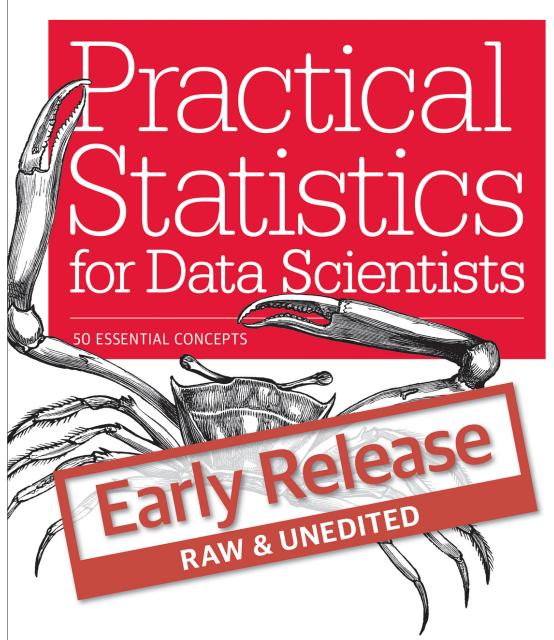


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Statistics for Data Scientists

1ST EDITION

50 Essential Concepts

Peter C. Bruce and Andrew G. Bruce



Practical Statistics for Data Scientists

by Peter Bruce and Andrew Bruce

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Preface

What to Expect

KEY TERMS

Data science is a fusion of multiple disciplines, including statistics, computer science, information technology and domain specific fields. As a result, a several different terms could be used to reference a given concept. Key terms and their synonyms will be highlighted throughout the book in a sidebar such as this.

Conventions Used in This Book

The following typographical conventions are used in this book:

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Indicates new terms, URLs, email addresses, filenames, and file extensions.

Constant width

Used for program listings, as well as within paragraphs to refer to program elements such as variable or function names, databases, data types, environment variables, statements, and keywords.

Constant width bold

Shows commands or other text that should be typed literally by the user.

Constant width italic

Shows text that should be replaced with user-supplied values or by values determined by context.



This element signifies a tip or suggestion.

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This element signifies a general note.

WARNING

This element indicates a warning or caution.

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Acknowledgments

Chapter 1. Exploratory Data Analysis

As a discipline, statistics has mostly developed in the past century. Probability theory — the mathematical foundation for statistics — was developed in the 17th to 19th centuries based on work by Thomas Bayes, Pierre-Simon Laplace and Carl Gauss. In contrast to the purely theoretical nature of probability, statistics is an applied science concerned with analysis and modeling of data. Modern statistics as a rigorous scientific discipline traces its roots back to the late 1800's and Francis Galton and Karl Pearson. R. A. Fischer, in the early 20th century, was a leading pioneer of modern statistics, introducing key ideas of *experimental design* and *maximum likelihood estimation*. These and many other statistical concepts live largely in the recesses of data science. The main goal of this book is to help illuminate these concepts and clarify their importance — or lack thereof — in the context of data science and big data.

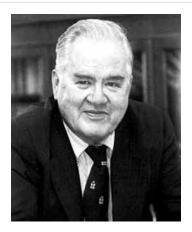


Figure 1-1. John Tukey, a preeminent statistician, whose ideas developed over fifty years ago form the foundation of data science.

This chapter focuses on the first step in any data science project: exploring the data. *Exploratory data analysis*, or *EDA*, is a comparatively new area of statistics. Classical statistics focused almost exclusively on *inference*, a sometimes complex set of procedures for drawing conclusons about large populations based on small samples. In 1962, John W. Tukey called for a reformation of statistics in his seminal paper "The Future of Data Analysis" [Link to Come]. He proposed a new scientific discipline called "Data Analysis" that included statistical inference as just one component. Tukey forged links to the engineering and computer science communities (he coined the terms "bit," short for binary digit, and "software"), and his original tenets are suprisingly durable and form part of the foundation for data science. The field of exploratory data analysis was established with Tukey's 1977 now classic book "Exploratory Data Analysis" [Link to Come].

With the ready availablility of computing power and expressive data analysis software, exploratory data analysis has evolved well beyond its original scope. Key drivers of this discipline have been the rapid development of new technology, access to more and bigger data, and the greater use of quantitative analysis in a variety of disciplines. David Donoho, professor of Statistics at Stanford University and undergraduate student of Tukey, authored an excellent article based on his

presentation at the Tukey Centennial workshop in Princeton, NJ [Link to Come]. Donoho traces the genesis of data science back to the Tukey's pioneering work in data analysis.

Elements of Structured Data

Data comes from many sources: sensor measurements, events, text, images, and videos. The *Internet of Things* is spewing out streams of information. Much of this data is unstructured: images are a collection of pixels with each pixel containing RGB color information. Texts are sequences of words and non-word characters, often organized by sections, sub-sections, etc.. Click streams are sequences of actions by a user interacting with an app or web page. In fact, a major challenge of data science is to harness this torrent of raw data into actionable information. To apply the statistical concepts covered in this book, unstructured raw data must be processed and manipulated into a structured form, as it might emerge from a relational database, or be collected for a study.

KEY TERMS FOR DATA TYPES Continuous Data that can take on any value in an interval. Synonyms interval, float, numeric Discrete Data that can only take on integer values, such as counts. Synonyms integer, count Categorical Data that can only take on a specific set of values. Synonyms enums, enumerated, factors, nominal, polychotomous A special case of categorical with just two categories (0/1, True, False). Synonyms dichotomous, logical, indicator **Ordinal** Categorical data that has an explicit ordering. Synonyms ordered factor

There are two basic types of structured data: numeric and categorical. Numeric data comes in two forms: *continuous*, such as wind speed or time duration, and *discrete*, such as the count of the occurence of an event. *Categorical* data takes only a fixed set of values, such as a type of TV screen (plasma, LCD, LED, ...) or a state name (Alabama, Alaska, ...). *Binary* data is an important special case of categorical data that takes on only one of two values, such as 0/1, yes/no or

true/false. Another useful type of categorical data is *ordinal* data in which the categories are ordered; an example of this is a numerical rating (1, 2, 3, 4, or 5).

Why do we bother with a taxonomy of data types? It turns out that for the purposes of data analysis and predictive modeling, the data type is important to help determine the type of visual display, data analysis or statistical model. In fact, data science software, such as R and Python, use these data types to improve computational performance. More important, the data type for a variable determines how software will handle computations for that variable.

Software engineers and database programmers may puzzle why we even need the notion of *categorical* and *ordinal* data for analytics. After all, categories are merely a collection of text (or numeric) values, and the underlying database automatically handles the internal representation. However, explicit identification of data as categorical, as distinct from text, does offer some advantages.

- 1. Knowing that data is categorical can act as a signal to tell software how statistical procedures, such as producing a chart or fitting a model, should behave. In particular, *ordinal* data can be represented as an ordered.factor in R and python, preserving a user-specified ordering in charts, tables and models.
- 2. Storage and indexing can be optimized (as in relational database).
- 3. The possible values a given categorical variable can take are enforced in the software (like an enum).

The third "benefit" can lead to unintended or unexpected behavior: the default behavior of data import functions in R (e.g., read.csv) is to automatically convert a text column into a factor. Subsequent operations on that column will assume that only the allowable values for that column are the ones originally imported, and assigning a new text value will introduce a warning and produce an NA (missing value).

KEY IDEAS

- 1. Data are typically classified in software by their type
- 2. Data types include continuous, discrete, categorical (which includes binary), and ordinal
- 3. Data-typing in software acts as a signal to the software on how to process the data

Further Reading

- 1. Data types can be confusing, since types may overlap, and the taxonomy in one software may differ from that in another. Here is a tutorial for the taxonomy for R: http://www.r-tutor.com/r-introduction/basic-data-types
- 2. Databases are more detailed in their classification of data types, incorporating considerations of precision levels, fixed or variable length fields, etc.; see this guide for SQL: http://www.w3schools.com/sql/sql_datatypes_general.asp

Rectangular Data

The typical frame of reference for an analysis in data science is a *rectangular data* object, like a spreadsheet or database table.

KEY TERMS FOR RECTANGULAR DATA

Data frame

Rectangular data (like a spreadsheet) is the basic data structure for statistical and machine learning models

Feature

A column in the table is commonly refered to as a *feature*.

Synonyms

attribute, input, predictor, variable

Outcome

Many data science projects involve predicting an *outcome* - often a yes/no outcome (in Table 1-1, it is "auction was competitive or not"). The *features* are sometimes used to predict the *outcome* in an experiment or study.

Synonyms

dependent variable, response, target, output

Records

A row in the table is commonly referred to as a record.

Synonyms

case, example, instance, observation, pattern, sample

Retangular data is essentially a 2-dimensional matrix with rows indicating records (cases) and columns indicating features (variables). The data don't always start in this form: unstructured data (e.g. text) must be processed and manipulated so that it can be represented as a set of features in the rectangular data (see "Elements of Structured Data"). Data that are in relational databases must be extracted and put into a single table for most data analysis and modeling tasks.

In Table 1-1 there is a mix of measured or counted data (e.g. duration and price), and categorical data (e.g. category and currency). A special form of categorical variable is a binary (yes/no or 0/1) variable, seen in the right-most column in Table 1-1 — an indicator variable showing whether an auction was competitive or not.

Table 1-1. A Typical Data Format

Category	currency	sellerRating	Duration	endDay	ClosePrice	OpenPrice	Competitive?
Music/Movie/Game	US	3249	5	Mon	0.01	0.01	0
Music/Movie/Game	US	3249	5	Mon	0.01	0.01	0
Automotive	US	3115	7	Tue	0.01	0.01	0
Automotive	US	3115	7	Tue	0.01	0.01	0
Automotive	US	3115	7	Tue	0.01	0.01	0
Automotive	US	3115	7	Tue	0.01	0.01	0
Automotive	US	3115	7	Tue	0.01	0.01	1

Category	currency	sellerRating	Duration	endDay	ClosePrice	OpenPrice	Competitive?
Automotive	US	3115	7	Tue	0.01	0.01	1

Data Frames and Indexes

Traditional database tables will have one or more columns designated as an index. This can vastly improve the efficiency of certain SQL queries. In *Python*, with the pandas library, the basic rectangular data structure is a DataFrame object. By default, an automatic integer index is created for a DataFrame based on the order of the rows. In pandas, it is also possible to set multilevel/hierarchical indexes to improve the efficiency of certain operations.

In *R*, the basic rectangular data structure is a data.frame object. A data.frame also has an implicit integer index based on the row order. While a custom key can be created through the row.names attribute, the native R data.frame does not support user-specified or multi-level indexes. To overcome this deficiency, two new packages are gaining widespread use: data.table and dplyr. Both support multi-level indexes and offer significant speed-ups in working with a data.frame.

TERMINOLOGY DIFFERENCES

Terminology for rectangular data can be confusing. Statisticians and data scientists use different terms for the same thing. For a statistician, *predictor variables* are used in a model to predict a *response* or *dependent variable*. For a data scientist, *features* are used to predict a *target*. One synonym is particularly confusing: computer scientists will use the term *sample* for a single row; a *sample* to a statistian means a collection of rows

Graph Data

In additional to rectangular data, another important data structure is *graph* or *network*. These are used to represent physical, social and abstract relationships. For example, a graph of a social network, such as Facebook or LinkedIn, may represent connections between people on the network. Distribution hubs connected by roads are an example of a physical network. Graph structures are useful for certain types of problems, such network optimization and recommender systems (see [Link to Come]). Nonetheless, the vast majority of applications in data science are based on the rectangular data structure.

GRAPHS IN STATISTICS

In computer science and information technology, the term *graph* typically refers to a depiction of the connections among entities, and to the underlying data structure. In statistics, *graph* is used to refer to a variety of plots and *visualizations*, not just of connections among entities, and the term applies just to the visualization, not to the data structure.

KEY IDEAS

- 1. The basic data structure in data science is a rectangular matrix in which rows are records and columns are variables (features).
- 2. Terminology can be confusing; there are a variety of synonyms arising from the different disciplines that contribute to data science (statistics, computer science, information technology).

Further Reading

- 1. Documentation on data frames in R: https://stat.ethz.ch/R-manual/R-devel/library/base/html/data.frame.html
- 2. Documentation on data frames in Python: http://pandas.pydata.org/pandas-docs/stable/dsintro.html#dataframe

Estimates of Location

Variables with measured or count data might have thousands of distinct values. A basic step in exploring your data is getting a "typical value" for each feature (variable): an estimate of where most of the data are located (i.e. their central tendency).

KEY TERMS FOR ESTIMATES OF LOCATION

Mean

The sum of all values divided by the number of values.

Synonyms

average

Weighted Mean

The sum of all values times a weight divided by the sum of the weights.

Synonyms

weighted average

Median

The value such that one-half of the data lies above and below.

Synonyms

50th percentile

Weighted Median

The value such that one-half of the sum of the weights lies above and below the sorted data.

Trimmed Mean

The average of all values after dropping a fixed number of extreme values.

Synonyms

truncated mean

Robust

Not sensitive to extreme values.

Synonyms

resistant

Outlier

A data value that is very different from most of the data.

Synonyms

extreme value

At first glance, summarizing data might seem fairly trivial: just take the *mean* of the data (see "Mean"). In fact, while the mean is easy to compute and expedient to use, it may not always be the best measure for a central value. For this reason, statisticians have developed and promoted several alternative estimates to the mean.

METRICS AND ESTIMATES

Statisticians often use the term *estimates* for values calculated from the data at hand, to draw a distinction between what we see from the data, and the theoretical true or exact state of affairs. Data scientists and business analysts are more likely to refer to such values as a *metric*. The difference reflects the approach of statistics versus data science: Accounting for uncertainty lies at the heart of the discipline of statistics, whereas concrete business or organizational objectives are the focus of data science. Hence, statisticians estimate, and data scientists measure.

Mean

The most basic estimate of location is the mean, or *average* value. The mean is the sum of all the values divided by the number of values. Consider the following set of numbers: $\{3 \ 5 \ 1 \ 2\}$. The mean is (3+5+1+2)/4=11/4=2.75. You will encounter the symbol \overline{X} to represent the mean of a sample from a population (pronounced x-bar). The formula to compute the mean for a set of N values x_1, x_2, \dots, x_N is

$$Mean = \overline{x} = \frac{\sum_{i}^{N} x_i}{N}$$

A variation of the mean is a *trimmed mean*, calculated by dropping a fixed number of sorted values at each end and then take an average of the remaining values. Representing the sorted by $x_{(1)}, x_{(2)}, \dots, x_{(N)}$ where $x_{(1)}$ is the smallest value and $x_{(N)}$, the formula to compute the trimmed mean with $x_{(N)}$ smallest and largest values omitted is

Trimmed Mean =
$$\bar{x} = \frac{\sum_{i=p+1}^{N-p} x_{(i)}}{N-2p}$$

A trimmed mean eliminates the influence of extreme values. For example, scoring for international diving is obtained dropping the top and bottom score from five judges and taking the average of the three remaining judges [Link to Come]> This makes it difficult for a single judge to manipulate the score, perhaps to favor their country's contestant. Trimmed means are widely used, and in many cases, are preferable to use instead of the ordinary mean: see "Median and Robust Estimates" for further discussion.

