

# Statistical Thinking for the 21st Century

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# Preface

## 0.1 Why does this book exist?

In 2018 I began teaching an undergraduate statistics course at Stanford (Psych 10/Stats 60). I had never taught statistics before, and this was a chance to shake things up. I have been increasingly unhappy with undergraduate statistics education in psychology, and I wanted to bring a number of new ideas and approaches to the class. In particular, I wanted to bring to bear the approaches that are increasingly used in real statistical practice in the 21st century. As Brad Efron and Trevor Hastie laid out so nicely in their book “Computer Age Statistical Inference: Algorithms, Evidence, and Data Science”, these methods take advantage of today’s increased computing power to solve statistical problems in ways that go far beyond the more standard methods that are usually taught in the undergraduate statistics course for psychology students.

The first year that I taught the class, I used Andy Field’s amazing graphic novel statistics book, “An Adventure in Statistics”, as the textbook. There are many things that I really like about this book – in particular, I like the way that it frames statistical practice around the building of models, and treats null hypothesis testing with sufficient caution (though insufficient disdain, in my opinion). Unfortunately, most of my students hated the book, primarily because it involved wading through a lot of story to get to the statistical knowledge. I also found it wanting because there are a number of topics (particular those from the field of artificial intelligence known as *machine learning*) that I wanted to include but were not discussed in his book. I ultimately came to feel that the students would be best served by a book that follows very closely to my lectures, so I started writing down my lectures into a set of computational notebooks that would ultimately become this book. The outline of this book follows roughly that of Field’s book, since the lectures were originally based in large part on the flow of that book, but the content is substantially different (and also much less fun and clever).

## 0.2 You’re not a statistician - why should we listen to you?

I am trained as a psychologist and neuroscientist, not a statistician. However, my research on brain imaging for the last 20 years has required the use of sophisticated statistical and computational tools, and this has required me to teach myself many of the fundamental concepts of statistics. Thus, I think that I have a solid feel for what kinds of statistical methods are important in the scientific trenches. There are almost certainly some things in this book that would annoy a real statistician (for example, I’m sure that there are places where I should have put a  $\hat{h}$  on a variable but did not).

Having said that, I welcome input from readers with greater statistical expertise than mine.

## 0.3 Why R?

In my course, students learn to analyze data hands-on using the R language. The question “Why R?” could be interpreted to mean “Why R instead of a graphical software package like (insert name here)?”. After all,

most of the students who enroll in my class have never programmed before, so teaching them to program is going to take away from instruction in statistical concepts. My answer is that I think that the best way to learn statistical tools is to work directly with data, and that working with graphical packages insulates one from the data and methods in way that impedes true understanding. In addition, for many of the students in my class this may be the only course in which they are exposed to programming; given that programming is an essential ability in a growing number of academic fields, I think that providing these students with basic programming literacy is critical to their future success, and will hopefully inspire at least a few of them to learn more.

The question could also be interpreted to mean “Why R instead of (insert language here)?”. On this question I am much more conflicted, because I deeply dislike R as a programming language (I greatly prefer Python). Why then do I use it? The first answer to the question is practical – nearly all of the potential teaching assistants (mostly graduate students in our department) have experience with R, since our graduate statistics course uses R. In fact, most of them have much greater skill with R than I do! On the other hand, relatively few of them have expertise in Python. Thus, if I want an army of skilled teaching assistants, it makes sense to use R.

The other reason is that the free Rstudio software makes using R relatively easy for new users. In particular, I like the RMarkdown Notebook feature that allows the mixing of narrative and executable code with integrated output. It’s similar in spirit to the Jupyter notebooks that many of us use for Python programming, but I find it easier to deal with because you edit it as a plain text file, rather than through an HTML interface. In my class, I give students a skeleton RMarkdown file for problem sets, and they submit the file with their solution added, which I then score using a set of automated grading scripts.

## 0.4 The golden age of data

Throughout this book I have tried when possible to use examples from real data. This is now very easy because we are swimming in open datasets, as governments, scientists, and companies are increasingly making data freely available. I think that using real datasets is important because it prepares students to work with real data rather than toy datasets, which I think should be one of the major goals of statistical training. It also helps us realize (as we will see at various points throughout the book) that data don’t always come to us ready to analyze, and often need *wrangling* to help get them into shape. Using real data also shows that the idealized statistical distributions often assumed in statistical methods don’t always hold in the real world – for example, as we will see in Chapter 4, distributions of some real-world quantities (like the number of friends on Facebook) can have very long tails that can break many standard assumptions.

