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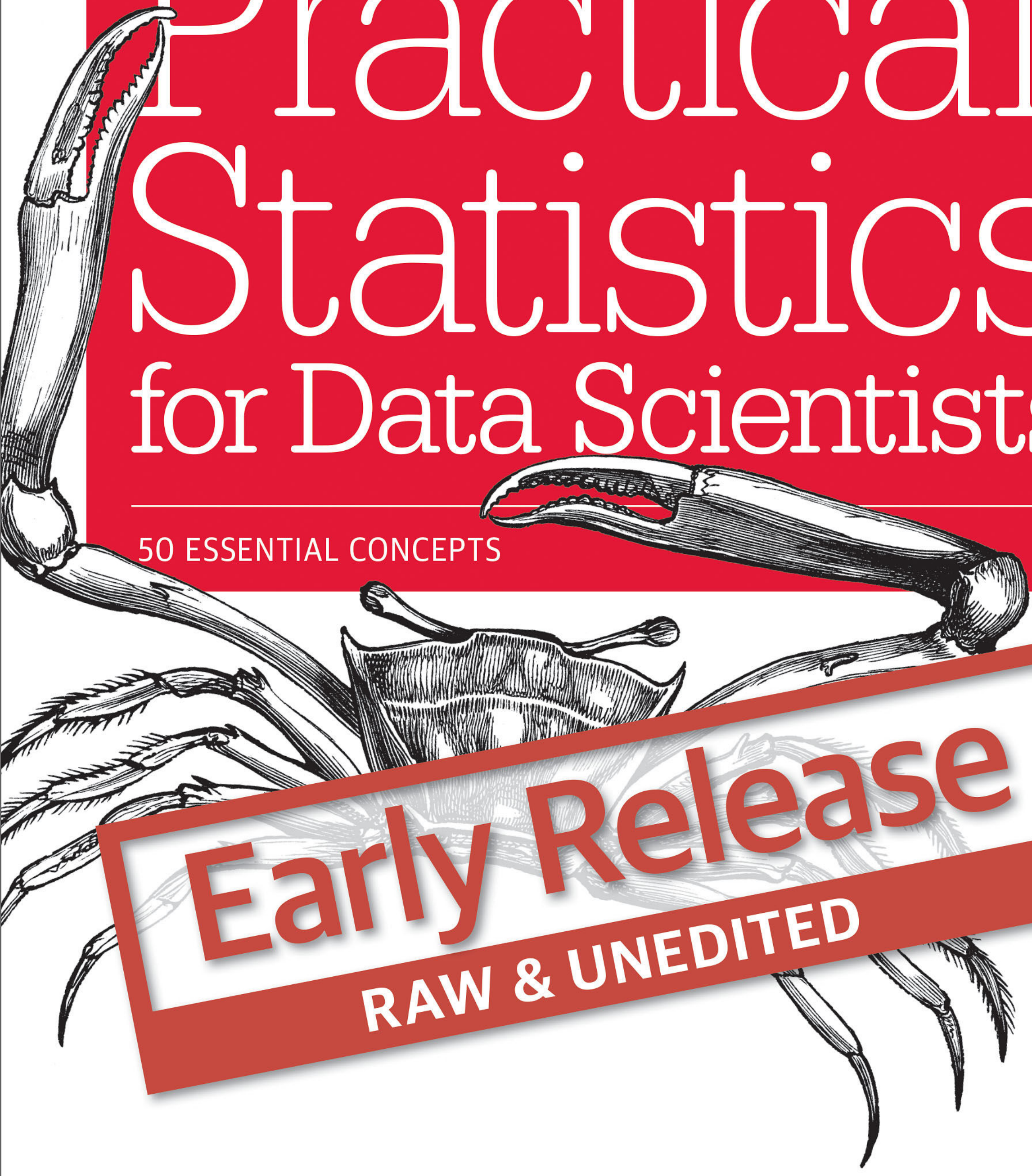
50 ESSENTIAL CONCEPTS



Peter Bruce & Andrew Bruce

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by Peter Bruce and Andrew Bruce

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1ST EDITION

Statistics for Data Scientists

50 Essential Concepts

Peter C. Bruce and Andrew G. Bruce

Beijing · Boston · Farnham · Sebastopol · Tokyo

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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" ???. 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" ???.

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 ???. 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

Binary

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" on page 11). 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
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 multi-level/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 ???). 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" on page 18). 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 $\bar{x}$ 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 $x_1, x_2, \ldots, x_N$ is

$$\text{Mean} = \bar{x} = \frac{\sum_i^N x_i}{N}$$

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 $x_{(1)}, x_{(2)}, \ldots, x_{(N)}$ where $x_{(1)}$ is the smallest value and $x_{(N)}$, the formula to compute the trimmed mean with p smallest and largest values omitted is

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

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 ???> 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" on page 19 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

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

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" on page 28). 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

	State	Population	Murder Rate
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
l2-norm, Euclidean norm

Mean Absolute Deviation
The mean of the absolute value of the deviations from the mean.

Synonyms
l1-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

$$\text{Mean Absolution Deviation} = \frac{\sum_{i=1}^{N} \left| x_i - \bar{x} \right|}{N}$$

where $\bar{x}$ 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.

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

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

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 ???).

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 refered 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 ???).

Neither the variance, the standard deviation nor the mean absolute deviation are *robust* to outliers and extreme values (see "Median and Robust Estimates" on page 19 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:

$$\text{Median Absolution Deviation} = \text{Median}\left(\left|x_1 - m\right|, \left|x_2 - m\right|, ..., \left|x_N - m\right|\right)$$

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 ???).

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 refered 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 ??? 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

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

Formally, the percentile is the weighted average

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

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 ??? 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 ??? for formulas and more details about skewness and kurtosis.

Percentiles and Boxplots

In "Estimates Based on Percentiles" on page 25, 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:

```
quantile(state[["Murder.Rate"]], p=c(.05, .25, .5, .75, .95))
   5%   25%   50%   75%   95%
1.600 2.425 4.000 5.550 6.510
```

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

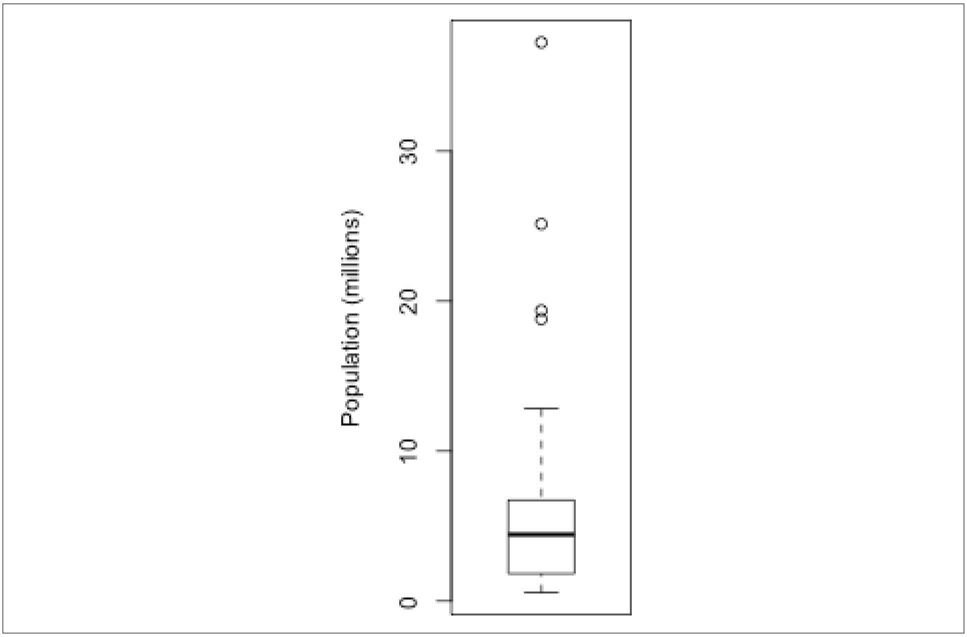


Figure 1-2. Boxplot of State Populations

Boxplots, introduced by Tukey ???, 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` ???. 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:

```
breaks <- seq(from=min(state[["Population"]]),
                to=max(state[["Population"]]), length=11)
pop_freq <- cut(state[["Population"]], breaks=breaks,
                   right=TRUE, include.lowest = TRUE)
table(pop_freq)
```

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.

> 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.

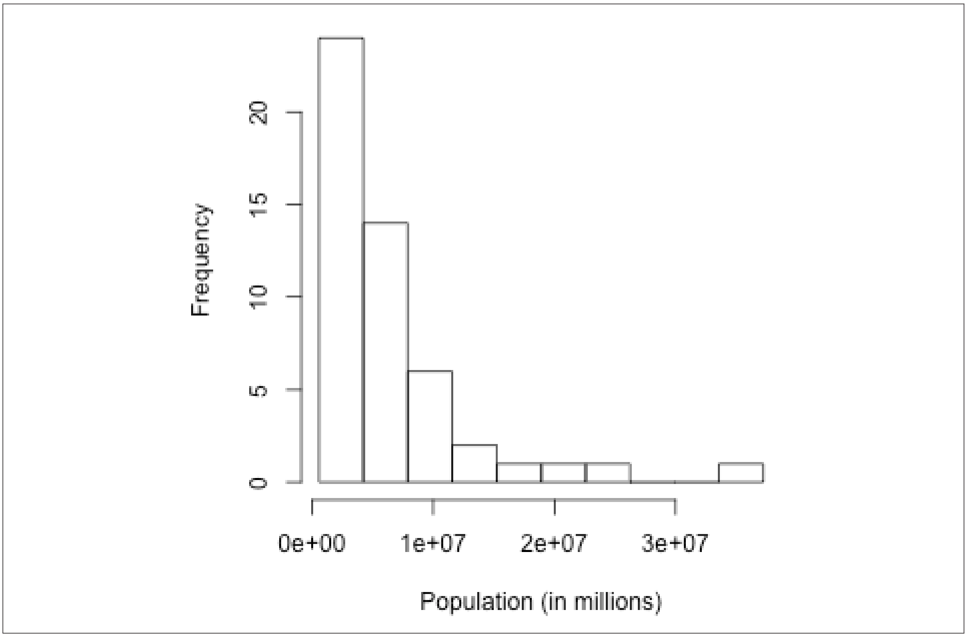


Figure 1-3. Histogram of State Populations

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 ??? 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`).

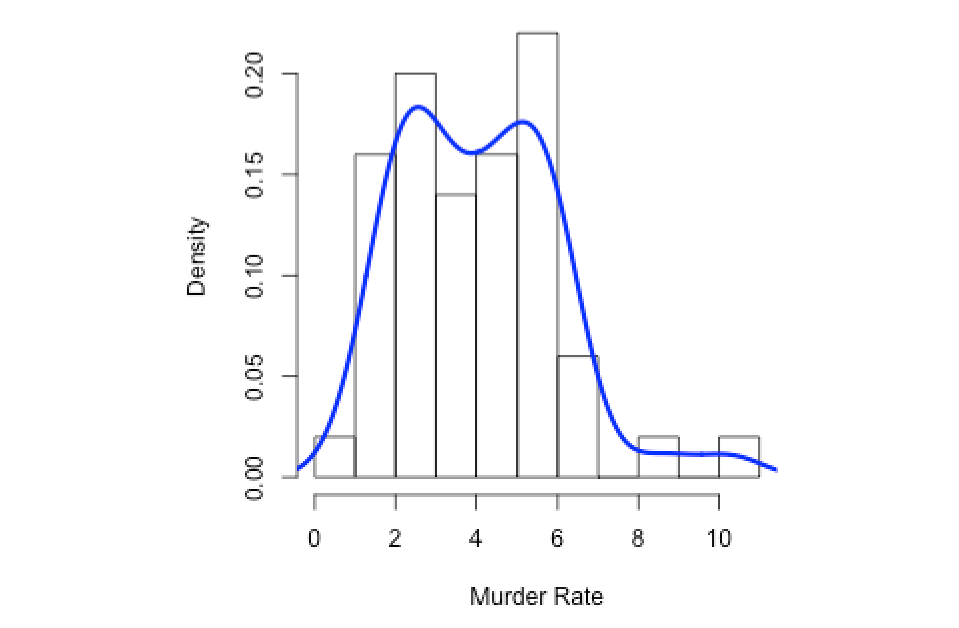


Figure 1-4. Density of State Murder Rates

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. ??? 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

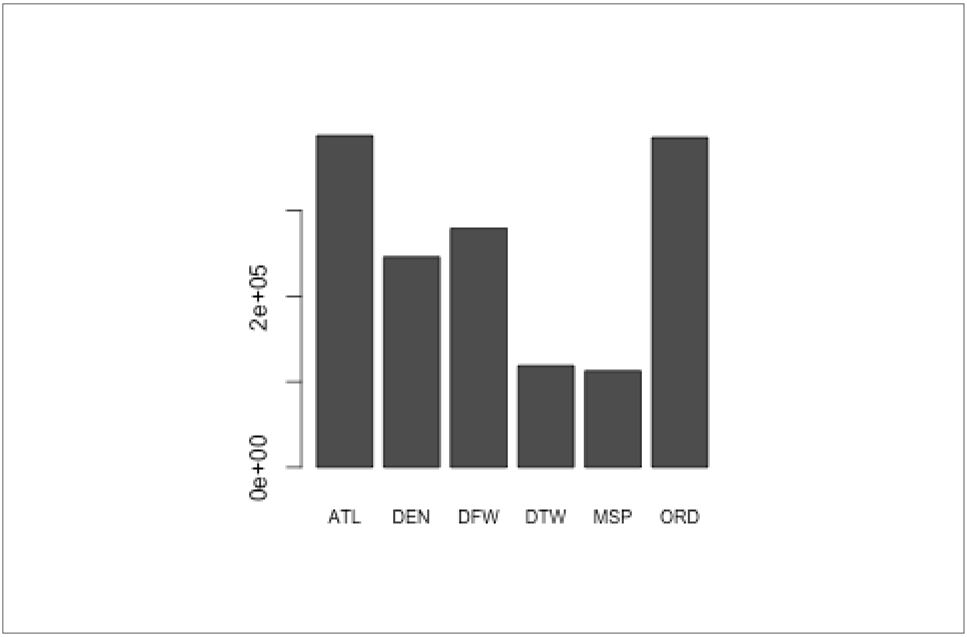


Figure 1-5. Bar plot airline delays by airport.

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 ???).

Numerical Data as Categorical Data

In “Exploring the Data Distribution” on page 27, 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:

V1: {1, 2, 3} V2: {4, 5, 6}

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 ???). 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:

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

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.

	T	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

	T	CTL	FTR	VZ	LVLT
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`:

```
etfs <- sp500_px[row.names(sp500_px)>"2012-07-01",
                 sp500_sym[sp500_sym$sector=="etf", 'symbol']]
library(corrplot, method = "ellipse")
corrplot(cor(etfs))
```

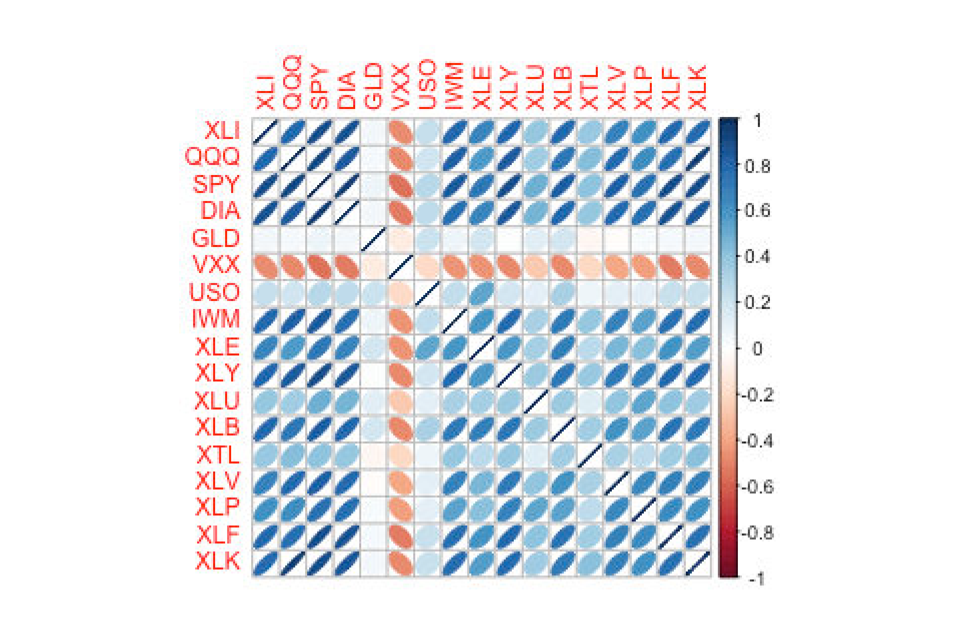


Figure 1-6. Correlation between ETF Returns

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 ???).

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).

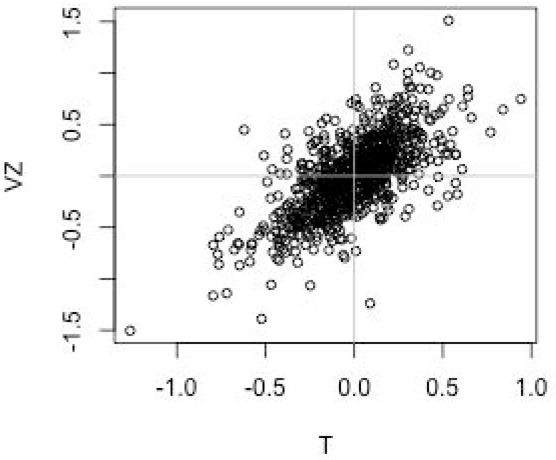


Figure 1-7. Scatter plot between returns for ATT and Verizon

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" on page 36) 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 assessde 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 ???. `ggplot2` is one of several new software libraries for advanced exploratory visual analysis of data: see "Visualizing Multiple Variables" on page 46.

```
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")
```

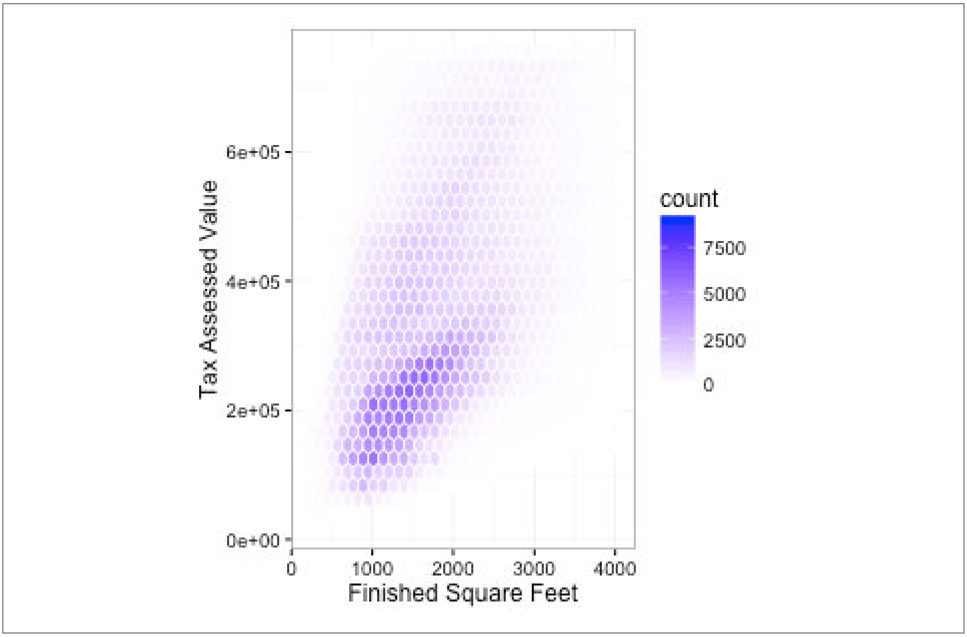


Figure 1-8. Hexagonal binning for tax assessed value versus finished square feet

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`:

```
library(ggplot)
house %>%
  filter(TaxAssessedValue < 750000, FinishedSquareFeet>100,
         FinishedSquareFeet<4000) %>%
  ggplot(aes(FinishedSquareFeet, TaxAssessedValue)) +
  theme_bw() +
  geom_point(colour="blue", alpha=0.2) +
  geom_density2d(colour="red") +
  labs(x="Finished Square Feet", y="Tax Assessed Value")
```

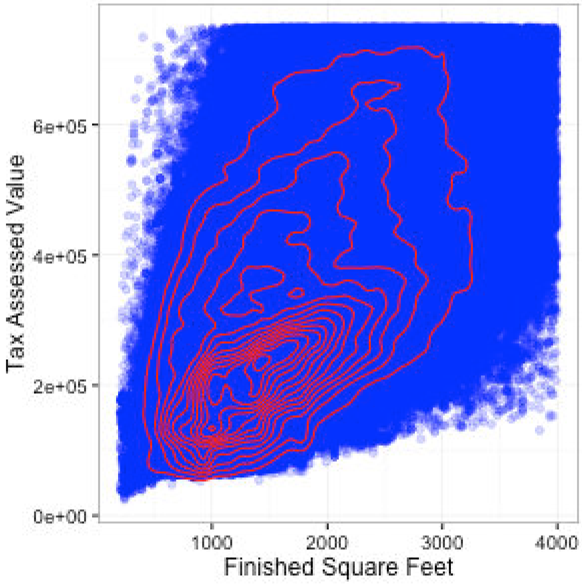


Figure 1-9. Contour plot for tax assessed value versus finished square feet

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:

```
library(descr)
CrossTable(loans$grade, loans$status, prop.c=FALSE,
                    prop.chisq=FALSE, prop.t=FALSE)
```

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
B	31785	97608	2149	5387	136929
	0.232	0.713	0.016	0.039	0.294
C	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
E	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
Total	99457	333472	10208	23150	466287

Categorical and Numeric Data

Boxplots (see "Percentiles and Boxplots" on page 28) 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))
```

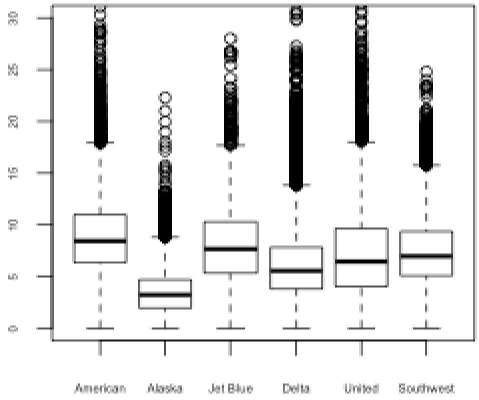


Figure 1-10. Boxplot of percent of airline delays by carrier.

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 ???, 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.

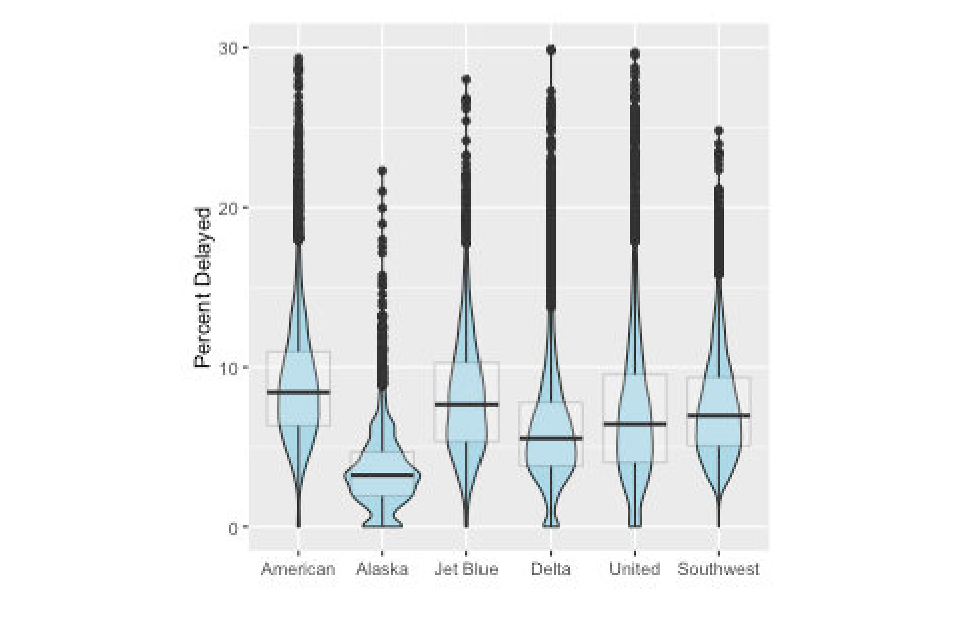


Figure 1-11. Combination of boxplot and violin plot of percent of airline delays by carrier.

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")
```

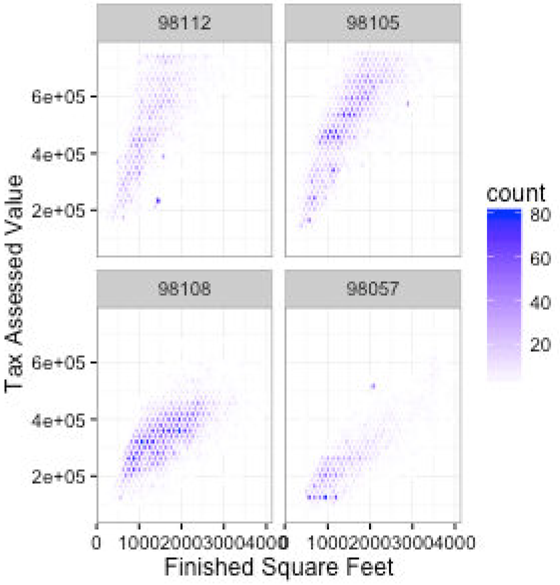


Figure 1-12. Tax assess value versus finished square feet by zip code.

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 ???. This idea has propogated to various modern graphics systems, such as the *lattice* (???) and *ggplot2* packages in R and the *Seaborn* (???) and *Bokeh* (???) 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).