Another type of mean is a *weighted mean*, calculated by multiplying each data value x_i by a weight w_i and dividing their sum by the sum of the weights. The formula for a weighted mean is

Weighted Mean =
$$\overline{x}_w = \frac{\sum_{i=1}^{N} w_i x_i}{\sum_{i=1}^{N} w_i}$$

There are two main motivations for using a weighted mean:

1. Some values are intrinsically more variable than others, and highly variable observations are given a lower weight. For example, if we are taking the average from multiple sensors and one of the sensors is less accurate, then we might downweight the data from that sensor.

2. The data collected does not equally represent the different groups that we are interested in measure. For example, because of the way an online experiment was conducted, we may not have a set of data that accurately reflects all groups in the user base. To correct that, we can give a higher weight to the values from the groups that were underrepresented.

Median and Robust Estimates

The *median* is the middle number on a sorted list of the data. If there is an even number of data values, the middle value is one that is not actually in the data set, but rather is the average of the two values that divide the sorted data into upper and lower halves. Compared to the mean, which uses all observations, the median only depends on the values in the center of the sorted data. While this might seem to be a disadvantage, since the mean is much more sensitive to the data, there are many instances in which the median is a better metric for location. Let's say we want to look at typical household incomes in neighborhoods around Lake Washington in Seattle. In comparing the Medina neighborhood to the Windermere neighborhood, using the mean would produce very different results because Bill Gates lives in Medina. If we use the median, it won't matter how rich Bill Gates is — the position of the middle observation will remain the same.

For the same reasons that one uses a weighted mean, it is also possible to compute a *weighted median*. As with the median, we first sort the data, although each data value has an associated weight. Instead of taking the middle number, the weighted median is the value such that sum of weights is equal for the lower and upper halves of the sorted list. Like the median, the weighted median is robust to outliers.

Outliers

The median is referred to as a *robust* estimate of location since it is not influenced by *outliers* (extreme cases) that could skew the results. An outlier is any value that is very distant from the other values in a dataset. The exact definition of an outlier is somewhat subjective, although certain conventions are used in various data summaries and plots (see "Percentiles and Boxplots"). Being an outlier in itself does not make a data value invalid or erroneous (as in the example above with Bill Gates). Still, outliers are often the result of data errors such as mixing data of different units (kilometers versus meters) or bad readings from a sensor. When outliers are the result of bad data, the mean will result in a poor estimate of location while the median will be still be valid. In any case, outliers should be identified and are often worthy of further investigation.

ANOMALY DETECTION

In contrast to typical data analysis, where outliers are sometimes informative and sometimes a nuisance, in *anomaly detection* the points of interest are the outliers, and the greater mass of data serves primarily to define the "normal" against which anomalies are measured.

The median is not the only robust estimate of location. In fact, a trimmed mean is widely used to avoid the influence of outliers. For example, trimming the bottom and top 10% (a common choice) of the data will provide protection against outliers in all but the smallest data sets. The trimmed

mean can be thought of as a compromise between the median and the mean: it is *robust* to extreme values in the data, but uses more data to calculate the estimate for location.

OTHER ROBUST METRICS FOR LOCATION

Statisticians have developed a plethora of other estimators for location, primarily with the goal of developing an estimator more robust than the mean but more *efficient* (i.e. better able to discern small location differences between datasets). While these methods are potentially useful for small data sets, they are not likely to provide added benefit for large or even moderately sized data sets.

Example: Location Estimates of Population and Murder Rates

Table 1-2 shows the first few rows in the data set containing population and murder rates (in units of murders per 100,000 people per year) for each state. Compute the mean, trimmed mean and median for the population using R:

```
> state <- read.csv(file="/Users/andrewbruce1/book/state.csv")
> mean(state[["Population"]])
[1] 6162876
> mean(state[["Population"]], trim=0.1)
[1] 4783697
> median(state[["Population"]])
[1] 4436370
```

Table 1-2. A few rows of the data. frame state of population and murder rate by state.

	State	Population	Murder Rate
1	Alabama	4,779,736	5.7
2	Alaska	710,231	5.6
3	Arizona	6,392,017	4.7
4	Arkansas	2,915,918	5.6
5	California	37,253,956	4.4
6	Colorado	5,029,196	2.8
7	Connecticut	3,574,097	2.4
8	Delaware	897,934	5.8

The mean is bigger than the trimmed mean which is bigger than the median. This is because the trimmed mean excludes the largest and smallest 5 states (trim=0.1 drops 10% from each end). If we want to compute the average murder rate for the country, we need to use a weighted mean or median to account for different populations in the states. Since base R doesn't have a function for weighted median, it is necessary to install a package such as matrixStats

```
> weighted.mean(state[["Murder.Rate"]], w=state[["Population"]])
[1] 4.445834
> library("matrixStats")
> weightedMedian(state[["Murder.Rate"]], w=state[["Population"]])
[1] 4.4
```

In this case, the weighted mean and median are about the same.

KEY IDEAS

- 1. The basic metric for location is the mean, but it can be sensitive to extreme values (outlier)
- 2. Other metrics (median, trimmed mean) are more robust

Further Reading

- 1. Michael Levine (Purdue) has posted some useful slides on basic calculations for measures of location: http://www.stat.purdue.edu/~mlevins/STAT511 2012/Lecture2standard.pdf
- 2. John Tukey's 1977 classic Exploratory Data Analysis (Pearson) is still widely read.

Estimates of Variability

Location is just one dimension in summarizing a feature. A second dimension, *variability*, also referred to as *dispersion*, measures whether the data values are tightly clustered or spread out. At the heart of statistics lies variability: measuring it, reducing it, distinguishing random from real variability, identifying the various sources of real variability and making decisions in the presence of it.

KEY TERMS FOR VARIABILITY METRICS

Deviations

The difference between the observed values and the estimate of location.

Synonyms

errors, residuals.

Variance

The sum of squared deviations from the mean divided by N-1 where N is the number of data values.

Synonyms

mean-squared-error.

Standard Deviation

The square root of the variance.

Synonyms

12-norm, Euclidean norm

Mean Absolute Deviation

The mean of the absolute value of the deviations from the mean.

Synonyms

11-norm, Manhattan norm

Median Absolute Deviation from the Median

The median of the absolute value of the deviations from the median.

Range

The difference between the largest and the smallest value in a data set.

Order Statistics

Metrics based on the data values sorted from smallest to biggest.

Synonyms

ranks

Percentile

The value such that P percent of the values take on this value or less and (100-P) percent take on this value or more.

Synonyms

quantile

Interquartile Range

The difference between the 75th percentile and the 25th percentile

Synonyms

IQR

Just as there are different ways to measure location (mean, median, ...) there are also different ways to measure variability.

Standard Deviation and Related Estimates

The most widely used estimates of variation are based on the the differences, or *deviations*, between the estimate of location and the observed data. For a set of data $\{1, 4, 4\}$, the mean is 3 and the median is 4. The deviations from the mean are the differences: 1 - 3 = -2, 4 - 3 = 1, 4 - 3 = 1. These deviations tell us how dispersed the data is around the central value.

One way to measure variability is to estimate a typical value for these deviations. Averaging the deviations themselves would not tell us much - the negative deviations offset the positive ones. In fact, the sum of the deviations from the mean is precisely zero. Instead, a simple approach is to take the average of the absolute values of the deviations from the mean. In the above example, the absolute value of the deviations is $\{2\ 1\ 1\}$ and their average is (2+1+1)/3 = 1.33. This is known as the *mean absolute deviation* and is computed using the formula

Mean Absolution Deviation =
$$\frac{\sum_{i=1}^{N} |x_i - \overline{x}|}{N}$$

where \overline{X} is the sample mean.

The best known estimates for variability are the *variance* and the *standard deviation* which are based on squared deviations. The variance is an average of the squared deviations and the standard deviation is the square root of the variance.

Variance =
$$s^2 = \frac{\sum (x - \overline{x})^2}{N - 1}$$

Standard Deviation =
$$s = \sqrt{\text{Variance}}$$

The standard deviation is much easier to interpret than the variance since it is on the same scale as the original data. Still, with its more complicated and less intuitive formula, it might seem peculiar that the standard deviation is preferred in statistics over the mean absolute deviation. Its owes its preeminence to statistical theory: mathematically, it turns out that working with squared values is much more convenient than absolute values, especially for statistical models (see [Link to Come]).

DEGREES OF FREEDOM, AND N OR N-1?

In statistics books, there is always some discussion of why we have N-1 in the denominator in the above formula, instead of N, leading into the concept of *degrees of freedom*. This distinction is not important since N is generally large enough so it won't make much difference whether you divide by N or N-1. But, in case you are interested, here is the story.

If you use the intuitive denominator of N in the above formula, you will underestimate the true value of the standard deviation in the population. This is referred to as a *biased* estimate. However, if you divide by N-1 instead of N, the standard deviation becomes an *unbiased* estimate.

To fully explain why using N leads to a biased estimate involves the notion of *degrees of freedom*, which takes into account the number of constraints in computing an estimate. In this case, there are N-1 degrees of freedom since there is one constraint: the standard deviation depends on calculating the sample mean. For many problems, data scientists do not need to worry about degrees of freedom, but there are cases where the concept is important (see [Link to Come]).

Neither the variance, the standard deviation nor the mean absolute deviation are *robust* to outliers and extreme values (see "Median and Robust Estimates" for a discussion of robust estimates for location). The variance and standard deviation are especially sensitive to outliers since they are based on the squared deviations.

An robust estimate of variability is the *median absolute deviation from the median*, sometimes denoted by MAD:

Median Absolution Deviation = Median
$$(|x_1 - m|, |x_2 - m|, ..., |x_N - m|)$$

where *m* is the median. Like the median, the MAD is not influenced by extreme values. It is also possible to compute a trimmed standard deviation analogous to the trimmed mean (see ???).

NOTE

The variance, the standard deviation, mean absolute deviation and median absolute deviation from the median are not equivalent estimates, even in the case where the data comes from a normal distribution. In fact, the standard deviation is always greater than the mean absolute deviation which itself is greater than the median absolute deviation. Sometimes, the median absolute deviation is multiplied by a factor of 1.4826: this puts MAD on the same scale as the standard deviation in the case of a normal distribution.

Estimates Based on Percentiles

A different approach to estimating dispersion is based on looking at the spread of the sorted data. Statistics based on sorted (ranked) data are referred to as *order statistics*. The most basic measure is the *range*: the difference between the largest and smallest number. The minimum and maximum values themselves are useful to know, and helpful in identifying outliers, but the range is extremely sensitive to outliers and not very useful as a general measure of dispersion in the data.

To avoid the sensitivity to outliers, we can look at the range of the data after dropping values from each end. Formally, these types of estimates are based on differences between *percentiles*. In a dataset, the P-th percentile is a value such that at least P percent of the values take on this value or less and at least (100-P) percent of the values take on this value or more. For example, to find the 80th percentile, sort the data. Then, starting with the smallest value, proceed 80 percent of the way to the largest value. Note that the median is the same thing as the 50th percentile. The percentile is essentially the same as a *quantile*, with quantiles indexed by fractions (so the .8 quantile is the same as the 80th percentile).

A common measurement of variability is the difference between the 25th percentile and the 75th percentile, called the *interquartile range* (or IQR). Here is a simple example: 3,1,5,3,6,7,2,9. We sort these to get 1,2,3,3,5,6,7,9. The 25th percentile is at 2.5, and the 75th percentile is at 6.5, so the interquartile range is 6.5 - 2.5 = 4. Software can have slightly differing approaches that yield different answers (see the note below.) Typically these differences are smaller.

For very large datasets, calculating exact percentiles can be computationally very expensive since it requires sorting all the data values. Machine learning and statistical software use special algorithms, such as [Link to Come] to calculate an approximate percentile that can be calculated very quickly and is guaranteed to have a certain accuracy.

PERCENTILE: PRECISE DEFINITION

If we have an even number of data (N is even), then the percentile is ambiguous under the above definition. In fact, we could take on any value between the order statistics X(j) and X(j+1) where j satisfies

$$100 * \frac{j}{N} \le P < 100 * \frac{j+1}{N}$$

Formally, the percentile is the weighted average

Percentile
$$(P) = (1 - w)x_{(j)} + wx_{(j+1)}$$

for some weight w between 0 and 1. Statistical software has slightly differing approaches to choose w In fact, the R function quantile offers nine different alternatives to compute the quantile: see [Link to Come] for a full discussion. Except for small datasets, you don't usually need to worry about the precise way a percentile is calculated.

Example: Variability Estimates of State Population

Table 1-2 shows the first few rows in the data set containing population and murder rates for each state. Using R's built-in functions for the standard deviation, interquartile range (IQR) and the median absolution deviation from the median (MAD), we can compute estimates of variability for the state population data:

```
> sd(state[["Population"]])
[1] 6848235
> IQR(state[["Population"]])
[1] 4847308
> mad(state[["Population"]])
[1] 3849870
```

The standard deviation is almost twice as large as the MAD (in R, by default, the scale of the MAD is adjusted to be on the same scale as the mean) This is not surprising since the standard deviation is sensitive to outliers.

KEY IDEAS

- 1. The variance and standard deviation are the most widespread and routinely reported statistics of variabilit
- 2. Both are sensitive to outliers
- 3. More robust metrics include mean and median absolute deviations from the mean, and percentiles (quantiles)

Further Reading

- 1. David Lane's online statistics resource has a section on percentiles here: http://onlinestatbook.com/2/introduction/percentiles.html
- 2. Kevin Davenport has a useful post on deviations from the median, and their robust properties in R-Bloggers: http://www.r-bloggers.com/absolute-deviation-around-the-median/

Exploring the Data Distribution

Each of the estimates described above sums up the data in a single number to describe the location or variability of the data. It is also useful to explore how the data are distributed overall.

KEY TERMS FOR EXPLORING THE DISTRIBUTION

Boxplot

A plot introduced by Tukey as a quick way to visualize the distribution of data.

