers have the information they need to make optimal energy consumption decisions in their homes and cars;
- Civil engineers can continuously monitor and identify at-risk man-made structures like bridges, moderate the impact of failures, and avoid disaster;
- Students and researchers have intuitive real-time tools to view, understand, and learn from publicly available large scientific data sets on everything from genome sequences to astronomical star surveys, from public health databases to particle accelerator simulations and their teachers and professors use student performance analytics to improve that learning; and
- Accurate predictions of natural disasters, such as earthquakes, hurricanes, and tornadoes, enable life-saving and cost-saving preventative actions."

Lovely. It would seem that there is nothing that cannot be accomplished with Big Data!

I know lots of scientists; the best of them lack self-confidence. They understand that their data may be flawed, their assumptions may be wrong, their methods might be inappropriate, their conclusions may be unrepeatable, and their most celebrated findings may one day be discredited. The worst scientists are just the opposite; confident of everything they do, say, or think [27].

The sad fact is that, among scientific disciplines, Big Data is probably the least reliable, providing major opportunities for blunders. Prior chapters covered limitations in measurement, data representation, and methodology. Some of the biases encountered in every Big Data analysis were covered in Chapter 14, "Special Considerations in Big Data Analysis." Apart from these limitations lies the ever-present dilemma that assertions based on Big Data analyses can sometimes be validated, but they can never be proven true. Confusing validation with proof is a frequently encountered manifestation of overconfidence. If you want to attain proof, you must confine your interests to pure mathematics. Mathematics is the branch of science devoted to truth. With math, you can prove that an assertion is true, you can prove that an assertion is false, you can prove that an assertion cannot be proven to be true or false. Mathematicians have the monopoly on proving things. None of the other sciences have the slightest idea what they're doing when it comes to proof.

In the non-mathematical sciences, such as chemistry, biology, medicine, and astronomy, assertions are sometimes demonstrably valid (true when tested), but assertions never attain the level of a mathematical truth (proven that it will always be true, and never false, forever). Nonetheless, we can do a little better than showing that an assertion is simply valid. We can sometimes explain why an assertion ought to be true for every test, now and forever. To do so, an assertion should have an underlying causal theory that is based on interactions of physical phenomena that are accepted as true. For example, $F = ma$ ought to be true, because we understand something about the concepts of mass and acceleration, and we can see why the product of mass and acceleration produce a force. Furthermore, everything about the assertion is testable in a wide variety of settings.

Big Data analysts develop models that are merely descriptive (e.g., predicting the behavior of variables in different settings), without providing explanations in terms of well-understood causal mechanisms. Trends, clusters, classes, and recommenders may appear to be valid over a limited range of observations; but may fail miserably in tests conducted over time, with a broader range of data. Big Data analysts must always be prepared to abandon beliefs that are not actually proven [21].

Finance has eagerly entered the Big Data realm, predicting economic swings, stock values, buyer preferences, the impact of new technologies, and a variety of market reactions, all based on Big Data analysis. For many financiers, accurate short-term predictions have been followed, in the long-run, with absolutely ruinous outcomes. In such cases, the mistake was overconfidence; the false belief that their analyses will always be correct [28].

In my own field of concentration, cancer research, there has been a major shift of effort away from small experimental studies toward large clinical trials and so-called

high-throughput molecular methods that produce vast arrays of data. This new generation of cancer research costs a great deal in terms of manpower, funding, and the time to complete a study. The funding agencies and the researchers are confident that a Big Data approach will work where other approaches have failed. Such efforts may one day lead to the eradication of cancer; who is to say? In the interim, we have already seen a great deal of time and money wasted on huge, data-intensive efforts that have produced predictions that are not reproducible, with no more value than a random throw of dice [4,29–32].

Despite the limitations of Big Data, the creators of Big Data cannot restrain their enthusiasm. The following is an announcement from the National Human Genome Research Institute concerning their own achievements [33]:

"In April 2003, NHGRI celebrated the historic culmination of one of the most important scientific projects in history: the sequencing of the human genome. In addition, April 2003 marked the 50th anniversary of another momentous achievement in biology: James Watson and Francis Crick's Nobel Prize winning description of the DNA double helix" and "To mark these achievements in the history of science and medicine, the NHGRI, the NIH and the DOE held a month-long series of scientific, educational, cultural and celebratory events across the United States."