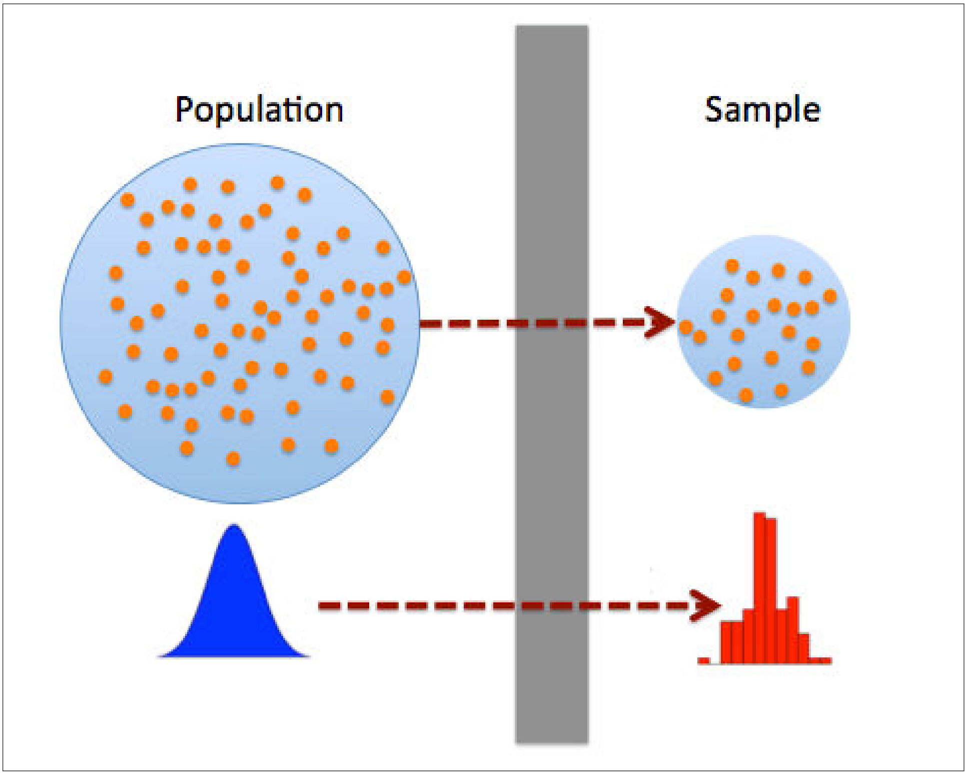


Figure 2-1. Population versus sample

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 socio-economic 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 non-random 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.

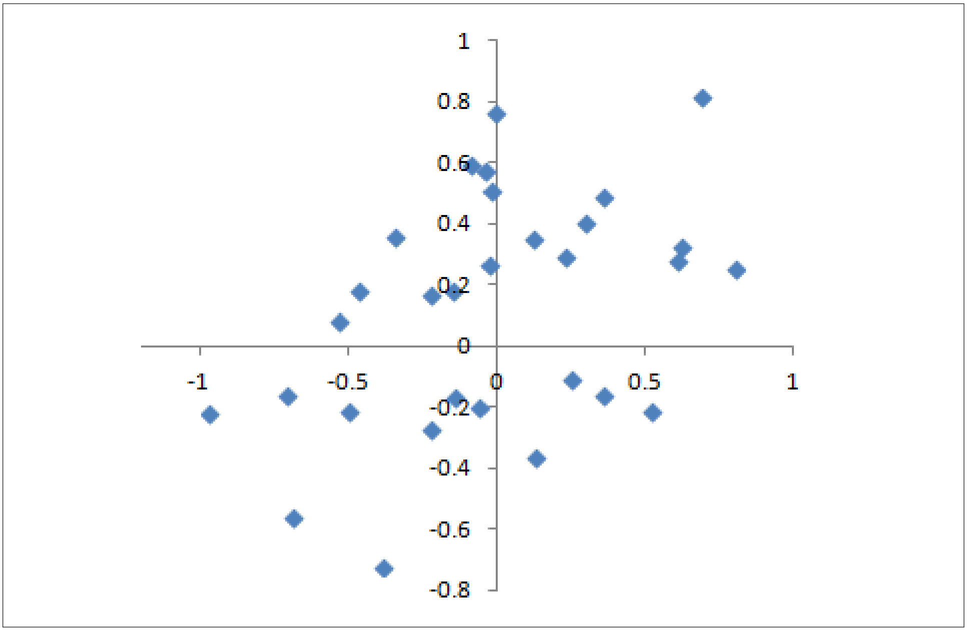


Figure 2-2. Scatter of shots from a gun with true aim

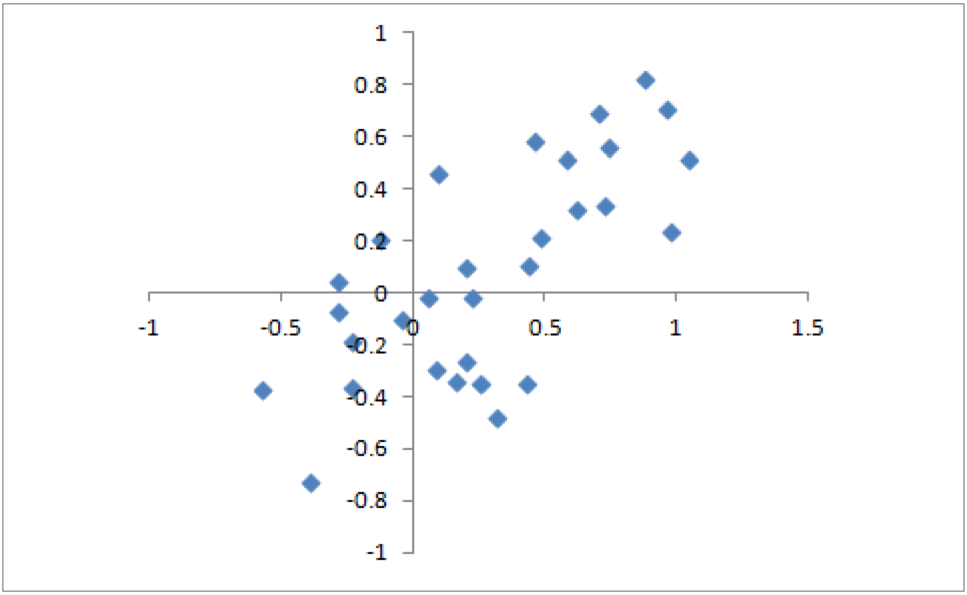


Figure 2-3. Scatterplot of shots from a gun with biased aim

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" on page 75.

Sample Mean Versus Population Mean

The symbol $\bar{x}$ 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 partiular 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 ???, 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.

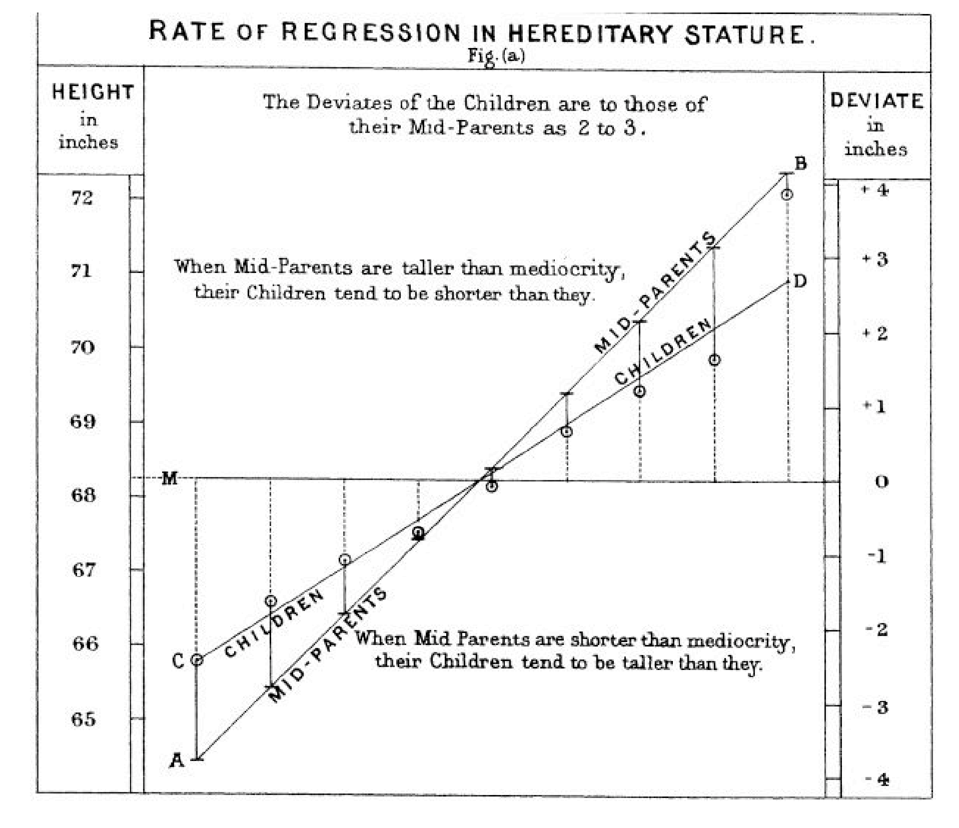


Figure 2-5. Galton's study that identified the phenomena of regression to the mean.

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.

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 annual income for loan applicants to Lending Club (see ??? 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.

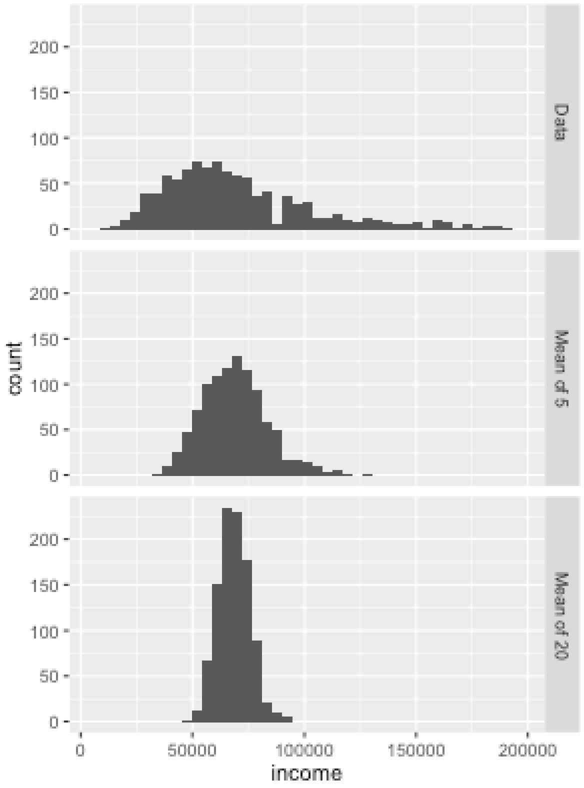


Figure 2-6. Histogram of annual incomes of 1000 loan applicants

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]
# take a simple random sample
samp_data <- data.frame(income=sample(loans_income, 1000),
                        type='data_dist')
# take a sample of means of 5 values
samp_mean_05 <- data.frame(
  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(
  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)
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" on page 72), 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*:

$$\text{Standard Error} = SE = \frac{s}{\sqrt{n}}$$

As the sample size increases, the standard error decreases, corresponding to 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" on page 63). 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" on page 65). 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.

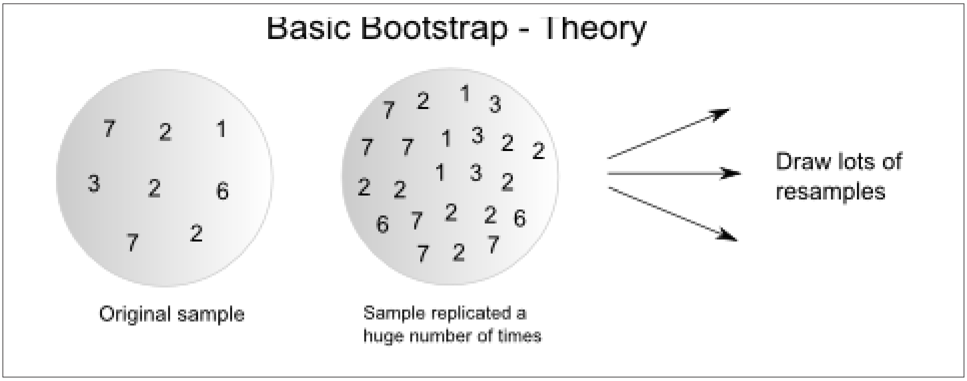


Figure 2-7. The idea of the bootstrap

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”).

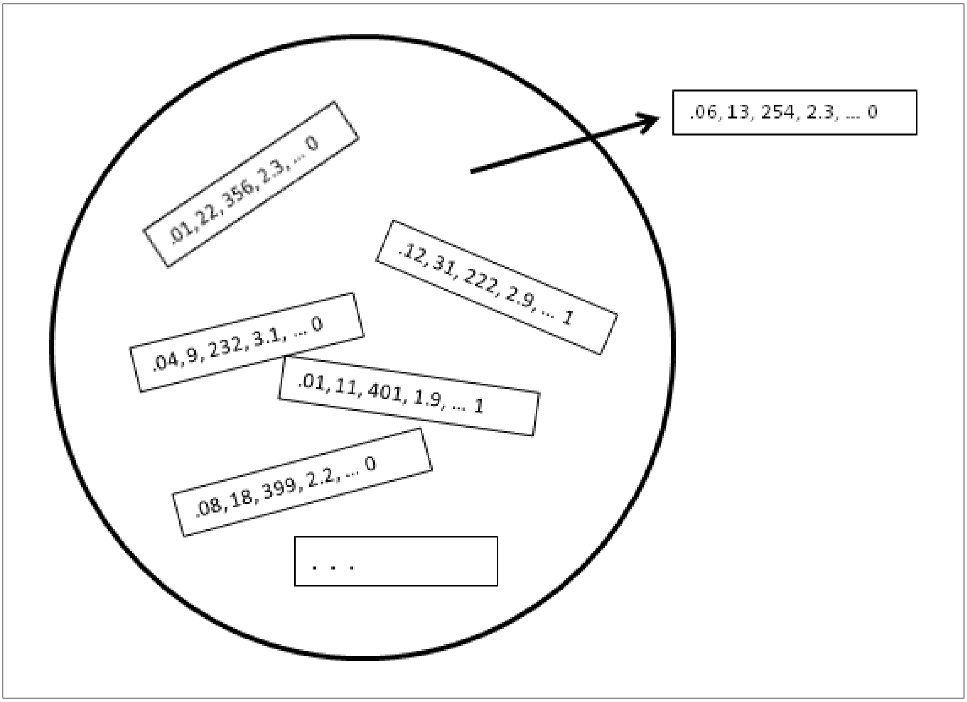


Figure 2-8. Multivariate bootstrap sampling

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.

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 how lots of additional samples would behave, 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 ???), 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 "Resampling" on page 96) 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 it is 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" on page 65). 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/100])/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.

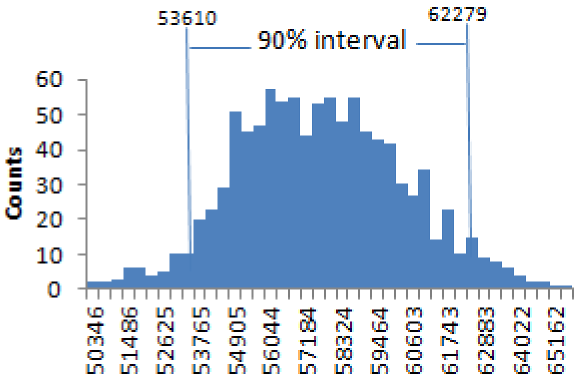


Figure 2-9. Bootstrap confidence interval for the annual income of loan applicants, based on a sample of 20

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" on page 77).

> 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.

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 a sample estimate will be.
3. The lower the level of confidence you can tolerate, the narrower the confidence interval will be.
4. 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.

[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."

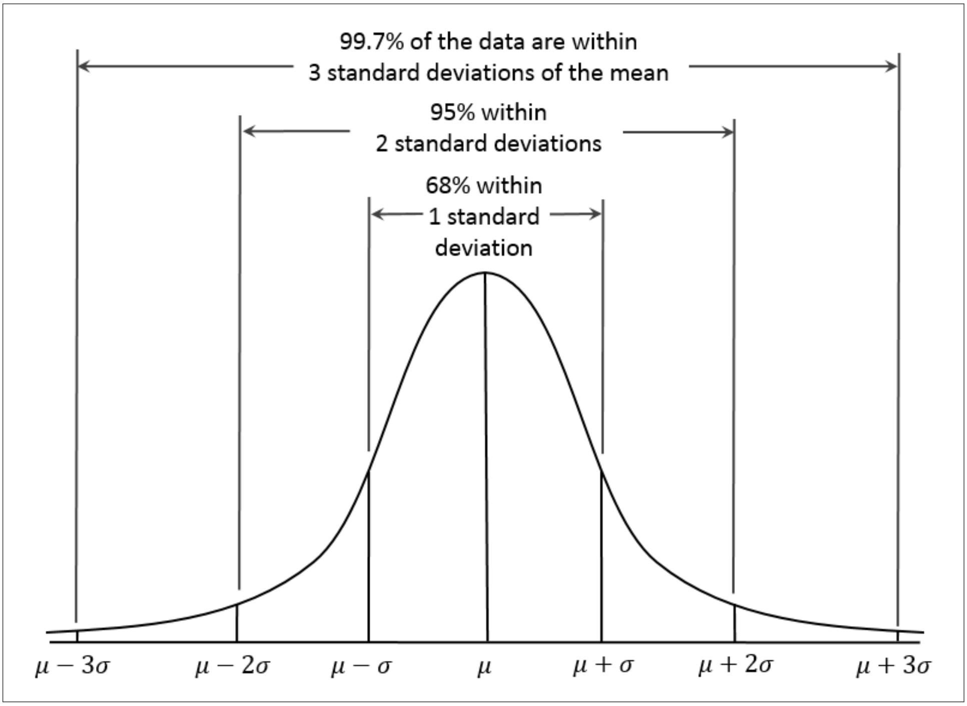


Figure 2-10. Normal curve

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" on page 75. 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.

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" on page 22) 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.

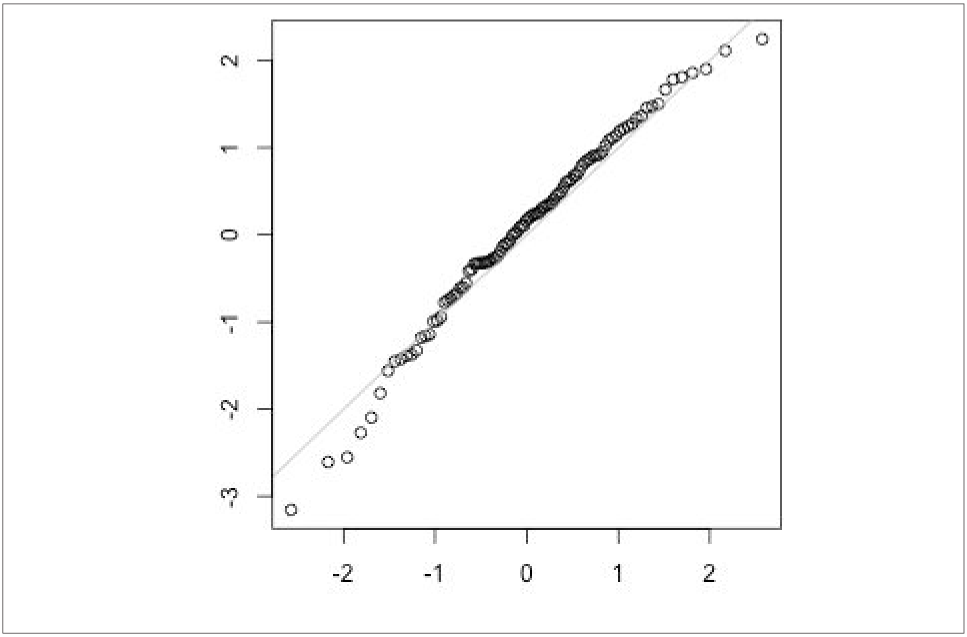


Figure 2-11. QQ-Plot of a sample of 100 values drawn from a normal distribution.