Synonyms

Box and whiskers plot

Frequency Table

A tally of the count of numeric data values that fall into a set of intervals (bins).

Histogram

A plot of the frequency table with the bins on the x-axis and the count (or proportion) on the y-axis.

Density Plot

A smoothed version of the histogram, often based on a kernal density estimate.

STATISTICAL MOMENTS

In statistical theory, location and variability are referred to as the first and second *moments* of a distribution. The third and fourth moments are called *skewness* and *kurtosis*. Skewness refers to whether the data is skewed to larger or small values and kurtosis indicates the propensity of the data to have extreme values. Generally, metrics are not used to measure skewness and kurtosis; instead, these are discovered using the visual displays such as Figure 1-2 and Figure 1-3. See [Link to Come] for formulas and more details about skewness and kurtosis.

Percentiles and Boxplots

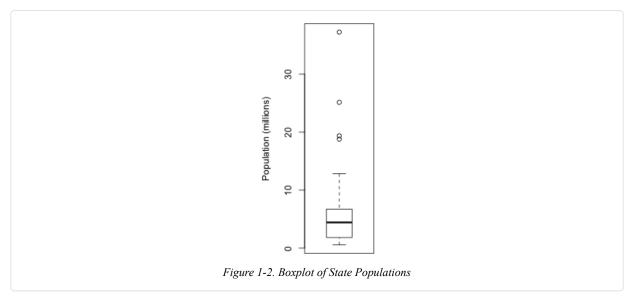
In "Estimates Based on Percentiles", we explored how percentiles can be used to measure the spread of the data. Percentiles are also valuable to summarize the entire distribution. It is common to report the quartiles (25th, 50th and 75th percentiles) and the deciles (the 10th, 20th, ..., 90th percentiles). Percentiles are especially valuable to summarize the *tails* (the outer range) of the distribution. Popular culture has coined the term *one-percenters* to refer to the people in the top 99th percentile of wealth.

Table 1-3. Percentiles of murder rate by state.

5% 25% 50% 75% 95% 1.60 2.42 4.00 5.55 6.51

Table 1-3 displays some percentiles of the murder rate by state. In R, this would be produced using the quantile function:

The median is 4 murders per 100,000 people although there is quite a bit of variability: the 5th percentile is only 1.6 and the 95th percentile is 6.51



Boxplots, introduced by Tukey [Link to Come], are based on percentiles and give a quick way to visualize the distribution of data. Figure 1-2 shows a boxplot of the population by state produced by R:

```
boxplot(state[["Population"]]/1000000, ylab="Population (millions)")
```

The top and bottom of the box are the 75th and 25th percentiles, respectively. The median is shown by the horizontal line in the box. The dashed lines, referred to as *whiskers*, extend from the top and bottom to indicate the range for the bulk of the data. There are many variations of a boxplot: see, for example, the documentation for the R function boxplot [Link to Come]. By default, the R function extends the whiskers to the furthest point beyond the box, except that it will not go beyond 1.5 times the IQR. Other software may use a different rule. Any data outside of the whiskers are plotted as single points.

Frequency Table and Histograms

A frequency table of a variable divides up the variable range into equally spaced segments, and tells us how many values fall in each segment. Table 1-4 shows a frequency table of the population by state computed using R:

Table 1-4. A frequency table of population by state.

BinNumber	BinRange	Count	States
1	563,626- 4,232,658	24	WY,VT,ND,AK,SD,DE,MT,RI,NH,ME,HI,ID,NE,WV,NM,NV,UT,KS,AR,MS,IA,CT,OK,OR
2	4,232,659- 7,901,691	14	KY,LA,SC,AL,CO,MN,WI,MD,MO,TN,AZ,IN,MA,WA
3	7,901,692- 11,570,724	6	VA,NJ,NC,GA,MI,OH
4	11,570,725- 15,239,757	2	PA,IL
5	15,239,758- 18,908,790	1	FL
6	18,908,791- 22,577,823	1	NY
7	22,577,824- 26,246,856	1	TX
8	26,246,857- 29,915,889	0	
9	29,915,890- 33,584,922	0	
10	33,584,923- 37,253,956	1	CA

The least populous is Wyoming, with 563,626 people (2010 Census) and the most populous is California, with 37,253,956 people. This gives us a range of 37,253,956 - 563,626 = 36,690,330 which we must divide up into equal size bins - let's say 10 bins. With 10 equal size bins, each bin will have a width of 3,669,033, so the first bin will span from 563,626 to 4,232,658. By contrast, the top bin, 33,584,923 to 37,253,956, has only one state - California. The two bins immediately below California are empty, until we reach Texas. It is important to include the empty bins - the fact that there are no values in those bins is useful information.

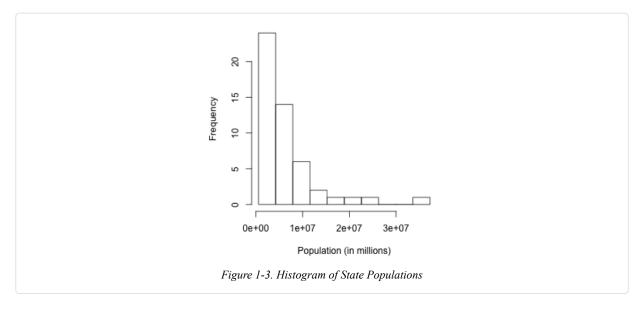
NOTE

Both frequency tables and percentiles summarize the data by creating bins. In general, quartiles and deciles will have the same count in each bin (equal-count bins) but the bin sizes will be different. The frequency table, by contrast, will have different counts in the bins (equal-size bins).

A histogram is a way to visualize a frequency table, with bins on the x-axis, and data count on the y-axis. To create a histogram corresponding to the frequency table Table 1-4 in R, use the hist function with the breaks argument:

```
hist(state[["Population"]], breaks=breaks)
```

The histogram is shown in Figure 1-3 In general, histograms are plotted such that - Empty bins are included in the graph - Bins are equal width - Number of bins (or, equivalently, bin size) is up to the user - Bars are contiguous — no empty space shows between bars, unless there is an empty bin.

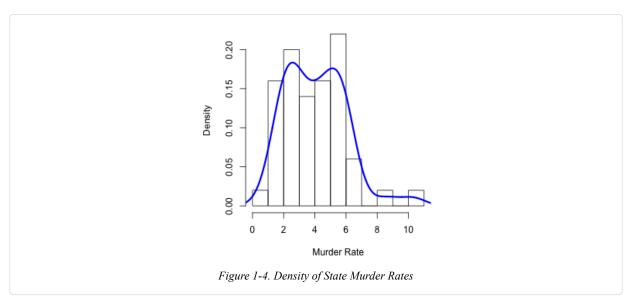


Density Estimates

Related to the histogram is a density plot which shows the distribution of data values as a continuous line. It can be thought of as a smoothed histogram, although it is typically computed directly from the data using a *kernal density estimate* (see [Link to Come] for a short tutorial). Figure 1-4 displays a density estimate superposed on a histogram. In R, a density estimate can be computed using the density function:

```
hist(state[["Murder.Rate"]], freq=FALSE)
lines(density(state[["Murder.Rate"]]), lwd=3, col="blue")
```

A key distinction from the histogram plotted in Figure 1-3 is the scale of the y-axis: a density plot corresponds to plotting the histogram as a proportion rather than counts (this is done in R using the argument freq=FALSE).



Example 1-1. Density Estimation

Density estimate is a rich topic with a long history in statistical literature. In fact, over twenty R packages have been published that offer functions for density estimation. [Link to come] give a comprehesive review of R packages, with a particular recommendation for ASH or KernSmooth. For many data science problems, there is no need to worry about the various types of densities estimates and it suffices to use the base functions.

KEY IDEAS

- 1. A frequency histogram plots frequency counts on the y-axis and variable values on the x-axis; it gives a sense of the distribution of the data at a glance.
- 2. A frequency table is a tabular version of the frequency counts in a histogram.
- 3. A boxplot, with the top and bottom of the box at the 75th and 25th percentiles, respectively, also gives a quick sense of the distribution of the data; it is often used in side-by-side displays to compare distributions.
- 4. A density plot is a smoothed version of a histogram; it requires a function to estimate a plot based on the data (multiple estimates are possible, of course).

Further reading

- 1. A step-by-step guide to creating a boxplot can be found here: http://www.oswego.edu/~srp/stats/bp_con.htm
- 2. Density estimation in R is covered in Henry Deng and Hadley Wickham's paper http://vita.had.co.nz/papers/density-estimation.pdf
- 3. R-Bloggers has a useful post on histograms in R, including customization elements, such as binning (breaks): http://www.r-bloggers.com/basics-of-histograms/
- 4. A similar post on box-plots in R can be found here: http://www.r-bloggers.com/box-plot-with-r-tutorial/

Exploring Binary and Categorical Data

For categorical data, simple proportions or percentages tell the story of the data.

KEY TERMS FOR EXPLORING CATEGORICAL DATA

Mode

The most commonly occurring category or value in a dataset.

Expected Value

When the categories can be associated with a numeric value, it gives an average value based on the probability of occurence of a category.

Bar Charts

The frequency or proportion for each category plotted as bars.

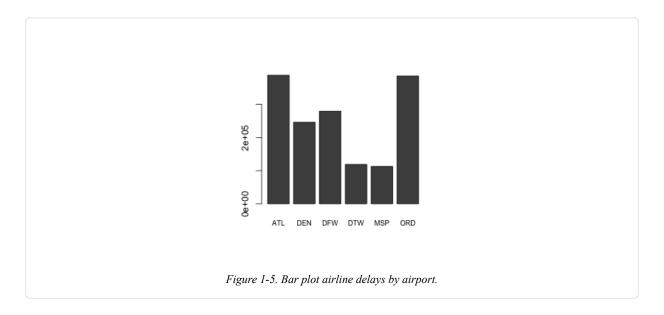
Pie Charts

The frequency or proportion for each category plotted as wedges in a pie.

Getting a summary of a binary variable, or a categorical variable with a few categories, is a fairly easy matter - we just figure out the proportion of 1's, or of the important categories. For example, Table 1-5 shows the percentage of delayed flights by the cause of delay at Dallas/Fort Worth airport since 2010. Delays are categorized as being due to factors under carrier control, air traffic control system delays (ATC), weather, security or a late inbound aircraft.

Table 1-5. Percentage of delays by cause of delay at Dallas-Ft. Worth airport.

Carrier	ATC	Weather	Security	Inbound
23.02	30.40	4.03	0.12	42.43



Bar charts are a common visual tool for displaying a single categorical variable, often seen in the popular press. Categories are listed on the x-axis, and frequencies or proportions on the y-axis. Figure 1-5 shows the airport delays per year by cause of delay for Dallas/ Fort Worth, and is produced with the R function barplot

```
barplot(as.matrix(dfw)/6, cex.axis=.5)
```

Note that a bar chart resembles a histogram; in a bar chart the x-axis represents different categories of a factor variable, while in a histogram the x axis represents values of a single variable on a numeric scales. In a histogram, the bars are typically shown touching each other, with gaps indicating values that did not occur in the data. In a bar chart, the bars are shown separate from one another

An alternative to bar charts are pie charts, although statisticians and data visualization experts generally eschew pie charts as less visually informative (see [Link to Come]).

NUMERICAL DATA AS CATEGORICAL DATA

In "Exploring the Data Distribution", we looked at frequency tables based on binning the data. This implicitly converts the numeric data to an ordered factor. In this sense, histograms and barcharts are similar, except that the categories on the x-axis in the bar chart are not ordered. Converting numeric data to categorical data is an important and widely used step in data analysis since it reduces the complexity (and size) of the data. This aids in the discovery of relationships between features, particularly at the initial stages of an analysis.

Mode

The mode is the value, or values in case of a tie, that appears most often in the data. For example, the mode of the cause of delay at Dallas/Fort Worth airport is "Inbound". As another example, in most parts of the United States, the mode for religious preference would be Christian. The mode is a simple summary statistic for categorical data, and it is generally not used for numeric data.

Expected Value

A special type of categorical data is data in which the categories represent, or can be mapped to, discrete values on the same scale. A marketer for a new cloud technology, for example, offers two levels of service, one priced at \$300/month and another at \$50/month. The marketer offers free webinars to generate leads, and the firm figures that 5% of the attendees will sign up for the \$300 service, 15% for the \$50 service, and 80% will not sign up for anything. These data can be summed up, for financial purposes, in a single "expected value," which is a form of weighted mean in which the weights are probabilities.

The expected value is calculated as follows

- 1. Multiply each outcome by its probability of occurring.
- 2. Sum these values.

In the cloud service example, the expected value of a webinar attendee is thus \$22.50 per month, calculated as follows:

$$EV = (0.05)(300) + (0.15)(50) + (0.80)(0) = 22.5$$

The expected value is really a form of weighted mean: it adds the ideas of future expectations and probability weights, often based on subjective judgment. Expected value is a fundamental concept in business valuation and capital budgeting, for example, the expected value of 5-years of profits from a new acquisition, or the expected cost savings from new patient management software at a clinic.

KEY IDEAS

- 1. Categorical data is typically summed up in proportions, and can be visualized in a bar chart.
- 2. Categories might represent distinct things (apples and oranges, male and female), they might represent levels of a factor variable (low, medium and high), or they might represent numeric data that has been binned.
- 3. Expected value is the sum of values times their probability of occurance, often used to sum up factor variable levels.

Further Reading

1. No statistics course is complete without a lesson on misleading graphs, which often involve bar charts and pie charts. Here's one: http://passyworldofmathematics.com/misleading-graphs/

Correlation

Exploratory data analysis in many modeling projects (whether in data science or in research) involves examining correlation among predictors, and between predictors and a target variable. Variables X and Y (each with measured data) are said to be positively correlated if high values of X go with high values of Y, and low values of X go with low values of Y. If high values of X go with low values of Y, and vice-versa, the variables are negatively correlated.

KEY TERMS FOR CORRELATION

Correlation coefficient

A metric that measures the extent to which numeric variables are associated with one another (ranges from -1 to +1).

Correlation matrix

A table where the variables are shown on both rows and columns, and the cell values are the correlations between the variables.

Scatterplot

A plot in which the x-axis is the value of one variable, and the y-axis the value of another.

Consider these two variables, perfectly correlated in the sense that each goes from low to high:

The vector sum of products is 4+10+18 = 32. Now try shuffling one of them and recalculating - the vector sum of products will never higher than 32. So this sum of products could be used as a metric - the observed sum of 32 could be compared to lots of random shufflings (in fact, this idea

relates to a resampling based estimate: see [Link to Come]). Values produced by this metric, though, are not that meaningful, except by reference to the resampling distribution.