In the years following this 2003 announcement, it has become obvious that the genome is much more complex than previously thought, that common human diseases are genetically complex, that the genome operates through mechanisms that cannot be understood by examining DNA sequences, and that much of the medical progress expected from the Human Genome Project will not be forthcoming anytime soon [29,34,35]. In a 2011 article, Eric Lander, one of the luminaries of the Human Genome Project, was quoted as saying, "anybody who thought in the year 2000 that we'd see cures in 2010 was smoking something" [35]. Monica Gisler and co-workers have hypothesized that large-scale projects create their own "social bubble," inflating the project beyond any rational measure [36]. It is important that Big Data proselytizers, myself included, rein in their enthusiasm.

Section 20.7. Case Study: The Citizen Scientists

> *There is no reason why someone would want a computer in their home.*
>
> *Ken Olson, President and founder of Digital Equipment Corporation, in 1977.*

In a sense, we have reached a post-information age. At this point, we have collected an awful lot of information, and we all have access too much more information than we can possibly analyze within our lifetimes. In fact, all the professional scientists and data analysts who are living today could not possibly exhaust the information available to anyone with Internet access. If we want to get the most out of the data that currently resides within our grasps, we will need to call upon everyone's talents, including amateurs. Lest we forget, every professional scientist enters the ranks of the amateur scientists on the day that he or she retires. Today, the baby boomer generation is amassing an army of

well-trained scientists who are retiring into a world that provides them with unfettered access to limitless data. Hence, we can presume that the number of amateur scientists will soon exceed the number of professional scientists.

Historically, some of the greatest advancements in science have come from amateurs. For example, Antonie van Leeuwenhoek (1632–1723), one of the earliest developers of the compound microscope, who is sometimes credited as the father of microbiology, was a janitor. Augustin-Jean Fresnel (1788–1827) was a civil engineer who found time to make significant and fundamental contributions to the theory of wave optics. Johann Jakob Balmer (1825–1898) earned his living as a teacher in a school for girls while formulating the mathematical equation describing the spectral emission lines of hydrogen. His work, published in 1885, led others, over the next four decades, to develop the new field of quantum mechanics. Of course, Albert Einstein was a paid patent clerk and an amateur physicist who found time, in 1905, to publish three papers that forever changed the landscape of science.

In the past few decades a wealth of scientific resources has been made available to anyone with Internet access. Many of the today's most successful amateurs are autodidacts with access to Big Data [37–42]. Here are a few examples:

– Amateurs identifying the genes that cause human disease

In the field of medicine, some of the most impressive data mining feats have come from individuals affected by rare diseases who have used publicly available resources to research their own conditions.

Jill Viles is a middle-aged woman who, when she was a college undergraduate, correctly determined that she was suffering from Emery-Dreifuss muscular dystrophy. The diagnosis of this very rare form of muscular dystrophy was missed by her physicians. After her self-diagnosis was confirmed, she noticed that her father, who had never been told he had any muscular condition, had a distribution of his muscle mass that was suggestive of Emery-Dreifuss. Jill's suspicions initiated a clinical consultation indicating that her father indeed had a mild form of the same disorder and that his heart had been affected. Her father received a needed pacemaker, and Jill's shrewd observations were credited with saving her father's life. Jill pursued her interest in her own condition and soon became one of the early beneficiaries of genome sequencing. A mutation of the lamin gene was apparently responsible for her particular variant of Emery-Dreifuss muscular dystrophy. Jill later realized that in addition to Emery-Dreifuss muscular dystrophy, she also exhibited some of the same highly distinctive features of partial lipodystrophy, a disease characterized by a decrease in the fat around muscles. When the fat around muscles is decreased, the definition of the muscles (i.e., the surface outline of musculature) is enhanced. She reasoned, correctly, that the lamin gene, in her case, was responsible for both conditions (i.e., Emery-Dreifuss muscular dystrophy and partial lipodystrophy).