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')
```

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.

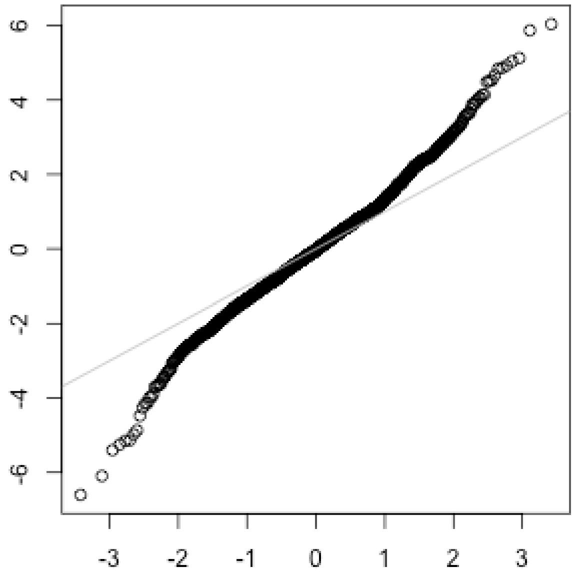


Figure 2-12. QQ-Plot of the returns for NFLX.

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 ???).

> 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" on page 83).

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).

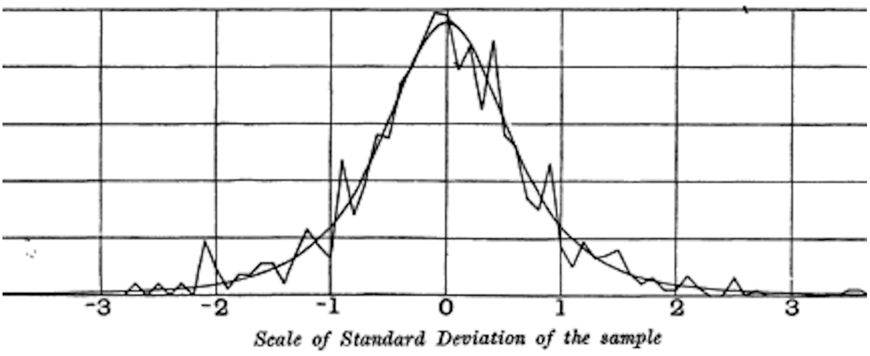


Figure 2-13. Gossett's resampling experiment results and fitted t-curve (from his 1908 Biometrika paper

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 ???), 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 ???).

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 probabiltiy *1-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 ???) 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 η, 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*

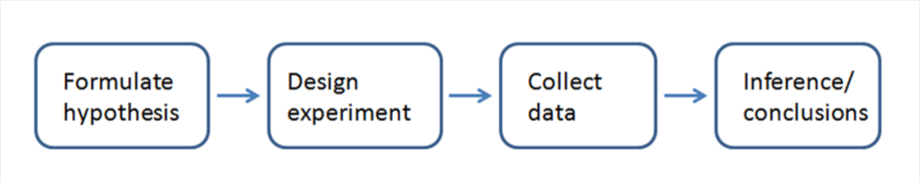
Summary

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.

CHAPTER 3

Statistical Experiments and Significance Testing

Design of experiments is a cornerstone of the practice of statistics, with applications in virtually all areas of research. The goal is to design an experiment in order to confirm or reject a hypothesis. Data scientists are faced with the need to conduct continual experiments, particularly regarding user interface and product marketing. This chapter reviews traditional experimental design, and discusses issues commonly faced in data science. It also covers some oft-cited concepts in statistical inference, and explains their meaning and relevance (or lack of relevance) to data science.



Whenever you see reference to statistical significance, t-tests, or p-values, it is typically in the context of the classical statistical inference “pipeline.” This process starts with a hypothesis (“drug A is better than the existing standard drug,” “price A is more profitable than the existing price B”). An experiment (it might be an A-B test) is designed to test the hypothesis - designed in such a way that, hopefully, the results will be conclusive. Data are collected and analyzed, then a conclusion is drawn. The term *inference* reflects the intention to apply the experiment results, which involve a limited set of data, to a larger process or population.

A-B Testing

An A-B test is an experiment with two groups to establish which of two treatments, products, procedures, etc. is superior. Often one of the two treatments is the standard existing treatment, or no treatment. If a standard (or no) treatment is used, it is called the control. A typical hypothesis is that treatment is better than control.

Key Terms for A-B Testing

Treatment
Something (drug, price, web headline) to which a subject is exposed

Treatment group
A group of subjects exposed to a specific treatment

Control group
A group of subjects exposed to no (or standard) treatment

Randomization
The process of randomly assigning subjects to treatments

Subjects
The items (web visitors, patients, etc.) that are exposed to treatments

Test statistic
The metric used to measure the effect of the treatment

A-B tests are common in web design and marketing, since results are so readily measured.

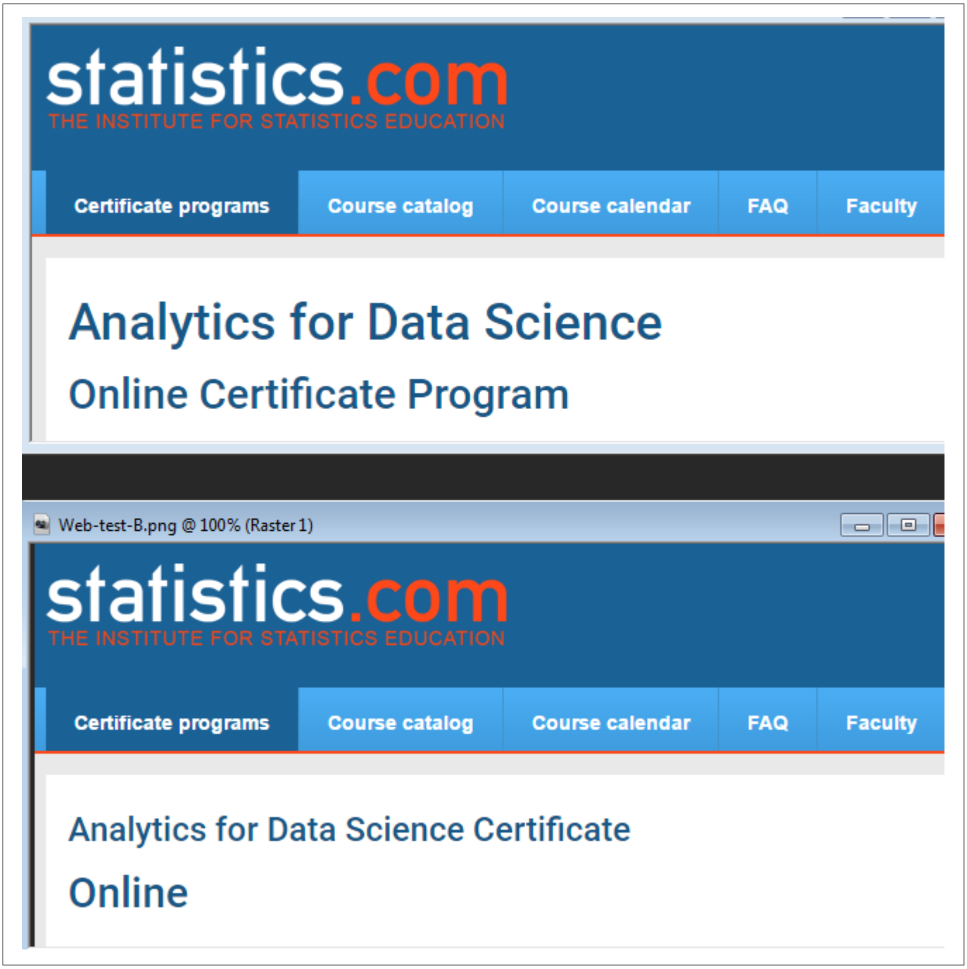


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Figure 3-1. Marketers continually test one web presentation against another

Some examples of A-B testing:

1. Testing two soil treatments to determine which produces better seed germination
2. Testing two therapies to determine which suppresses cancer more effectively
3. Testing two prices to determine which yields more net profit
4. Testing two web headlines to determine which produces more clicks
5. Testing two web ads to determine which generates more conversions

A proper A-B test has *subjects* that can be assigned to one treatment or another. The subject might be a person, a plant seed, a web visitor; the key is that the subject is exposed to the treatment. Ideally, subjects are *randomized* (assigned randomly) to treatments. In this way, you know that any difference between the treatment groups is due to one of two things:

1. The effect of the different treatments, or
2. Luck of the draw in which subjects are assigned to which treatments (i.e. the random assignment may have resulted in the naturally better performing subjects being concentrated in A, or B).

You also need to pay attention to the *test statistic* or metric you use to compare group A to group B. Perhaps the most common metric in data science is a binary variable - click or no-click, buy or don't buy, fraud or no fraud, etc. Those results would be summed up in a 2x2 table. Here's a 2x2 table for an actual price test:

[[2x2]] .2x2 table - eCommerce experiment results

Outcome	Price A	Price B
Conversion	200	182
No conversion	23539	22406

If the metric is a continuous variable (purchase amount, profit, etc.), or a count (e.g. days in hospital, pages visited) the result might be displayed differently. If one were interested not in conversion, but in revenue per page view, the results of the above price test might look like this in typical default software output:

Revenue/page-view with Price A: mean = 3.87, SD = 51.10

Revenue/page-view with Price B: mean = 4.11, SD = 62.98

"SD" refers to the standard deviation of the values within each group.

Just because statistical software - including R - generates output by default does not mean that all the output is useful or relevant. You can see that the standard deviations above are not that useful - on their face they suggest that numerous values might be negative, when negative revenue is not feasible. These data consist of a small set of relatively high values (page views with conversions) and a huge number of 0-values (page views with no conversion). It is difficult to sum up the variability of such data with a single number, though the mean absolute deviation from the mean (7.68 for A and 8.15 for B) is more reasonable than the standard deviation.

Why have a control group?

Why not skip the control group and just run an experiment applying the treatment of interest to just one group, and compare the outcome to prior experience?

Without a control group, there is no assurance that “other things are equal” and that any difference is really due to the treatment (or to chance). When you have a control group, it is subject to the same conditions (except for the treatment of interest) as the treatment group. If you simply make a comparison to “baseline” or prior experience, other factors, besides the treatment, might differ.

Blinding in studies

A *blinded study* is one in which the subjects are unaware of whether they are getting Treatment A or Treatment B. Awareness of receiving a particular treatment can affect response. A *double blind* study is one in which the investigators and facilitators (e.g. doctors and nurses in a medical study) are unaware which subjects are getting which treatment. Blinding is not possible when the nature of the treatment is transparent - e.g. cognitive therapy from a computer vrs. a psychologist.

The use of A-B testing in data science is typically in a web context. Treatments might be the design of a web page, the price for a product, the wording of a headline, or some other item. Some thought is required to preserve the principles of randomization. Typically the subject in the experiment is the web visitor, and the outcomes we are interested in measuring are clicks, purchases, visit duration, number of pages visited, whether a particular page is visited, etc. In a standard A-B experiment, you need to decide on one metric ahead of time. Multiple behavior metrics might be collected, and be of interest, but, if the experiment is expected to lead to a decision between treatment A and treatment B, a single metric, or *test statistic*, needs to be established beforehand. Selecting a test statistic *after* the experiment is conducted opens the door to researcher bias.

Why just A-B? Why not C, D, etc.?

A-B tests are popular in the marketing and ecommerce worlds, but are far from the only type of statistical experiment. Additional treatments can be included. Subjects might have repeated measurements taken. Pharmaceutical trials where subjects are scarce, expensive and acquired over time, are sometimes designed with multiple opportunities to stop the experiment and reach a conclusion.

Traditional statistical experimental designs focus on answering a static question about the efficacy of specified treatments. Data scientists are less interested in the question

"Is the difference between price A and price B statistically significant?"

than in the question

"Which, out of multiple possible prices, is best?"

For this, a relatively new type of experimental design is used - the *multi-arm bandit* (see "Multi-arm bandit algorithm" on page 124).

Getting Permission

In scientific and medical research involving human subjects, it is typically necessary to get their permission, and obtain the approval of an "Institutional Review Board." Experiments in business that are done as a part of ongoing operations almost never do this. In most cases (e.g. pricing experiments, experiments about which headline to show or which offer should be made), this practice is widely accepted. Facebook, however, ran afoul of this general acceptance in 2014 when it experimented with the emotional tone in users' newsfeeds. Facebook used sentiment analysis to classify newsfeed posts as positive or negative, then altered the positive/negative balance in what it showed users. Some randomly selected users experienced more positive posts, others experienced more negative posts. Facebook found that the users who experienced a more positive newsfeed were more likely to post positively themselves, and vice-versa. The magnitude of the effect was small, however, and Facebook faced much criticism for conducting the experiment without users' knowledge. Some users speculated that Facebook might have pushed some extremely depressed users over the edge, if they got the negative version of their feed.

Key ideas

1. Subjects are assigned to two (or more) groups that are treated exactly alike, except that the treatment under study differs from one to another.
2. Ideally, subjects are assigned randomly to the groups.

For Further Reading

1. Two group comparisons (A-B tests) are a staple of traditional statistics, and just about any introductory statistics text will have extensive coverage of design principles and inference procedures. For a discussion that places A-B tests in more of a data science context and uses resampling, see *Introductory Statistics and Analytics: A Resampling Perspective* by Peter Bruce (Wiley, 2014).

2. For web-testing, the logistical aspects of testing can be just as challenging as the statistical ones. A good place to start is the Google Analytics help section on Experiments, *https://support.google.com/analytics/answer/1745149?hl=en&ref_topic=1745207*
3. Beware advice found in the ubiquitous guides to A-B testing that you see on the web, such as these words in one such guide: "wait for about 1,000 total visitors and make sure you run the test for a week." Such general rules of thumb are not statistically meaningful, see ??? for more detail.

Hypothesis Test

Hypothesis tests, also called *significance tests*, are ubiquitous in the traditional statistical analysis of published research. Their purpose is to help learn whether random chance might be responsible for an observed effect.

Key Terms

Null hypothesis
The hypothesis that chance is to blame

Alternative hypothesis
Counterpoint to the null (what you hope to prove)

One-way test
Hypothesis test that counts chance results only in one direction

Two-way test
Hypothesis test that counts chance results in two directions

An A-B test (see "A-B Testing" on page 88) is typically constructed with a hypothesis in mind. For example, the hypothesis might be that Price B produces higher profit. Why do we need a hypothesis? Why not just look at the outcome of the experiment and go whichever treatment does better?

The answer lies in the tendency of the human mind to underestimate the scope of natural random behavior. One manifestation of this is the failure to anticipate extreme events - so-called "black swans" (see "Long-Tailed Distributions" on page 75). Another manifestation is the tendency to misinterpret random events as having patterns of some significance. Statistical hypothesis testing was invented as a way to protect researchers from being fooled by random chance.

Misinterpreting Randomness

You can observe the human tendency to underestimate randomness in this experiment. Ask several friends to invent a series of 50 coin flips - have them write down a series of random H's and T's. Then ask them to actually flip a coin fifty times and write down the results. Have them put the real coin flip results in one pile, and the made-up in another. It is easy to tell which are real - the real ones will have longer runs of H's or T's in a row. In a set of 50 *real* coin flips, it is not at all unusual to see runs of 5 or 6 H's or T's in a row. However, when most of us are inventing random coin flips and we have gotten 3 or 4 H's in a row, we tell ourselves that, for the series to look random, we had better switch to T.

The other side of this coin, so to speak, is that when we *do* see the real world equivalent of 6 H's in a row (e.g. when one headline outperforms another by 10%) we are inclined to attribute it to something real, not just chance.

In a properly designed A-B test, you collect data on treatments A and B in such a way that any observed difference between A and B must be due to either

1. Random chance in assignment of subjects, or
2. A true difference between A and B

A statistical hypothesis test is further analysis of an A-B test, or any randomized experiment, to assess whether random chance is a reasonable explanation for the observed difference between groups A and B.

The Null Hypothesis

Hypothesis tests use the following logic: "Given the human tendency to react to unusual but random behavior and interpret it as something meaningful and real, in our experiments we will require proof that the difference between groups is more extreme than what chance might reasonable produce." This involves a baseline assumption that the treatments are equivalent, and any difference between the groups is due to chance. This baseline assumption is termed the *null hypothesis*. Our hope is then that we can, in fact, prove the null hypothesis *wrong*, and show that the outcomes for groups A and B are more different than what chance might produce.

One way to do this is via a resampling permutation procedure, in which we shuffle together the results from groups A and B and then repeatedly deal out the data in groups of similar sizes, then observe how often we get a difference as extreme as the observed difference. See "Resampling" on page 96 for more detail.

Alternative hypothesis

Hypothesis tests by their nature involve not just a null hypothesis, but also an offsetting alternative hypothesis. Here are some examples:

- Null = “no difference between the means of group A and group B,” alternative = “A is different from B” (could be bigger or smaller)
- Null = “A ⇐ B,” alternative = “B > A”
- Null = “B is not X% greater than A,” alternative = “B is X% greater than A”

Taken together, the null and alternative hypotheses must account for all possibilities. The nature of the null hypothesis determines the structure of the hypothesis test.

One-way, two-way hypothesis test

Often, in an A-B test, you are testing a new option, say B, against an established default option, (A), and the presumption is that you will stick with the default option unless the new option proves itself definitively better. In such a case, you want a hypothesis test to protect you from being fooled by chance in the direction favoring B. You don’t care about being fooled by chance in the other direction, because you would be sticking with A unless B proves definitively better. So you want a *directional* alternative hypothesis (B is better than A). In such a case, you use a *one-way* (or one-tail) hypothesis test. This means that extreme chance results in only one direction direction count towards the p-value.

If you want a hypothesis test to protect you from being fooled by chance in either direction, the alternative hypothesis is *bi-directional* (A is different from B, could be bigger or smaller). In such a case, you use a *two-way* (or two-tail) hypothesis. This means that extreme chance results in either direction count towards the p-value.

A one-tail hypothesis test often fits the nature of A-B decision-making, in which a decision is required and one option is typically assigned “default” status unless the other proves better. Software, however, including R, typically provides a two-tail test in its default output, and many statisticians opt for the more conservative 2-tail test just to avoid argument. One-tail versus two-tail is a confusing subject, and not that relevant for data science, where the precision of p-value calculations is not terribly important.

Key Ideas

1. A *null hypothesis* is a logical construct embodying the notion that nothing special has happened, and any effect you observe is due to random chance

2. The *hypothesis test* assumes that the null hypothesis is true, creates a “null model” (a probability model) and tests whether the effect you observe is a reasonable outcome of that model

Further Reading

1. *The Drunkard’s Walk* by Leonard Mlodinow (2008, Vintage Books) is a readable survey of the ways in which “randomness rulles our lives.”
2. The classic statistics text *Statistics* by Freedman, et al (4th ed., 2007, W. W. Norton) has excellent non-mathematical treatments of most statistics topics, including hypothesis testing.
3. *Introductory Statistics and Analytics: A Resampling Perspective* by Peter Bruce (Wiley, 2014) develops hypothesis testing concepts using resampling.

Resampling

Resampling in statistics means to repeatedly sample values from observed data, with a general goal of assessing random variability in a statistic. It can also be used to assess and improve the accuracy of some machine-learning models (e.g. the predictions from decision tree models built on multiple bootstrapped datasets can be averaged in a process known as *bagging*).

Key Terms

1. ***Bootstrap***:: The procedure of randomly selecting a sample, with replacement, from an existing sample
2. ***Permutation test***:: The procedure of combining two or more samples together, and randomly (or exhaustively) reallocating the observations to resamples

   Synonyms

   Randomization test, random permutation test, exact test
3. ***With or without replacement***:: In sampling, whether or not an item is returned to the sample before the next draw

There are two main branches of resampling:

- The *bootstrap*
- Permutation

In the *bootstrap*, values are sampled with replacement from a dataset, to assess how reliable an estimate based on the dataset is - how much it might be in error due to sampling variation. The dataset might be a collection of cards with 0's and 1's (representing a binary variable like purchase/don't purchase), or it might be a multivariate dataset from which a model is built. In the latter case, each record is represented as a unit - e.g. a strip of paper with one row, and a value for each variable (feature). The bootstrap sampling process proceeds as follows:

1. Draw the card, or the slip of paper, record its value(s), then replace the card
2. Repeat the draw, usually N times (where N = number of records in the sample); this yields one bootstrap sample
3. Record the estimate, or model parameters, from the bootstrap sample; his constitutes one bootstrap iteration.
4. Repeat the above steps B times, where B is some arbitrarily large number - big enough to yield stable sampling results, and small enough to be computationally feasible; thus, there are a total of N*B draws

The result from this procedure is a bootstrap set of sample statistics, or estimated model parameters, which can then be examined to see how variable they are.

R combines these multiple steps in one command `boot`, as follows:

```
boot(data= , statistic= , R=, …)
```

`data` is a vector, matrix or dataframe `statistic` is a function to calculate a statistic, or *k* statistics `R` is the number of bootstrap resamples to be collected

The command can also accept, at the end, parameters that are to be passed to the function to calculate the statistic.

In a *permutation* procedure, two or more samples are involved, typically the groups in an A-B or other hypothesis test. *Permute* means to change the order of a set of values. The first step in a *permutation test* of a hypothesis is to combine the results from groups A and B (and, if used, C, D, …) together. This is the logical embodiment of the null hypothesis that the treatments to which the groups were exposed do not differ. We then test that hypothesis by randomly drawing groups from this combined set, and seeing how much they differ from one another. The permutation procedure is as follows:

1. Combine the results from the different groups in a single dataset
2. Shuffle the combined data, randomly draw (without replacing) a resample of the same size as group A
3. From the remaining data, randomly draw (without replacing) a resample of the same size as group B

4. Same for groups C, D, …
5. Whatever statistic or estimate was calculated for the original samples (e.g. difference in group proportions), calculate it now for the resamples, and record; this constitutes one permutation iteration
6. Repeat the above steps B times, yields a permutation distribution of the test statistic

Now compare the observed difference between groups, and compare it to the set of permuted differences. If the observed difference lies well within the set of permuted differences, then we have not proven anything - the observed difference is within the range of what chance might produce. However, if the observed difference lies outside most of the permutation distribution, then we conclude that chance is *not* responsible. In technical terms, the difference is *statistically significant*. See "statistical significance."

In addition to the above random shuffling procedure, also called a *random permutation test* or a *randomization test*, there are two variants of the permutation test:

- An *exhaustive permutation test*
- A *bootstrap permutation test*

In an exhaustive permutation test, instead of just randomly shuffling and dividing the data, we actually figure out all the possible ways it could be divided. This is practical only for relatively small sample sizes. With a large number of repeated shufflings, the random permutation test results approximate those of the exhaustive permutation test, and approach them in the limit. Permutation tests are also sometimes called *exact tests*, due to their statistical property of guaranteeing that the null model will not test as "significant" more than the alpha level of the test (see ???).

In a bootstrap permutation test, the draws outlined above in steps 2 and 3 of the random permutation test are made *with replacement* instead of without replacement. In this way the resampling procedure models not just the random element in the assignment of treament to subject, but also the random element in the selection of subjects from a population. Both procedures are encountered in statistics, and the distinction between them is somewhat convoluted and not of consequence in the practice of data science.

Resampling: The Bottom Line for Data Science

There are two key concepts in resampling:

1. Resampling with replacement (bootstrapping) from a dataset to assess possible random sampling error, and

2. Shuffling (permutation) of one variable relative to another, to assess whether random assignment might account for observed differences or associations.

Both are useful as heuristic procedures for exploring the role of random variation. Both are relatively easy to code, interpret and explain, and offer a useful detour around the formalism and "false determinism" of formula-based statistics.

One virtue of resampling, in contrast to formula approaches, is that it comes much closer to a "one size fits all" approach to inference. Data can be numeric, or binary. Sample sizes can be the same or different. Assumptions about normally-distributed data are not needed.

1. Key ideas

1. Sampling with replacement from an existing sample (the bootstrap) is an effective way to model sampling variability without using traditional formulas
2. The bootstrap is often used with multivariate data to assess stability in models, where the entire record is drawn (or not drawn) for the resample
3. Combining samples, then shuffling the values and drawing new resamples (permutation), allows you to judge whether an observed difference between samples might occur by chance

For 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. *Randomization Tests* by Edgington and Onghena (4th ed., Chapman Hall, 2007), but don't get too drawn into the thicket of non-random sampling
3. The retrospective on the bootstrap in the May, 2003 issue of *Statistical Science*, (v. 18, #2), which discusses (among other antecedents, in Peter Hall's "Prehistory") Julian Simon's first publication of the bootstrap in 1969.

Statistical Significance and P-values

Statistical significance is how statisticians measure whether an experiment (or even a study of existing data) yields a result more extreme than what chance might produce.

If the result is beyond the realm of chance variation, it is said to be statistically significant.

Key Terms

1. ***P-value***:: Given a chance model that embodies the null hypothesis, the p-value is the probability of obtaining results as unusual or extreme as the observed results
2. ***Alpha***:: The probability threshold of "unusualness" that chance results must surpass, for actual outcomes to be deemed statistically significant
3. ***Type 1 error***:: Mistakenly concluding an effect is real (when it is due to chance)
4. ***Type 2 error***:: Mistakenly concluding an effect is due to chance (when it is real)

Consider the results of the web test shown earlier:

Table 3-1. 2x2 table - eCommerce experiment results

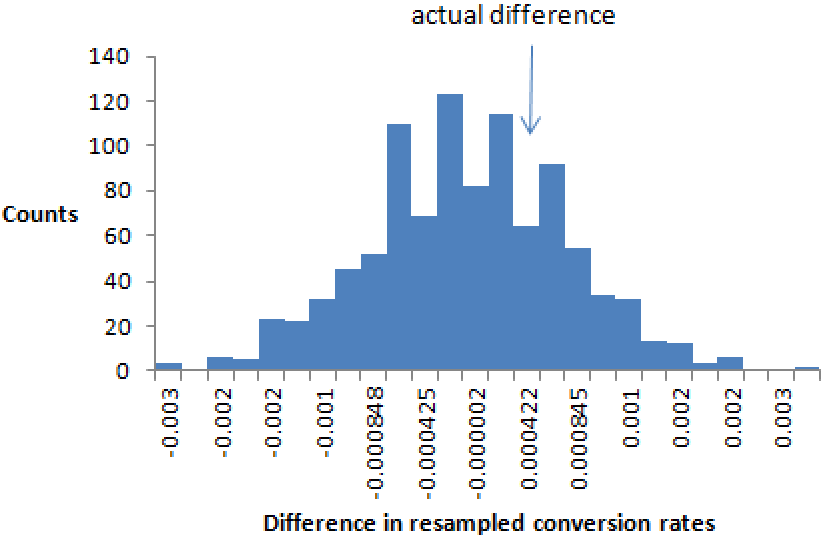
Outcome	Price A	Price B
Conversion	200	182
No conversion	23539	22406

Price A converts almost 5% better than price B (0.8425% versus 0.8057% - a difference of 0.368 percentage points), big enough to be meaningful in a high volume business. We have over 45,000 data points here, and it is tempting to consider this as "big data," not requiring tests of statistical significance (needed mainly to account for sampling variability in small samples). However, the conversion rates are so low (less than 1%) that the actual meaningful values - the conversions - are only in the 100's, and the sample size needed is really determined by these conversions. We can test whether the difference in conversions between prices A and B is within the range of chance variation, using a resampling procedure. By "chance variation," we mean the random variation produced by a probability model that embodies the null hypothesis that there is no difference between the rates (see ???). The following permutation procedure asks "if the two prices share the same conversion rate, could chance variation produce a difference as big as 5% just by chance?"

1. Create an urn with all sample results - this represents the supposed shared conversion rate of 382 1's and 45,945 0's = 0.008246 = 0.8246%.
2. Shuffle and draw out a resample of size 23,739 (same N as Price A), record how many 1's
3. Record the number of 1's in the remaining 22,588 (same N as Price B)

4. Record the difference in proportion 1's
5. Repeat steps 2-4.
6. How often was the difference >= 0.368?

As it happens, in this case the observed difference of 0.368% is well within the range of chance variation. See the histogram of 1000 resampled results (Figure).



Most software will compute this by approximating the proportions with a normal distribution; here is the R code for comparing two proportions (the first vector is the number of successes, the second is the number of trials):

```
prop.test(c(200,182),c(23739,22588))
```

P-value

Simply looking at the graph is not a very precise way to measure statistical significance, so of more interest is the *p-value*. This is the frequency with which the chance model produces a result more extreme than the observed result. We can estimate a p-value from our permutation test: it is the proportion of times that the permutation test produces a difference equal to or greater than 0.36. The permutation test we did above involved 10,000 repetitions, of which exceeded 0.36, so the p-value is

Alpha

Statisticians frown on the practice of leaving it to the researcher's discretion to determine whether a result is "too unusual" to happen by chance. Rather, a threshold is specified in advance, as in "more extreme than 5% of the chance (null hypothesis) results." Typical levels are 5% and 1%. Any chosen level is an arbitrary decision - there is nothing about the process that will guarantee correct decisions x% of the time. This is because the probability question being answered is *not* "what is the probability that this happpened by chance," but rather "given a chance model, what is the probability of a result this extreme." We then deduce backwards about the appropriateness of the chance model, but that judgement does not carry a probability. This point has been the subject of much confusion.

Value of the p-value

Considerable controversy has surrounded the use of the p-value in recent years. One psychology journal has gone so far as to "ban" the use of p-values in submitted papers, on the grounds that publication decisions based solely on the p-value were resulting in the publication of poor research. Too many researchers, only dimly aware of what a p-value really means, root around in the data and among different possible hypotheses to test, until a combination is found that yields a significant p-value and, hence, a paper suitable for publication.

The real problem is that people want more meaning from the p-value than it contains. Here's what we would *like* the p-value to convey:

"The probability that the result is due to chance."

We hope for a low value, so we can conclude that we've proved something. This is how many journal editors were interpreting the p-value. But here's what the p-value *actually* represents:

"The probability that, *given a chance model*, results as extreme as the observed results could occur."

The difference is subtle, but real. A significant p-value does not carry you quite as far along the road to "proof" as it seems to promise. The logical foundation for the conclusion "statistically significant" is somewhat weaker when the real meaning of the p-value is understood.

In March, 2016, the American Statistical Association, after much internal deliberation, revealed the extent of misunderstanding about the p-value when it issued a cautionary statement regarding their use.

American Statistical Association statement on using p-values

The ASA statement stressed six principles for researchers and journal editors:

1. P-values can indicate how incompatible the data are with a specified statistical model.
2. P-values do not measure the probability that the studied hypothesis is true, or the probability that the data were produced by random chance alone.
3. Scientific conclusions and business or policy decisions should not be based only on whether a p-value passes a specific threshold.
4. Proper inference requires full reporting and transparency.
5. A p-value, or statistical significance, does not measure the size of an effect or the importance of a result.
6. By itself, a p-value does not provide a good measure of evidence regarding a model or hypothesis.

Type 1 and Type 2 Error

In assessing statistical significance, two types of error are possible:

1. Type 1 error, in which you mistakenly conclude an effect is real, when it is really just due to chance
2. Type 2 error, in which you mistakenly conclude that an effect is not real (i.e. not due to chance), when it really is real.

Actually, is not so much an error as a judgement that the sample size is too small to detect the effect. When a p-value falls short of statistical signiciance (e.g. it exceeds 5%), what we are really saying is "effect not proven." It could be that a larger sample would yield a smaller p-value.

The basic function of significance tests (also called hypothesis tests) is to protect against being fooled by random chance, thus they are typically structured to minimize Type 1 error.

Data Science and P-Values

The work that data scientists do is typically not destined for publication in scientific journals, so the debate over the value of a p-value is somewhat academic. For a data scientist, a p-value is a useful metric in situations where you want to know whether a model result that appears interesting and useful is within the range of normal chance variability. As a decision tool in an experiment, a p-value should not be considered controlling, but merely another point of information bearing on a decision. For example, p-values are sometimes used as intermediate inputs in some statistical or machine learning models - a feature night be included in or excluded from a model depending on its p-value.

1. Key Ideas

1. Significance tests are used to determine whether an observed effect is within the range of chance variation for a null hypothesis model
2. The p-value is the probability that results as extreme as the observed results might occur, given a null hypothesis model
3. The alpha value is the threshold of "unusualness" in a null hypothesis chance model
4. Significance testing has been much more relevant for formal reporting of research than for data science (but has been fading recently even for the former)

Further Reading

1. "Fisher and the 5% Level" in *Chance* (2008, v. 21, issue 4) is a short commentary on Fisher's 1925 book *Statistical Methods for Research Workers*, and his emphasis on the 5% level of significance.
2. See also ??? and the reading mentioned there.

t-test

There are numerous types of significance tests, depending on whether the data are count data or measured data, how many samples there are, and what's being measured. A very common one is the *t-test*, named after Student's t-distribution, originally developed by W.S. Gossett to approximate the distribution of a single sample mean (see <t-distribution>).

1. Key Terms

1. ***Test statistic*** A metric for the difference or effect of interest
2. ***t-statistic*** A standardized version of the test statistic
3. ***t distribution*** A reference distribution (in this case derived from the null hypothesis), to which the observed t-statistic can be compared

All significance tests require that you specify a *test statistic* to measure the effect you are interested in, and help you determine whether that observed effect lies within the range of normal chance variation. In a resampling test (see the discussion of permutation in "Resampling" on page 96), the scale of the data does not matter. You create the reference (null hypothesis) distribution from the data themselves, and use the test statistic as is.

In the 1920's and 30's, when statistical hypothesis testing was being developed, it was not feasible to randomly shuffle data thousands of times to do a resampling test. Statisticians found that a good approximation to the permutation (shuffled) distribution was the t-test, based on Gossett's t-distribution. It is used for the very common two-sample comparison - A-B test - in which the data are numeric. But in order for the t-distribution to be used without regard to scale, a standardized form of the test statistic must be used.

A classic statistics text would show various formulas at this stage - formulas that incorporate Gossett's distribution and show how to standardize your data to compare it to the standard t-distribution. These formulas are not shown here because all statistical software, as well as R and Python, have commands that embody the formula. In R the command is