More useful is a standardized variant: the *correlation coefficient*, which gives an estimate of the correlation between two variables that always lies on the same scale. *Pearson's correlation coefficient* is computed by multiplying deviations from the mean for variable 1 times those for variable 2, and dividing by the product of the standard deviations:

$$r = \frac{\sum_{i=1}^{N} (x_i - \overline{x})(y_i - \overline{y})}{(N-1)s_x s_y}$$

Note that we divide by N-1 instead of N: see Degrees of Freedom, and N or N-1? for more details. The correlation coefficient always lies between +1 (perfect positive correlation) and -1 (perfect negative correlation); 0 indicates no correlation.

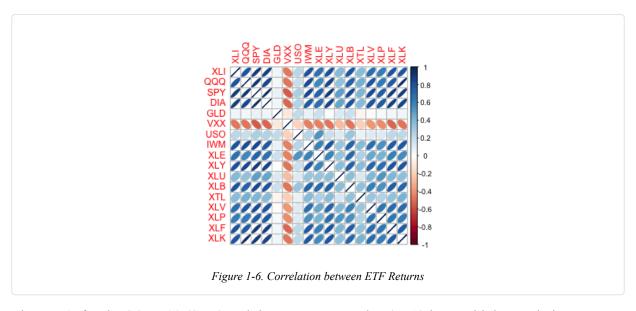
Variables can have an association that is not linear, in which case the correlation coefficient may not be a useful metric. The relationship between tax rates and revenue raised is an example - as tax rates increase from 0, the revenue raised also increases. However, once tax rates reach a high level, and approach 100%, tax avoidance increases and tax revenue actually declines.

Table 1-6. Correlation between telecommunication stock returns.

	Т	CTL	FTR	VZ	LVLT
T	1.000	0.475	0.328	0.678	0.279
CTL	0.475	1.000	0.420	0.417	0.287
FTR	0.328	0.420	1.000	0.287	0.260
VZ	0.678	0.417	0.287	1.000	0.242
LVLT	0.279	0.287	0.260	0.242	1.000

Table 1-6, called a *correlation matrix*, shows the correlation between the daily returns for telecommunication stocks from July, 2012 through June 2015. From the table, you can see that Verizon (VZ) and ATT (T) have the highest correlation. Level Three (LVLT), which is an infrastructure company, has the lowest correlation.

A table of correlations, such as Table 1-6, is commonly plotted to give a visual display of the relationship between multiple variables. Figure 1-6 shows the correlation between the daily returns for major exchange traded funds (ETF's). In R, this is easily created using the package corrplot:



The ETF's for the S&P 500 (SPY) and the Dow Jones Index (DIA) have a high correlation. Similary, the QQQ and the XLK, composed mostly of technology companies, are postively correlated. Defensive ETF's, such as those tracking gold prices (GLD), oil prices (USO), or market volatility (VXX) tend to be negatively correlated with the other ETF's. The orientation of the ellipse indicates whether two variables are positively correlated (ellipse is pointed right) or negatively correlated (ellipse is pointed left). The shading and width of the ellipse indicate the strength of the association: thinner and darker ellipses correspond to stronger relationships.

Like the mean and standard deviation, the correlation coefficient is sensitive to outliers in the data. Software packages offer robust alternatives to the classical correlation coefficient. For example, the R function cor has a trim argument similar to that for computing a trimmed mean (see [Link to Come]).

Example 1-2. Other Correlation Estimates

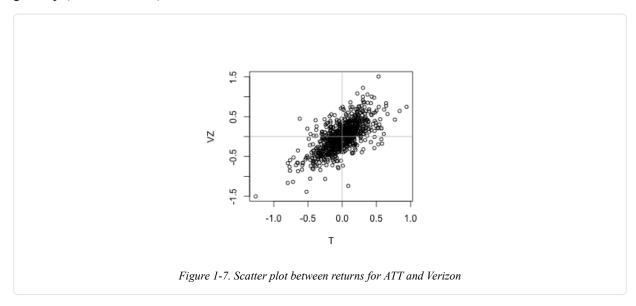
Statisticians have long ago proposed other types of correlation coefficients, such as *Spearman's rho* or *Kendall's tau*. These are correlation coefficients based on the rank of the data. Since they work with ranks rather than values, these estimates are robust to outliers and can handle certain types of non-linearities. However, data scientists can generally stick to Pearson's correlation coefficient, and its robust alternatives, for exploratory analysis. The appeal of rank-based estimates is mostly for smaller data sets, and specific hyphothesis tests.

Scatterplots

The standard way to visualize the relationship that two measured data variables have is with a scatterplot. The x-axis represents one variable, the y-axis another, and each point on the graph is a record. See Figure 1-7 for a plot between the daily returns for ATT and Verizon. This is produced in R with the command

```
plot(telecom$T, telecom$VZ, xlab="T", ylab="VZ")
```

The returns have a strong positive relationship: on most days, when both stocks go up or go down in tandem. There are very few days where one stock goes down significantly while the other stock goes up (and visa versa).



KEY IDEAS FOR CORRELATION

- 1. The correlation coefficient measures the extent to which two variables are associated with one another
- 2. When high values of v1 go with high values of v2, v1 and v2 are positively associated
- 3. When high values of v1 are associated with low values of v2, v1 and v2 are negatively associated
- 4. The correlation coefficient is a standardized metric so that it always ranges from -1 (perfect negative correlation) to +1 (perfect positive correlation
- 5. 0 indicates no correlation, but be aware that random arrangements of data will produce both positive and negative valies for the correlation coefficient just by chance

Exploring Two or More Variables

Familiar estimators like mean and variance look at variables one at a time (*univariate analysis*). Correlation analysis (see "Correlation") is an important method that compare two variables (*bivariate analysis*). In this section we look at additional estimates and plots, and at more than two variables (*multivariate analysis*).

KEY TERMS FOR EXPLORING TWO OR MORE VARIABLES

Contingency Tables

A tally of counts between two or more categorical variables.

Hexagonal Binning

A plot of two numeric variables with the records binned into hexagons.

Contour Plots

A plot showing the density of two numeric variables like a topographical map.

Violin Plots

Similar to a boxplot but showing the density estimate.

As in a univariate analysis, bivariate analysis involves both computing summary statistics and producing visual displays. The appropriate type of bivariate or multivariate analysis depends on the nature of the data: numeric versus categorical.

Hexagonal Binning and Contours (plotting numeric vs. numeric)

Scatterplots are fine when there are a relatively small number of data values. The plot of stock returns in Figure 1-7 only involves about 750 points. For data sets with hundreds of thousands or millions of records, a scatterplot will be too dense and we need a different way to visualize the relationship.

Figure 1-8 is a *hexagon binning* plot of the relationship between the finished square feet versus the tax assessed value for homes in King County, Washington. Rather than plotting points, which would appear as a monolithic dark cloud, the records are grouped into hexagonal bins and the hexagons are plotted with a color indicating the number of records in that bin. In this chart, the positive relationship between square feet and tax assessed value is clear. An interesting feature is the presence of a second cloud above the main cloud where homes have the same square footage as those in the main cloud, but a higher tax assessed value.

Figure 1-8 was generated by the powerful R package ggplot2 developed by Hadley Wickham [Link to Come]. ggplot2 is one of several new software libraries for advanced exploratory visual analysis of data: see "Visualizing Multiple Variables".

```
library(ggplot)
  ggplot(house0, aes(x=FinishedSquareFeet, y=TaxAssessedValue)) +
  stat_binhex(colour="white") +
  theme_bw() +
  scale_fill_gradient(limits=c(0, 9000), low="white", high="blue") +
  labs(x="Finished Square Feet", y="Tax Assessed Value")
```

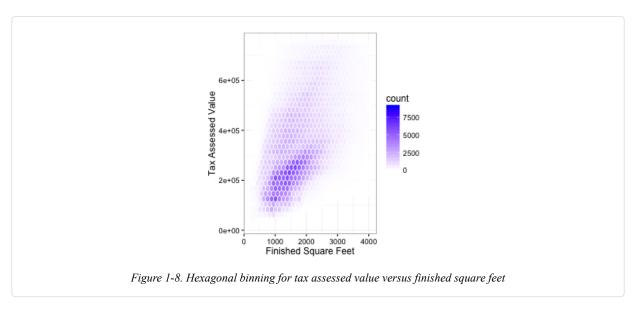
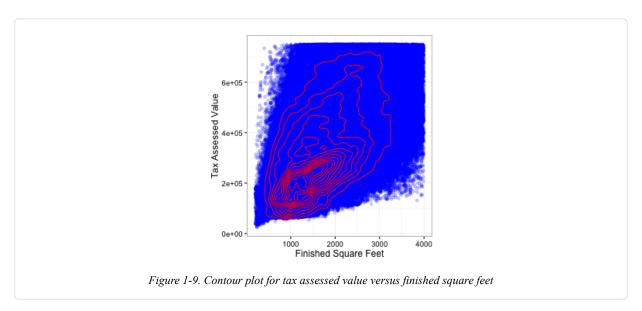


Figure 1-9 uses contours overlaid on a scatterplot to visualize the relationship between two numeric variables. The contours are essentially a topographical map to two variables; each contour band represents a specific density of points, increasing as one nears a "peak." This plot shows a similar story as Figure 1-8: there is a secondary peak "north" of the main peak. This chart was also created using ggplot2:



Other types of charts are used to show the relationship between two numeric variables, such as *heat maps*. Heat maps, hexagonal binning and contour plots all give a visual representation of a two-dimensional density. In this way, they are natural analogs to histograms and density plots.

Two Categorical Variables

A useful way to summarize two categorical variable is a contingency table - a table of counts by category. Table 1-7 shows the contingency table between the grade of a personal loan and the outcome of that loan. This is taken from data provided by Lending Club, a leader in the peer-to-peer lending business (provide reference here). The grade goes from A (high) to G (low). The outcome is either paid off, current, late or charged off (the balance of the loan is not expected to be collected). This table shows the count and row percentages. High grade loans have a very low late/charge-off percentage as compared with lower grade loans. Contingency tables can look at just counts, or also include column and total precentages. Pivot tables in Excel are perhaps the most common tool used to create contingency table. Table 1-7 was created in R using the CrossTable function in the descr package:

Table 1-7. Contingency table of loan grade and status

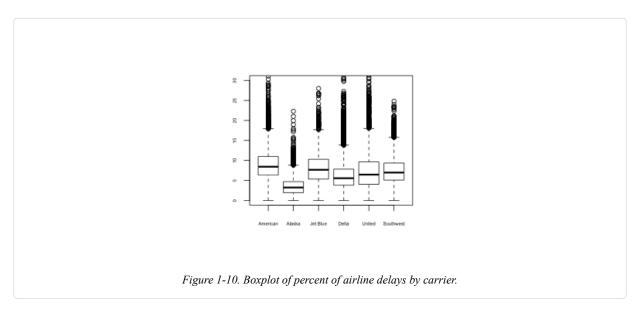
Grade	Fully Paid	Current	Late	Charged Off	Total
A	20726	52059	494	1588	74867
	0.277	0.695	0.007	0.021	0.161
В	31785	97608	2149	5387	136929
	0.232	0.713	0.016	0.039	0.294
С	23784	92448	2895	6166	125293
	0.190	0.738	0.023	0.049	0.269
D	14040	55293	2421	5135	76889
	0.183	0.719	0.031	0.067	0.165
Е	6091	25346	1421	2899	35757
	0.170	0.709	0.040	0.081	0.077
F	2376	8676	622	1556	13230
	0.180	0.656	0.047	0.118	0.028
G	655	2042	206	419	3322
	0.197	0.615	0.062	0.126	0.007

Grade	Fully Paid	Current	Late	Charged Off	Total
Total	99457	333472	10208	23150	466287

Categorical and Numeric Data

Boxplots (see "Percentiles and Boxplots") are a simple way to visually compare the distributions of a numeric variable grouped according to a categorical variable. For example, we might want to compare how the percentage of flight delays varies across different airlines. Figure 1-10 shows the percentage of flights in a month that were delayed where the delay was within control of the carrier.

boxplot(pct_delay ~ airline, data=airline_stats, ylim=c(0,30))

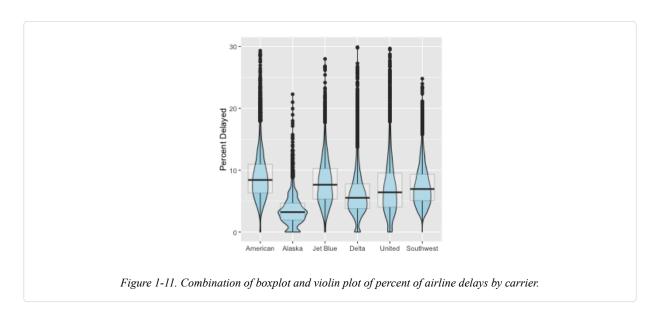


Alaska stands out as having the fewest delays while American has the most delays: the lower quartile for American is higher than the upper quartile for Alaska.

A *violin plot*, introduced by [Link to Come], is an enhancement to the boxplot and plots the density estimate with the density on the y-axis. A mirror image of the density is flipped over and the resulting shape is filled in creating an image resembling a violin. The advantage of a violin plot is that it can show nuances in the distribution not perceptible in a boxplot. Often, a violin plot is combined with a boxplot, as in Figure 1-11. This was created using ggplot2:

```
ggplot(data=airline_stats, aes(airline, pct_delay)) +
  geom_violin(fill="lightblue") +
  geom_boxplot( alpha=.2) +
  ylim(0, 30)
```

The violin plot shows a concentration in the distribution near zero for Alaska, and to a lesser extent, Delta. This phenomenon is not as obvious in the boxplot.

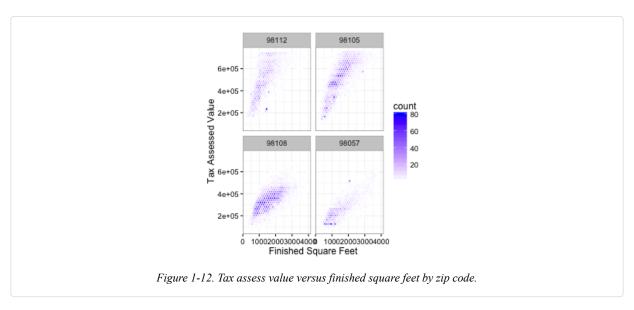


Visualizing Multiple Variables

The types of charts used to compare two variables - scatterplots, hexagonal binning, and boxplots - are readily extended to more variables using the notion of *conditioning*. As an example, consider the Figure 1-8 that shows the relationship between finished square feet and tax assessed value. We observed that there appears to be a cluster of homes that have higher tax assessed value per square foot. Diving deeper, Figure 1-12 accounts for the effect of location by plotting the data for a set of zip codes. Now the picture is much clearer: tax assessed value is much higher in certain zip code (98112, 98105) as opposed to other (98108, 98057). This disparity gives rise to the clusters observed in Figure 1-8.