## 0.5 An open source book

This book is meant to be a living document, which is why its source is available online at <https://github.com/poldrack/psych10-book>. If you find any errors in the book or want to make a suggestion for how to improve it, please open an issue on the Github site. Even better, submit a pull request with your suggested change.

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# Chapter 1

## Introduction

“Statistical thinking will one day be as necessary for efficient citizenship as the ability to read and write.” - H.G. Wells

### 1.1 What is statistical thinking?

Statistical thinking is a way of understanding a complex world by describing it in relatively simple terms that nonetheless capture essential aspects of its structure, and that also provide us some idea of how uncertain we are about our knowledge. The foundations of statistical thinking come primarily from mathematics and statistics, but also from computer science, psychology, and other fields of study.

We can distinguish statistical thinking from other forms of thinking that are less likely to describe the world accurately. In particular, human intuition often tries to answer the same questions that we can answer using statistical thinking, but often gets the answer wrong. For example, in recent years most Americans have reported that they think that violent crime was worse compared to the previous year (Pew Research Center). However, a statistical analysis of the actual crime data shows that in fact violent crime has steadily *decreased* since the 1990’s. Intuition fails us because we rely upon best guesses (which psychologists refer to as *heuristics*) that can often get it wrong. For example, humans often judge the prevalence of some event (like violent crime) using an *availability heuristic* – that is, how easily can we think of an example of violent crime. For this reason, our judgments of increasing crime rates may be more reflective of increasing news coverage, in spite of an actual decrease in the rate of crime. Statistical thinking provides us with the tools to more accurately understand the world and overcome the fallibility of human intuition.

### 1.2 What can statistics do for us?

There are three major things that we can do with statistics:

- *Describe*: The world is complex and we often need to describe it in a simplified way that we can understand.
- *Decide*: We often need to make decisions based on data, usually in the face of uncertainty.
- *Predict*: We often wish to make predictions about new situations based on our knowledge of previous situations.

Let’s look at an example of these in action, centered on a question that many of us are interested in: How do we decide what’s healthy to eat?

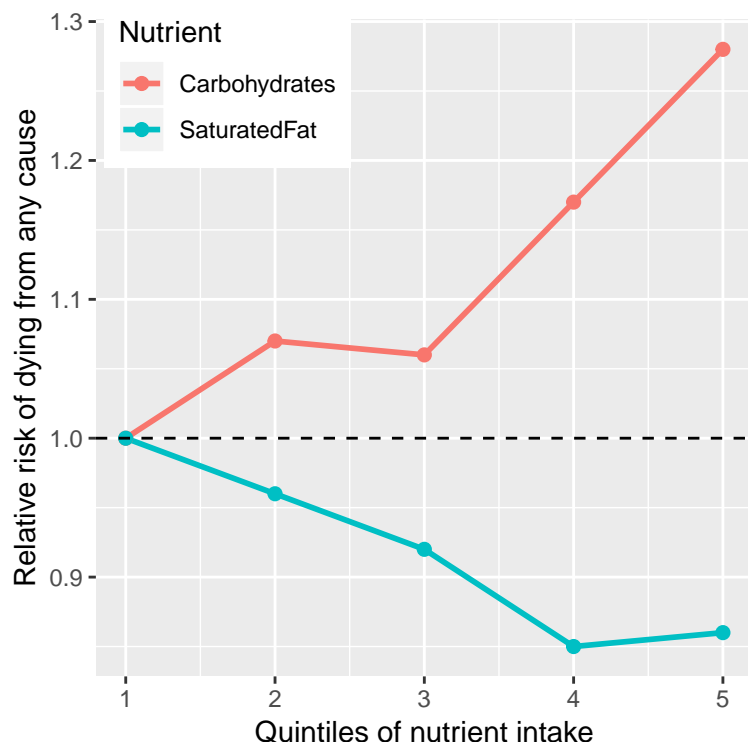


Figure 1.1: A plot of data from the PURE study, showing the relationship between death from any cause and the relative intake of saturated fats and carbohydrates.

There are many different sources of guidance, from government dietary guidelines to diet books to bloggers. Let's focus in on a specific question: Is saturated fat in our diet a bad thing?