Jill's story does not end here. While looking at photographs of Priscilla Lopes-Schlief, an Olympic athlete known for her hypertrophied muscles, Jill noticed something very peculiar. The athlete had a pattern of fat-deficient muscle definition on her shoulders, arms,

hips, and butt, that was identical to Jill's; the difference being that Priscilla's muscles were large, and Jill's muscles were small. Jill contacted the Olympian, and the discussions that followed eventually led to Priscilla's diagnosis of lipodystrophy due to a mutation on the lamin gene, at a locus different from Jill's. Lipodystrophy can produce a dangerous elevation in triglycerides, and Priscilla's new diagnosis prompted a blood screen for elevated lipids. Priscilla had high levels of triglyceride, requiring prompt treatment. Once again, Jill had made a diagnosis that was missed by physicians, linked the diagnosis to a particular gene and uncovered a treatable and overlooked secondary condition (i.e., hypertriglyceridemia). And it was all done by an amateur with Internet access [43]!

Jill Viles' story is not unique. Kim Goodsell, a patient with two rare diseases, Charcot-Marie-Tooth disease and arrhythmogenic right ventricular cardiomyopathy, searched the available gene datasets until she found a single gene that might account for both of her conditions. After much study, she determined that a point mutation in the LMNA gene was the most likely cause of her condition. Kim paid $3000 for gene sequencing of her own DNA, and a rare point mutation on LMNA was confirmed to be responsible for her dual afflictions [44]. In Kim's case, as in Jill's case, a persistent and motivated amateur can be credited with a significant advance in the genetics of human disease.

– 36-year-old satellite resurrected

The International Space/Earth Explorer 3 (ISEE-3) spacecraft was launched in 1978 and proceeded on a successful mission to monitor the interaction between the solar wind and the earth's magnetic field. In 1985, ISEE-3 visited the comet Giacobini-Zinner, and was thereupon given a new name, ICE (the International Cometary Explorer). In 1999 NASA, short of funds, decommissioned ICE. In 2008, NASA tried to contact ICE and found that all but one of its 13 observational experiments were still in operation, and that the spacecraft had not yet exhausted its propellant.

In April 2014, a citizens group of interested scientists and engineers announced their intention to reboot ICE [38]. In May, 2014, NASA entered into a Non-Reimbursable Space Act Agreement with the citizen group, which would provide the reboot team with NASA advisors, but no funding. Later in May, the team successfully commanded the probe to broadcast its telemetry (i.e., its recorded data). In September, the team lost contact with ICE. ICE will return to a near-earth position, in 17 years (Fig. 20.1). There is reason to hope that scientists will eventually recover ICE telemetry, and, with it, find new opportunities for data analysis [45].

In the past, the term "amateurish" was used to describe products that are unprofessional and substandard. In the realm of Big Data, where everyone has access to the same data, amateurs and professionals can now compete on a level playing field. To their credit, amateurs are unsullied by the kind of academic turf battles, departmental jealousies, and high-stakes grantsmanship ploys that produce fraudulent, misleading, or irreproducible results [46]. Because amateurs tend to work with free and publicly available data sets, their research tends to be low-cost or no-cost. Hence, on a cost-benefit analysis, amateur scientist may actually have more value, in terms of return on investment, than professional