Figure 1-12 was created using ggplot2 using the idea of *facets*, or a conditioning variable (in this case zip code):

```
ggplot(house1, aes(x=FinishedSquareFeet, y=TaxAssessedValue)) +
stat_binhex(colour="white") +
theme_bw() +
scale_fill_gradient( low="white", high="blue") +
labs(x="Finished Square Feet", y="Tax Assessed Value") +
facet_wrap("zip")
```



The concept of conditioning variables in a graphics system was pioneered with *Trellis graphics* developed by Rick Becker, Bill Cleveland and others at Bell Labs [Link to Come]. This idea has propogated to various modern graphics systems, such as the *lattice* ([Link to Come]) and *ggplot2* packages in R and the *Seaborn* ([Link to Come]) and *Bokeh* ([Link to Come]) modules in python. Conditioning variables are also integral to business intelligence platforms such as Tableau and Spotfire. With the advent of vast computing power, modern visualization platforms have moved well beyond the humble beginnings of exploratory data analysis. However, key concepts and tools developed over the years still form a foundation for these systems.

KEY IDEAS

- 1. Hexagonal binning and contour plots are useful tools that permit graphical examination of two numeric variables at a time, without being overwhelmed by huge amounts of data.
- 2. Contingency tables are the standard tool for looking at the counts of two categorical variables.
- 3. Box plots and violin plots allow you to plot a numeric variable against a categorical variable.

Further Reading

- 1. *Ggplot2: Elegant Graphics for Data Analysis*, by Hadley Wickham, the creator of ggplot2 (Springer, 2009)
- 2. Josef Fruehwald has a web-based tutorial on ggplot2: http://www.ling.upenn.edu/~joseff/avml2012/

Conclusion

With the development of exploratory data analysis (EDA), pioneered by John Tukey, statistics set a foundation that was a precursor to the field of data science. The key idea of EDA: the first and most important step in any project based on data is to **look at the data**. By summarizing and visualizing the data, you can gain valuable intuition and understanding of the project.

This chapter has reviewed several concepts, ranging from simple metrics, such as estimates of location and variability, to rich visual displays to explore the relationships between multiple variables as in Figure 1-12. The rich set of tools and techniques being developed by the open source community, combined with the expressiveness of the R and Python languages, has created a plethora of ways to explore and analyze data. Exploratory analysis should be a cornerstone of any data science project.

Chapter 2. Data and Sampling Distributions

A popular misconception holds that the era of Big Data means the end of a need for sampling. In fact, the proliferation of data of varying quality and relevance reinforces the need for sampling as a tool to work efficiently with a variety of data, and minimize bias. Even in a Big Data project, predictive models are typically developed and piloted with samples. Samples are also used in tests of various sorts (e.g. pricing, web treatments).

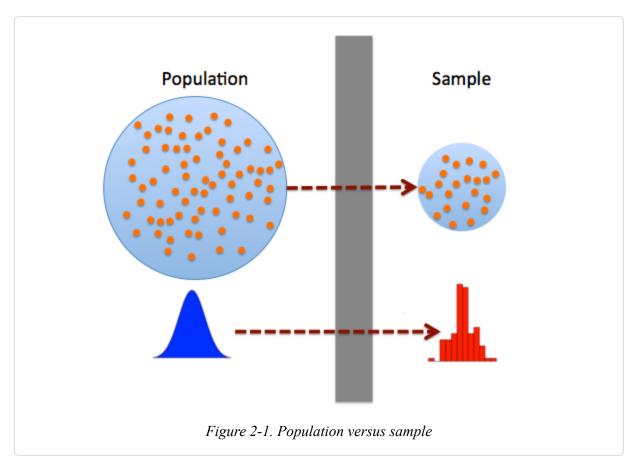


Figure Figure 2-1 shows a schematic that underpins the concepts in this chapter. The left-hand side represents a population which, in statistics, is assumed to follow an underlying but **unknown** distribution. The only thing

available is the *sample* data, and its empirical distribution, shown on the right-hand side. To get from the left-hand side to the right-hand side, a *sampling* procedure is used represented by red-dash arrows. Traditional statistics focused very much on the left-hand side, using theory based on strong assumptions about the population. Modern statistics has moved to the right-hand side where such assumptions are not needed.

In general, data scientists need not worry about the theoretical nature of the left-hand side, and instead focus on the sampling procedures and the data at hand. There are some notable exceptions. Sometimes data is generated from a physical process that can be modeled. The simplest example is flipping a coin: this follows a binomial distribution. In these cases, we can gain additional insight by using our understanding of the population.

Random sampling and sample bias

A *sample* is a subset of data from a larger dataset; statisticians call this larger dataset the *population*. A population in statistics is not the same thing as in biology - it is a large, defined but sometimes theoretical or imaginary, set of data.

KEY TERMS FOR RANDOM SAMPLING

Sample

A subset from a larger dataset

Population

The larger dataset, or idea of a dataset

N(n)

The size of the population (sample)

Random sampling

Drawing elements into a sample at random

Stratified sampling

Dividing the population into strata and randomly sampling from each strata.

Simple random sample

The sample that results from random sampling without stratifying the population.

Sample bias

A sample that misrepresents the population

Random sampling is a process in which each available member of the population being sampled has an equal chance of being chosen for the sample at each draw. The sample that results is called a *simple random sample*. Sampling can be done *with replacement*, in which observations are put back in the population after each draw for possible future reselection. Or it can be done *without replacement*, in which case observations, once selected, are unavailable for future draws.

Data quality often matters more than data quantity when making an estimate or a model based on a sample. Data quality in data science involves completeness, consistency of format, cleanliness and accuracy of individual data points. Statistics adds the notion of *representativeness*.

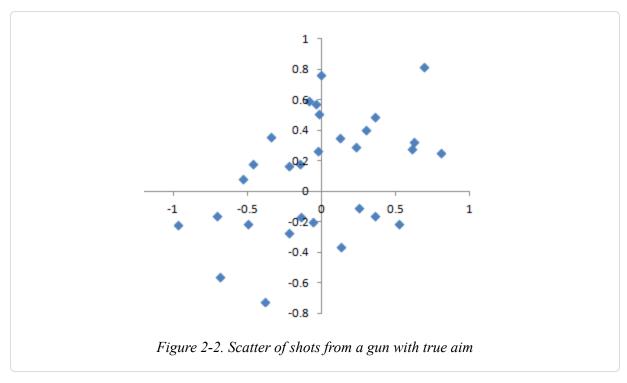
The classic example is the *Literary Digest* poll of 1936 that predicted a victory of Al Landon against Franklin Roosevelt. The *Literary Digest*, a leading periodical of the day, polled its entire subscriber base, plus additional lists of individuals, a total of over 10 million, and predicted a

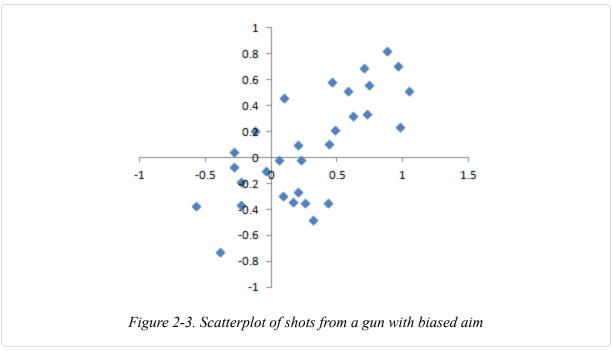
landslide victory for Landon. George Gallup, founder of the Gallup Poll, conducted bi-weekly polls of just 2000, and accurately predicted a Roosevelt victory. The difference lay in the selection of those polled.

The *Literary Digest* opted for quantity, paying little attention to the method of selection. They ended up polling those with relatively high socioeconomic status (their own subscribers, plus those who, by virtue of owning luxuries like telephones and automobiles, appeared in marketers' lists). The result was *sample bias*- the sample was different in some meaningful nonrandom way from the larger population it is meant to represent. The term "non-random" is important - hardly any sample, including random samples, will be exactly representative of the population. Sample bias occurs when the difference is meaningful, and can be expected to continue for other samples drawn in the same way as the first.

Bias

Statistical bias refers to measurement or sampling errors that are systematic and produced by the measurement or sampling process. An important distinction should be made between errors due to random chance, and errors due to bias. Consider the physical process of a gun shooting at a target. It will not hit the absolute center of the target every time, or even much at all. An unbiased process will produce error, but it is random and does not tend strongly in any direction (see Figure 2-2). The results shown in Figure 2-3 show a biased process - there is still random error in both the x and y direction, but there is also a bias. Shots tend to fall in the right upper quadrant.





Bias comes in different forms, and may be observable or invisible. When a result does suggest bias (e.g. by reference to a benchmark, or actual values), it is often an indicator that a statistical or machine learning model has been misspecified, or an important variable left out.

Random Selection

To avoid the problem of sample bias that led the *Literary Digest* to predict Landon over Roosevelt, George Gallup opted for more scientifically-chosen methods to achieve a sample that was representative of the US voter. There are now a variety of methods to achieve representativeness, but at the heart of all of them lies *random sampling*.



Figure 2-4. George Gallup, catapaulted to fame by the Literary Digest's "big data" failure

Random sampling is not always easy. Proper definition of an accessible population is key. Suppose we want to generate a representative profile of customers and we need to conduct a pilot customer survey. The survey needs to be representative but is labor intensive.

First we need to define who is a customer. We might select all customer records where purchase amount > 0. Do we include all past customers? Do we include refunds? Internal test purchases? Resellers? Both billing agent and customer?

Next we need to specify a sampling procedure. It might be "select 100 customers at random." Where a sampling from a flow is involved (e.g. realtime customer transactions, or web visitors), timing considerations ma be important (e.g. a web visitor at 10 am on a weekday may be different from a web visitor at 10 pm on a weekend).

In *stratified sampling*, the population is divided up into *strata*, and random samples are taken from each stratum. Political pollsters might seek to learn the electoral preferences of whites, blacks and hispanics. A simple random sample taken from the population would yield too few blacks and hispanics, so those strata could be overweighted in stratified sampling to yield equivalent sample sizes.

Size Versus Quality

Time and effort spent on random sampling not only reduce bias, but also allow greater attention to data quality. For example, missing data and outliers may contain useful information. It might be prohibitively expensive to track down missing values, or evaluate outliers, in millions of records, but doing so in a sample of several thousand records may be feasible.

The flip side of this effect is when you have sparse data. Consider the search queries received by Google, where columns are terms, rows are individual search queries, and cell values are either 0 or 1, depending on whether a query contains a term. The goal is to determine the best predicted search destination for a given query. There are over 150,000 words in the English language, and Google processes over 1 trillion queries per year. This yields a huge matrix, the vast majority of whose entries are "0."

This is a true Big Data problem - only when such enormous quantities of data are accumulated can effective search results be returned for most queries. And the more data accumulates, the better the results. For popular search terms this is not such a problem - effective data can be found fairly quickly for the handful of extremely popular topics trending at a particular time. The real value of modern search technology lies in the ability to return detailed and useful results for a huge variety of search queries, including those that occur only with a frequency, say, of one in a million.

Consider the search phrase "Ricky Ricardo and Little Red Riding Hood." In the early days of the internet, this query would probably have returned results on Ricky Ricardo the band leader, the television show *I Love Lucy* in which he starred, and the children's story *Little Red Riding Hood*. Later, now that trillions of search queries have been accumulated, this search

query returns the exact *I Love Lucy* episode in which Ricky narrates, in dramatic fashion, the Little Red Riding hood story to his infant son in a comic mix of English and Spanish.

Keep in mind that the number of actual *pertinent* records - ones in which this exact search query, or something very similar, appears (together with information on what link people ultimately clicked on) might need only be in the thousands to be effective. However, many trillions of data points are needed in order to obtain these pertinant records (and random sampling, of course will not help). See also "Long-Tailed Distributions".

Sample Mean Versus Population Mean

The symbol \overline{X} is used to represent the mean of a sample from a population (pronounced x-bar), whereas μ is used to represent the mean of a population. Why make the distinction? Information about samples is observed, and information about large populations is often inferred from smaller samples. Statisticians like to keep the two things separate in the symbology.

KEY IDEAS

- 1. Even in the era of Big Data, random sampling remains an important arrow in the data scientist's quiver
- 2. Bias occurs when measurements or observations are systematically in error because they are not representative of the full population
- 3. Data quality is often more important than data quantity, and random sampling can reduce bias and facilitate quality improvement that would be prohibitively expensive

Further Reading

1. A useful review of sampling procedures can be found in Ronald Fricker's chapter "Sampling Methods for Web and E-mail Surveys," found in the *Sage Handbook of Online research Methods*. This chapter includes a review of the modifications to random sampling that are often used for practical reasons of cost or feasibility.

2. The story of the Literary Digest poll failure can be found here: http://www.capitalcentury.com/1935.html

Selection bias

To paraphrase Yogi Berra, "If you don't know what you're looking for, look hard enough, and you'll find it."

Selection bias refers to the practice of selectively choosing data - consciously or unconsciously - in a way that that leads to a conclusion that is misleading or ephemeral.

KEY TERMS

Bias

Systematic error

Data snooping

Extensive hunting through data in search of something interesting

Massive search effect

Bias or non-reproducibility resulting from repeated data modeling, or modeling data with large numbers of predictor variables

If you specify a hypothesis and conduct a well-designed experiment to test it, you can have high confidence in the conclusion. Such is often not the case, however. Often, one looks at available data and tries to discern patterns. But is the pattern for real, or just the product of "data snooping," or extensive hunting through the data until something interesting emerges? There is a saying among statisticians, "if you torture the data long enough, sooner or later it will confess."

The difference between a phenomenon that you verify when you test a hypothesis using an experiment, versus a phenomenon that you discover by perusing available data, can be illuminated with this thought experiment:

Imagine that a person tells you she can flip a coin and have it land heads on the next 10 tosses. You challenge her (the equivalent of an experiment), and she proceeds to toss it 10 times, all landing heads. Clearly you ascribe some special talent to her - the probabilty that 10 coin tosses will land heads just by chance is 1 in 1000.