```
t.test(y1,y2)
```

where y1 and y2 are variables containing the numeric data from groups A and B. The result may include various output, but it will always contain a p-value.

Often data will be coded so that y1 and y2 are not listed in separate variables (columns) but are in the same column y, and there is another column x, a binary variable that indicates which group each value is in. In this case the R code is

```
t.test(y~x)
```

In a resampling mode, we structure the solution to reflect the observed data and the hypothesis to be tested, not worrying about whether the data are numeric or binary, sample sizes are balanced or not, sample variances, or a variety of other factors. In the formula world, many variations present themselves, and can be bewildering. Statisticians need to navigate that world and learn its map, but data scientists do not. They are typically not in the business of sweating the details of hypothesis tests and confidence intervals the way a researcher preparing a paper for presentation might.

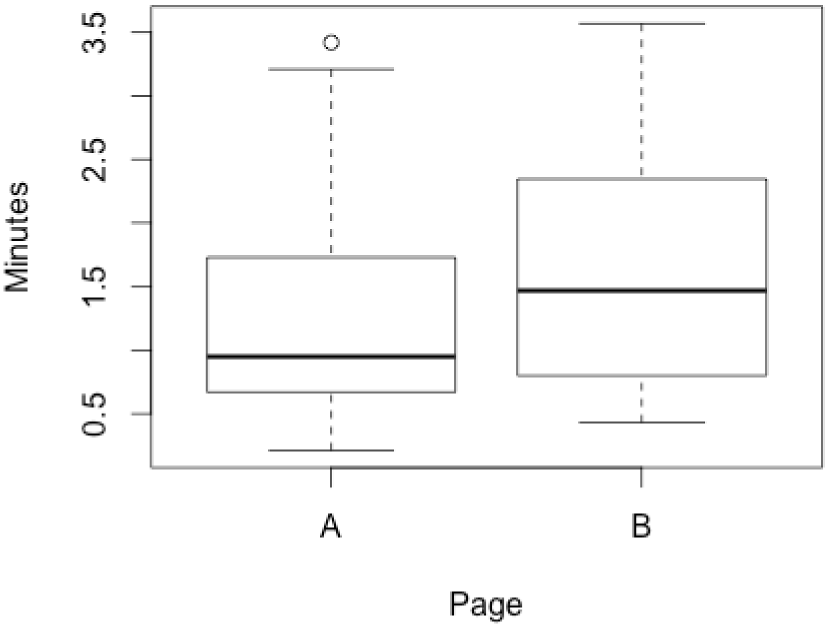
Example

A company selling a relatively high value service wants to test which of two web presentations does a better selling job. Due to the high value of the service being sold, sales are infrequent and the sales cycle is lengthy - it would take too long to accumulate enough sales to know which presentation is superior. So the company decides to measure the results with a proxy variable, using the detailed interior page that describes the service.

A *proxy* variable is one that stands in for the true variable of interest, which may be unavailable, too costly, or too time-consuming to measure. In climate research, for example, the oxygen content of ancient ice cores is used as a proxy for temperature. It is useful to have at least *some* data on the true variable of interest, so the strength of its association with the proxy can be assessed.

One potential proxy variable for our company is the number of clicks on the detailed landing page. A better one is how long people spend on the page. It is reasonable to think that a web presentation that holds people's attention longer will lead to more sales.

Our metric is average session time, comparing presentation A to presentation B. Due to the fact that this is an interior, special purpose page, it does not receive a huge number of visitors. Also note that Google Analytics, which is how we measure session time, cannot measure session time for the last session a person visits. Instead of deleting that session from the data, though, GA records it as a zero, so the data requires additional processing to remove those sessions. As a result, we have a relatively small amount of data (plus extra effort involved in collecting it), with the following result:



Page A mean session time: 1.26 minutes

Page B mean session time: 1.62 minutes

Difference in means: 0.36 minutes

It looks like page B is stickier by 0.36 minutes.

We can test whether that difference is *statistically significant* with a permutation test (see permutation test), in which we repeatedly shuffle together all the values from groups A and B and deal out samples of 21 and 15, and find the difference. In our example, figure Figure 3-2 is a frequency histogram of these results. You can see that they range from roughly -0.8 to +0.8.

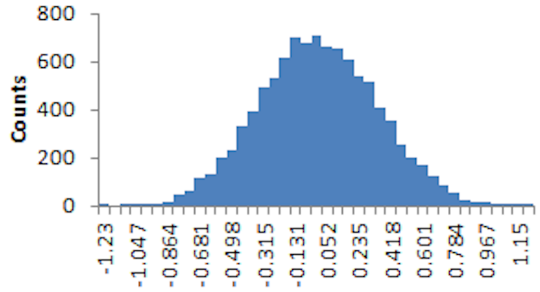


Figure 3-2. Permutation test of page stickiness

The observed result difference was 0.36, and we can see that the chance model can produce a difference that big or bigger with some regularity, and therefore the result is not statistically significant.

1. Key Ideas

1. Before the advent of computers, resampling tests were not practical and statisticians used standard reference distributions
2. A test statistic could then be standardized and compared to the reference distribution
3. One such widely-used standardized statistic is the t-statistic

Further Reading

1. Any introductory statistics text will have illustrations of the t-statistic and its uses; two good ones are *Statistics* by Freedman, et al (4th ed., 2007, W. W. Norton) and *The Basic Practice of Statistics* by David S. Moore (2010, Palgrave Macmillan).
2. For a treatment of both the t-test and resampling procedures in parallel, 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).

Multiple Testing

There is a saying in statistics, "torture the data long enough and it will confess." This means that if you look at the data through enough different perspectives, and ask enough questions, you can almost invariably find a statistically significant effect.

1. Key Terms

1. ***Type 1 error*** Mistakenly concluding that an effect is statistically significant
2. ***Adjustment of p-values*** To account for doing multiple tests on the same data
3. ***Overfitting*** Or fitting the noise

For example, if you have 20 predictor variables and one outcome variable, all *randomly* generated, the odds are pretty good that at least one predictor will (falsely) turn out to be "statistically significant." This is called *Type 1 error*. You can calculate this probability via the back door of first finding the probability that all will correctly test non-significant at the 0.05 level. This probability is found using the multiplication rule[1] as 0.95^{20} or 0.36. The probability that at least one will test significant is 1 - (probability that all will be non-significant) or 0.64.

This issue is related to the problem of overfitting in data mining, or "fitting the model to the noise." The more variables you add, or the more models you run, the greater the probability that something will emerge as "significant" just by chance.

In supervised learning tasks, a holdout set where models are assessed on data that the model has not seen before mitigates this risk. In statistical and machine learning tasks not involving a labeled holdout set, the risk of reaching conclusions based on statistical noise persists.

In statistics, there are some procedures intended to deal with this problem in very specific circumstances. For example, if you are comparing results across multiple treatment groups you might ask multiple questions. Say, for treatments A-C you might ask

1. Is A different from B?
2. Is B different from C?

[1] The multiplication rule states that the probability of *n* independent events all happening is the product of the individual probabilities. For example, if you and I each flip a coin once, the probability that your coin and my coin will both land heads is 0.5 x 0.5 = 0.25

3. Is A different from C?

Or, in a clinical trial, you might want to look at results from a therapy at multiple stages. In each case, you are asking multiple questions, and, with each question, you are increasing the chance of being fooled by chance. Adjustment procedures in statistics can compensate for this by setting the bar for statistical significance more stringently than it would be for a single hypothesis test. These adjustment procedures typically involve "dividing up the alpha" according to the number of tests. This results in a smaller alpha (i.e. a more stringent bar for statistical significance) for each test. One such procedure, the Bonferroni adjustment, simply divides the alpha by the number of observations *n*.

However, the problem of multiple comparisons goes beyond these highly structured cases and is related to the phenomenon of repeated data "dredging" that gives rise to the saying about torturing the data. Another way of putting it is to say that, given sufficiently complex data, if you haven't found something interesting, you simply haven't looked long and hard enough. More data is available now than ever before, and the number of journal articles published nearly doubled between 2002 and 2010. This gives rise to lots of opportunities to find something interesting in the data, including multiplicity issues such as

1. Checking for multiple pairwise differences across groups
2. Looking at multiple sub-group results ("we found no significant treatment effect overall, but we did find an effect for unmarried women younger than 30")
3. Trying lots of statistical models
4. Including lots of variables in models
5. Asking a number of different questions (i.e. different possible outcomes)

For a variety of reasons, including especially this general issue of "multiplicity," more research does not necessarily mean better research - the pharmaceutical company Bayer found in 2011 that when it tried to replicate 67 scientific studies, it could fully replicate only 14 of them. Nearly two-thirds could not be replicated at all.

In any case, the adjustment procedures for highly defined and structured statistical tests are too specific and inflexible to be of general use to data scientists. The bottom line for data scientists on multiplicity is:

1. For predictive modeling, the risk of getting an illusory model whose apparent efficacy is largely a product of random chance is mitigated by cross-validation, and use of a holdout sample.
2. For other procedures without a labeled holdout set to check the model, you must rely on

   a. Awareness that, the more you query and manipulate the data, the greater the role that chance might play; and
   b. Resampling and simulation hueristics to provide random chance benchmarks against which observed results can be compared.

3. Key Ideas

1. Multiplicity in a research study or data mining project (multiple comparisons, many variables, many models, etc.) increases the risk of concluding that something is significant just by chance
2. For situations involving multiple statistical comparisons (i.e. multiple tests of significance) there are statistical adjustment procedures
3. In a data mining situation, use of a holdout sample with labeled outcome variables can help avoid misleading results

Further Reading

1. For a short exposition of one procedure (Dunnett's) to adjust for multiple comparisons, see David Lane's online statistics text *http://davidmlane.com/hyperstat/B112114.html*
2. Megan Goldman offers a slightly longer treatment of the Bonferroni adjustment procedure in this paper: *http://www.stat.berkeley.edu/~mgoldman/Section0402.pdf*
3. For an in-depth treatment of more flexible statistical procedures to adjust p-values, see *Resampling-Based Multiple Testing* by Westfall and Young (Wiley, 1993)
4. For a discussion of data partitioning and the use of holdout samples in predictive modeling, see *Data Mining for Business Intelligence*, chapter 2, by Shmueli, Bruce and Patel (Wiley, 2016)

Degrees of freedom

In the documentation and settings to many statistical tests, you will see reference to the concept of "degrees of freedom." The concept is applied to statistics calculated from sample data, and refers to the number of values free to vary. For example, if you know the mean for a sample of 10 values, and you also know 9 of the values, you also know the 10th value. Only 9 are free to vary.

1. Key Terms

1. ***n* or sample size_** The number of observations (also called rows or records) in the data
2. ***d.f.*** Degrees of freedom,

The number of degrees of freedom is an input to many statistical tests. For example, degrees of freedom is the name given to the *n-1* denominator that is seen in calculations for variance and standard deviation. Why does it matter? When you use a sample to estimate the variance for a population, you will end up with an estimate that is slightly biased downward if you use *n* in the denominator. If you use *n-1* in the denominator, the estimate will be free of that bias.

A large share of a traditional statistics course or text is consumed by various standard tests of hypotheses (t-test, F-test, etc.). When sample statistics are standardized for use in traditional statistical formulas, degrees of freedom is part of the standardization calculation to ensure that your standardized data match the appropriate reference distribution (t distribution, F distribution, etc.).

Is it important for data science? Not really, at least in the context of significance testing.

For one thing, formal statistical tests are used only sparingly in data science. For another, the data size is usually large enough that it rarely makes a real difference for a data scientist whether, for example, the denominator has *n* or *n-1*.

There is one context, though, in which it does have relevance - the use of factored variables in regression (including logistic regression). Regression algorithms choke if exactly redundant predictor variables are present. This most commonly occurs when factoring categorical variables into binary indicators (dummies). Consider day-of-week. Although there are 7 days of the week, there are only 6 degrees of freedom in specifying day-of-week. For example, once you know that day-of-week is not Monday through Saturday, you know it must be Sunday. Inclusion of the Mon-Sat indicators thus means that *also* including Sunday would cause the regression to fail, due to a *multicollinearity* error.

1. Key Ideas

1. The number of degrees of freedom (d.f.) forms part of the calculation to standardize test statistics so they can be compared to reference distributions (t distribution, F distribution, etc.)
2. The concept of degrees of freedom lies behind the factoring of categorical variables into n-1 indicator or dummy variables when doing a regression (to avoid multicollinearity)

Further Reading

1. There are several web tutorials on degrees of freedom; here's one: *http://blog.minitab.com/blog/statistics-and-quality-data-analysis/what-are-degrees-of-freedom-in-statistics*

ANOVA

Suppose that, instead of an A-B test, we had a comparison of multiple groups, say A-B-C-D, each with numeric data. The statistical procedure that tests for a statistically significant difference among the groups is called *Analysis of Variance* or *ANOVA*.

1. Key Terms for ANOVA

1. ***Pairwise comparison*** A hypothesis test (e.g. of means) between two groups among multiple groups
2. ***Omnibus test*** A single hypothesis test of the overall variance among multiple group means
3. ***Decomposition of variance*** Separation of components contributing to an inidividual value (e.g. from the overall average, from a treatment mean, and from a residual error)
4. ***F statistic*** A standardized statistic that measures the extent to which differences among group means exceeds what might be expected in a chance model.
5. ***SS*** "Sum of squares," referring to deviations from some average value.

In ??? we show the stickiness of four web pages, in numbers of seconds spent on the page. The four pages are randomly switched out so that each web visitor receives one at random. There are a total of five visitors for each page, and, in ???, each column is an independent set of data. The first viewer for Page 1 has no connection to the first viewer for Page 2. Note that in a web test like this, we cannot fully implement the classic randomized sampling design in which each visitor is selected at ranomd from some huge population. We must take the visitors as they come. Visitors may systematically differ depending on time of day, time of week, season of the year, conditions of their internet, what device they are using, etc. These factors should be considered as potential bias when reviewing the experiment results.

[[4-groups]] .Stickiness (in seconds) for 4 Web Pages

	Page 1	Page 2	Page 3	Page 4
	164	178	175	155
	172	191	193	166
	177	182	171	164
	156	185	163	170
	195	177	176	168
Average	172	185	176	162
Grand average				173.75

Boxplots of the 4 groups show considerable differences among them:

[[4groups]] image::images/4-groups.png[images/4-groups.png]

Now, we have a conundrum. When we were comparing just two groups, it was a simple matter; we merely looked at the difference between the means of each group. With four means, there are six possible comparisons between groups.

- Page 1 compared to Page 2
- Page 1 compared to Page 3
- Page 1 compared to Page 4
- Page 2 compared to Page 3
- Page 2 compared to Page 4
- Page 3 compared to Page 4

The more such *pairwise* comparisons we make, the greater the potential for being fooled by random chance (see "Multiple Testing" on page 109). Instead of worrying about all the different comparisons between individual pages we could possibly make, we can do a single overall *omnibus* test that addresses the question, "Could all the pages have the same underlying stickiness, snd the differences among them be due to the random way in which a common set of session times got allocated among the four pages?"

The procedure used to test this is called *Analysis of Variance* or *ANOVA*. The basis for it can be seen in the following resampling procedure (specified here for the A-B-C-D test of web page stickiness): . Combine all the data together in a single box . Shuffle and draw out four resamples of 5 values each . Record the mean of each of the four groups . Record the variance among the four group means . Repeat steps 2-4 many times (say 1000) . What proportion of the time did the resampled variance exceed the observed variance? This is the p-value.

Most ANOVA procedures in software will scale the variance so that the statistic being tracked is really the ratio of the variance across group means (i.e. the treatment effect) to the variance due to residual error. The higher this ratio, also called the F-statistic, the more statistically significant the result.

Decomposition of Variance

Observed values in a data set can be considered sums of different components. For any observed data value within a data set, we can break it down into the grand average, the treatment effect, and the residual error. We call this a "decomposition of variance."

1. Start with grand average (173.75 for doughnut data)
2. Add treatment effect, which might be negative (independent variable = fat type)
3. Add residual error, which might be negative

For any observed data value within a data set, we can break it down into the grand average, the treatment effect, and the residual error. We call this a "decomposition" of the variance. The decomposition of the variance for the top left value in the A-B-C-D test table is as follows:

Start with grand average: 173.75

Add treatment (group) effect: -1.75 (172-173.75)

Add residual: -8 (164-172)

Equals: 164

We can see the development of the F-test in the *ANOVA table*, which we will look at for the web page stickiness data:

Table 3-2. ANOVA Table for the Web Stickiness 4-Group Example

Source of Variability	SS	df	MS	F
Grand Average	724537.5	1		
Treatment	1636.5	3	545.5	5.4117.13
Residual error	2018	20	100.9	
Total	728192	24		

SS is “sum of squares,” *df* is “degrees of freedom,” *MS* is “mean squares” (short for mean squared deviations), and *F* is the F statistic (a standardized version of the resampled statistic described above). For the grand average, SS is the departure of the grand average from 0, squared, times 20 (the number of observations). The degrees of freedom for the grand average is 1, by definition. For the treatment means, the degrees of freedom is 3 (once three values are set, and the grand average is set, the other treatment mean cannot vary). SS for the treatment means is the sum of squared departures between the treatment means and the grand average. For the residuals, degrees of freedom is 20 (all observations can vary), and SS is the sum of squared difference between the individual observations and the treatment means. Mean squares (MS) is SS/df. The F statistic is MS(treatment)/MS(error). The F value thus depends only on this ratio, and can be compared to a standard F distribution to determine whether the differences among treatment means is greater than would be expected in random chance variation.

2-way ANOVA

The A-B-C-D test described above is a “one-way” ANOVA, in which we have one factor (group) that is varying. We could have a second factor involved - say “weekend vs. weekday,” with data collected on each combination (group A weekend, group A weekday, group B weekend, etc.). This would be a “two-way ANOVA,” and would be handled in similar fashion to the one-way ANOVA by identifying the “interaction effect.” After identifying the grand average effect, and the treatment effect, we then separate the weekend and the weekday observations for each group, and find the difference between the averages for those subsets and the treatment average.

You can see that ANOVA, then two-way ANOVA, are the first steps on the road towards a full statistical model, such as regression and logistic regression, in which multiple factors and their effects can be modeled (see ???).

1. Key Ideas

1. ANOVA is a statistical proecdure for analyzing the results of an experiment with multiple groups.
2. It is the extension of similar procedures for the A-B test, used to assess whether the overall variation among groups is within the range of chance variation.
3. A useful outcome of an ANOVA is the identification of variance components associated with group treatments, interaction effects, and errors.

Further Reading

1. *Introductory Statistics: A Resampling Perspective* by Peter Bruce (Wiley 2014) has a chapter on ANOVA.
2. *Introduction to Design and Analysis of Experiments* by George Cobb (Wiley, 2008) is a comprehensive and readable treatment of its subject.

Chi-square test

The chi-square test is used with count data to test how well they fit some expected distribution.

1. Key Terms

1. ***Chi-square statistic*** A measure of the extent to which some observed data depart from expectation
2. ***Expectation* or *expected*** How we would expect the data to turn out under some assumption, typically the null hypothesis
3. ***d.f.*** Degrees of freedom

The most common use of the chi-square statistic in statistical practice is with r x c contingency tables, to assess whether the null hypothesis of independence among variables is reasonable.

"r x c" means "rows by columns" - a 2 x 3 table has two rows and three columns

For example, web testing often goes beyond A-B testing and tests multiple treatments at once. Suppose you are testing three different headlines, A, B and C, and you run them each on 1,000 visitors with the following results:

Table 3-3. Web testing results of 3 different headlines

	Headline A	Headline B	Headline C
Click	14	8	12
No-click	986	992	988

The headlines certainly appear to differ - A returns nearly twice the click rate of B. The actual numbers are small, though. A resampling procedure can test whether the click rates differ to an extent greater than chance might cause. For this test, we need to have the concept of the "expected" distribution of clicks, and, in this case, that would be under the null hypothesis assumption that all three headlines share the same click rate, for an overall click rate of 34/3000. Under this assumption, our contingency table would look like this:

Table 3-4. Expected if all 3 headlines have the same click rate (null hypothesis)

	Headline A	Headline B	Headline C
Click	11.33	11.33	11.33
No-click	988.67	988.67	988.67

We can measure the extent to which the actual counts differ from these expected counts by squaring the deviations (to render them positive), then summing.

Table 3-5. Squared deviations (observed - expected)

	Headline A	Headline B	Headline C
Click	$(14-11.33)^2$	$(8-11.33)^2$	$(12-11.33)^2$
No-click	$(986-988.67)^2$	$(992-988.67)^2$	$(988-988.67)^2$

The sum of squared deviations in this example is 37.33. Is that more than could reasonably occur in a chance model?

We can test with this resampling algorithm:

1. Constitute a box with 34 1's (clicks) and 2966 0's (no clicks).
2. Shuffle, take three separate samples of 1000, count the clicks in each.
3. Find the squared differences between the shuffled counts and the expected counts, sum them
4. Repeat steps 2 and 3, say, 1000 times.
5. How often does the resampled sum of squared deviations exceed the observed? That's the p-value.

(Show histogram, result)

The *chi-square test* is a standardized version of the resampling procedure described above. After each value's departure from expectation is squared, it is divided by its expected value. It is then summed across all values, yielding the *chi-square statistic*.

\begin{equation*} {Ξ = \sum_i\frac{(obs_i-exp_i)^2}{exp_i}} \end{equation*}

This allows it to be compared to a standard *chi-square distribution*, or, more precisely, to the appropriate member of the family of chi-square distributions. The appropriate standard chi-square distribution is determined by the *degrees of freedom* (see ???), which, in a contingency table is related to the number of rows (r) and columns (s) as follows:

d.f. = (r-1)(c-1)

They are typically shaped like the above resampling distribution, long-tailed to the right. The further out on the chi-square distribution the observed statistic is, the lower the p-value.

The R code for a chi-square test is

```
> chisq.test(tbl)
```

where *tbl* is a contingency table (matrix) of counts. R can create such a table from the raw (0/1) data, where each row is a case, the columns are variables (v1, v2), and the cell values are either 0 or 1 for each variable + case.