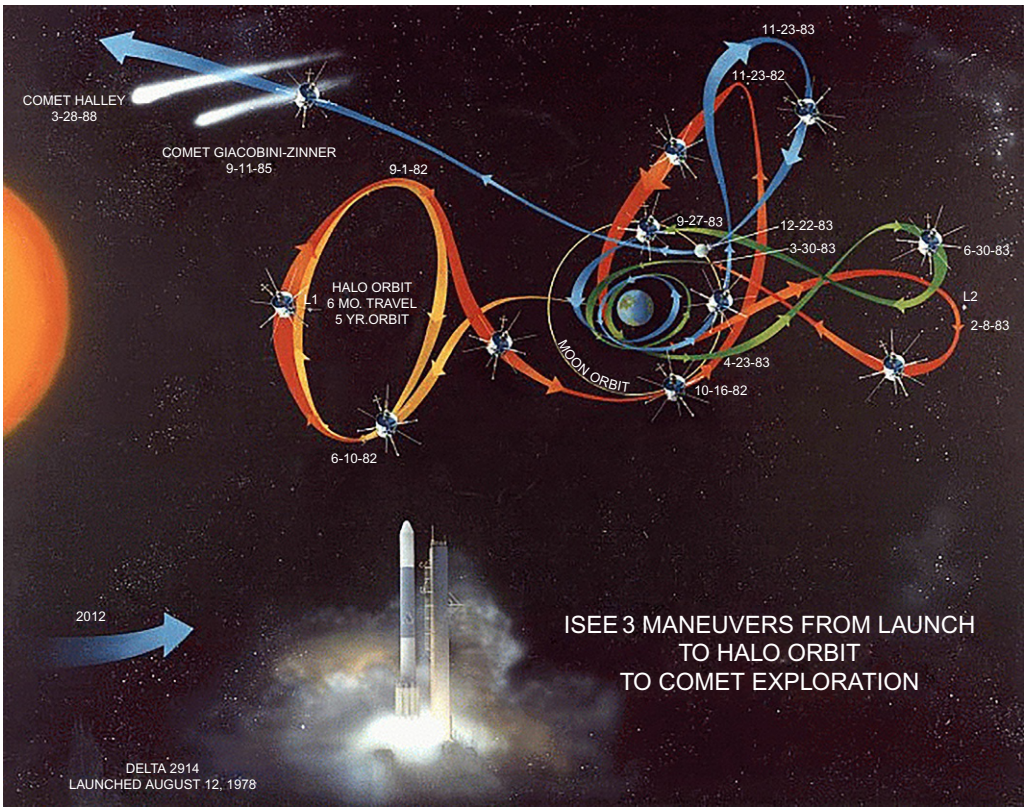

FIG. 20.1 Trajectory of the International Cometary Explorer. *From NASA, public domain.*

scientists. Moreover, there are soon to be many more amateur scientists than there are professionals, making it likely that these citizen scientists, who toil for love, not money, will achieve the bulk of the breakthroughs that come from Big Data science. Of course, none of these breakthroughs, from citizen scientists, would be possible without free and open access to Big Data resources.

Section 20.8. Case Study: 1984, by George Orwell

> *He who controls the past controls the future.*
>
> *George Orwell*

When you have access to Big Data, you feel liberated; when Big Data has access to you, you feel enslaved. Everyone is familiar with the iconic image, from Orwell's 1984, of a totalitarian government that spies on its citizens from telescreens [47]. The ominous

phrase, "Big Brother is watching you," evokes an important thesis of Orwell's masterpiece; that an evil government can use an expansive surveillance system to crush its critics.

Lest anyone forget, Orwell's book had a second thesis, that was, in my opinion, more insidious and more disturbing than the threat of governmental surveillance. Orwell was concerned that governments could change the past and the present by inserting, deleting, and otherwise distorting the information available to citizens. In Orwell's 1984, previously published reports of military defeats, genocidal atrocities, ineffective policies, mass starvation, and any ideas that might foment unrest among the proletariat, were deleted and replaced with propaganda pieces. Such truth-altering activities were conducted undetected, routinely distorting everyone's perception of reality to suit a totalitarian agenda. Aside from understanding the dangers in a surveillance-centric society, Orwell was alerting us to the dangers inherent with mutable Big Data.

Today, our perception of reality can be altered by deleting or modifying electronic data distributed via the Internet. In 2009, Amazon was eagerly selling electronic editions of a popular book, much to the displeasure of the book's publisher. Amazon, to mollify the publisher, did something that seemed impossible. Amazon retracted the electronic books from the devices of readers who had already made their purchase. Where there was once a book on a personal eBook reader, there was now nothing. Amazon rectified their action by crediting customer accounts for the price of the book. So far as Amazon and the publisher were concerned, the equilibrium of the world was restored [48].

The public reaction to Amazon's vanishing act was a combination of bewilderment ("What just happened?"), shock ("How was it possible for Amazon to do this?"), outrage ("That book was mine!"), fear ("What else can they do to my eBook reader?"), and suspicion ("Can I ever buy another eBook?"). Amazon quickly apologized for any misunderstanding and promised never to do it again.

To add an element of irony to the episode, the book that was bought, then deleted, to suit the needs of a powerful entity, was George Orwell's 1984.