One way that we might answer this question is common sense.

If we eat fat then it's going to turn straight into fat in our bodies, right?

And we have all seen photos of arteries clogged with fat, so eating fat is going to clog our arteries, right?

Another way that we might answer this question is by listening to authority figures. The Dietary Guidelines from the US Food and Drug Administration have as one of their Key Recommendations that "A healthy eating pattern limits saturated fats". You might hope that these guidelines would be based on good science, and in some cases they are, but as Nina Teicholz outlined in her book "Big Fat Surprise" (Teicholz 2014), this particular recommendation seems to be based more on the dogma of nutrition researchers than on actual evidence.

Finally, we might look at actual scientific research. Let's start by looking at a large study called the PURE study, which has examined diets and health outcomes (including death) in more than 135,000 people from 18 different countries. In one of the analyses of this dataset (published in *The Lancet* in 2017; Dehghan et al. (2017)), the PURE investigators reported an analysis of how intake of various classes of macronutrients (including saturated fats and carbohydrates) was related to the likelihood of dying during the time that people were followed. People were followed for a *median* of 7.4 years, meaning that half of the people in the study were followed for less and half were followed for more than 7.4 years. Figure 1.1 plots some of the data from the study (extracted from the paper), showing the relationship between the intake of both saturated fats and carbohydrates and the risk of dying from any cause.

This plot is based on ten numbers. To obtain these numbers, the researchers split the group of 135,335 study participants (which we call the "sample") into 5 groups ("quintiles") after ordering them in terms of their intake of either of the nutrients; the first quintile contains the 20% of people with the lowest intake, and the 5th quintile contains the 20% with the highest intake. The researchers then computed how often people

in each of those groups died during the time they were being followed. The figure expresses this in terms of the *relative risk* of dying in comparison to the lowest quintile: If this number is greater than 1 it means that people in the group are *more* likely to die than are people in the lowest quintile, whereas if it's less than one it means that people in the group are *less* likely to die. The figure is pretty clear: People who ate more saturated fat were *less* likely to die during the study, and the more they ate, the bigger this effect was. The opposite is seen for carbohydrates; the more carbs a person ate, the more likely they were to die during the study. This example shows how we can use statistics to *describe* a complex dataset in terms of a much simpler set of numbers; if we had to look at the data from each of the study participants at the same time, we would be overloaded with data and it would be hard to see the pattern that emerges when they are described more simply.

The numbers in Figure 1.1 seem to show that deaths decrease with saturated fat and increase with carbohydrate intake, but we also know that there is a lot of uncertainty in the data; there are some people who died early even though they ate a low-carb diet, and, similarly, some people who ate a ton of carbs but lived to a ripe old age. Given this variability, we want to *decide* whether the relationships that we see in the data are large enough that we wouldn't expect them to occur randomly if there was not truly a relationship between diet and longevity. Statistics provide us with the tools to make these kinds of decisions, and often people from the outside view this as *the* main purpose of statistics. But as we will see throughout the book, this need for black-and-white decisions based on fuzzy evidence has often led researchers astray.

Based on the data we would also like to make predictions about future outcomes. For example, a life insurance company might want to use data about a particular person's intake of fat and carbohydrate to predict how long they are likely to live. An important aspect of prediction is that it requires us to generalize from the data we already have to some other situation, often in the future; if our conclusions were limited to the specific people in the study at a particular time, then the study would not be very useful. In general, researchers must assume that their particular sample is representative of a larger *population*, which requires that they obtain the sample in a way that is unbiased. For example, if the PURE study had recruited all of its participants from religious sects that practice vegetarianism, then we probably wouldn't want to generalize the results to people who follow different dietary standards.

## 1.3 Fundamental concepts of statistics

There are a number of very basic ideas that cut through nearly all aspects of statistical thinking. Several of these are outlined by Stigler (2016) in his outstanding book "The Seven Pillars of Statistical Wisdom", which I have augmented here.