```
table(v1, v2)
```

Fisher's Exact Test

The chi-square distribution is a good approximation of the shuffled resampling test described above, except when counts are extremely low (single digits, especially 5 or fewer). In such cases, the resampling procedure will yield more accurate p-values. In fact, most statistical software has a procedure to actually enumerate *all* the possible rearrangements (permutations) that can occur, tabulate their frequencies, and determine exactly how extreme the observed result it. This is called *Fisher's Exact Test* after the great statistician R. A. Fisher.

R code for Fisher's exact test is simple in its basic form:

```
fisher.test(x)
```

Where *x* is either a two-dimensional contingency table in matrix form or a factor object

Where some counts are very low but others are quite high (e.g. the denominator in a conversion rate), it may be necessary to do a shuffled permutation test instead of a full exact test, due to the difficulty of calculating all possible permutations. In such cases, some software will automatically switch to the permutation test, sometimes called a Monte Carlo or approximation option. The above R function has several arguments that control whether to use this approximation (simulate.p.value=TRUE or FALSE), how many iterations should be used (B=…), and a computational constraint (workspace=…) that limits how far calculations for the *exact* result should go.

Detecting Scientific Fraud

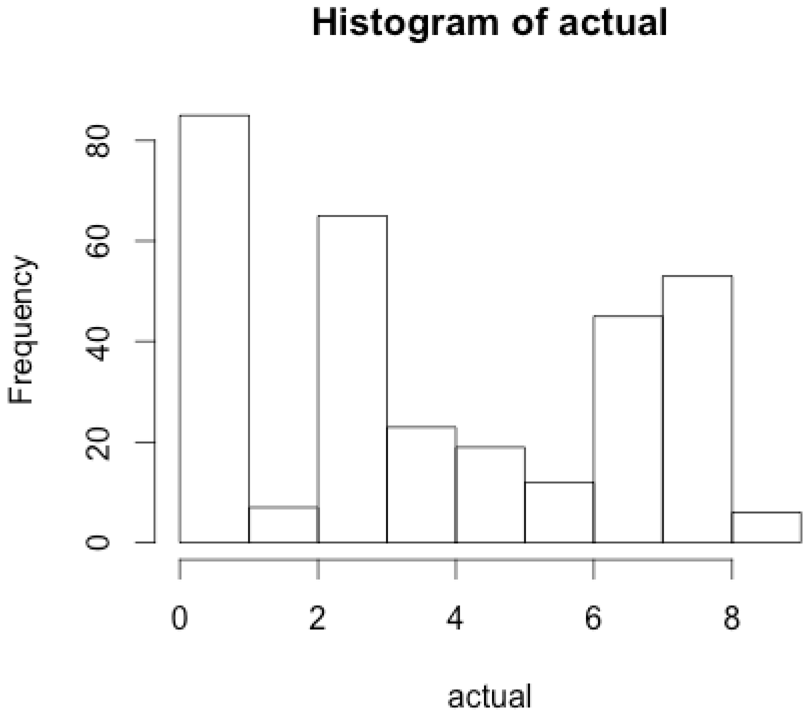
An interesting example is provided by Tufts University researcher Thereza Imanishi-Kari, who was accused in 1991 of fabricating data in her research. Congressman John Dingell became involved, and the case eventually led to the resignation of her colleague, David Baltimore, from the presidency of Rockefeller University.

Imanishi-Kari was ultimately exonerated after a lengthy proceeding. However, one element in the case rested on statistical evidence regarding the expected distribution of digits in her laboratory data, where each observation had many digits. Investigators focused on the *interior* digits, which would be expected to follow a *uniform random* distribution. That is, they would occur randomly, with each digit having equal probability of occurring (the lead digit might be predominantly one value, and the final digits might be affected by rounding). Here are some interior digits from the actual data in the case:

Table 3-6. Central digit in laboratory data

Digit	Frequency
0	14
1	71
2	7
3	65
4	23
5	19
6	12
7	45
8	53
9	6

The distribution of the 315 digits certainly looks non-random:



Investigators calculated the departure from expectation (31.5 - that's how often each digit would occur in a strictly uniform distribution) and used a chi-square test (a resampling procedure could equally have been used) to show that the actual distribution was well beyond the range of normal chance variation.

Relevance for data science

Most standard uses of the chi-square test, or Fisher's exact test, are not terribly relevant for data science. In most experiments, whether A-B or A-B-C…, the goal is not simply to establish statistical significance, but rather to arive at the best treatment. For this purpose, multi-armed bandits (see "Multi-arm bandit algorithm" on page 124) offer a more complete solution.

One data science application of the chi-square test, especially Fisher's exact version, is in determining appropriate sample sizes for web experiments. These experiments often have very low click rates and, despite thousands of exposures, count rates might be too small to yield definitive conclusions in an experiment. In such cases, Fisher's exact test, the chi square test, and other tests can be useful as a component of power and sample sie calculations (see ???).

A chi-square test could be used to assess whether algorithms A, B and C really differ, or whether the differences in the test could be just a product of random variation.

A more likely approach to this problem, though, is via a multi-arm bandit algorithm, see below.

Chi-square tests are used widely in research, by investigators in search of the elusive statistically-significant p-value that will allow publication. Chi-square tests, or similar resampling simulations, are used in data science applications, more as a filter to determine whether an effect or feature is worth of further consideration than as a formal test of significance. For example, they are used in spatial statistics and mapping to determine whether spatial data conforms to a specified null distribution (e.g. are crimes concentrated in a certain area to a greater degree than random chance would allow). They can also be used in automated feature selection in machine learning, to assess class prevalence across features and identify features where the prevalence of a certain class is unusually high or low, in a way that is not compatible with random variation.

1. Key Ideas

1. A common procedure in statistics is to test whether observed data counts are consistent with an assumption of independence (e.g. propensity to buy a particular item is independent of gender)
2. The chi-square distribution is the reference distribution to which the observed calculated chi-square statistic must be compared

Further Reading

1. R.A. Fisher famous "Lady Tasting Tea" example from the beginning of the 20th century remains a simple and effective illustration of his exact test - Google "Lady Tasting Tea" and you will find a number of good writeups.
2. A good tutorial on the Chi Square test can be found at *http://stattrek.com/chi-square-test/independence.aspx?Tutorial=AP*

Multi-arm bandit algorithm

Multi-arm bandits offer an approach to testing, especially web testing, that allows explicit optimization and more rapid decision-making than the traditional statistical approach to designing experiments.

1. Key Terms

1. ***Multi-arm bandit*** An imaginary slot machine with multiple arms for the customer to choose from, each with different payoffs, here taken to be an analogy for a multi-treatment experiment
2. ***Arm*** A treatment in an experiment, e.g. "headline A in a web test"
3. ***Win*** The experimental analog of a win at the slot machine, e.g. "customer clicks on the link"

A traditional A-B test involves data that are collected in an experiment, according to a specified design, to answer a specific question, e.g. "Which is better, treatment A or treatment B?" The presumption is that, once we get an answer to that question, the experimenting is over and we proceed to act on the results.

You can probably perceive several difficulties with that approach. First, our answer may be inconclusive: "effect not proven." In other words, the results from the experiment may suggest an effect, but, if there is an effect, we don't have a big enough sample to prove it (to the satisfaction of the traditional statistical standards). What decision do we take? Second, we might want to begin taking advantage of results that come in prior to the conclusion of the experiment. Third, we might want the right to change our minds, or try something different, based on additional data that comes in after the experiment is over. The traditional approach to experiments and hypothesis tests dates from the 1920's, and is rather inflexible. The advent of computer power and software has made possible more powerful flexible approaches. Moreover, data science, and business in general, is not so worried about statistical significance, but more concerned with optimizing overall effort and results.

Bandit algorithms, which are very popular in web testing, allow you to test multiple treatments at once and reach conclusions faster than traditional statistical designs. They take their name from slot machines used in gambling, also termed one-armed bandits (since they are configured in such a way that they extract money from the gambler in a steady flow). If you imagine a slot machine with more than one arm, and each arm paid out at a different rate, you would have a multi-armed bandit, and that is the full name for this algorithm.

Your goal is to win as much money as possible, and, more specifically, to identify and settle on the winning arm sooner rather than later. The challenge is that you don't know at what rate the arms pay out – you only know the results of pulling the arm. Suppose each "win" is for the same amount, no matter which arm. What differs is the probability of a win. Suppose further that you initially try each arm 100 times and get the following results:

Arm A: 10 wins out of 50 Arm B: 2 win out of 50 Arm C: 4 wins out of 50

One extreme approach is to say "Looks like arm A is a winner – let's quit trying the other arms and stick with A. This takes full advantage of the information from the initial trial. If A is truly superior, we get the benefit of that early on. On the other hand, if B or C are truly better, we lose any opportunity to discover that. Another extreme approach is to say "This all looks to be within the realm of chance – let's keep pulling them all equally. This gives maximum opportunity for alternates to A to show themselves. However, in the process, we are deploying what seem to be inferior treatments. How long do we permit that? Bandit algorithms take a hybrid approach: We start pulling A more often, to take advantage of its apparent superiority, but we don't abandon B and C. We just pull them less often. If A continues to outperform, we continue to shift resources (pulls) away from B and C and pull A more often. If, on the other hand, C starts to do better, and A starts to do worse, we can shift pulls from A back to C. If one of them turns out to be superior to A and this was hidden in the initial trial due to chance, it now has a chance to emerge with further testing.

Now think of applying this to web testing. Instead of multiple slot machine arms, you might have multiple offers, headlines, colors, etc. being tested on a web site. Customers either click (a "win" for the merchant) or don't click. Initially, the offers are shown randomly and equally. If, however, one offer starts to outperform the others, it can be shown ("pulled") more often. But what should be the parameters of the algorithm that modifies the pull rates? What "pull rates" should we change to, and when should we change?

Here is one simple algorithm, the epsilon-greedy algorithm for an A-B test:

1. Generate a random number between 0 and 1.
2. If the number lies between 0 and epsilon (where epsilon is a number between 0 and 1, typically fairly small), flip a fair coin (50/50 probability), and
    a. If the coin is heads, show offer A
    b. If the coin is tails, show offer B
3. If the number is >= epsilon, show whichever offer has had the highest response rate to date.

Epsilon is the single parameter that governs this algorithm. If epsilon is 1, we end up with a standard simple A-B experiment (random allocation between A and B for each subject). If epsilon is 0, we end up with a purely *greedy* algorithm - it seeks no further experimentation, simply assigning subjects (web visitors) to the best performing treatment.

A more sophisticated algorithm uses "Thompson's sampling." This procedure "samples" (pulls a bandit arm) at each stage to maximize the probability of choosing the best arm. Of course you don't know which is the best arm (that's the whole problem!), but, as you observe the payoff with each successive draw, you gain more information about which is the best. Thompson's sampling uses a Bayesian approach - some prior distribution of rewards is assumed initially, using what is called a Beta distribution (this is a common mechanism for specifying prior information in a Bayesian problem). As information accumulates from each draw, this information can be updated, allowing the selection of the next draw to be better optimized as far as choosing the right arm.

Bandit algorithms can efficiently handle 3+ treatments and move towards optimal selection of the "best." For traditional statistical testing procedures, the complexity of decision- making for 3+ treatments far outstrips that for the traditional A-B test, and the advantage of bandit algorithms is much greater.

1. Key Ideas

1. Traditional A-B tests envision a random sampling process, which can lead to excessive exposure to the inferior treatment
2. Multi-arm bandits, in contrast, alter the sampling process to incorporate information learned during the experiment, and reduce the frequency of the inferior treatment
3. They also facilitate efficient treatment of more than two treatments
4. There are different algorithms for shifting sampling probability away from the inferior treatment(s) and to the (presumed) superior one

Further Reading

1. An excellent short treatment of multi-arm bandit algorithms is found in *Bandit Algorithms*, by John Myles White, O'Reilly, 2012. White includes Python code, as well as the results of simulations to assess the performance of bandits.
2. For more (somewhat technical) information about Thompson Sampling, see "Analysis of Thompson Sampling for the Multi-armed Bandit Problem" by

Agrawal and Goyal, *http://jmlr.org/proceedings/papers/v23/agrawal12/agrawal12.pdf*

Power and sample size

If you run a web test, how do you decide how long it should run (i.e. how many impressions per treatment are needed)? Despite what you may read in many guides to web testing on the web, there is no good general guidance - it depends, mainly, on the frequency with which the desired goal is attained.

1. Key Terms

1. ***Effect size*** The minimum size of the effect that you hope to be able to detect in a statistical test, e.g. "a 20% improvement in click rates"
2. ***Power*** The probability of detecting a given effect size with a given sample size
3. ***Significance level*** The significance level at which the test will be conducted

One step in statistical calculations for sample size is to ask whether a hypothesis test will actually reveal a difference between treatments A and B? The outcome of a hypothesis test - the p-value - depends on what the real difference is between treatment A and treatment B. It also depends on the luck of the draw, in who gets selected for the groups in the experiment. But it makes sense that, the bigger the actual difference between treatments A and B, the greater the probability that our experiment will reveal it. And, the smaller the difference, the more data will be needed to detect it. To distinguish between a .350 hitter in baseball, and a .200 hitter, not that many at-bats are needed. To distinguish between a .300 hitter and a .280 hitter, a good many more at-bats will be needed.

Power is the probability of detecting a specified *effect size* with specified sample characteristics (size and variability). For example, we might say (hypothetically) that the probability of distinguishing between a .330 hitter and a .200 hitter in 25 at bats is 0.75. The effect size here is a difference of .130. And "detecting" means that a hypothesis test will reject the null hypothesis of "no difference" and conclude there is a real effect. So the experiment of 25 at-bats (N=25) for two hitters, with an effect size of . 130, has (hypothetical) power of 0.75 or 75%.

You can see that there are several moving parts here, and it is easy to get tangled up with the numerous statistical assumptions and formulas that will be needed (to specify sample variability, effect size, sample size, alpha-level for the hypothesis test, etc., and to calculate power). Indeed, there is special purpose statistical software to calculate power. Most data scientists will not need to go through all the formal steps needed to report power, e.g. in a published paper. However, they may face occasions where they want to collect some data for an A-B test, and collecting or processing the data involves some cost. In that case, knowing approximately how much data to collect can help avoid the situation where you collect data at some effort, and the result ends up being inconclusive. Here's a fairly intuitive alternative approach:

1. Start with some hypothetical data that represent your best guess about the data that will result (perhaps based on prior data). For example, a box with 20 ones and 80 zeros to represent a .200 hitter. Or a box with some observations of "time spent on web site."
2. Create a second sample simply by adding the desired effect size to the first sample. For example, a second box with 33 ones and 67 zeros. Or a second box with 25 seconds added to each initial "time spent on web site."
3. Draw a bootstrap sample of size N from each box.
4. Conduct a permutation (or formula-based) hypothesis test on the two bootstrap samples and record whether the difference between them is statistically significant.
5. Repeat the above two steps many times and determine how often the difference was significant - that's the estimated power.

Sample Size

The most common use of power calculations is to estimate how big a sample you will need.

For example, suppose you are looking at click-through rates (clicks as a percentage of exposures), and testing a new ad against an existing ad. How many clicks do you need to accumulate in the study? If you are only interested in results that show a huge difference (say a 50% difference), a relatively small sample might do the trick. If, on the other hand, even a minor difference would be of interest, then a much larger sample is needed. A standard approach is to establish a policy that a new ad must do better than an existing ad by some percentage, say 10%, otherwise the existing ad will remain in place. This goal, the "effect size," then drives the sample size.

For example, suppose current click-through rates are about 1.1%, and you are seeking a 10% boost to 1.21%. So we have two boxes, Box A with 1.1% ones (say 110 ones and 9890 zeros), and a Box B with 1.21% ones (say 121 ones and 9879 zeros). For starters, let's try 300 draws from each box (this would be like 300 "impressions" for each ad). Suppose our first draw yields the following: Box A: 3 ones Box B: 5 ones

Right away we can see that any hypothesis test would reveal this difference (5 vrs. 3) to be well within the range of chance variation. This combination of sample size (N=300 in each group) and effect size (10% difference) is too small for any hypothesis test to reliably show a difference.

So we can try increasing the sample size (let's try 2000 impressions), and require a larger improvement (30% instead of 10%).

For example, suppose current click-through rates are still 1.1%, but we are now seeking a 50% boost to 1.65%. So we have two boxes, Box A still with 1.1% ones (say 110 ones and 9890 zeros), and a Box B with 1.65% ones (say 165 ones and 9868 zeros). Now we'll try 2000 draws from each box. Suppose our first draw yields the following: Box A: 19 ones Box B: 34 ones

A significance test on this difference (34-19) still shows it registers as "not significant" (though much closer to significance than the earlier difference of 5-3). To calculate power, we would need to repeat the above procedure many times, or use statistical software that can calculate power, but our initial draw suggest to us that even detecting a 50% improvement will require several thousand ad impressions.

In summary: For calculating power or required sample size, you can see that there are four moving parts:

1. Sample size
2. Effect size you want to detect
3. Significance level (alpha) at which the test will be conducted
4. Power

Specify any three of them, and the fourth can be calculated. Most commonly, you would want to calculate sample size, so you must specify the other three. Here is R code for a test involving two proportions, where both samples are the same size (this uses the pwr package):

```
pwr.2p.test(h = ..., n = ..., sig.level = ..., power = )

h= effect size (as a proportion)
n = sample size
sig.level = the significance level (alpha) at which the test will be conducted
power = power (probability of detecting the effect size)
```

1. Key Ideas

1. Finding out how big a sample size you need requires thinking ahead to the statistical test you plan to conduct

2. You must specify the minimum size of the effect that you want to detect
3. You must also specify the required probability of detecting that effect size (power)
4. Finally, you must specify the significance level (alpha) at which the test will be conducted

For Further Reading

1. *Sample Size Determination and Power* by Tom Ryan (2013, Wiley) is a comprehensive and readable review of this subject.
2. Steve Simon, a statistical consultant, has written a very engaging narrative-style post on the subject: *http://www.pmean.com/09/AppropriateSampleSize.html*

Summary

The principles of experimental design - randomization of subjects into two or more groups receiving different treatments - allow us to draw valid conclusions about how well the treatments work. It is best to include a control treatment of "making no change." The subject of formal statistical inference - hypothesis testing, p-values, t-tests, and much more along these lines - occupies much time and space in a traditional statistics course or text, and the formality is mostly unneeded from a data science perspective. However, it remains important to recognize the role that random variation can play in fooling the human brain. Intuitive resampling procedures (permutation and bootstrap) allow data scientists to gauge the extent to which chance variation can play a role in their data analysis.

CHAPTER 4

Regression and Prediction

Perhaps the most common goal in statistics is to answer the question: Is the variable X (or more likely, $X_1, ..., X_p$ associated with a variable Y, and, if so, what is the relationship and can we use it to predict Y?

Nowhere is the nexus between statistics and data science stronger than in the realm of prediction - specifically the prediction of an outcome (target) variable based on the values of other "predictor" variables. Another important connection is in the area of *anomaly detection*, where regression diagnostics originally intended for data analysis and improving the regression model can be used to detect unusual records. The antecedents of correlation and linear regression date back over a century.

Simple Linear Regression

Simple linear regression models the relationship between the magnitude of one variable and that of a second — e.g. as X increases, Y also increases. Or as X increases, Y decreases. Correlation is another way measure how two variables are related: see section "Correlation" on page 36. The difference is that, while correlation measures the strength of an association between two variables, regression quantifies the nature of the relationship.

Key Terms for Simple Linear Regression

Response
The variable we are trying to predict.

Synonyms
dependent variable, Y-variable, target, outcome

Independent Variable

The variable used to predict the response.

Synonyms

independent variable, X-variable, feature, attribute

Intercept

The intercept of the regression line; i.e., the predicted value when $X = 0$.

Synonyms

b_0, β_0

Regression Coefficient

The slope of the regression line.

Synonyms

slope, b_1, β_1

Fitted Values

The estimates [$\hat{Y}_i$] obtained from the regression line.

Synonyms

predicted values

Residuals

The difference between the observed values and the fitted values.

Synonyms

errors

Least Squares

The method of fitting a regression by minimizing the sum of squared residuals.

Synonyms

ordinary least squares

The Regression Equation

Simple linear regression estimates exactly how much Y will change when X changes by a certain amount. With the correlation coefficient, the variables X and Y are interchangable. With regression, we are trying to predict the Y variable from the X using a linear relationship (i.e., a line):

$$Y = b_0 + b_1 X$$

We read this as "`Y equals b_1 times X, plus a constant b_0.`" The symbol b_0 is known as the *intercept* and the symbol b_1 is known as the coefficient for X. The Y

variable is known as the *response* or *dependent* variable since it depends on *X*. The *X* variable is known as the *predictor* or *independent* variable The machine learning community tends to use different terminology, calling *Y* as the *target* and *X* as a *feature* vector.

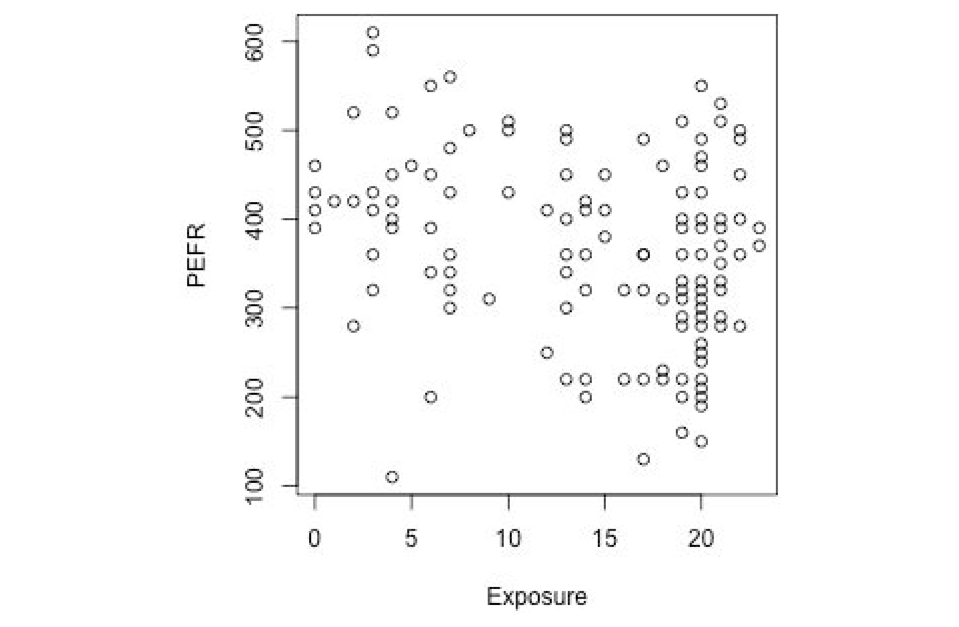


Figure 4-1. Cotton exposure vs. lung capacity

Consider the scatterplot in Figure Figure 4-1 displaying the number of years a worker was exposed to cotton dust (`Exposure`) versus a measure of lung capacity (`PEFR` or "`peak expiratory flow rate`“). How is `PEFR` related to `Exposure`? It’s hard to tell, just based on the picture.

Simple linear regression tries to fine the "`best`" line to predict the response `PEFR` as a function of the predictor variable `Exposure`.

$$\text{PEFR} = b_0 + b_1\text{Exposure}$$

The `lm` function in R can be used to fit a linear regression.

```
model <- lm(PEFR ~ Exposure, data=lung)
```

`lm` standards for *linear model* and the ~ symbol denotes that `PEFR` is predicted by `Exposure`.

Printing the `model` object produces the following output:

```
Call:
lm(formula = PEFR ~ Exposure, data = lung)

Coefficients:
(Intercept)     Exposure
    424.583       -4.185
```

The intercept, or b_0, is 424.583 and can be interpreted as the predicted PEFR for a worker with zero years exposure. The regression coefficient, or b_1, can be interpreted as follows: for each additional year that a worker is exposed to cotton dust, their PEFR measurement is reduced by -4.185.

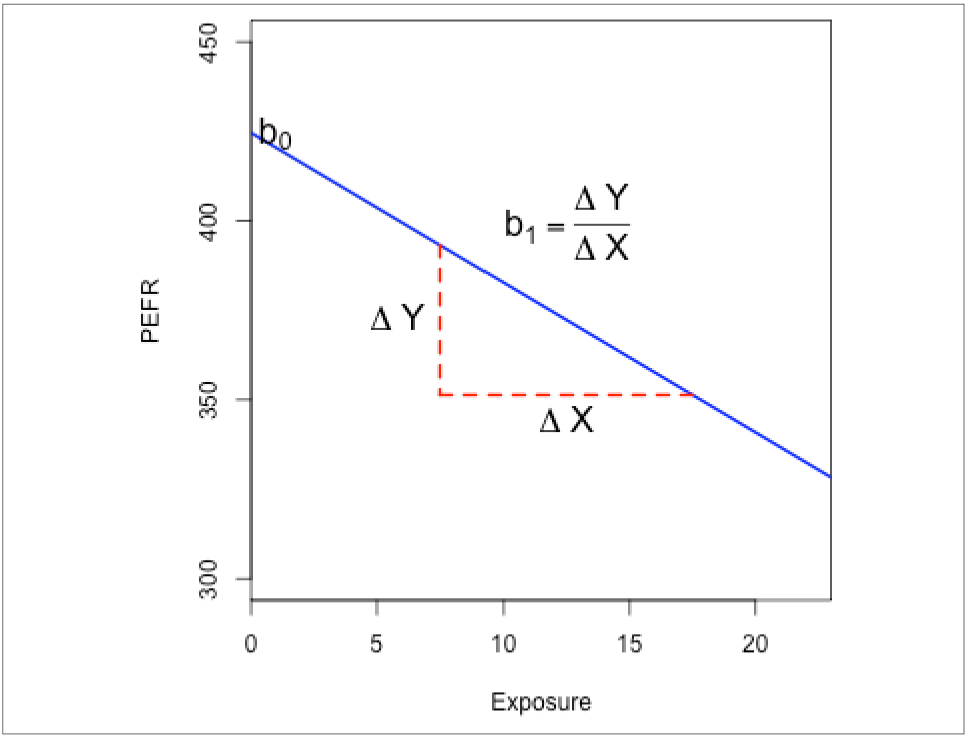


Figure 4-2. Slope and intercept for the regression fit to the lung data.

The regression line from this model is displayed in Figure 4-2.

Fitted Values and Residuals

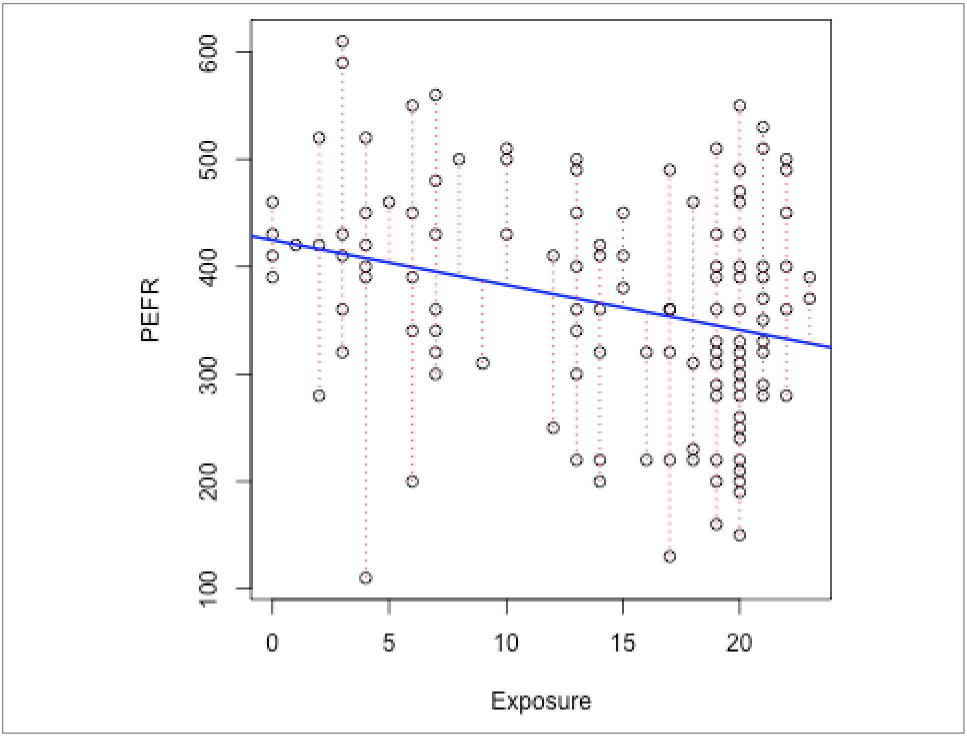


Figure 4-3. Residuals from a regression line (note the different y-axis scale from Figure 4-2, hence the apparently different slope)

Important concepts in regression analysis are the *fitted* values and *residuals*. In general, the data don't fall exactly on a line, so the regression equation should include an explicit error term e_i:

$$Y_i = b_0 + b_1 X_i + e_i$$

The *fitted* values, also referred to as the *predicted* values, are typically denoted by $\hat{Y}_i$ (Y-hat). These are given by

$$\hat{Y}_i = \hat{b}_0 + \hat{b}_1 X_i$$

The notation $\hat{b}_0$ and $\hat{b}_1$ indicates the coefficients are estimated versus known: see Hat Notation: Estimates Versus Known Values The residuals $\hat{e}_i$ are computed by subtracting the *predicted* values from the original data.

$$\hat{e}_i = Y_i - \hat{Y}_i$$

In R, the fitted values and residuals can be obtained using the functions predict and residuals