One of the purposes of this book is to describe the potential negative consequences of Big Data when data is not collected ethically, prepared thoughtfully, analyzed openly, or subjected to constant public review and correction. These lessons are important because the future reality of our Big Data universe will be determined by some of the people who are reading this book today.

Glossary

Artificial intelligence Artificial intelligence is the field of computer science that seeks to create machines and computer programs that seem to have human intelligence. The field of artificial intelligence sometimes includes the related fields of machine learning and computational intelligence. Over the past few decades, the term "artificial intelligence" has taken a battering from professionals inside and outside the field, for good reasons. First and foremost is that computers do not think in the way that humans think. Though powerful computers can now beat chess masters at their own game, the algorithms for doing so do not simulate human thought processes. Furthermore, most of the predicted benefits from artificial intelligence have not come to pass, despite decades of generous

funding. The areas of neural networks, expert systems, and language translation have not met expectations. Detractors have suggested that artificial intelligence is not a well-defined sub discipline within computer science as it has encroached into areas unrelated to machine intelligence, and has appropriated techniques from other fields, including statistics and numerical analysis. Some of the goals of artificial intelligence have been achieved (e.g., speech-to-text translation), and the analytic methods employed in Big Data analysis should be counted among the enduring successes of the field.

Checksum An outdated term that is sometimes used synonymously with one-way hash or message digest. Checksums are performed on a string, block or file yielding a short alphanumeric string intended to be specific for the input data. Ideally, If a single bit were to change, anywhere within the input file, then the checksum for the input file would change drastically. Checksums, as the name implies, involve summing values (typically weighted character values), to produce a sequence that can be calculated on a file before and after transmission. Most of the errors that were commonly introduced by poor transmission could be detected with checksums. Today, the old checksum algorithms have been largely replaced with one-way hash algorithms. A checksum that produces a single digit as output is referred to as a check digit.

Machine learning Refers to computer systems and software applications that learn or improve as new data is acquired. Examples would include language translation software that improves in accuracy as additional language data is added to the system, and predictive software that improves as more examples are obtained. Machine learning can be applied to search engines, optical character recognition software, speech recognition software, vision software, neural networks. Machine learning systems are likely to use training data sets and test data sets.

Semantics The study of meaning. In the context of Big Data, semantics is the technique of creating meaningful assertions about data objects. A meaningful assertion, as used here, is a triple consisting of an identified data object, a data value, and a descriptor for the data value. In practical terms, semantics involves making assertions about data objects (i.e., making triples), combining assertions about data objects (i.e., merging triples), and assigning data objects to classes; hence relating triples to other triples. As a word of warning, few informaticians would define semantics in these terms, but I would suggest that most definitions for semantics would be functionally equivalent to the definition offered here.

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About the Author:

Jules J. Berman holds two Bachelor of Science degrees from MIT (in mathematics, and in earth and planetary sciences), a PhD from Temple University, and an MD from the University of Miami. His post-doctoral studies were completed at the US National Institutes of Health, and his residency was completed at the George Washington University Medical Center in Washington, D.C. Dr. Berman served as chief of Anatomic Pathology, Surgical Pathology, and Cytopathology at the Veterans Administration Medical Center in Baltimore, Maryland, where he held joint appointments at the University of Maryland Medical Center and at the Johns Hopkins Medical Institutions. In 1998, he transferred to the US National Institutes of Health as a medical officer and as the program director for pathology informatics in the Cancer Diagnosis Program at the National Cancer Institute. Dr. Berman is a past president of the Association for Pathology Informatics and the 2011 recipient of the association's Lifetime Achievement Award.

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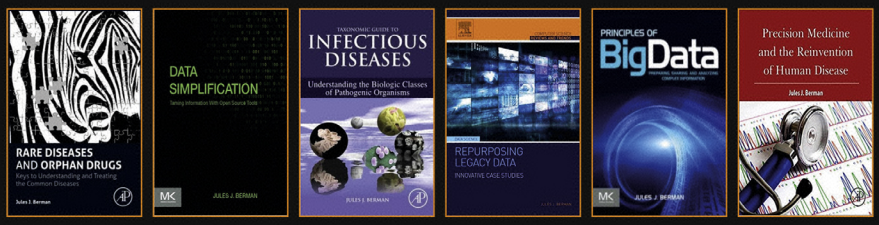

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