### 1.3.1 Learning from data

One way to think of statistics is as a set of tools that enable us to learn from data. In any situation, we start with a set of ideas or *hypotheses* about what might be the case. In the PURE study, the researchers may have started out with the expectation that eating more fat would lead to higher death rates, given the prevailing negative dogma about saturated fats. Later in the course we will introduce the idea of *prior knowledge*, which is meant to reflect the knowledge that we bring to a situation. This prior knowledge can vary in its strength, often based on our amount of experience; if I visit a restaurant for the first time I am likely to have a weak expectation of how good it will be, but if I visit a restaurant where I have eaten ten times before, my expectations will be much stronger. Similarly, if I look at a restaurant review site and see that a restaurant's average rating of four stars is only based on three reviews, I will have a weaker expectation than I would if it was based on 300 reviews.

Statistics provides us with a way to describe how new data can be best used to update our beliefs, and in this way there are deep links between statistics and psychology. In fact, many theories of human and animal learning from psychology are closely aligned with ideas from the new field of *machine learning*. Machine learning is a field at the interface of statistics and computer science that focuses on how to build computer

algorithms that can learn from experience. While statistics and machine learning often try to solve the same problems, researchers from these fields often take very different approaches; the famous statistician Leo Breiman once referred to them as “The Two Cultures” to reflect how different their approaches can be (Breiman 2001). In this book I will try to blend the two cultures together because both approaches provide useful tools for thinking about data.

### 1.3.2 Aggregation

Another way to think of statistics is “the science of throwing away data”. In the example of the PURE study above, we took more than 100,000 numbers and condensed them into ten. It is this kind of *aggregation* that is one of the most important concepts in statistics. When it was first advanced, this was revolutionary: If we throw out all of the details about every one of the participants, then how can we be sure that we aren’t missing something important?

As we will see, statistics provides us ways to characterize the structure of aggregates of data, and with theoretical foundations that explain why this usually works well. However, it’s also important to keep in mind that aggregation can go too far, and later we will encounter cases where a summary can provide a misleading picture of the data being summarized.

### 1.3.3 Uncertainty

The world is an uncertain place. We now know that cigarette smoking causes lung cancer, but this causation is probabilistic: A 68-year-old man who smoked two packs a day for the past 50 years and continues to smoke has a 15% (1 out of 7) risk of getting lung cancer, which is much higher than the chance of lung cancer in a nonsmoker. However, it also means that there will be many people who smoke their entire lives and never get lung cancer. Statistics provides us with the tools to characterize uncertainty, to make decisions under uncertainty, and to make predictions whose uncertainty we can quantify.

One often sees journalists write that scientific researchers have “proven” some hypothesis. But statistical analysis can never “prove” a hypothesis, in the sense of demonstrating that it must be true (as one would in a mathematical proof). Statistics can provide us with evidence, but it’s always tentative and subject to the uncertainty that is always present in the real world.

### 1.3.4 Sampling

The concept of aggregation implies that we can make useful insights by collapsing across data – but how much data do we need? The idea of *sampling* says that we can summarize an entire population based on just a small number of samples from the population, as long as those samples are obtained in the right way. For example, the PURE study enrolled a sample of about 135,000 people, but its goal was to provide insights about the billions of humans who make up the population from which those people were sampled. As we already discussed above, the way that the study sample is obtained is critical, as it determines how broadly we can generalize the results. Another fundamental insight from statistics about sampling is that while larger samples are always better (in terms of their ability to accurately represent the entire population), there are diminishing returns as the sample gets larger. In fact, the rate at which the benefit of larger samples decreases follows a simple mathematical rule, growing as the square root of the sample size.

## 1.4 Causality and statistics

The PURE study seemed to provide pretty strong evidence for a positive relationship between eating saturated fat and living longer, but this doesn’t tell us what we really want to know: If we eat more saturated fat, will that cause us to live longer? This is because we don’t know whether there is a direct causal relationship

between eating saturated fat and living longer. The data are consistent with such a relationship, but they are equally consistent with some other factor causing both higher saturated fat and longer life. For example, it is likely that people who are richer eat more saturated fat and richer people tend to live longer, but their longer life is not necessarily due to fat intake — it could instead be due to better health care, reduced psychological stress, better food quality, or many other factors. The PURE study investigators tried to account for these factors, but we can't be certain that their efforts completely removed the effects of other variables. The fact that other factors may explain the relationship between saturated fat intake and death is an example of why introductory statistics classes often teach that “correlation does not imply causation”, though the renowned data visualization expert Edward Tufte has added, “but it sure is a hint.”