```
fitted <- predict(model)
resid <- residuals(model)
```

Figure 4-3 illustrates the residuals from the regression line fit to the lung data. The residuals are the length of the vertical dashed lines from the data to the line.

Least Squares

How is the model fit to the data? When there is a clear relationship, you could imagine fitting the line by hand. In practice, the regression line is the estimate that minimizes the sum of squared residual values, also called the *residual sum of squares* or *RSS*:

$$\begin{aligned} RSS &= \sum_{i=1}^{n} \left(Y_i - \hat{Y}_i\right)^2 \\ &= \sum_{i=1}^{n} \left(Y_i - \hat{b}_0 - \hat{b}_1 X_i\right)^2 \end{aligned}$$

The estimates $\hat{b}_0$ and $\hat{b}_1$ are the values that minimize RSS.

The method of minimizing the sum of the squared residuals is termed *least squares* regression, or *ordinary least squares* (OLS) regression. It is attributed by Gauss ??? but first published by Legendre ??? in 1805. Least squares regression leads to a simple formula to compute the coefficients:

$$\begin{aligned} \hat{b}_1 &= \frac{\sum_{i=1}^{n} \left(Y_i - \bar{Y}\right)\left(X_i - \bar{X}\right)}{\sum_{i=1}^{n} \left(X_i - \bar{X}\right)^2} \\ \hat{b}_0 &= \bar{Y} - \hat{b}_1 \bar{X} \end{aligned}$$

Historically, computational convenience is one reason for the widespread use of least squares in regression. With the advent of big data, computational speed is still an important factor. Least squares, like the mean (see "Median and Robust Estimates" on page 19), is sensitive to outliers, although this tends to be a signicant problem only in small or moderate sized problems. See "Outliers" on page 158 for a discussion of outliers in regression.

Example 4-1. Regression terminology

When analysts and researchers use the term "`regression`" by itself they are typically referring to linear regression, and the focus is usually on developing a linear model to explain the relationship between predictor variables and a numeric outcome variable. In its formal statistical sense, regression also includes nonlinear models that yield a functional relationship between predictors and outcome variables. In the machine learning community, the term is also occasionally used loosely to refer to the use of any predictive model that produces a predicted numeric outcome (standing in distinction from classification methods that predict a binary or categorical outcome).

Hat Notation: Estimates Versus Known Values

The ““hat”” notation is used to differentiate between estimates and known values. So the symbol $\hat{b}$ (“b-hat”) is an estimate of the unknown parameter b. Why do statisticians differentiate between the estimate and the true value? The estimate has uncertainty whereas the true value is a fixed value.[1]

Prediction Versus Explanation (Profiling)

Historically, a primary use of regression was to illuminate a supposed linear relationship between predictor variables and an outcome variable. The goal has been to understand a relationship and explain it, using the data that the regression was fit to. In this case, the primary focus is on the estimated slope of the regression equation, $\hat{b}$. Economists want to know the relationship between consumer spending and GDP growth. Public health officials might want to measure the decline in tobacco use over time, where time is a predictor variable.

With the advent of big data, regression is widely used to form a model to predict outcomes for new data, rather than explain data in hand - i.e. a predictive model. In this instance, the main items of interest are the fitted values $\hat{Y}$. In marketing, regression can be use to predict the change in revenue in response to the size of an ad campaign. Universities use regression to predict a student’s GPA based on their SAT scores.

A regression model that fits the data well is set up in the form that changes in X lead to changes in Y. However, by itself, the regression equation itself does not prove the direction of causation. Conclusions about causation must come from a broader context of understanding about the relationship. For example, a regression equation might show a definite relationship between number of clicks on a web ad, and num-

[1] In Bayesian statistics, the true value is assumed to be a random variable with a specified distribution. In the Bayesian context, instead of estimates of unknown parameters, there are posterior and prior distributions.

ber of conversions. It is our knowledge of the marketing process, not the regression equation, that leads us to the conclusion that clicks on the ad lead to sales, and not vice versa.

Key ideas

1. The regression equation models the relationship between a response variable Y and a predictor variable X as a line.
2. A regression model yields fitted values and residuals --- predictions of the response and the errors of the predictions.
3. Regression models are typically fit by the method of least squares.
4. Regression is used both for prediction and explanation.

Further Reading

1. For an in-depth treatment of profiling vs. explanation, see Galit Shmueli's article *To Explain or to Predict* *https://projecteuclid.org/euclid.ss/1294167961*

Multiple Linear Regression

When there are multiple predictors, the equation is simply extended to accommodate them:

$$Y = b_0 + b_1 X_1 + b_2 X_2 + ... + b_p X_p + e$$

Instead of a line, we now have a linear model - the relationship between each coefficient and its variable (feature) is linear.

Key Terms for Multiple Linear Regression

Root Mean Square Error
The square root of the average squared error of the regression and the most widely used metric to compare models.

Synonyms
RMSE

Residual Standard Error
The same as the root mean squared error, but adjusted for degrees of freedom.

Synonyms
RSE

R-Squared
The proportion of variance explained by the model, from 0 to 1.

Synonyms
coefficient of determination, R^2.

t-statistic
the coefficient divided by the standard error of the coefficient, giving a metric to compare the importance of variables in the model.

Weighted Regression
Regression with the records having different weights.

All of other concepts in simple linear regression, such as fitting by least squares and the definition of fitted values and residuals, extend to the multiple linear regression setting. For example, the fitted values are given by

$$\hat{Y}_i = \hat{b}_0 + \hat{b}_1 X_{1,i} + \hat{b}_2 X_{2,i} + \ldots + \hat{b}_p X_{p,i}$$

Example: King County Housing Data

An example of using regression is in estimating value of houses. County assessors must estimate the value of a house for the purposes of assessing taxes. Real estate consumers and professionals consult popular websites such as zillow.com to ascertain a fair price. Here are a few rows of data from King County (Seattle) Washington housing data, from the `house data.frame`:

```
head(house[, c("AdjSalePrice", "SqFtTotLiving", "SqFtLot", "Bathrooms",
               "Bedrooms", "BldgGrade")])
Source: local data frame [6 x 6]

  AdjSalePrice SqFtTotLiving SqFtLot Bathrooms Bedrooms BldgGrade
         (dbl)         (int)   (int)     (dbl)    (int)     (int)
1       300805          2400    9373      3.00        6         7
2      1076162          3764   20156      3.75        4        10
3       761805          2060   26036      1.75        4         8
4       442065          3200    8618      3.75        5         7
5       297065          1720    8620      1.75        4         7
6       411781           930    1012      1.50        2         8
```

The goal is to predict the sales price from the other variables. The `lm` handles the multiple regression case simply by including more terms on the right-hand side of the equation:

```
house_lm <- lm(AdjSalePrice ~ SqFtTotLiving + SqFtLot + Bathrooms +
                 Bedrooms + BldgGrade,
               data=house, na.action=na.omit)
```

Printing `house_lm` object produces the following output:

```
house_lm

Call:
lm(formula = AdjSalePrice ~ SqFtTotLiving + SqFtLot + Bathrooms +
    Bedrooms + BldgGrade, data = house, na.action = na.omit)

Coefficients:
  (Intercept)  SqFtTotLiving        SqFtLot      Bathrooms
   -5.219e+05      2.288e+02     -6.051e-02     -1.944e+04
     Bedrooms      BldgGrade
   -4.778e+04      1.061e+05
```

The interpretation of the coefficients is as with simple linear regression: the predicted value $\hat{Y}$ changes by the coefficient b_j for each unit change in X_j assuming all the other variables, X_k for $k \neq j$, remain the same. For example, adding an extra finished square foot to a house increases the estimated value by roughly $229; adding 1,000 finished square feet implies the value will increase by $228,800.

Assessing the Model

The most important performance metric from a data science perspective is *root mean squared error* or *RMSE*. RMSE is the square root of the average squared error in the predicted $\hat{Y}_i$ values:

$$\hat{Y}_i = \sqrt{\frac{\Sigma_{i=1}^{N}\left(Y_i - \hat{Y}_i\right)^2}{N}}$$

This measures the overall accuracy of the model, and is a basis for comparing it to other models (including models fit using machine learning techniques). Similar to RMSE is the *residual standard error* or *RSE*. In this case we have P predictors, the RSE is given by

$$RSE = \sqrt{\frac{\Sigma_{i=1}^{N}\left(Y_i - \hat{Y}_i\right)^2}{(N - P - 1)}}$$

The only difference is that the denominator is the degrees of freedom, as opposed to number of records (see ???). In practice, for linear regression, the difference between RMSE and RSE is very small, particularly for big data applications.

The summary function in R computes RSE as well as other metrics for a regression model:

```
summary(house_lm)

Call:
lm(formula = AdjSalePrice ~ SqFtTotLiving + SqFtLot + Bathrooms +
    Bedrooms + BldgGrade, data = house, na.action = na.omit)

Residuals:
     Min       1Q   Median       3Q      Max
-1199508  -118879   -20982    87414  9472982

Coefficients:
                Estimate Std. Error t value Pr(>|t|)
(Intercept)   -5.219e+05  1.565e+04 -33.349  < 2e-16 ***
SqFtTotLiving  2.288e+02  3.898e+00  58.699  < 2e-16 ***
SqFtLot       -6.051e-02  6.118e-02  -0.989    0.323
Bathrooms     -1.944e+04  3.625e+03  -5.362 8.32e-08 ***
Bedrooms      -4.778e+04  2.489e+03 -19.194  < 2e-16 ***
BldgGrade      1.061e+05  2.396e+03  44.287  < 2e-16 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 261200 on 22683 degrees of freedom
Multiple R-squared:  0.5407,    Adjusted R-squared:  0.5406
F-statistic:  5340 on 5 and 22683 DF,  p-value: < 2.2e-16
```

Another useful metric that you will see in software output is the *coefficient of determination*, also called the *R-squared* statistic or R^2. R-squared ranges from 0 to 1 and measures the proportion of variation in the data that is accounted for in the model. It is useful mainly in explanatory uses of regression where you want to assess how well the model fits the data. The formula for R^2 is

$$R^2 = 1 - \frac{\sum_{i=1}^{N} \left(Y_i - \hat{Y}_i\right)^2}{\sum_{i=1}^{N} \left(Y_i - \bar{Y}\right)^2}$$

The denominator is proportional to the variance of Y. The output from R also reports an *adjusted R-squared* which adjust for the degrees of freedom; seldom is this significantly different in multiple regression.

Along with the estimated coefficients, R reports the standard error of the coefficients (SE) and a *t-statistic*:

$$t_b = \frac{\hat{b}}{\mathrm{SE}\left(\hat{b}\right)}$$

The t-statistic, and its mirror image the p-value, measure the extent to which a coefficient is “statistically significant” - i.e. outside the range of what a random chance arrangement of predictor and target variable might produce. The higher the t-statistic (and the lower the p-value) the more significant the predictor. Since parsimony is a valuable model feature, it is useful to have a tool like this to guide choice of variables to include as predictors (see “Model Selection and Stepwise Regression” on page 142).

In addition to the t-statistic, `R` and other packages will often report a *p-value* (`Pr(>|t|)` in the `R` output) an *F-statistic*. Data scientists do not generally get too involved with the interpretation of these statistics, nor with the issue of statistical significance. Data scientists primarily focus on the t-statistic as a useful guide for whether to include a predictor in a model or not. High t-statistics (which go with p-values near 0) indicate a predictor should be retained in a model, very low t-statistics indicate a predictor could be dropped. See “P-value” on page 101 for more discussion.

Model Selection and Stepwise Regression

In some problems, many variables could be used as predictors in a regression. For example, to predict house value, additional variables such as the basement size or year built could be used. In `R`, these are easy to add to the regression equation:

```
house_full <- lm(AdjSalePrice ~ SqFtTotLiving + SqFtLot + Bathrooms +
                 Bedrooms + BldgGrade + PropertyType + NbrLivingUnits +
                 SqFtFinBasement + YrBuilt + YrRenovated +
                 NewConstruction,
               data=house, na.action=na.omit)
```

Adding more variables, however, does not necessarily mean we have a better model. Statisticians use the principle of *Occam’s razor* to guide the choice of a model: all things being equal, a simpler model should be used in preference to a more complicated model.

Including additional variables always improves reduces RMSE and increases R^2. Hence, these are not appropriate to help guide the model choice. In the 1970’s, Hirotugu Akaike, the preeminent Japanese statistician, deveoped a metric called *AIC* (Akaike’s Information Criteria) that penalizes adding terms to a model. In the case of regression, AIC has the form

$$\mathtt{AC} \quad = 2P + N \log \left(\mathrm{RS} \ \ / N\right)$$

where P is the number of variables and N is the number of records. The goal is to find the model that minimizes AIC; models with k more extra variables are penalized by 2k.

How do we find the model that minimizes AIC? One approach to search through all possible models, called *all subsets regression*. This is computationally expensive and is not feasible for problems with large data and many variables. An attractive alternative is to use *stepwise regression*, which successively adds and drops predictors to find a model that lowers AIC. The MASS package by Venebles and Ripley ??? offers a stepwise regression function stepAIC.

```
library(MASS)
step <- stepAIC(house_full, direction="both")
step

Call:
lm(formula = AdjSalePrice ~ SqFtTotLiving + Bathrooms + Bedrooms +
    BldgGrade + PropertyType + SqFtFinBasement + YrBuilt, data = house0,
    na.action = na.omit)

Coefficients:
              (Intercept)              SqFtTotLiving
               6227632.22                     186.50
                Bathrooms                   Bedrooms
                 44721.72                  -49807.18
                BldgGrade  PropertyTypeSingle Family
                139179.23                   23328.69
    PropertyTypeTownhouse            SqFtFinBasement
                 92216.25                       9.04
                  YrBuilt
                 -3592.47
```

The function chose a model in which several variables were dropped from house_full: SqFtLot, NbrLivingUnits, YrRenovated and NewConstruction

Penalized regression is similar in spirit to AIC. Instead of explicitly searching through a set of discrete set of models, a constraint is incorporated into the model fitting fitting equation that penalizes the model for too many variables (parameters). Common penalized regression methods are *ridge regression* and *lasso regression*. See ??? for details.

In-Sample Versus Cross Validation

Stepwise regression and all subset regression are *in-sample* methods to assess and tune models. This means the model selection is possibly subject to over-fitting and may not perform as well when applied to new data. One common approach to avoid this is to use *cross-validation* to validate the models. Cross-validation involves successively holding out part of the data when fitting the model and evaluating the model on the holdout set. In linear regression, over-fitting is typically not a major issue, due to the simple (linear) global structure imposed on the data. For more sophisticated types of models, particularly iterative procedures that respond to local data structure, cross validation is a very important tool: see ??? for details.

AIC, BIC and Mallows Cp

The formula for AIC may seem a bit mysterious, but in fact is based on asymptotic results in information theory. There are several variants to AIC:

1. AICc: a version of AIC corrected for small sample sizes.
2. BIC or Bayesian information criteria: similar to AIC with a stronger penalty for including additional variables to the model.
3. Mallows Cp: A variant of AIC developed by Colin Mallows ???.

Data scientists generally do not need to worry about these different metrics and the underlying theory behind them.

Weighted Regression

Weighted regression is used by statisticians for a variety of purposes; in paricular, it is important for analysis of complex surveys. Data scientists may find weighted regression useful in two cases:

1. Inverse-variance weighting when different observations have been measured with different precision.
2. Analysis of data in an aggregated form such that the weight variable encodes how many original observations each row in the aggregated data represents.

For example, with the housing data, older sales are less reliable than more recent sales. Using the `DocumentDate` to determine the year of the sale, a `Weight` can be computed as the number of years since 2005 (the beginning of the data).

```
house <-  house %>%
  mutate(Year = year(DocumentDate),
         Weight = (Year - 2005))
```

A weighted regression can be computed with the `lm` function using the `weight` argument.

```
house_wt <- lm(AdjSalePrice ~ SqFtTotLiving + SqFtLot + Bathrooms +
                 Bedrooms + BldgGrade,
               data=house, weight=Weight)
round(cbind(house_lm=house_lm$coefficients,
            house_wt=house_wt$coefficients), digits=3)

                 house_lm    house_wt
(Intercept)   -521924.722 -584265.244
SqFtTotLiving     228.832     245.017
SqFtLot            -0.061      -0.292
Bathrooms      -19438.099  -26079.171
```

```
Bedrooms       -47781.153  -53625.404
BldgGrade      106117.210  115259.026
```

The coefficents in the weighted regression are slightly different from the original regression.

Key ideas

1. Multiple linear regression equation models the relationship between a response variable Y and muliple predictor variables $X_1, ..., X_p$.
2. The most important metrics to evaluate a model are root mean squared error and R-squared.
3. The standard error of the coefficients can be used to measure the reliability of a variable's contribution to a model.
4. Stepwise regression is a way to automatically determine which variables should be included in the model.
5. Weighted regression is used to give certain records more or less weight in fitting the equation.
6. A regression model should not be used to extrapolate beyond the range of the data.

Prediction Using Regression

The Dangers of Extrapolation

Regression models should not be used to extrapolate beyond the range of the data. The model is valid only for predictor values for which the data has sufficient values (even in the case that sufficient data is available, there could be other problems: see "Testing the Assumptions - Regression Diagnostics" on page 157). As an extreme case, suppose `model_lm` is used to predict the value of a 5,000 square foot empty lot. In this case, all the predictors related to the building would have a value of zero and the regression equation would yield an absurd prediction of -521,900 + 5,000 * -.0605 = -$522,202. Why did this happen? The data only contains parcels with buildings --- there are no records corresponding to vacant land. Consequently, the model has no information to tell it how to predict the sales price for vacant land.

Confidence and Prediction Intervals

Much of statistics involves understanding and measuring variability (uncertainty). The t-statistics and p-values reported in regression output deal with this in a formal way, which is sometimes useful for variable selection (see "Assessing the Model" on page 140). More useful metrics are confidence intervals, which are uncertainty intervals placed around regression coefficients and predictions. An easy way to understand this is via the bootstrap (see ???) for more details about the general bootstrap procedure). The most common regression confidence intervals encountered in software output are those for regression parameters (coefficients). Here is a bootstrap algorithm for generating confidence intervals for regression parameters (coefficients) for a dataset with P predictors and N records (rows):

1. Consider each row (including outcome variable) as a single "ticket" and place all the N tickets in a box.
2. Draw a ticket at random, record the values, replace it in the box
3. Repeat step 2 N times, you now have one bootstrap resample
4. Fit a regression to the boostrap sample, record the estimated coefficients
5. Repeat steps 2-4, say, 1000 times
6. You now have 1000 bootstrap values for each coefficient; find the appropriate percentiles for each one (e.g. 5th and 95th for a 90% confidence interval)

Of greater interest to data scientists are intervals around predicted y values ($\hat{Y}_i$). The uncertainty around $\hat{Y}_i$ comes from two sources:

- Uncertainty about what the regression parameters are (see the above bootstrap algorithm)
- Additional error inherent in individual data points

The individual data point error can be thought of as follows: even if we knew for certain what the regression equation was (e.g. if we had a huge number of records to fit it), the *actual* outcome values for a given set of predictor values will vary. We can model this individual error with the residuals from the fitted values. The bootstrap algorithm for modeling both the regression model error and the individual data point error would look as follows:

1. Take a bootstrap sample from the data (spelled out in greater detail above)
2. Fit the regression, and predict the new value
3. Take a single residual at random from the original regression fit, add it to the predicted value, record the result
4. Repeat steps 1-3, say, 1000 times
5. Find the 2.5th and the 97.5th percentiles of the results

Prediction Interval or Confidence Interval?

A prediction interval pertains to uncertainty around a single value, while a confidence interval pertains to a mean or other statistic calculated from multiple values. Thus, a prediction interval will typically be much wider than a confidence interval for the same value. We model this individual value error in the bootstrap model by selecting an individual residual to tack on to the predicted value. Which should you use? That depends on the context and the purpose of the analysis, but, in general, data scientists are interested in specific individual predictions, so a prediction interval would be more appropriate. Using a confidence interval when you should be using a prediction interval will greatly underestimate the uncertainty in a given predicted value.

Most software, R included, will produce prediction and confidence intervals in default or specified output. They will typically not use the bootstrap approach outlined above, but rather a formula approach based on normal approximation theory. The math is more complex, but the idea is the same.

Factor Variables in Regression

Factor variables, also termed *categorical* variables, take on a limited number of discrete values. For example, a loan purpose can be "debt consolidation", "wedding", "car" etc. The binary (yes/no) variable, also called an *indicator* variable, is a special case of a factor variable. Regression requires numerical inputs, so factor variables need to be recoded to use in the model. The most common approach is to convert a variable into a set of binary *dummy* variables.

Key Terms for Factor Variables

Dummy Variables

Binary 0-1 variables derived by recoding factor data for use in regression and other models.

Reference Coding

The most common type of coding used by statisticians which one level of a factor as a reference and other factors are compared to that level.

Synonyms

treatment coding

One Hot Encoder

A common type of coding used in the machine learning community in which all factors levels are retained. While useful for certain machine learning algorithms, this is not appropriate for multiple linear regression.

Deviation Coding

A type of coding that compares each level against the overall mean as opposed to the reference level. This is commonly used in ANOVA.

Synonyms

sum contrasts

ANOVA

A regression involving only factor variables. Synonyms: Analysis of variance.

Dummy Variables Representation

In the King County housing data, there is a factor variable for the property type.

```
head(house[, 'PropertyType'])
Source: local data frame [6 x 1]

   PropertyType
         (fctr)
1     Multiplex
2 Single Family
3 Single Family
4 Single Family
5 Single Family
6     Townhouse
```

There are three possible values: 'Multiplex', 'Single Family' and 'Townhouse'. To use this factor variable, we need to convert it to a set of binary variables. This is done creating a binary variable for each possible value of the factor variable. This can be done in R using the `model.matrix` function: [1]

```
prop_type_dummies <- model.matrix(~PropertyType -1, data=house)
head(prop_type_dummies)
  PropertyTypeMultiplex PropertyTypeSingle Family PropertyTypeTownhouse
1                     1                         0                     0
2                     0                         1                     0
3                     0                         1                     0
4                     0                         1                     0
```

[1] The `-1` argument in the `model.matrix` removes the intercept term from the model. This is the way to extract the one hot encoding representation. The default in R is to produce a matrix with P-1 columns with the first factor level as a reference.

```
5                      0                          1                      0
6                      0                          0                      1
```

The factor variable `PropertyType`, which has three distinct levels, is represented as a matrix with three columns. In the machine learning community, this representation is referred to as *one hot encoding*. In certain machine learning algorithms, such as nearest neighbors and tree models, one hot encoding is the standard way to represent factor variables (for example, see ???).

In the regression setting, a factor variable with P distinct levels is usually represented by a matrix with only P-1 columns. This is because a regression model typically includes an intercept term. With an intercept, once you have defined the values for P-1 binaries, the value for the Pth is known and could be considered redundant. Adding the Pth column will cause a multicollinearity error (see "Multicollinearity" on page 154).

The default way in R is to use the first factor level as a *reference* and the remaining levels are interpreted relative to that factor.

```
lm(AdjSalePrice ~ SqFtTotLiving + SqFtLot + Bathrooms +
+       Bedrooms +  BldgGrade + PropertyType, data=house)

Call:
lm(formula = AdjSalePrice ~ SqFtTotLiving + SqFtLot + Bathrooms +
    Bedrooms + BldgGrade + PropertyType, data = house)

Coefficients:
              (Intercept)            SqFtTotLiving
               -4.469e+05                2.234e+02
                  SqFtLot                Bathrooms
               -7.041e-02               -1.597e+04
                 Bedrooms                BldgGrade
               -5.090e+04                1.094e+05
PropertyTypeSingle Family     PropertyTypeTownhouse
               -8.469e+04               -1.151e+05
```

The output from the R regression shows two coefficients corresponding to `PropertyType`: `PropertyTypeSingle Family` and `PropertyTypeTownhouse`. There is no coefficient of `Multiplex` since it is implicitly defined when `PropertyTypeSingle Family == 0` and `PropertyTypeTownhouse == 0`. The coefficients are interpreted as relative to `Multiplex` with a home of `Single Family` is worth almost $85,000 less and a home of `Townhouse` worth over $150,000 less. [1]

[1] This is unintuive, but can be explained by the impact of location as a confounding variable: see "Confounding Variables" on page 154.

Different factor codings

There are several different ways to encode factor variables, known as *contrast coding* systems. For example, *deviation coding* , also know as *sum contrasts* compare each level against the overall mean. and is commonly used in ANOVA: see section "ANOVA" on page 113. Another contrast is *polynomial coding* which is appropriate for ordered factors: see section "Ordered factor variables" on page 151. With the exception of ANOVA and ordered factors, data scientists will generally not encounter any type of coding besides reference coding or one hot encoder. See ??? for a comprehensive discussion of different factor codings.

Factor Variables With Many Levels

Some factor variables can produce a huge number of binary dummies --- zip codes are a factor variable and there are 43,000 zip codes in the US. In such cases, it is useful to explore the data, and the relationships between predictor variables and the outcome, to determine whether useful information is contained in the categories. If so, it must be further decided whether it is useful to retain all factors, or whether the levels should be consolidated.

In King County, there are 82 zip codes with a house sale:

```
table(house$ZipCode)

 9800 89118 98001 98002 98003 98004 98005 98006 98007 98008 98010 98011
    1     1   358   180   241   293   133   460   112   291    56   163
98014 98019 98022 98023 98024 98027 98028 98029 98030 98031 98032 98033
   85   242   188   455    31   366   252   475   263   308   121   517
98034 98038 98039 98040 98042 98043 98045 98047 98050 98051 98052 98053
  575   788    47   244   641     1   222    48     7    32   614   499
98055 98056 98057 98058 98059 98065 98068 98070 98072 98074 98075 98077
  332   402     4   420   513   430     1    89   245   502   388   204
98092 98102 98103 98105 98106 98107 98108 98109 98112 98113 98115 98116
  289   106   671   313   361   296   155   149   357     1   620   364
98117 98118 98119 98122 98125 98126 98133 98136 98144 98146 98148 98155
  619   492   260   380   409   473   465   310   332   287    40   358
98166 98168 98177 98178 98188 98198 98199 98224 98288 98354
  193   332   216   266   101   225   393     3     4     9
```

`ZipCode` is an important variable, since it is a proxy for the effect of location on the value of a house. Including all levels requires 81 coefficients corresponding to 81 degrees of freedom. The original model `house_lm` has only 5 degress of freedom: see "Assessing the Model" on page 140. Moreover, several zip codes have only one sale. In some problems, zip code can be consolidated using the the first two or three digits, corresponding to a sub-metropolitan geographic region. For King County, almost all of the sales occur in 980xx or 981xx, so this doesn't help.

An alternative approach is to group the zipcodes according to another variable, such as sale price. Even better is to form zip code groups using the residuals from an initial model. The following dplyr code consolidates the 82 zip codes into five groups based on the median of the residual from the house_lm regression.