Now imagine that the announcer at a sports stadium asks the 20,000 people in attendance each to toss a coin 10 times, and report to an usher if they get 10 head in a row. The chance that *somebody* in the stadium will get 10 heads is extremely high (more than 99% - it's 1 minus the probability that nobody gets 10 heads). Clearly, selecting, after the fact, the person (or persons) who get 10 heads at the stadium does not indicate they have any special talent - it's most likely luck.

Since repeated review of large data sets is a key value proposition in data science, selection bias is something to worry about. A form of selection bias of particular concern to data scientists is what John Elder (founder of Elder Research, a respected data mining consultancy) calls the "*massive search effect*." If you repeatedly run different models and ask different questions with a large data set, you are bound to find something interesting. Is the result you found truly something interesting, or is it the chance outlier?

We can guard against this by using a holdout set, and sometimes more than one holdout set, against which to validate performance. Elder also advocates the use of what he calls "target shuffling" (a permutation test, in essence) to test the validity of predictive associations that a data mining model suggests.

Typical forms of selection bias in statistics, in addition to the massive search effect, include non-random sampling (see *sampling bias*), cherry-picking data, selection of time intervals that accentuate a partial statistical effect and stopping an experiment when the results look "interesting."

Regression to the mean

Regression to the mean refers to a phenomenon involving successive measurements on a given variable: extreme observations tend to be followed be more central ones. Attaching special focus and meaning to the extreme value can lead to a form of selection bias.

Sports fans are familiar with the "Rookie of the year, sophomore slump" phenomenon. Among the athletes who begin their career in a given season (the rookie class), there is always one who performs better than all the rest. Generally, this "rookie of the year" does not do as well in his second year. Why not?

In nearly all major sports, at least those played with a ball or puck, there are two elements that play a role in overall performance:

- skill
- luck

Regression to the mean is a consequence of a particular form of selection bias. When we select the rookie with the best performance, skill and good luck are probably contributing. In his next season, the skill will still be there but, in most cases, the luck will not, so his performance will decline - it will regress. The phenomenon was first identified by Francis Galton in 1886 [Link to Come], who wrote of it in connection with genetic tendencies: e.g., the children of extremely tall men tend not to be as tall as their father.

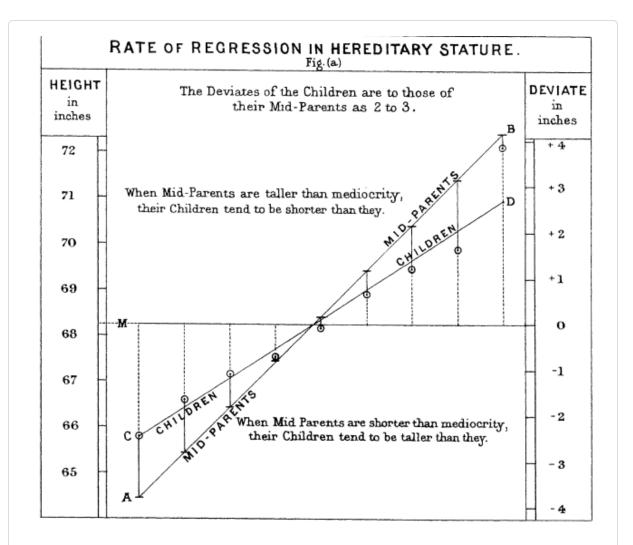


Figure 2-5. Galton's study that identified the phenomena of regression to the mean.

WARNING

Regression to the mean, meaning to "go back," is distinct from the statistical modeling method of linear regression, in which a linear relationship is estimated between predictor variables and an outcome variable.

KEY IDEAS

- 1. Specifying a hypothesis, then collecting data following randomization and random sampling principles ensures against bias.
- 2. All other forms of data analysis run the risk of bias resulting from the data collection/analysis process (repeated running of models in data mining, data snooping in research, after-the-fact selection of interesting events).

Further Reading

- 1. Christopher J. Pannucci and Edwin G. Wilkins' article "Identifying and Avoiding Bias in Research" in (surprisingly) *Plastic and Reconstructive Surgery* (August 2010) has an excellent review of various types of bias that can enter into research, including selection bias
- 2. Michael Harris's article "Fooled by Randomness Through Selection Bias" (http://systemtradersuccess.com/fooled-by-randomness-through-selection-bias/) provides an interesting review of selection bias considerations in stock market trading schemes, from the perspective of traders.

Sampling Distribution of a Statistic

The term *sampling distribution* of a statistic refers to the distribution of some sample statistic, over many samples drawn from the same population. Much of classical statistics is concerned with making inference from (small) samples to (very large) populations.

KEY TERMS

Sample statistic

A metric calculated for a sample of data drawn from a larger population

Data distribution

The frequency distribution of individual values in a data set

Sampling distribution

The frequency distribution of a *sample statistic* over many samples or resamples

Central Limit Theorem

The tendency of the sampling distribution to take on a normal shape as sample size rises

Standard error

The variability (standard deviation) of a sample *statistic* over many samples (not to be confused with *standard deviation*, which, by itself, refers to variability of individual data *values*)

Typically a sample is drawn with the goal of measuring something (with a *sample statistic*) or modeling something (with a statistical or machine learning model). Since our estimate or model is based on a sample, it might be in error - it might be different if we were to draw a different sample. We are therefore interested in how different it might be - a key concern is *sampling variability*. If we had lots of data, we could draw additional samples and observe the distribution of a sample statistic, directly. Typically, we will calculate our estimate or model using as much data as are easily available, so the option of drawing additional samples from the population is not readily available.

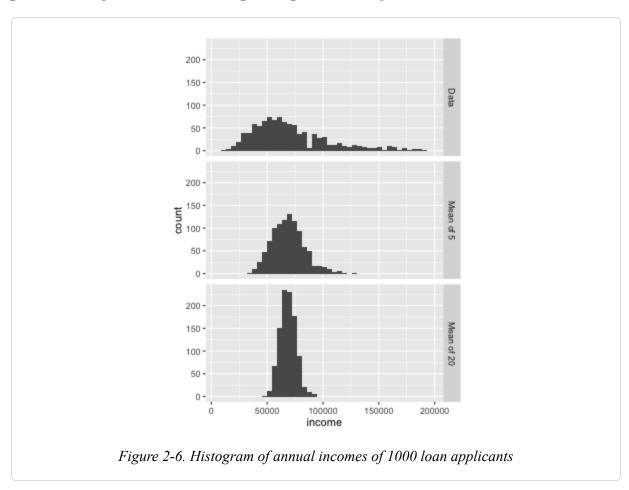
WARNING

It is important to distinguish between the distribution of the individual data points - *the data distribution*, and the distribution of a sample statistic - the *sampling distribution*.

The distribution of a sample statistic such as the mean is likely to be more regular and bell-shaped than the distribution of the data themselves. The

larger the sample that the statistic is based on, the more this is true. Also, the larger the sample, the narrower the distribution of the sample statistic.

This is illustrated in the following example using a annual income for loan applicants to Lending Club (see [Link to Come] for a description of the data). Take three samples from this data: a sample of 1000 values, a sample of 1000 means of 5 values and a sample of 1000 means of 20 values. Then plot a histogram of each sample to produce Figure 2-6.



The histogram of the individual data values is broadly spread out and skewed towards higher values as is to be expected with income data. The histograms of the means of 5 and 20 are increasingly compact and more bell-shaped. Here is the R code to generate these histograms, using the visualization backage ggplot2.

```
library(ggplot2)
loans_income <- read.csv("/Users/andrewbruce1/book/loans_income.csv")[,1]</pre>
# take a simple random sample
samp_data <- data.frame(income=sample(loans_income, 1000),</pre>
                         type='data dist')
# take a sample of means of 5 values
samp mean 05 <- data.frame(</pre>
  income = tapply(sample(loans_income, 1000*5),
                  rep(1:1000, rep(5, 1000)), FUN=mean),
  type = 'mean_of_5')
# take a sample of means of 20 values
samp mean 20 <- data.frame(</pre>
  income = tapply(sample(loans_income, 1000*20),
                   rep(1:1000, rep(20, 1000)), FUN=mean),
  type = 'mean_of_20')
# bind the data.frames and convert type to a factor
income <- rbind(samp_data, samp_mean_05, samp_mean_20)</pre>
income$type = factor(income$type,
                      levels=c('data_dist', 'mean_of_5', 'mean_of_20'),
                      labels=c('Data', 'Mean of 5', 'Mean of 20'))
# plot the histograms
ggplot(income, aes(x=income)) +
  geom_histogram(bins=40) +
  facet_grid(type ~ .)
```

Central Limit Theorem

This phenomenon is termed the *Central Limit Theorem*. It says that the means drawn from multiple samples will be shaped like the familiar bell-shaped normal curve (see "Normal distribution"), even if the source population is not normally-distributed, provided that the sample size is large enough and the departure of the data from normality is not too great. The Central Limit Theorem allows normal-approximation formulas like the t-distribution to be used in calculating sampling distributions for inference, i.e., confidence intervals and hypothesis tests.

The Central Limit Theorem receives much attention in traditional statistics texts because it underlies the machinery of hypothesis tests and confidence intervals, which themselves consume half the space in such texts. Data scientists should be aware of this role, but, since formal hypothesis tests and confidence intervals play a small role in data science, and the bootstrap is

available in any case, the Central Limit Theorem is not so central in the practice of data science.

Standard error

The *standard error* is a single metric that sums up the variability in the sampling distribution for a statistic. The standard error can be estimated using a statistic based on the standard deviation s of the sample values, and the sample size n:

Standard Error =
$$SE = \frac{S}{\sqrt{n}}$$

As the sample size increases, the standard error decreases, corresponding what was observed in Figure 2-6. The relationship between standard error and sample size is sometimes referred to as the *square-root of n* rule: in order to reduce the standard error by a factor of 2, the sample size must be increased by a factor of 4.

The validity of the standard error formula arises from the *central limit theorem* (see "Central Limit Theorem"). In fact, you don't need to rely on the central limit theorem to understand standard error. Consider the following approach to measure standard error:

- 1. Collect a number of brand new samples from the population.
- 2. For each new sample, calculate the statistic (e.g., mean).
- 3. Estimate the standard error by the standard deviation of the statistics computed in step 2.

In practice, the above approach of collecting new samples to estimate the standard error is typically not feasible (and statistically very wasteful). Fortunately, it turns out that it is not necessary to draw brand new samples; instead it is possible to use *bootstrap* resamples (see "The bootstrap"). In modern statistics, the bootstrap has become the standard way to to estimate standard error. It can be used for virtually any statistic and does not rely on the central limit theorem or other distributional assumptions.

STANDARD DEVIATION VS. STANDARD ERROR

Do not confuse standard deviation (which measures the variability of individual data points) with standard error (which measures the variability of a sample metric).

KEY IDEAS

- 1. The frequency distribution of a sample statistic tells us how that metric would turn out differently from sample to sample
- 2. This sampling distribution can be estimated via the bootstrap, or via formulas that rely on the central limit theorem
- 3. A key metric that sums up the variability of a sample statistic is its standard error

Further Reading

1. David Lane's online multimedia resource in statistics has a useful simulation that allows you to select a sample statistic, a sample size and number of iterations and visualize a histogram of the resulting frequency distribution:

http://onlinestatbook.com/stat_sim/sampling_dist/

The bootstrap

One easy and effective way to estimate the sampling distribution of a statistic, or of model parameters, is to draw additional samples, with replacement, from the sample itself, and recalculate the statistic or model for each resample. This procedure is called the *bootstrap*, and it does not necessarily involve any assumptions about the data, or the sample statistic, being normally-distributed.

KEY TERMS

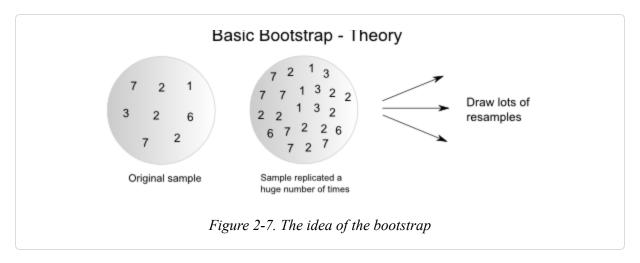
Bootstrap sample

A sample taken with replacement from an observed dataset

Resampling

The process of taking repeated samples from observed data; includes both bootstrap and permutation (shuffling) procedures

Conceptually, you can imagine the bootstrap as replicating the original sample thousands or millions of times so that you have a hypothetical population that embodies all the knowledge from your original sample (it's just larger). You can then draw samples from this hypothetical population for the purpose of estimating a sampling distribution.



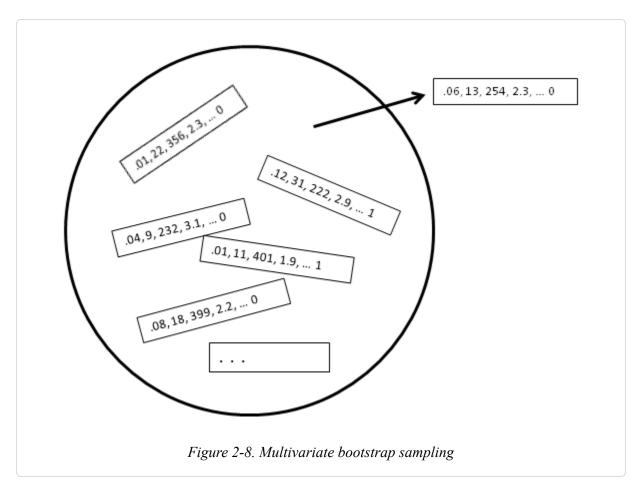
In practice, it is not necessary to actually replicate the sample a huge number of times. We simply replace each observation after each draw - we *sample with replacement*. In this way we effectively create an infinite population in which the probability of an element being drawn remains unchanged from draw to draw. The algorithm for a bootstrap resampling of the mean is as follows, for a sample of size N:

- 1. Draw a sample value, record, replace it
- 2. Repeat N times
- 3. Record the mean of the N resampled values

- 4. Repeat steps 1-3 B times
- 5. Use the B results to:
 - a. Calculate their standard deviation (this estimates sample mean standard error)
 - b. Produce a histogram or boxplot
 - c. Find a confidence interval

B, the number of iterations of the bootstrap, is set somewhat arbitrarily. The more iterations you do, the more accurate the estimate of the standard error, or the confidence interval.

The bootstrap can be used with multivariate data, where the rows are sampled as units (see Figure 2-8). A model might then be run on the bootstrapped data, for example, to estimate the stability (variability) of model parameters, or to improve predictive power. With classification and regression trees (also called decision trees), running multiple trees on bootstrap samples and then averaging their predictions (or, with classification, taking a majority vote) generally performs better than using a single tree. This process is called *bagging* (short for "bootstrap aggregating").