Although observational research (like the PURE study) cannot conclusively demonstrate causal relations, we generally think that causation can be demonstrated using studies that experimentally control and manipulate a specific factor. In medicine, such a study is referred to as a *randomized controlled trial* (RCT). Let's say that we wanted to do an RCT to examine whether increasing saturated fat intake increases life span. To do this, we would sample a group of people, and then assign them to either a treatment group (which would be told to increase their saturated fat intake) or a control group (who would be told to keep eating the same as before). It is essential that we assign the individuals to these groups randomly. Otherwise, people who choose the treatment might be different in some way than people who choose the control group – for example, they might be more likely to engage in other healthy behaviors as well. We would then follow the participants over time and see how many people in each group died. Because we randomized the participants to treatment or control groups, we can be reasonably confident that there are no other differences between the groups that would *confound* the treatment effect; however, we still can't be certain because sometimes randomization yields treatment versus control groups that *do* vary in some important way. Researchers often try to address these confounds using statistical analyses, but removing the influence of a confound from the data can be very difficult.

A number of RCTs have examined the question of whether changing saturated fat intake results in better health and longer life. These trials have focused on *reducing* saturated fat because of the strong dogma amongst nutrition researchers that saturated fat is deadly; most of these researchers would have probably argued that it was not ethical to cause people to eat *more* saturated fat! However, the RCTs have shown a very consistent pattern: Overall there is no appreciable effect on death rates of reducing saturated fat intake.

## 1.5 Suggested readings

- *The Seven Pillars of Statistical Wisdom*, by Stephen Stigler
- *The Lady Tasting Tea: How Statistics Revolutionized Science in the Twentieth Century*, by David Salsburg
- *Naked Statistics: Stripping the Dread from the Data*, by Charles Wheelan





## Chapter 2

# Working with data

### 2.1 What are data?

The first important point about data is that data *are* - meaning that the word “data” is plural (though some people disagree with me on this). You might also wonder how to pronounce “data” – I say “day-tah” but I know many people who say “dah-tah” and I have been able to remain friends with them in spite of this. Now if I heard them say “the data is” then that would be bigger issue. . .

#### 2.1.1 Qualitative data

Data are composed of *variables*, where a variable reflects a unique measurement or quantity. Some variables are *qualitative*, meaning that they describe a quality rather than a numeric quantity. For example, in my stats course I generally give an introductory survey, both to obtain data to use in class and to learn more about the students. One of the questions that I ask is “What is your favorite food?”, to which some of the answers have been: blueberries, chocolate, tamales, pasta, pizza, and mango. Those data are not intrinsically numerical; we could assign numbers to each one (1=blueberries, 2=chocolate, etc), but we would just be using the numbers as labels rather than as real numbers; for example, it wouldn’t make sense to add the numbers together in this case. However, we will often code qualitative data using numbers in order to make them easier to work with, as you will see later.

#### 2.1.2 Quantitative data

More commonly in statistics we will work with *quantitative* data, meaning data that are numerical. For example, here Table 2.1 shows the results from another question that I ask in my introductory class, which is “Why are you taking this class?”

Table 2.1: Counts of the prevalence of different responses to the question "Why are you taking this class?"

| Why are you taking this class?                      | Number of students |
|---|--------------------|
| It fulfills a degree plan requirement               | 105                |
| It fulfills a General Education Breadth Requirement | 32                 |
| It is not required but I am interested in the topic | 11                 |
| Other   | 4                  |

Note that the students' answers were qualitative, but we generated a quantitative summary of them by counting how many students gave each response.

### 2.1.2.1 Types of numbers

There are several different types of numbers that we work with in statistics. It's important to understand these differences, in part because programming languages like R often distinguish between them.

**Binary numbers.** The simplest are binary numbers – that is, zero or one. We will often use binary numbers to represent whether something is true or false, or present or absent. For example, I might ask 10 people if they have ever experienced a migraine headache. If their answers were:

```
# create variable containing responses to migraine question
```

```
everHadMigraine <- c('Yes', 'No', 'Yes', 'No', 'No', 'No', 'Yes', 'No', 'No', 'No')
everHadMigraine
```

```
## [1] "Yes" "No" "Yes" "No" "No" "No" "Yes" "No" "No" "No"
```

we could instead recode these into truth values, using the `==` symbol which is a test for equality, returning the logical value TRUE if the two things are equal and FALSE if they are not:

```
# create truth values from everHadMigraine variable
```

```
everHadMigraineTF <- everHadMigraine == 'Yes'
everHadMigraineTF
```

```
## [1] TRUE FALSE TRUE FALSE FALSE FALSE TRUE FALSE FALSE FALSE
```