```
zip_groups <- house %>%
  mutate(resid = residuals(house_lm)) %>%
  group_by(ZipCode) %>%
  summarize(med_resid = median(resid),
            cnt = n()) %>%
  arrange(med_resid) %>%
  mutate(cum_cnt = cumsum(cnt),
         ZipGroup = ntile(cum_cnt, 5))
house <- house %>%
  left_join(select(zip_groups, ZipCode, ZipGroup), by='ZipCode')
```

See "Confounding Variables" on page 154 for an example of how this is used as a term in a regression improving upon the original fit.

The concept of using the residuals to help guide the regression fitting is a fundamental step in the modeling process: see "Testing the Assumptions - Regression Diagnostics" on page 157.

Ordered factor variables

Table 4-1. A Typical Data Format

Value	Description
1	Cabin
2	Substandard
5	Fair
10	Very good
12	Luxury
13	Mansion

Some factor variables reflect levels of a factor; these are termed ordered factor variables or ordered categorical variables. For example, the loan grade could be A, B, C, etc. - each grade carries more risk than the prior grade. Ordered factor variables can typically be converted to numerical values and used as is. For example, the variable BldgGrade is an ordered factor variable. Several of the types of grades are shown in Table 4-1. While the grades have specific meaning, the numeric value is ordered from low to high corresponding to higher grade homes. With the regression model `house_lm`, fit in "Multiple Linear Regression" on page 138, `BldgGrade` was treated as a numeric variable.

Treating ordered factors as a numeric variable preserves the information contained in the ordering would be lost that would be lost if it were converted to a factor.

Key ideas

1. Factor variables need to be converted into numeric variables for use in a regression.
2. The most common method to encode a factor variable with P distinct values is to represent them using P-1 dummy variables.
3. A factor variable with many levels, even in very big datasets, may need to be consolidated into a variable with fewer levels.
4. Some factors have levels that are ordered and can be represented as a single numeric variable.
5. ANOVA is a special case of regression with just factor variables as predictors.

Interpreting the Regression Equation

In data science, the most important use of regression is to predict some dependent (outcome) variable. In some cases, however, gaining insight from the equation itself to understand the nature of the relationship between the predictors and the outcome can be of value.

Key Terms for Confounding Variables and Interactions

Correlated Variables
When the predictor variables are highly correlated, it is difficult to interpret the individual coefficients.

Multicollinearity
When the predictor variables have perfect, or near perfect, correlation, the regression can be unstable or impossible to compute.

Synonyms
collinearity

Confounding Variables
An important predictor that, when omitted, leads to spurious relationships in a regression equation.

Main Effects
: The relationship between a predictor and the outcome variable, independent from other variables.

Interactions
: An interdependent relationship between two or more predictors and the response.

Correlated Predictors

In multiple regression, the predictor variables are often correlated with each other. As an example, examine the regression coefficients for the model `step_lm`, fit in "Model Selection and Stepwise Regression" on page 142:

```
step_lm$coefficients
              (Intercept)             SqFtTotLiving
             6.227632e+06              1.865012e+02
                Bathrooms                  Bedrooms
             4.472172e+04             -4.980718e+04
                BldgGrade PropertyTypeSingle Family
             1.391792e+05              2.332869e+04
    PropertyTypeTownhouse            SqFtFinBasement
             9.221625e+04              9.039911e+00
                  YrBuilt
            -3.592468e+03
```

The coefficient for `Bedrooms` is negative! This implies that adding an adding a bedroom to a house will reduce its value. How can this be? This is because the predictor variables are correlated: larger houses tend to have more bedrooms, and it is the size that drives house value, not the number of bedrooms. Consider two homes of the exact same size: it is reasonable to expect that a home with more, but smaller, bedrooms would be considered less desirable.

Having correlated predictors can make it difficult to interpret the sign and value of regression coefficients (and can inflate the standard error of the estimates). The variables for bedrooms, house size, and number of bathrooms are all correlated. This is illustrated by fitting another regression removing the variables `SqFtTotLiving`, `SqFtFinBasement`, and `Bathrooms` from the equation:

```
update(step_lm, . ~ . -SqFtTotLiving - SqFtFinBasement - Bathrooms)

Call:
lm(formula = AdjSalePrice ~ Bedrooms + BldgGrade + PropertyType +
    YrBuilt, data = house0, na.action = na.omit)

Coefficients:
              (Intercept)                   Bedrooms
                  4834680                      27657
```

```
                    BldgGrade  PropertyTypeSingle Family
                       245709                     -17604
        PropertyTypeTownhouse                    YrBuilt
                       -47477                      -3161
```

Now the coefficient for bedrooms positive --- in-line with what we would expect (though it is really acting as a proxy for house size, now that those variables have been removed).

Correlated variables are only one issue with interpreting regression coefficients. In `house_lm`, there is no variable to account for the location of the home, and the model is mixing together very different types of regions. Location may be a *confounding* variables: see "Confounding Variables" on page 154 for further discussion.

Multicollinearity

Multicollinearity is a condition in which there is redundance among the predictor variables. Perfect multicollinearity occurs when one predictor variable can be expressed as a linear combination of others. Multicollinearity occurs when

1. A variable is included multiple times by error.
2. P dummies, instead of P-1 dummies, are created from a factor variable (see "Factor Variables in Regression" on page 147).
3. Two variables are nearly perfectly correlated with one another

Multicollinearity in regression must be addressed — variables should be removed until the multicollinearity is gone. A regression does not have a well defined solution in the presence of perfect multicollinearity. Many software packages, including `R`, automatically handle certain types of multicollieарity. For example, if `SqFtTotLiving` is included twice in the regression of the `house` data, the results are the same as for the `house_lm` model. In the case of non-perfect multicollinearity, the software may obtain a solution but the results may be unstable.

> Multicollinearity is not such a problem for non-regression methods like trees, clustering and nearest-neighbors, and in such methods it may be advisable to retain P dummies (instead of P-1). That said, even in those methods, non-redundancy in predictor variables is still a virtue.

Confounding Variables

With correlated variables, the problem is one of commission: including different variables that have a similar predictive relationship with the response. With *confounding variables*, the problem is one of omission: an important variable is not included in the regression equation. Naive interpretation of the equation coefficients can lead to invalid conclusions.

Take, for example, the King County regression equation `house_lm` from "Example: King County Housing Data" on page 139. The regression coefficients of `SqFtLot`, `Bathrooms` and `Bedrooms` are all negative. The original regression model does not contain a variable to represent location --- a very important predictor of house price. To model location, include a variable `ZipGroup` that categorizes the zip code into one of five groups, from least expensive (1) to most expense (5). [1]

```
lm(AdjSalePrice ~  SqFtTotLiving + SqFtLot +
     Bathrooms + Bedrooms +
     BldgGrade + PropertyType + ZipGroup,
   data=house, na.action=na.omit)

Coefficients:
              (Intercept)              SqFtTotLiving
               -6.709e+05                  2.112e+02
                  SqFtLot                  Bathrooms
                4.692e-01                  5.537e+03
                 Bedrooms                  BldgGrade
               -4.139e+04                  9.893e+04
PropertyTypeSingle Family      PropertyTypeTownhouse
                2.113e+04                 -7.741e+04
                ZipGroup2                  ZipGroup3
                5.169e+04                  1.142e+05
                ZipGroup4                  ZipGroup5
                1.783e+05                  3.391e+05
```

`ZipGroup` is clearly an important variable: a home in the most expensive zip code group is estimated to have a higher sales price by almost $340,000. The coefficients of `SqFtLot` and `Bathrooms` are now positive and adding a bathroom increases the sale price by $7,500.

The coefficient for `Bedrooms` is still negative. While this is unintuitive, this is a well-known phenomenon in real-estate. For homes of the same livable area and number of bathrooms, having more, and therefore smaller, bedrooms is associated with less valuable homes.

Interactions and Main Effects

Statisticians like to distinguish between *main effects*, or independent variables, and the *interactions* between the main effects. Main effects are what are often referred to

[1] There are 82 zip codes in King County, several with just a handful of sales. An alternative to directly using zip code as a factor variable, `ZipGroup` clusters similar zip codes into a single group. See "Factor Variables With Many Levels" on page 150 for details

as the predictor variables in the regression equation. An implicit assumption when using only main effects in a model is that the relationship between a predictor variable and the response is independent of the other predictor variables. This is often not the case.

For example, the model fit to the King County Housing Data in "Confounding Variables" on page 154 includes several variables as main effects, including ZipCode. Location in real estate is everything and it is natural to presume that the relationship between, say, house size and the sale price depends on location. Building a big house in a low-rent district is not going to retain the same value as building a big house in an expensive area. Interactions between variables in R are included using the * operator. For the King County data, the following fits an interaction between SqFtTotLiving and ZipGroup:

```
lm(AdjSalePrice ~  SqFtTotLiving*ZipGroup + SqFtLot +
     Bathrooms + Bedrooms + BldgGrade + PropertyType,
   data=house, na.action=na.omit)

 Coefficients:
              (Intercept)              SqFtTotLiving
               -4.919e+05                  1.176e+02
                ZipGroup2                  ZipGroup3
               -1.342e+04                  2.254e+04
                ZipGroup4                  ZipGroup5
                1.776e+04                 -1.555e+05
                  SqFtLot                  Bathrooms
                7.176e-01                 -5.130e+03
                 Bedrooms                  BldgGrade
               -4.181e+04                  1.053e+05
PropertyTypeSingle Family      PropertyTypeTownhouse
                1.603e+04                 -5.629e+04
  SqFtTotLiving:ZipGroup2    SqFtTotLiving:ZipGroup3
                3.165e+01                  3.893e+01
  SqFtTotLiving:ZipGroup4    SqFtTotLiving:ZipGroup5
                7.051e+01                  2.298e+02
```

The resulting model has four new terms: SqFtTotLiving:ZipGroup2, SqFtTotLiving:ZipGroup3, etc..

Location and house size appear to have a strong interaction. For a home in the lowest ZipGroup, the slope is the same as the slope for the main effect SqFtTotLiving, which is $177 per square foot (this is because R uses *reference* coding for factor variables: see "Factor Variables in Regression" on page 147). For a home in the highest ZipGroup, the slope is the sum of the main effect plus SqFtTotLiving:ZipGroup5, or $177 + $230 = $447 per square foot. In other words, adding a square foot in the most expensive zip code group boosts the predicted sale price by a factor of almost 2.7, compared to the boost in the least expensive zip code group.

Model Selection with Interaction Terms

In problems involving many variables, it can be challenging to decide which interaction terms should be included in the model. Several different approaches are commonly taken:

1. In some problems, prior knowledge and intuition can guide the choice of which interaction terms to include in the model.
2. Stepwise selection (see "Model Selection and Stepwise Regression" on page 142) can be used to sift through the various models.
3. Penalized regression (see ???) can automatically fit to a large set of possible interaction terms.
4. Perhaps the most common approach is the use *tree models*, and their descendents *random forest* and *gradient boosted trees*. This class of models automatically searches for optimal interaction terms: see ???.

Key ideas

1. Because of correlation between predictors, care must be taken in the interpretation of the coefficients in multiple linear regression.
2. Multicollinearity can cause numerical instability in fitting the regression equation.
3. A confounding variable is an important predictor that is omitted from a model and can lead to a regression equation with spurious relationships.
4. An interaction term between two variables is needed if the relationship between the variables and the response is interdependent.

Testing the Assumptions - Regression Diagnostics

In explanatory modeling (i.e. in a research context), various steps, in addition to the metrics mentioned above (see "Assessing the Model" on page 140) are taken to assess how well the model fits the data. Most are based on analysis of the residuals, which can test the assumptions underlying the model.

Key Terms for Regression Diagnostics

Standardized Residuals
: Residuals divided by the standard error of the residuals

Outliers

Records (or outcome values) that are distant from the rest of the data (or the predicted outcome)

Influential Value

A value or record whose presence or absence makes a big difference in the regression equation

Leverage

The degree of influence that a single record has on a regression equation

Synonyms

Hat-value

Non-Normal Residuals

Non-normally distributed residuals can invalidate some technical requirements of regression, but are usually not a worry in data science

Heteroskedasticity

When some ranges of the outcome experience residuals with higher variance (may indicate a predictor missing from the equation)

Partial Residual Plots

A diagnostic plot to illuminate the relationship between the outcome variable and a single predictor.

Synonyms

Added variables plot

Outliers

Generally speaking, an extreme value, also called an *outlier*, is one that is distant from most of the other observations. Just as outliers need to be handled for estimates of location and variability (see "Estimates of Location" on page 16 and "Estimates of Variability" on page 22), outliers can cause problems with regression models. In regression, an outlier is a record whose actual y-value is distant from the predicted value. Outliers can be detected by examining the *standardized residual*, which is the residual divided by the standard error of the residuals.

There is no statistical theory that separates outliers from non-outliers. Rather, there are (arbitrary) rules of thumb for how distant from the bulk of the data an observation needs to be in order to be called an outlier. For example, with the boxplot, outliers those data points that are more than 1.5 times the inter-quartile range above or below the box boundaries (see "Percentiles and Boxplots" on page 28). In regression, the standardized residual is the metric that is typically used to determine whether a record is classified as an outlier. Standardized residuals can be interpreted as "the number of standard errors away from the regression line."

Let's fit a regression to the King County house sales data for all sales in zip code 98105

```
house_98105 <- house[house$ZipCode == 98105,]
lm_98105 <- lm(AdjSalePrice ~ SqFtTotLiving + SqFtLot + Bathrooms +
                 Bedrooms + BldgGrade, data=house_98105)
```

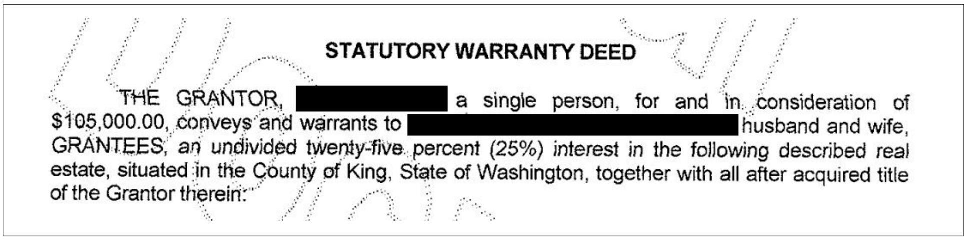
The standardized residuals are extracted using the `rstandard` function and the index of the smallest residual can be obtained using the `order` function.

```
sresid <- rstandard(lm_98105)
idx <- order(sresid)
sresid[idx[1]]
    20431
-4.326732
```

The biggest overestimate from the model is more than four standard errors above the regression line corresponding to an overestimate of $757,753. The original data record corresponding to this outlier is as follows:

```
house_98105[idx[1], c('AdjSalePrice', 'SqFtTotLiving', 'SqFtLot',
              'Bathrooms', 'Bedrooms', 'BldgGrade')]

AdjSalePrice SqFtTotLiving SqFtLot Bathrooms Bedrooms BldgGrade
         (dbl)         (int)   (int)     (dbl)    (int)     (int)
1       119748          2900    7276         3        6         7
```



STATUTORY WARRANTY DEED

THE GRANTOR, [redacted] a single person, for and in consideration of $105,000.00, conveys and warrants to [redacted] husband and wife, GRANTEES, *an undivided twenty-five percent (25%) interest in the following described real* estate, situated in the County of King, State of Washington, together with all after acquired title of the Grantor therein:

Figure 4-4. Statutory warrant of deed for the largest negative residual

In this case, it appears that there is something wrong with the record: a house of that size typically sells for much more than $110,748 in that zip code. Figure 4-4 shows an excerpt from the statuatory deed from this sales: it is clear that the sale involved only partial interest in the property. In this case, the outlier corresonds to a sale that is anomalous and should not be included in the regression. Outliers could also be the result of other problems, such as a "fat-finger" data entry or a mismatch of units (e.g., reporting a sale in thousands of dollars versus simply dollars).

For big data problems, outliers are generally not a problem in fitting the regression to be used in predicting new data. However, outliers are central to anomaly detection, where finding outliers is the whole point. The outlier could also correspond to a case of fraud or an accidental action. In any case, detecting outliers can be a critical business need.

Influential values

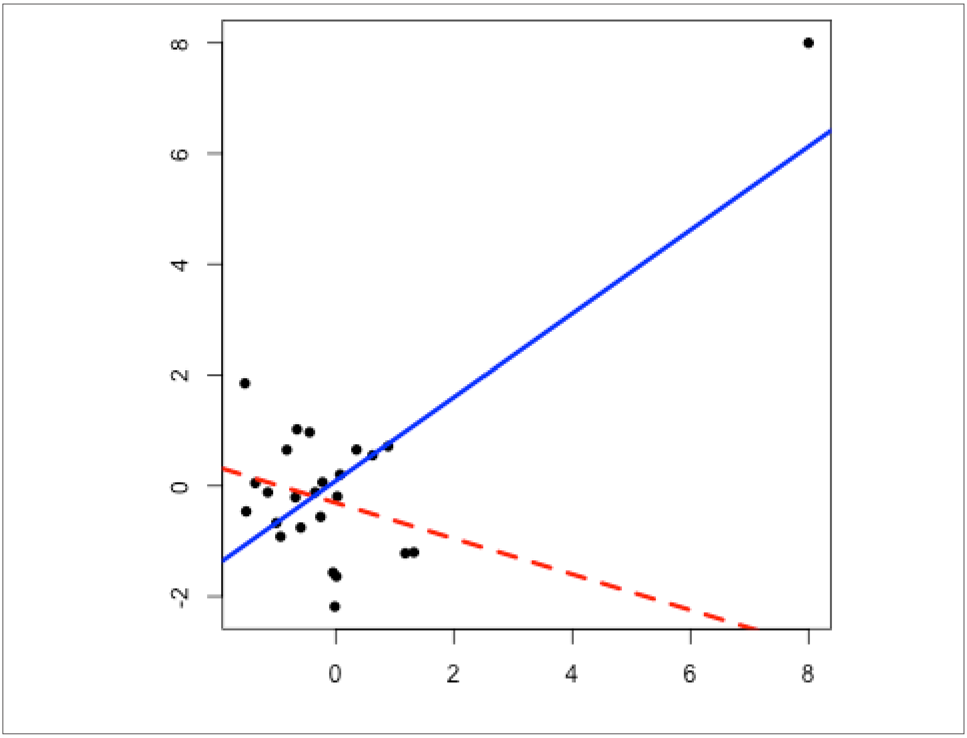


Figure 4-5. An example of an influential data point in regression

A value whose absence would significantly change the regression equation is termed an *infuential observation*. In regression, such a value need not be associated with a large residual. As an example, consider the regression lines in Figure 4-5. The solid blue line corresponds to the regression with all the data while the red dashed line corresonds to the regression with the point in the upper right removed. Clearly that data value has huge influence on the regression even it is not associated with a large outlier (from the full regression). This data value is considered to have high *leverage* on the regression.

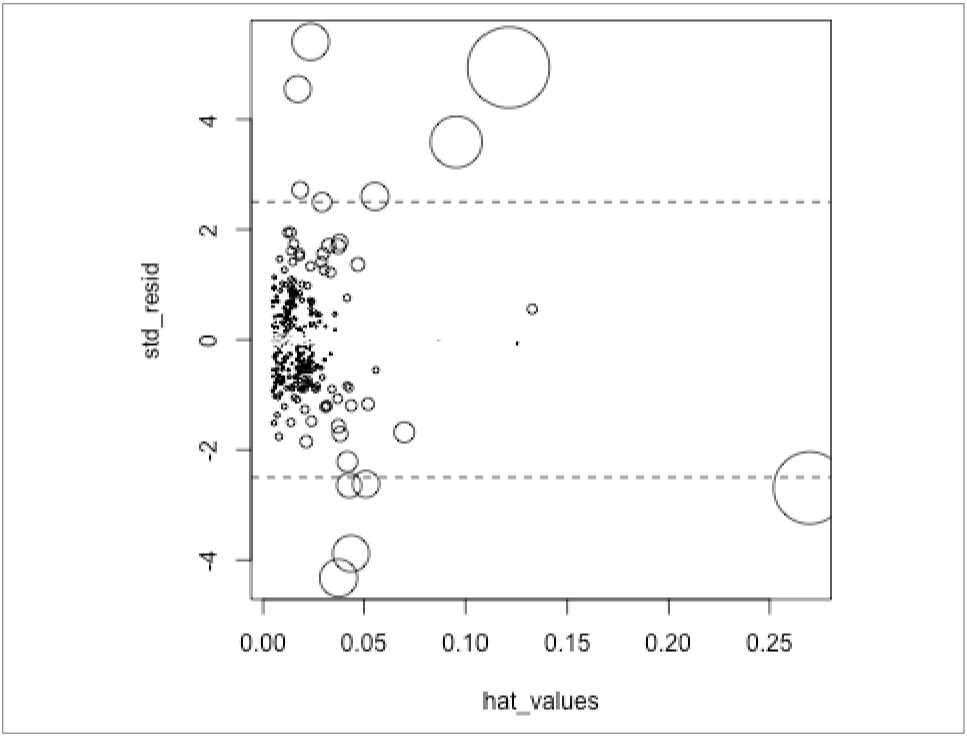


Figure 4-6. A plot to determine which observations have high influence

In addition to standardized residuals (see "Outliers" on page 158), statisticians have developed several metrics to determine the influence of a single record on a regression. A common measure of leverage is the *hat-value*; values above $2(P + 1)/N$ indicate a high-leverage data value. [1]

Another metric is *Cook's distance* which defines influence as a combination of leverage and residual size. A rule of thumb is that an observation has high influence if Cook's distance exceeds $4/(N - P - 1$.

An *influence plot* or *bubble plot* combines standardized residuals, the hat-value and Cook's distance in a single plot. Figure 4-6 shows the influence plot for the King County house data, and can be created by the following R code.

```
std_resid <- rstandard(lm_98105)
cooks_D <- cooks.distance(lm_98105)
hat_values <- hatvalues(lm_98105)
```

[1] The term hat-value comes from the notion of the hat matrix in regression. Multiple linear regression can be expressed by the formula $\hat{Y} = HY$ where H is the hat matrix. The hat values correspond to the diagonal of H.

```
plot(hat_values, std_resid, cex=10*sqrt(cooks_D))
abline(h=c(-2.5, 2.5), lty=2)
```

There are apparently several data points that exhibit large influence in the regression.

Table 4-2. Comparison of regression coefficients with the full data and with influential data removed

	Original	Influential Removed
(Intercept)	-772550	-647137
SqFtTotLiving	210	230
SqFtLot	39	33
Bathrooms	2282	-16132
Bedrooms	-26320	-22888
BldgGrade	130000	114871

Table 4-2 compares the regression with the full data set and with highly influential data points removed. The regression coefficient for `Bathrooms` changes quite dramatically. [1]

For purposes of fitting a regression that reliably predicts future data, identifying influential observations is only useful in smaller data sets. For regressions involving many records, it is unlikely that any one observation will carry sufficient weight to cause extreme influence on the fitted equation (although the regression may still have big outliers). For purposes of anomaly detection, though, identifying influential observations can be very useful.

Heteroskedasticity, Non-normality and Correlated Errors

Statisticians pay considerable attention to the distribution of the residuals. It turns out that ordinary least squares (see "Least Squares" on page 136) is unbaised, and in some cases the "optimal" estimator, under a wide range of distributional assumptions. This means that, in most problems, data scientists do not need be too concerned with the distribution of the residuals.

[1] The coefficient for `Bathrooms` becomes negative, which is unintuitive. Location has not been taken into account and the zip code 98105 contains areas of disparate types homes. See "Confounding Variables" on page 154 for a discussion of confounding variables.

The distribution of the residuals is relevant mainly for the validity of formal statistical inference (hypothesis tests and p-values) that is of minimal importance to data scientists concerned mainly with predictive accuracy. For formal inference to be fully valid, the residuals are assumed to be normally distributed, have the same variance and be independent. One area where this may be of concern to data scientists is the standard calculation of condidence intervals for predicted values, which are based upon the assumptions about the residuals (see "Confidence and Prediction Intervals" on page 145).

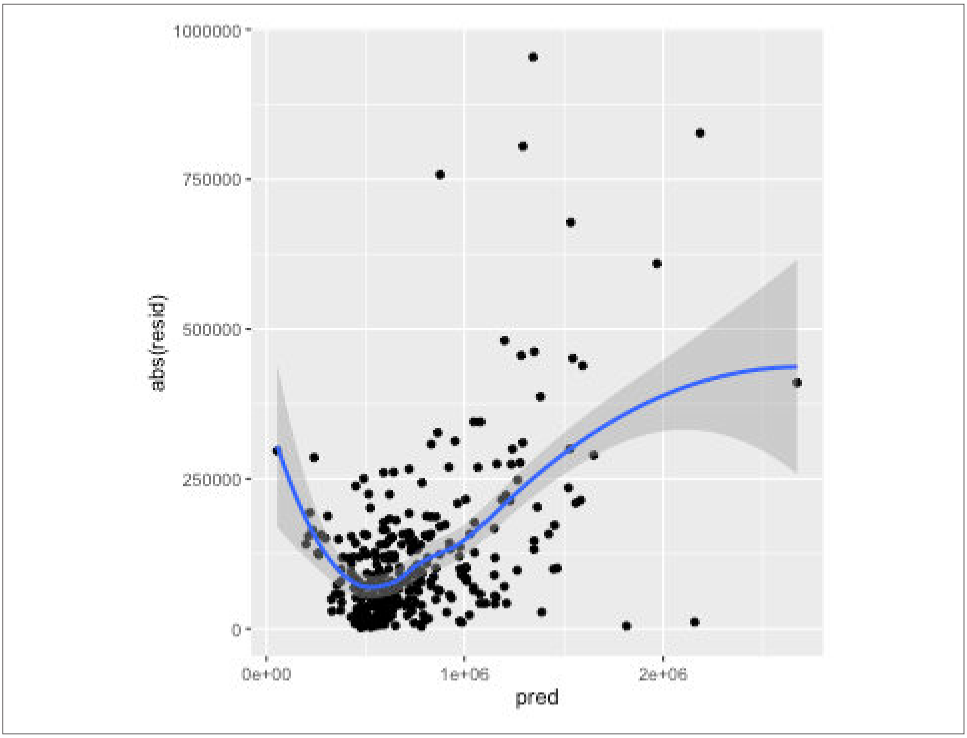


Figure 4-7. A plot of the absolute value of the residuals versus the predicted values

Heteroskedasticity is the lack of constant residual variance across the range of the predicted values. In other words, errors are greater for some portions of the range than for others. The `ggplot2` package has some convenient tools to analyze residuals.

The following code plots the absolute residuals versus the predicted values for the `lm_98105` regression fit in "Outliers" on page 158.