The repeated resampling of the bootstrap is conceptually simple, and Julian Simon, an economist and demographer, published a compendium of resampling examples, including the bootstrap, in his 1969 text *Basic Research Methods in Social Science*. However, it is also computationally intensive, and was not a feasible option before the widespread availability of computing power. The technique gained its name and took off with the publication of several journal articles and a book by Stanford statistician Bradley Efron in the late 1970's and early 1980's. It was particularly popular among researchers who use statistics but are not statisticians, and for use with metrics or models where mathematical approximations are not readily available. The sampling distribution of the mean has been well established since 1908; the sampling distribution of many other metrics has not. The bootstrap can be used for sample size determination - experiment with different values for N to see how the sampling distribution is affected.

The bootstrap met with considerable skepticism when it was first introduced; it had the aura to many of spinning gold from straw. This skepticism stemmed from a misunderstanding of the bootstrap's purpose.

WARNING

The bootstrap does not compensate for a small sample size - it does not create new data, nor does it fill in holes in an existing dataset. It merely informs us about lots of additional samples would be have, when drawn from a population like our original sample.

Resampling versus bootstrapping

Sometimes the term resampling is used synonymously with the term bootstrapping, as outlined above. More often, the term resampling also includes permutation procedures (see [Link to Come]), where multiple samples are combined, and the sampling may be done without replacement. In any case, the term *bootstrap* always implies sampling with replacement from an observed dataset.

KEY IDEAS

- 1. The bootstrap (sampling with replacement from a dataset), is a powerful tool for assessing the variability of a sample statistic.
- 2. The bootstrap can be applied in similar fashion in a wide variety of circumstances, without extensive study of mathematical approximations to sampling distributions.
- 3. It also allows us to estimate sampling distributions for statistics where no mathematical approximation has been developed.
- 4. When applied to predictive models, aggregating multiple bootstrap sample predictions (bagging) outperforms the use of a single model

Further Reading

1. *An Introduction to the Bootstrap* by Efron and Tibshirani (Chapman Hall, 1993); the first book-length treatment of the bootstrap, and still widely read

2. The section on resampling in Chapter 4 (see [Link to Come]) also discusses the bootstrap and permutation procedures.

Confidence intervals

Frequency tables, histograms, boxplots and standard errors are all ways to understand the potential error in a sample estimate. Confidence intervals are another.

KEY TERMS

Confidence level

The percentage of confidence intervals, constructed in the same way from the same population, expected to contain the statistic of interest

Interval endpoints

The top and bottom of the confidence interval

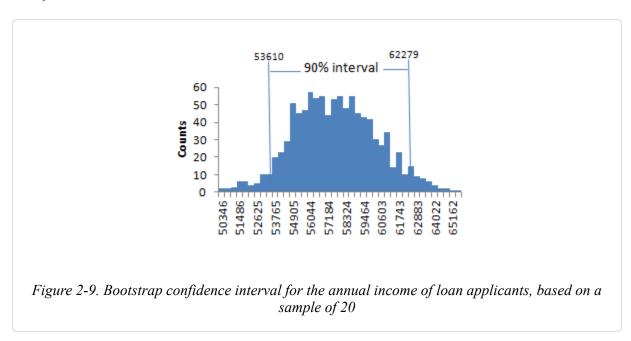
There is a natural human aversion to uncertainty - people (especially experts) say "I don't know" far too rarely. Analysts and managers, while acknowledging uncertainty, nonetheless place undue faith in an estimate when presented as a single number (a *point estimate*). Presenting an estimate not as a single number but as a range is one way to counteract this tendency. Confidence intervals do this in a manner grounded in statistical sampling principles.

Confidence intervals always come with a coverage level, expressed as a (high) percentage, say 90% or 95%. One way to think of a 90% confidence interval is as follows: it is the interval that encloses the central 90% of the bootstrap sampling distribution of a sample statistic (see "The bootstrap"). More generally, an x% confidence interval around a sample estimate should, on average, contain similar sample estimates x% of the time (when a similar sampling procedure is followed).

Given a sample of size n, and a sample statistic of interest, the algorithm for a bootstrap confidence interval is as follows:

- 1. Draw a random sample of size *n* with replacement from the data (a resample)
- 2. Record the statistic of interest for the resample
- 3. Repeat steps 1-2 many times, call it B times
- 4. For an x% confidence interval, trim [(1-x)/2]% of the B resample results from either end of the distribution.
- 5. The trim points are the endpoints of an x% bootstrap confidence interval

Figure 2-9 shows a a 90% confidence interval for the mean annual income of loan applicants, based on a sample of 20 for which the mean was \$57,573.



The bootstrap is a general tool that can be used to generate confidence intervals for most statistics, or model parameters. Statistical textbooks and software, with roots in over a half-century of computer-less statistical analysis, will also reference confidence intervals generated by formulas, especially the t-distribution (see "Student's t distribution").

NOTE

Of course, what we are really interested in when we have a sample result is "what is the probability that the true value lies within a certain interval?" This is not really the question that a confidence interval answers, but it ends up being how most people interpret the answer.

The probability question associated with a confidence interval starts out with the phrase "Given a sampling procedure and a population, what is the probability that..." To go in the opposite direction, "Given a sample result, what is the probability that (something is true about the population)," involves more complex calculations and deeper imponderables.

The percentage associated with the confidence interval is termed the *level of confidence*. The higher the level of confidence, the wider the interval. Also, the smaller the sample, the wider the interval (i.e. the more uncertainty). Both make sense: the more confident you want to be, and the less data you have, the wider you must make the confidence interval to be sufficiently assured of capturing the true value.

NOTE

For a data scientist, a confidence interval is a tool to get an idea of how variable a sample result might be. Data scientists would use this information not to publish a scholarly paper or submit a result to a regulatory agency (as a researcher might), but most likely to communicate the potential error in an estimate, and, perhaps, learn whether a larger sample is needed.

KEY IDEAS

- 1. Confidence intervals are the typical way to present estimates as an interval range.
- 2. The more data you have, the less variable it is, and the lower the level of confidence you can tolerate, the narrower the confidence interval.
- 3. The bootstrap is an effective way to construct confidence intervals

Further reading

- 1. For a bootstrap approach to confidence intervals see *Introductory Statistics and Analytics: A Resampling Perspective* by Peter Bruce (Wiley, 2014) or *Statistics* by Robin Lock and four other Lock family members (Wiley, 2012).
- 2. Engineers, with a need to understand the precision of their measurements, use confidence intervals perhaps more than most disciplines, and *Modern Engineering Statistics* by Tom Ryan (2007, Wiley) discusses confidence intervals. It also reviews a tool that is just as useful and gets less attention: prediction intervals (intervals around a single value, as opposed to a mean or other summary statistic)

Normal distribution

The bell-shaped normal distribution is iconic in traditional statistics.¹ The fact that distributions of sample statistics are often normally shaped provided a powerful tool in the development of mathematical formulas that approximate those distributions.

KEY TERMS

Error

The difference between a data point and a predicted or average value

Standardize

Subtract the mean and divide by the standard deviation

Z score

The result of standardizing an individual data point

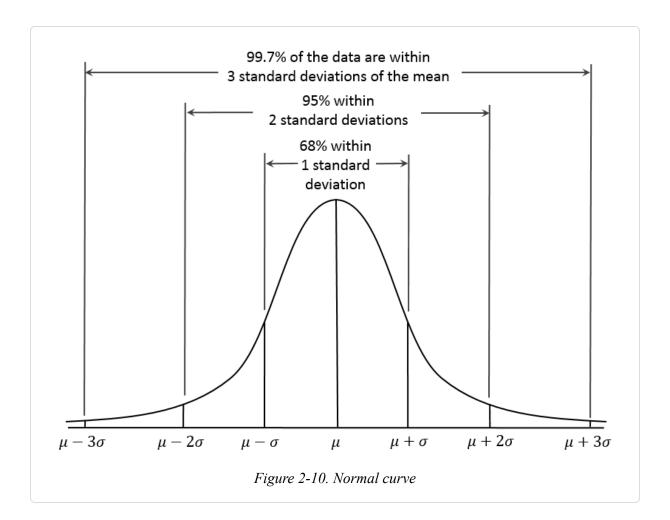
Standard normal

A normal distribution with mean = 0 and standard deviation = 1

QQ-Plot

A plot to visualize how close a sample distribution is to a normal distribution.

In a normal distribution (Figure 2-10) 68% of the data lie within one standard deviation of the mean, and 95% lie within two standard deviations.



WARNING

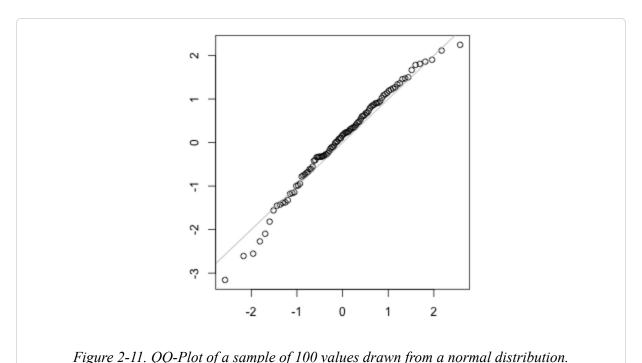
It is a common misconception that the normal distribution is called that because most data follow a normal distribution, i.e. it is the normal thing. Most of the variables used in a typical data science project, in fact most raw data as a whole, are *not* normally distributed: see "Long-Tailed Distributions". The utility of the normal distribution derives from the fact that many statistics *are* normally distributed in their sampling distribution. Even so, assumptions of normality are generally a last resort, used when empirical probability distributions, or bootstrap distributions, are not available.

NOTE

The normal distribution is also referred to as a *Gaussian* distribution after Carl Friedrich Gauss, a prodigous German mathematician from the late 18th and early 19th century. Another name previously used for the normal distribution was the "error" distribution. Statistically speaking, an *error* is the difference between an actual value and a statistical estimate like the sample mean. For example, the standard deviation (see "Estimates of Variability") is based on the errors from the mean of the data. Development of the normal distribution by Gauss came from study of the errors of astronomical measurements that were found to be normally-distributed.

Standard Normal and QQ-Plots

A *standard normal* distribution is one in which the units on the x-axis are expressed in terms of standard deviations away from the mean. To compare data to a standard normal distribution you subtract the mean then divide by the standard deviation; this is also called *normalization* or *standardization*. Note that "standardization" in this sense is unrelated to database record standardization (conversion to a common format). The transformed value is termed a *z*-score, and the normal distribution is sometimes called the *z*-distribution.



A QQ-Plot is used to visually determine how close a sample is to the normal distribution. The QQ-Plot orders the *z*-scores from low to high, and plots each value's z-score on the y-axis; the x-axis is the corresponding quantile of a normal distribution for that value's rank. Since the data are normalized, the units correspond to the number of standard deviations away of the data from the mean. If the points roughly fall on the diagonal line, then the sample distribution can be considered close to normal. Figure 2-11 shows a QQ-Plot for a sample of 100 values randomly generated from a normal distribution: as expected, the points closely follow the line. This figure can easily be produced in R:

```
norm_samp <- rnorm(100)
qqnorm(norm_samp)
abline(a=0, b=1, col='grey')</pre>
```

WARNING

Converting data to z-scores (i.e. standardizing or normalizing the data) does **not** make the data normally distributed. It just puts the data on the same scale as the standard normal distribution, often for comparison purposes.

KEY IDEAS

- 1. The normal distribution was essential to the historical development of statistics as it permitted mathematical approximation of uncertainty and variability.
- 2. While raw data are typically not normally-distributed, errors often are.
- 3. Data are often converted to z-scores by subtracting the mean of the data, and dividing by the standard deviation; the data can then be compared to a normal distribution.

Long-Tailed Distributions

Despite the importance of the normal distribution historically in statistics, and in contrast to what the name would suggest, data are generally not normally distributed.

KEY TERMS FOR LONG-TAIL DISTRIBUTION

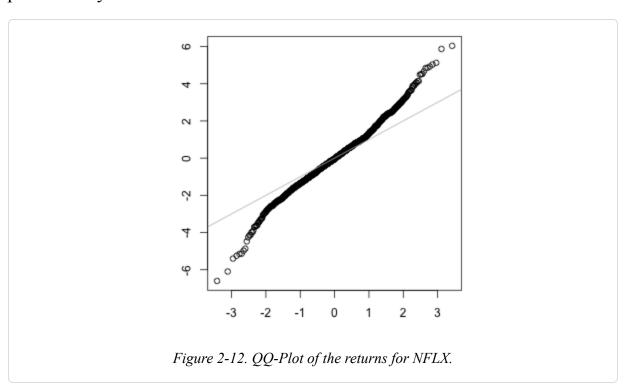
Tail

The long narrow portion of a frequency distribution, where relatively extreme values occur at low frequency

Skew

Where one tail of a distribution is longer than the other

While the normal distribution is often appropriate and useful with respect to the distribution of errors and sample statistics, it typically does not characterize the distribution of raw data. Sometimes, the distribution is highly *skewed* (asymmetric), such as with income data, or the distribution can be discrete, as with binomial data. Both symmetric and asymmetric distributions may have *long tail(s)*. The tails of a distribution correspond to the extreme values (small and large). Long-tails, and guarding against them, are widely recognized in practical work. Nassim Taleb has proposed the *black swan* theory which predicts that anamolous events, such as a stock market crash, are likely to occur in much greater likelihood than would be predicted by the normal distribution.



To illustrate the long-tailed nature of data, a good example is to look at stock returns. Figure 2-12 shows the QQ-Plot for the daily stock returns for Netflix (NFLX), generated in R by

```
sp500_px <- read.csv("/Users/andrewbruce1/book/sp500_data.csv", row.names = 1)
nflx <- sp500_px[,'NFLX']
nflx <- diff(log(nflx[nflx>0]))
qqnorm(nflx)
abline(a=0, b=1, col='grey')
```

In contrast to Figure 2-11, the points are far below the line for low values and far above the line for high values. This means that we are much more likely to observe extreme values than would be expected if the data had a normal distribution. Figure 2-12 shows another common phenomena: the points are close to the line for the data within one standard deviation of the mean. Tukey calls this phenomena as data being "normal in the middle", but having much longer tails (see [Link to Come]).