R treats truth values and binary numbers equivalently:

```
# evaluate truth of a set of assertions
```

```
# 1 is equal to TRUE - should return TRUE
TRUE == 1
```

```
## [1] TRUE
```

```
# 0 is equal to FALSE - should return TRUE
FALSE == 0
```

```
## [1] TRUE
```

```
# 0 is equal to true - should return FALSE
TRUE == 0
```

```
## [1] FALSE
```

And we can also turn our list of truth values into integers explicitly:

```
# create integer values from truth values using as.integer()
```

```
everHadMigraineBinary <- as.integer(everHadMigraineTF)
everHadMigraineBinary
```

```
## [1] 1 0 1 0 0 0 1 0 0 0
```

When we get to probability theory we will see a way in which this kind of representation can be very useful.

**Integers.** Integers are whole numbers with no fractional or decimal part. We most commonly encounter integers when we count things, but they also often occur in psychological measurement. For example, in my introductory survey I administer a set of questions about attitudes towards statistics (such as “Statistics

seems very mysterious to me.”), on which the students respond with a number between 1 (“Disagree strongly”) and 7 (“Agree strongly”).

**Real numbers.** Most commonly in statistics we work with real numbers, which have a fractional/decimal part. For example, we might measure someone’s weight, which can be measured to an arbitrary level of precision, from whole pounds down to micrograms.

## 2.2 Scales of measurement

All variables must take on at least two different possible values (otherwise they would be a *constant* rather than a variable), but different values of the variable can relate to each other in different ways, which we refer to as *scales of measurement*. There are four ways in which the different values of a variable can differ.

- *Identity*: Each value of the variable has a unique meaning.
- *Magnitude*: The values of the variable reflect different magnitudes and have an ordered relationship to one another — that is, some values are larger and some are smaller.
- *Equal intervals*: Units along the scale of measurement are equal to one another. This means, for example, that the difference between 1 and 2 would be equal in its magnitude to the difference between 19 and 20.
- *Absolute zero*: The scale has a true meaningful zero point. For example, for many measurements of physical quantities such as height or weight, this is the complete absence of the thing being measured.

There are four different scales of measurement that go along with these different ways that values of a variable can differ.

*Nominal scale.* A nominal variable satisfies the criterion of identity, such that each value of the variable represents something different, but the numbers simply serve as qualitative labels as discussed above. For example, we might ask people for their political party affiliation, and then code those as numbers: 1 = “Republican”, 2 = “Democrat”, 3 = “Libertarian”, and so on. However, the different numbers do not have any ordered relationship with one another.

*Ordinal scale.* An ordinal variable satisfies the criteria of identity and magnitude, such that the values can be ordered in terms of their magnitude. For example, we might ask a person with chronic pain to complete a form every day assessing how bad their pain is, using a 1-7 numeric scale. Note that while the person is presumably feeling more pain on a day when they report a 6 versus a day when they report a 3, it wouldn’t make sense to say that their pain is twice as bad on the former versus the latter day; the ordering gives us information about relative magnitude, but the differences between values are not necessarily equal in magnitude.

*Interval scale.* An interval scale has all of the features of an ordinal scale, but in addition the intervals between units on the measurement scale can be treated as equal. A standard example is physical temperature measured in Celsius or Fahrenheit; the physical difference between 10 and 20 degrees is the same as the physical difference between 90 and 100 degrees, but each scale can also take on negative values.

*Ratio scale.* A ratio scale variable has all four of the features outlined above: identity, magnitude, equal intervals, and absolute zero. The difference between a ratio scale variable and an interval scale variable is that the ratio scale variable has a true zero point. Examples of ratio scale variables include physical height and weight, along with temperature measured in Kelvin.