```
df <- data.frame(
  resid = residuals(lm_98105),
  pred = predict(lm_98105))
ggplot(df, aes(pred, abs(resid))) +
  geom_point() +
  geom_smooth()
```

Figure 4-7 shows the resulting plot. Using `geom_smooth`, it is easy to superpose a smooth of the absolute residuals. The function calls the `loess` method to produce a visual smooth to estimate between the variables on the *x*-axis and *y*-axis in a scatterplot (see: ???).

Evidently, the variance of the residuals tends to increase for higher valued homes, but is also large for lower valued homes. This plot indicates that `lm_98105` has *heteroskedastic* errors, which can indicate that the regression may have left something unaccounted for in high and low range homes.

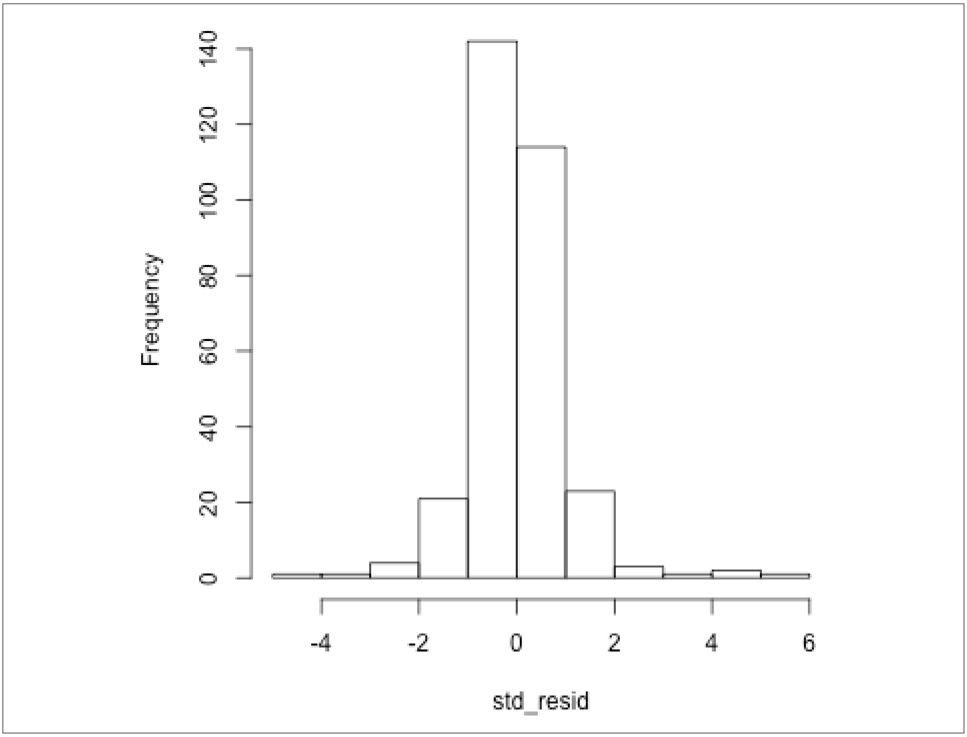


Figure 4-8. A histogram of the residuals from the regression of the housing data

Figure 4-8 is a histogram of the standarized residuals for the `lm_98105` regression. The distribution has decidely longer tails than the normal distribution, and exhibits mild skewness toward larger residuals.

Statisticians may also check the assumption that the errors are independent. This is particular true for data that is collected over time. The *Durbin-Watson* statistic can be used to detect if there is significant autocorrelation in a regression involving time series data.

Even though a regression may violate one of the distributional assumptions, should we care? Most often in data science, where the interest is primarily in predictive accuracy, the answer is no. As long as we are not doing formal inference, then the distribution of the residuals is not that important.

Scatterplot Smoothers

Regression is about modeling the relationship between the response and predictor variables. In evaluating a regression model, is useful to use a *scatterplot smoother* to visually highlight relationships between two variables. Scatterplot smoothers are empirical estimates and operate in an analogous manner to the smoothing for density estimation (see: ???), except that it works in two-dimensionals.

For example, in Figure 4-7, a smooth of the relationship between the absolute residuals and the predicted value shows that the variance of the residuals depends on the value of the residual. In this case, the `loess` function was used; `loess` works by repeatedly fitting a series of local regressions to contiguous subsets to come up with a smooth. While `loess` is probably the most commonly used smoother, other scatterplot smoothers are available in R, such as super smooth (`supsmu`) and kernal smoothing (`ksmooth`). For the purposed of evaluating a regression model, there is typically no need to worry about the details of these scatterplot smoothes.

Partial Residual Plots and Nonlinearity

Partial residual plots are a way to visualize how well the estimated fit explains the relationship between a predictor and the outcome. Along with detection of outliers, this is probably the most important diagnostic for data scientists. The basic idea of a partial residual plot is to isolate the relationship between a predictor variable and the response *taking into account all of the other predictor variables*. A partial residual might be thought of as a “synthetic outcome” value, combining the prediction based on a single predictor with the actual residual from the full regression equation. A partial residual for predictor X_i is the ordinary residual plus the regression term associated with X_i:

$$\text{Partial Residual} = \text{Residual} + \hat{b}_i X_i$$

where $\hat{b}_i$ is the estimated regression coefficient. The `predict` function in R has an option to return the individual regression terms $\hat{b}_i X_i$:

```
terms <- predict(lm_98105, type='terms')
partial_resid <- resid(lm_98105) + terms
```

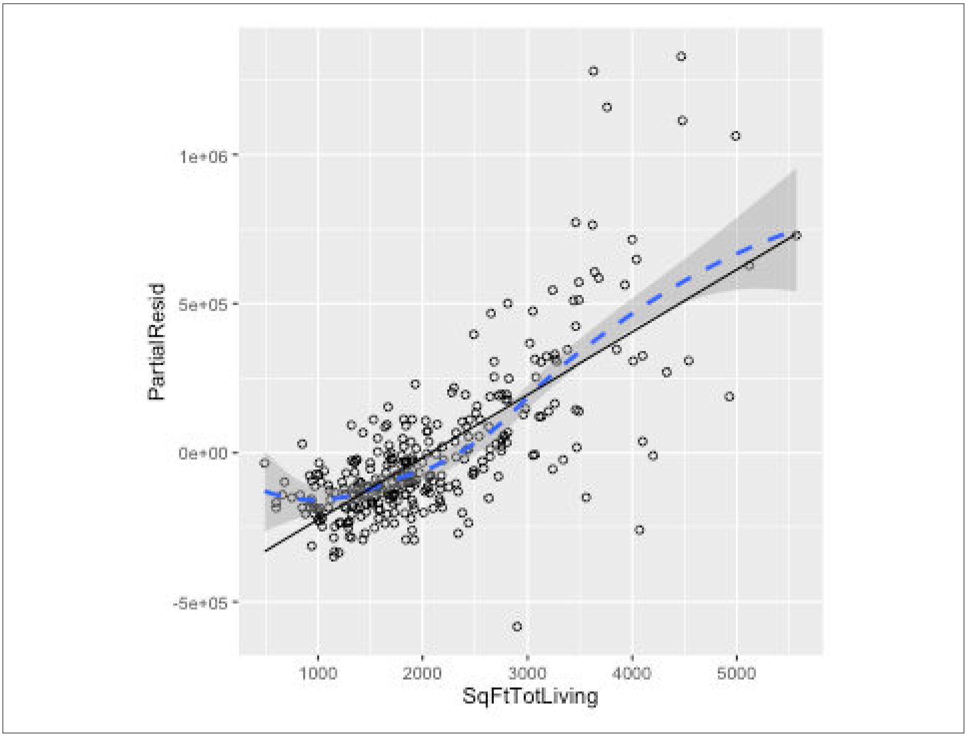


Figure 4-9. A partial residual plot of for the variable `SqFtTotLiving`

The partial residual plot displays the X_i on the x-axis and the partial residuals on the y-axis. Using `ggplot2` makes it easy to superpose a smooth of the partial residuals.

```
df <- data.frame(SqFtTotLiving = house_98105[, 'SqFtTotLiving'],
                 Terms = terms[, 'SqFtTotLiving'],
                 PartialResid = partial_resid[, 'SqFtTotLiving'])
ggplot(df, aes(SqFtTotLiving, PartialResid)) +
  geom_point(shape=1) + scale_shape(solid = FALSE) +
  geom_smooth(linetype=2) +
  geom_line(aes(SqFtTotLiving, Terms))
```

The resulting plot is shown in Figure 4-9. The partial residual is an estimate of the contribution that `SqFtTotLiving` adds to the sales price. The relationship between `SqFtTotLiving` and the sales price is evidently non-linear. The regression line underestimates the sales price for homes less than 1000 square feet and over estimates the price for homes between 2000 and 3000 square feet. There are too few data points above 4000 square feet to draw conclusions for those homes.

This non-linearity makes sense in this case: adding 500 feet in a small home makes a much bigger difference than adding 500 feet in a large home. This suggests that, instead of a simple linear term for `SqFtTotLiving`, a non-linear term should be considered (see "Polynomial and Spline Regression" on page 167).

Key ideas

1. While outliers can cause problems for small datasets, the primary interest with outliers is to identify problems with the data, or locate anomalies.
2. Single records (including regression outliers) can have a big influence on a regression equation with small dat3a, but this effect washes out in big data.
3. If the regression model is used for formal inference (p-values, etc.), then certain assumptions about the distribution of the residuals should be checked. In general, however, the distribution of residuals is critical in data science.
4. The partial residuals plot can be used to qualitatively assess the fit for each regression term, possibly leading to alternative model specification.

Polynomial and Spline Regression

The relationship between the response and a predictor variable is not necessarily linear. The response to the dose of a drug is often nonlinear: doubling the dosage generally doesn't lead to a double in the response. The demand for a product is not a linear function of marketing dollars spent since, at some point, demand is likely to be saturated. There are several ways that regression can be extended to capture these nonlinear effects.

Key Terms for Non-Linear Regression

Polynomial Regression
Adds polynomial terms - squares, cubes, etc. - to a regression

Spline Regression
Fitting a smooth curve with a series of polynomial segments

Knots
Values that separate spline segments

Generalized Additive Models
Spline models with automated selection of knots

Synonyms
GAM

Nonlinear Regression

When statisticians talk about *nonlinear regression*, they are referring to models that can't be fit using least squares. What kind of models are nonlinear? Essentially all models where the response cannot be expressed as a linear combination of the predictors or some transform of the predictors. Nonlinear regression models are harder and computationally more intensive to fit, since they require numerical optimization. For this reason, it is generally preferred to use a linear model if possible.

Polynomial

Polynomial regression involves including polynomial terms to a regression equation. The use of polynomial regression dates back almost to the development of regression itself with a paper by ??? in 1815. For example, a quadratic regression between the response Y and the predictor X would take the form

$$Y = b_0 + b_1 X + b_2 X^2 + e$$

Polynomial regression can be fit in R using the `poly` function. For example, the following fits a quadratic polynomial for `SqFtTotLiving` with the King County housing data:

```
lm(AdjSalePrice ~  poly(SqFtTotLiving, 2) + SqFtLot +
                BldgGrade +  Bathrooms +  Bedrooms,
                    data=house_98105)

Call:
lm(formula = AdjSalePrice ~ poly(SqFtTotLiving, 2) + SqFtLot +
    BldgGrade + Bathrooms + Bedrooms, data = house_98105)

Coefficients:
            (Intercept)  poly(SqFtTotLiving, 2)1
             -402530.47               3271519.49
poly(SqFtTotLiving, 2)2                  SqFtLot
              776934.02                    32.56
              BldgGrade                Bathrooms
              135717.06                 -1435.12
               Bedrooms
               -9191.94
```

There are now two coefficients associated with SqFtTotLiving: one for the linear term and one for the quadratic term.

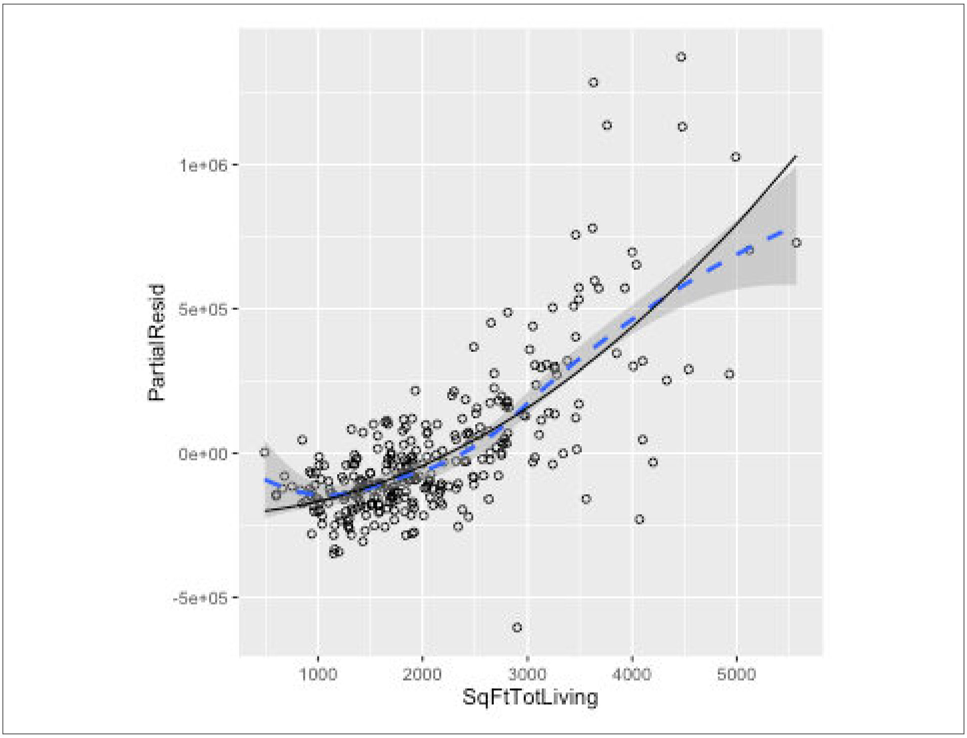


Figure 4-10. A polynomial regression fit for the variable SqFtTotLiving (solid line) versus a smooth (dashed line, see "Splines" on page 170)

The partial residual plot (see "Partial Residual Plots and Nonlinearity" on page 165) indicates some curvature in the regression equation associated with SqFtTotLiving. The fitted line more closely matches the smooth (see "Splines" on page 170) of the partial residuals as compared to a linear fit (see Figure 4-9).

Splines

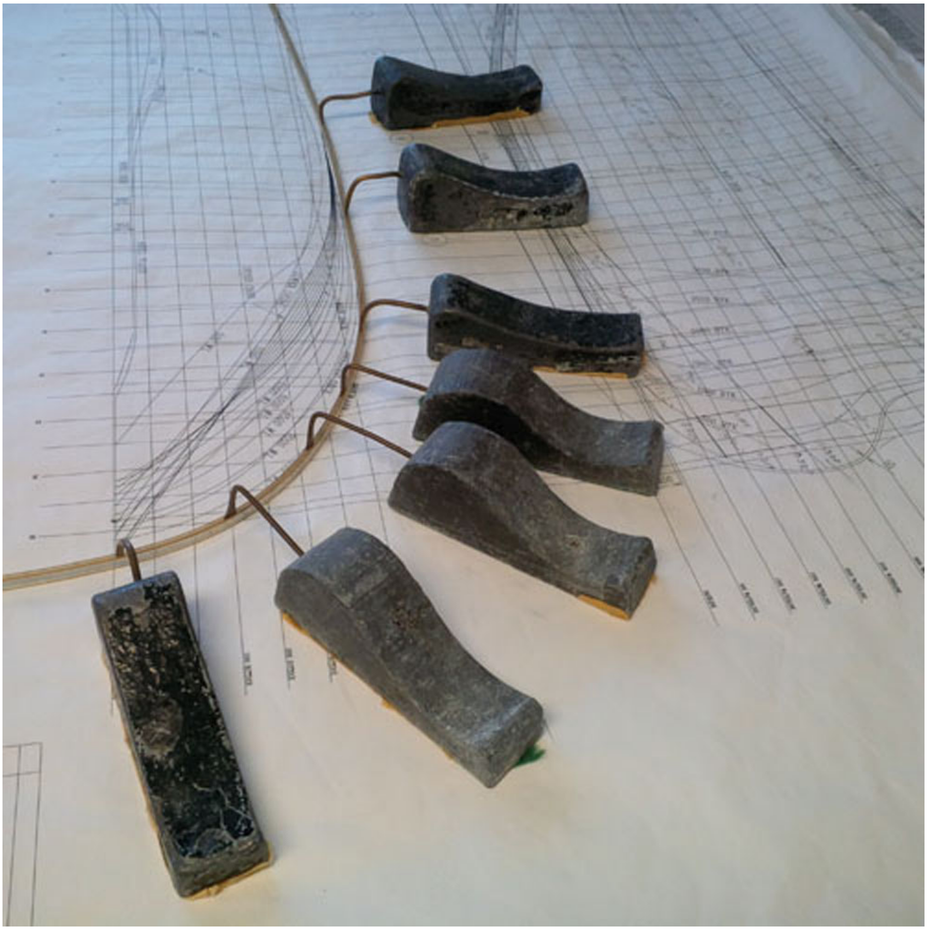


Figure 4-11. Splines were originally created using bendable wood and "ducks", and were used as a draftsmen tool to fit curves.

Polynomial regression only captures a certain amount of curvature in a non-linear relationship. Adding in higher order terms, such as a cubic quartic polynomial, often leads to undesirable "wiggliness" in the regression equation. An alternative, and often superior, approach to modeling non-linear relationships is to use *splines.*(splines *Splines* provide a way to smoothly interpolate between fixed points. Splines were originally used as a draftsman technique to draw a smooth curve, particularly in ship and aircraft building. The splines were created by bending a thin piece of wood using using weights, referred to as "ducks": see Figure 4-11.

The technical definition of a spline is a series of piecewise continuous polynomial. They were first developed during World War II at the U.S. Aberdeen Proving Grounds by I. J. Schoenberg, a Roumanian mathematician. The polynomial pieces are smoothly connected at a series of fixed points, referred to as *knots*. Formulation of splines is much more complicated than polynomial regression; statistical software usually handles the details of fitting a spline. The R package `splines` includes the function `bs` to create a *b-spline* term in a regression model. For example, the following adds a b-spline term to the house regression model:

```
library(splines)
knots <- quantile(house_98105$SqFtTotLiving, p=c(.25, .5, .75))
lm_spline <- lm(AdjSalePrice ~ bs(SqFtTotLiving, knots=knots, degree=3) +   SqFtLot + Bathrooms +
```

Two parameters need to be specified: the degree of the polynomial and the location of the knots. In this case, `SqFtTotLiving` is modeled using a cubic spline (`degree=3`). By default, `bs` places knots at the boundaries; in addition, knots were also placed at the lower quartile, the median and the upper quartile.

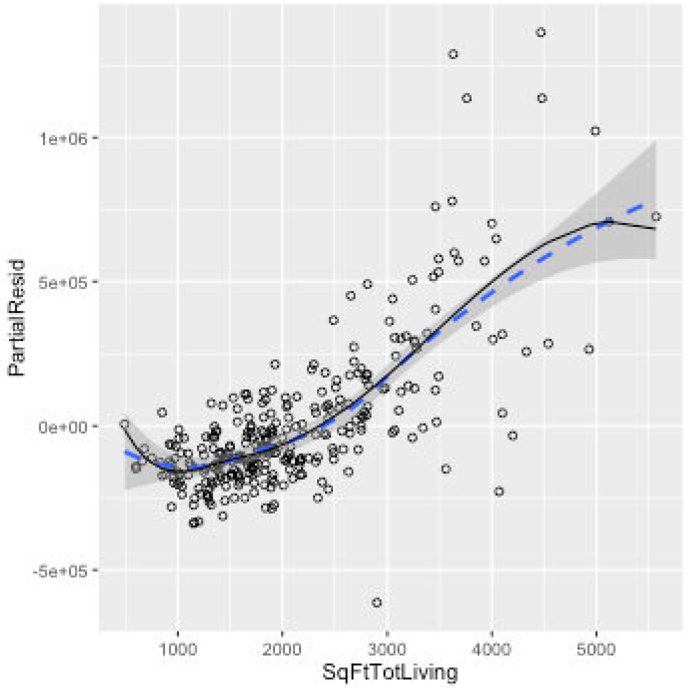


Figure 4-12. A spline regression fit for the variable `SqFtTotLiving` (solid line) compared to a smooth (long dashed line) and a polynomial fit (short dashed line)

In contrast to a linear term, for which the coefficient has a direct meaning, the coefficients for a spline term are not interpretable. Instead, it is more useful to use the visual display to reveal the nature of the spline fit. Figure 4-12 displays the partial residual plot from the regression. In contrast to the polynomial model, the spline model more closely matches the smooth, demonstrating the greater flexibility of splines. In this case, the line more closely fits the data. Does this mean the spline regression is a better model? Not necessarily: it doesn't make economic sense that very small homes (less than 1000 square feet) would have higher value than slightly larger homes. This is possibly an artifact of a confounding variable: see "Confounding Variables" on page 154.

Generalized Additive Models

Suppose you suspect a non-linear relationship between the response and a predictor variable, either by *a priori* knowledge or by examining the regression diagnostics. Polynomial terms may not flexible enough to capture the relationship and spline terms require specifying the knots. *Generalized additive models* ???, or *GAM*, is a technique to automatically fit a spline regression. The `gam` package in R can be used to fit a GAM model to the housing data:

```
library(gam)
lm_gam <- gam(AdjSalePrice ~ s(SqFtTotLiving) + SqFtLot +
                      Bathrooms +  Bedrooms + BldgGrade,
                    data=house_98105)
```

The term `s(SqFtTotLiving)` tells the `gam` function to find the "best" knots for a spline term.

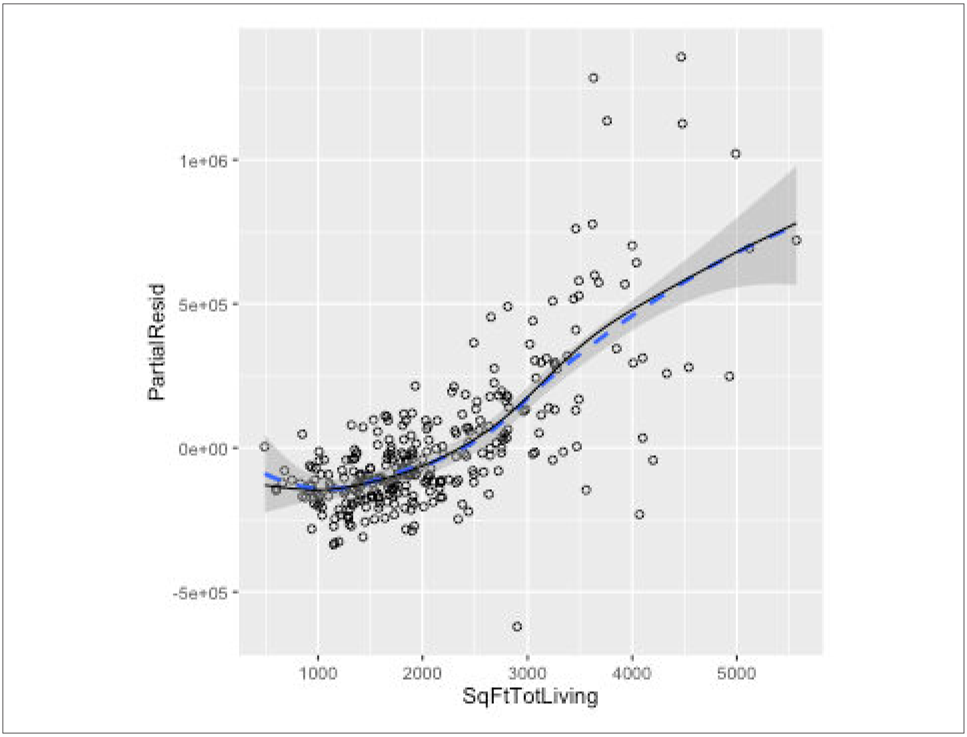


Figure 4-13. A GAM regression fit for the variable `SqFtTotLiving` (solid line) compared to a smooth (long dashed line) and a spline fit (short dashed line)

Key ideas

1. Outliers in a regression are records with a large residual
2. Multicollinearity can cause numerical instability in fitting the regression equation
3. A confounding variable is an important predictor that is omitted from a model and can lead to a regression equation with spurious relationships.
4. An interaction term between two variables is needed if the effect of one variable depends on the *level* of the other.
5. Polynomial regression can fit nonlinear relationships between predictors and the outcome variable
6. Splines are series of polynomial segments strung together, joining at knots
7. Generalized Additive Models (GAM) automate the process of specifying the knots in splines