NOTE

There is much statistical literature about the task of fitting statistical distributions to observed data. Beware an excessively data-centric approach to this job, which is as much art as science. Data are variable, and often consistent, on their face, with more than one shape and type of distribution. It is typically the case that domain and statistical knowledge must be brought to bear to determine what type of distribution is appropriate to model a given situation. For example, we might have data on the level of internet traffic on a server over many consecutive 5-second periods. It is useful to know that the best distribution to model "events per time period" is the Poisson (see "Poisson Distributions").

KEY IDEAS FOR LONG-TAIL DISTRIBUTION

- 1. Most data are not normally distributed
- 2. Assuming a normal distribution can lead to underestimation of extreme events ("black swans")

Further Reading

- 1. The Black Swan by Nassim Taleb (2010, 2nd ed., Random House)
- 2. *Handbook of Statistical Distributions with Applications*, by K. Krishnamoorthy (2016, 2nd ed., CRC Press)

Student's t distribution

The *t-distribution* is a normally-shaped distribution, but a bit thicker and longer on the tails. It is used extensively in depicting distributions of sample statistics. Distributions of sample means are typically shaped like a t-distribution, and there is a family of t-distributions that differ depending on how large the sample is. The larger the sample, the more normally-shaped the t-distribution becomes.

KEY TERMS FOR STUDENT'S T-DISTRIBUTION

n

Sample size

degrees of freedom

A parameter that allows the t-distribution to adjust to different sample sizes, statistics, and number of groups. *_

The t-distribution is often called *Student's t* because it was published in 1908 in *Biometrika* by W. S. Gossett under the name "Student." Gossett's employer, the Guiness brewery, did not want competitors to know that they were using statistical methods, so insisted that Gossett not use his name on the article.

Gossett wanted to answer the question "what is the sampling distribution of the mean of a sample, drawn from a larger population." He started out with a resampling experiment - drawing random samples of four from a dataset of 3000 measurements of criminals' height and left middle finger lengths. (This being the era of eugenics, there was much interest in data on criminals, and in discovering correlations between criminal tendencies and

physical or psychological attributes.) He plotted the standardized results (the z-scores) on the x-axis, and the frequency on the y-axis. Separately, he had derived a function - now known as *Student's t*, and he fit this function over the sample results, plotting the comparison (see Figure 2-13).

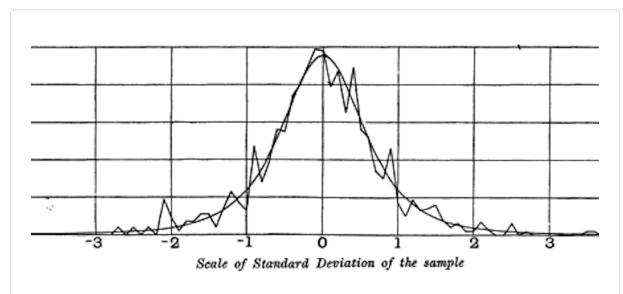


Figure 2-13. Gossett's resampling experiment results and fitted t-curve (from his 1908 Biometrika paper

A number of different statistics can be compared, after standardization, to the t-distribution, to estimate confidence intervals in light of sampling variation. Consider a sample of size n for which the sample mean, x-bar, has been calculated. We can estimate a 90% confidence interval around the sample mean by adding and subtracting the following:

$$t(n-1).05*(s/sqrt n)$$

where t(n-1).05 is the value of the t-statistic, with (n-1) degrees of freedom (see [Link to Come]), that "chops off" 5% of the t-distribution at either end.

The t-distribution has been used as a reference for the distribution of a sample mean, of the difference between two sample means, of regression parameters, and more.

Had computing power been widely available in 1908, statistics would no doubt have relied much more heavily on computationally intensive resampling methods from the start. Lacking computers, statisticians turned

to mathematics, and functions such as the t-distribution, to approximate sampling distributions. Computer power enabled practical resampling experiments in the 1980's but, by then, use of the t-distribution and similar distributions had become deeply embedded in textbooks and software.

The *t*-distribution's accuracy in depicting the behavior of a sample statistic requires that the distribution of that statistic for that sample be shaped like a normal distribution. It turns out that sample statistics *are* often normally distributed, even when the underlying population data are not (a fact which led to widespread application of the *t*-distribution). This phenomenon is termed the *Central Limit Theorem* (see [Link to Come]).

NOTE

What do data scientists need to know about the t-distribution, and the central limit theorem? Not a whole lot. These distributions are used in classical statistical inference, but are not as central to the purposes of data science. Understanding and quantifying uncertainty and variation are important to data scientists, but empirical bootstrap sampling can answer most questions about sampling error. However, data scientists will routinely encounter *t*-statistics in output from statistical software and statistical procedures in R, e.g. in A-B tests and regressions, so familiarity with its purpose is helpful.

KEY IDEAS FOR T-DISTRIBUTION

- 1. The t-distribution is actually a family of distributions resembling the normal distribution, but with thicker tails
- 2. It is widely used as a reference basis for the distribution of sample means, differences between two sample means, regression parameters, and more.

Further Reading

1. The original Gossett paper in Biometrica from 1908 can be found here:

http://seismo.berkeley.edu/~kirchner/eps_120/Odds_n_ends/Students_original_paper.pdf

2. A standard treatment of the t-distribution can be found in David Lane's online resource:

http://onlinestatbook.com/2/estimation/t_distribution.html

Binomial distribution

KEY TERMS FOR BINOMIAL DISTRIBUTION

Trial

An event with a discrete outcomes, e.g. a coin flip

Success

The outcome of interest for a trial

Synonyms

"1" (as opposed to "0")

Binomial

Having two outcomes

Synonyms

yes/no, 0/1, binary

Binomial trial

A trial with two outcomes

Synonym

Bernoulli trial

Binomial distribution

Distribution of number of successes in x trials Synonym::: Bernoulli distribution

Yes/no (binomial) outcomes lie at the heart of analytics since they are often the culmination of a decision or other process - buy/don't buy, click/don't click, survive/die, etc. Central to understanding the binomial distribution is the idea of a set of *trials*, each trial having two possible outcomes with definite probabilities.



Image courtesy of CCF Numismaticsfootnote[Public domain or CC BY-SA 3.0 (http://creativecommons.org/licenses/by-sa/3.0), via Wikimedia Commons]

For example, flipping a coin ten times is a binomial experiment with ten trials, each trial having two possible outcomes (heads or tails). Such yes/no or 0/1 outcomes are termed *binary* outcomes, and they need not have 50/50 probabilities. Any probabilities that sum to 1.0 are possible. It is conventional in statistics to term the "1" outcome the *success* outcome; it is also common practice to assign "1" to the more rare outcome. Use of the term "success" does not imply that the outcome is desirable or beneficial; it does tend to indicate the outcome of interest. For example, a loan default or a fraudulent transaction are relatively uncommon events that we may be interested in predicting, so are termed "1's" or "successes."

The binomial distribution is the frequency distribution of the number of successes (x) in a given number of trials (n) with specified probability (p) of success oin each trial. There is a family of binomial distributions, depending on the values of x, n and p. The binomial distribution would answer a question like this:

"If the probability of a click converting to a sale is 0.02, what is the probability of observing 0 sales in 200 clicks?"

The R code to calculate binomial probabilities is

> dbinom(x, n, p)

For example,

```
> dbinom(2, 5, 0.1)
```

would return 0.0729, the probability of observing exactly 2 successes in 5 trials, where the probability of success for each trial is 0.1.

Often we are interested in determining the probability of x or fewer successes in n trials, the code for that is

```
> pbinom(x, n, p)
```

For example

```
> pbinom(2, 5, 0.1)
```

would return 0.9914, the probability of observing 2 or fewer successes in 5 trials, where the probability of success for each trial is 0.1.

The mean of a binomial distribution is np; you can also think of this as the expected number of successes in n trials, for success probability = p.

The variance is as follows:

$$np(1-p)$$

With a large enough number of trials (particularly when *p* is close to 0.50), the binomial distribution is virtually indistinguishable from the normal distribution. In fact, calculating binomial probabilities with large sample sizes is computationally demanding, and most statistical procedures use the normal distribution, with mean and variance as above, as an approximation.

KEY IDEAS

- 1. Binomial outcomes are important to model, since they represent, among other things, fundamental decisions (buy or don't buy, click or don't click, survive or die, etc.)
- 2. Binomial trial is an experiment with two possible outcomes, one with probability p and the other with probability l-p
- 3. With large *n*, and provided *p* is not too close to 0 or 1, the binomial distribution can be approximated by the normal distribution

Further Reading

- 1. An easy read can be found at https://www.mathsisfun.com/data/binomial-distribution.html . Check out the section on the "quincunx," a pinball-like simulation device for illustrating the binomial distribution.
- 2. The binomial distribution is a staple of introductory statistics, and all introductory statistics texts will have a chapter or two on it.

Poisson and Related Distributions

Many processes produce events randomly at a given overall rate - visitors arriving at a web site, cars arriving at a toll plaza (events spread over time), imperfections in a square meter of fabric, or typos per 100 lines of code (events spread over space).

KEY TERMS FOR POISSON AND RELATED DISTRIBUTIONS

Lambda

The rate (per unit of time or space) at which events occur

Poisson distribution

The frequency distribution of the number of events in sampled units of time or space Synonyms

"1" (as opposed to "0")

Exponential distribution

The frequency distribution of the time or distance from one event to the next event Synonyms

yes/no, 0/1, binary

Weibull distribution

A generalized version of the exponential, in which the event rate is allowed to shift over time

Poisson Distributions

From prior data we can estimate the average number of events per unit of time or space, but we might also want to know how different this might be from one unit of time/space to another. The Poisson distribution tells us the distribution of events per unit of time or space, when we sample many such units. It is useful when addressing queuing questions like "how much capacity do we need to be 95% sure of fully processing the internet traffic that arrives on a server in any 5 second period."

The key parameter in a Poisson distribution is λ , or lambda. This is the mean number of events that occurs in a specified interval of time or space. The variance for a Poisson distribution is also λ .

A common technique is to generate random numbers from a Poisson distribution as part of a queuing simulation. The rpois function in R does this, taking only two arguments - the quantity of random numbers sought, and lambda:

```
>rpois(100, lambda = 2)
```

This code will generate 100 random numbers from a Poisson distribution with $\lambda = 2$. For example, if incoming customer service calls average two per minute, this code will simulate 100 minutes, returning the number of calls in each of those 100 minutes.

Exponential distribution

Using the same parameter λ that we used in the Poisson distribution, we can also model the distribution of the time between events: time between visits to a web site or between cars arriving at a toll plaza. It is also used in engineering to model time to failure, and in process management to model, for example, the time required per service call. The R code to generate random numbers from an exponential distribution takes two arguments, n (the quantity of numbers to be generated), and rate, the number of events per time period. For example:

```
rexp(n = 100, rate = .2)
```

This code would generate 100 random numbers from an exponential distribution where the mean number of events per time period is 2. So you could use it to simulate 100 intervals, in minutes, between service calls, where the average rate of incoming calls is 0.2 per minute.

A key assumption in any simulation study for either the Poisson or exponential distribution is that the rate, λ , remains constant over the period being considered. This is rarely reasonable in a global sense; for example, traffic on roads or data networks varies by time of day, and day of week. However, the time periods, or areas of space, can usually be divided into segments that are sufficiently homogeneous so that analysis or simulation within those periods is valid.

Inference

In many applications, the event rate, λ , is known or can be estimated from prior data. However, for rare events, this is not necessarily so. Aircraft engine failure, for example, is sufficiently rare (thankfully) that, for a given engine type, there may be little data on which to base an estimate of time between failures. With no data at all, there is little basis on which to estimate an event rate. However, you can make some guess - if no events have been seen after 20 hours, you can be pretty sure that the rate is not 1 per hour. Via simulation, or direct calculation of probabilities, you can assess different hypothetical event rates and estimate threshold values below which the rate is very unlikely to fall. If there is some data but not enough to provide a precise, reliable estimate of the rate, a goodness-of-fit test (see [Link to Come]) can be applied to various rates to determine how well they fit the observed data.

Weibull distribution

In many cases, the event rate does not remain constant over time. If the period over which it changes is much longer than the typical interval between events, there is no problem - you just subdivide the analysis into the segments where rates are relatively constant, as mentioned above. If,

however, the event rate changes over the time of the interval, the exponential (or Poisson) distributions are no longer useful. This is likely to be the case in mechanical failure - the risk of failure increases as time goes by. The *Weibull* distribution is an extension of the exponential distribution, in which the event rate is allowed to change, as specified by a *shape* paramenter, β . If β is > 1, the probability of an event increases over time, if β is < 1, it decreases. Because the Weibull distribution is used with time-to-failure analysis, instead of event rate, the second parameter is expressed in terms of characteristic life, rather than in terms of the rate of events per interval. The symbol used is γ , the Greek letter eta. It is also called the *scale* parameter.

With the Weibull, the estimation task now includes estimation of both parameters, β and η . Software is used to model the data and yield an estimate of the best fitting Weibull distribution.

The R code to generate random numbers from a Weibull distribution takes three arguments, n (the quantity of numbers to be generated), shape and scale. For example, the following code would generate 100 random numbers (lifetimes) from a Weibull distribution with shape = 1.5 and characteristic life of 5000:

rweibull(100,1.5,5000)

KEY IDEAS

- 1. For events that occur at a constant rate, the number of events per unit of time or space can be modeled as a Poisson distribution
- 2. In this scenario, you can also model the time or distance between one event and the next as an exponential distribution
- 3. A changing event rate over time (e.g. an increasing probability of device failure) can be modeled with the Weibull distribution

Further reading

- 1. *Modern Engineering Statistics* by Tom Ryan (2007, Wiley) has a chapter devoted to the probability distributions used in engineering applications
- 2. Further reading on the use of the Weibull distribution (mainly from an engineering perspective):

http://www.sascommunity.org/sugi/SUGI88/Sugi-13-43%20Kay%20Price.pdf http://www.ipedr.com/vol75/29_ICQM2014-051.pdf

Summary

In the era of big data, the principles of random sampling remain important in cases where accurate estimates are needed. Random selection of data can reduce bias, and yield a higher quality dataset than would result from simply using all the conveniently-available data. Knowledge of various sampling and data generating distributions can allow us to quantify the potential error in an estimate that might be due to random variation. At the same time, the bootstrap (sampling with replacement from an observed dataset) is an attractive "one size fits all" method of determining potential error in sample estimates.

¹ Iconic but perhaps overrated. George W. Cobb, the Mount Holyoke statistician noted for his contribution to the philosophy of teaching introductory statistics, argued in a November 2015 editorial in the *American Statistician* that the "standard introductory course, which puts the normal distribution at its center, had outlived the usefulness of its centrality."