### 2.2.1 Why do scales of measurement matter?

There are two important reasons that we must pay attention to the scale of measurement of a variable. First, the scale determines what kind of mathematical operations we can apply to the data (see Table 2.2). A nominal variable can only be compared for equality; that is, do two observations on that variable have the

Table 2.2: Different scales of measurement admit different types of numeric operations

|          | Equal/not equal | Greater than/less than | Add/subtract | Multiply/divide |
|----------|-----------------|------------------------|--------------|-----------------|
| Nominal  | OK              |                        |              |                 |
| Ordinal  | OK              | OK                     |              |                 |
| Interval | OK              | OK                     | OK           |                 |
| Ratio    | OK              | OK                     | OK           | OK              |

same numeric value? It would not make sense to apply other mathematical operations to a nominal variable, since they don't really function as numbers in a nominal variable, but rather as labels. With ordinal variables, we can also test whether one value is greater or lesser than another, but we can't do any arithmetic. Interval and ratio variables allow us to perform arithmetic; with interval variables we can only add or subtract values, whereas with ratio variables we can also multiply and divide values.

These constraints also imply that there are certain kinds of statistics that we can compute on each type of variable. Statistics that simply involve counting of different values (such as the most common value, known as the *mode*), can be calculated on any of the variable types. Other statistics are based on ordering or ranking of values (such as the *median*, which is the middle value when all of the values are ordered by their magnitude), and these require that the value at least be on an ordinal scale. Finally, statistics that involve adding up values (such as the average, or *mean*), require that the variables be at least on an interval scale. Having said that, we should note that it's quite common for researchers to compute the mean of variables that are only ordinal (such as responses on personality tests), but this can sometimes be problematic.

## 2.3 What makes a good measurement?

In many fields such as psychology, the thing that we are measuring is not a physical feature, but instead is an unobservable theoretical concept, which we usually refer to as a *construct*. For example, let's say that I want to test how well you understand the distinction between the four different scales of measurement described above. I could give you a pop quiz that would ask you several questions about these concepts and count how many you got right. This test might or might not be a good measurement of the construct of your actual knowledge — for example, if I were to write the test in a confusing way or use language that you don't understand, then the test might suggest you don't understand the concepts when really you do. On the other hand, if I give a multiple choice test with very obvious wrong answers, then you might be able to perform well on the test even if you don't actually understand the material.

It is usually impossible to measure a construct without some amount of error. In the example above, you might know the answer but you might mis-read the question and get it wrong. In other cases there is error intrinsic to the thing being measured, such as when we measure how long it takes a person to respond on a simple reaction time test, which will vary from trial to trial for many reasons. We generally want our measurement error to be as low as possible.

Sometimes there is a standard against which other measurements can be tested, which we might refer to as a “gold standard” — for example, measurement of sleep can be done using many different devices (such as devices that measure movement in bed), but they are generally considered inferior to the gold standard of polysomnography (which uses measurement of brain waves to quantify the amount of time a person spends in each stage of sleep). Often the gold standard is more difficult or expensive to perform, and the cheaper method is used even though it might have greater error.

When we think about what makes a good measurement, we usually distinguish two different aspects of a good measurement.

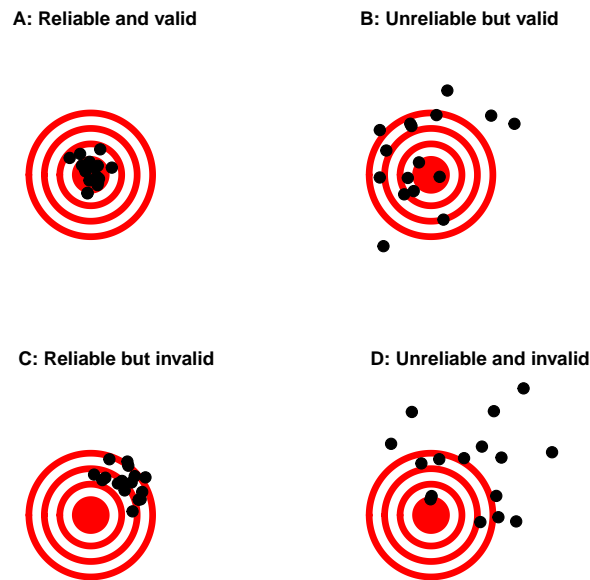


Figure 2.1: A figure demonstrating the distinction between reliability and validity, using shots at a bullseye. Reliability refers to the consistency of location of shots, and validity refers to the accuracy of the shots with respect to the center of the bullseye.

### 2.3.1 Reliability

Reliability quantifies the consistency of our measurements. One common form of reliability, known as “test-retest reliability”, measures how well the measurements agree if the same measurement is performed twice. For example, I might give you a questionnaire about your attitude towards statistics today, repeat this same questionnaire tomorrow, and compare your answers on the two days; we would hope that they would be very similar to one another, unless something happened in between the two tests that should have changed your view of statistics (like reading this book!).

Another way to assess reliability comes in cases where the data includes subjective judgments. For example, let’s say that a researcher wants to determine whether a treatment changes how well an autistic child interacts with other children, which is measured by having experts watch the child and rate their interactions with the other children. In this case we would like to make sure that the answers don’t depend on the rater — that is, we would like for there to be high *inter-rater reliability*. This can be assessed by having more than one rater perform the rating, and then comparing their ratings to make sure that they agree well with one another.

Reliability is important if we want to compare one measurement to another. The relationship between two different measurements can’t be any stronger than the relationship between either of the measurements and itself (i.e., its reliability). This means that an unreliable measure can never have a strong statistical relationship with any other measure. For this reason, researchers developing a new measurement (such as a new survey) will often go to great lengths to test its reliability.

### 2.3.2 Validity

Reliability is important, but on its own it’s not enough: After all, I could create a highly reliable measurement on a personality test by coding every answer using a single number, regardless of how the person answers. We want our measurements to also be *valid* — that is, we want to make sure that we are actually measuring the construct that we think we are measuring (Figure 2.1). There are many different types of validity that are commonly discussed; we will focus on three of them.

*Face validity.* Does the measurement make sense on its face? If I were to tell you that I was going to measure

a person's blood pressure by looking at the color of their tongue, you would probably think that this was not a valid measure on its face. On the other hand, using a blood pressure cuff would have face validity. This is usually a first reality check before we dive into more complicated aspects of validity.

*Construct validity.* Is the measurement related to other measurements in an appropriate way? This is often subdivided into two aspects. *Convergent validity* means that the measurement should be closely related to other measures that are thought to reflect the same construct. Let's say that I am interested in measuring how extroverted a person is using a questionnaire or an interview. Convergent validity would be demonstrated if both of these different measurements are closely related to one another. On the other hand, measurements thought to reflect different constructs should be unrelated, known as *divergent validity*. If my theory of personality says that extraversion and conscientiousness are two distinct constructs, then I should also see that my measurements of extraversion are *unrelated* to measurements of conscientiousness.

*Predictive validity.* If our measurements are truly valid, then they should also be predictive of other outcomes. For example, let's say that we think that the psychological trait of sensation seeking (the desire for new experiences) is related to risk taking in the real world. To test for predictive validity of a measurement of sensation seeking, we would test how well scores on the test predict scores on a different survey that measures real-world risk taking.

## 2.4 Suggested readings

- *An introduction to psychometric theory with applications in R* - A free online textbook on psychological measurement

# Chapter 3

## Probability

Probability theory is the branch of mathematics that deals with chance and uncertainty. It forms an important part of the foundation for statistics, because it provides us with the mathematical tools to describe uncertain events. The study of probability arose in part due to interest in understanding games of chance, like cards or dice. These games provide useful examples of many statistical concepts, because when we repeat these games the likelihood of different outcomes remains (mostly) the same. However, there are deep questions about the meaning of probability that we will not address here; see Suggested Readings at the end if you are interested in learning more about this fascinating topic and its history.

### 3.1 What is probability?

Informally, we usually think of probability as a number that describes the likelihood of some event occurring, which ranges from zero (impossibility) to one (certainty). Sometimes probabilities will instead be expressed in percentages, which range from zero to one hundred, as when the weather forecast predicts a twenty percent chance of rain today. In each case, these numbers are expressing how likely that particular event is.

To formalize probability theory, we first need to define a few terms:

- An **experiment** is any activity that produces or observes an outcome. Examples are flipping a coin, rolling a 6-sided die, or trying a new route to work to see if it's faster than the old route.
- The **sample space** is the set of possible outcomes for an experiment. For a coin flip, the sample space is  $\{H, T\}$  where the brackets represent the sample space and H/T represent heads/tails respectively. For the die, the sample space is  $\{1, 2, 3, 4, 5, 6\}$ . For the amount of time it takes to get to work, the sample space is all possible real numbers greater than zero (since it can't take a negative amount of time to get somewhere, at least not yet).
- An **event** is a subset of the sample space. Here we will focus primarily on *elementary events* which consist of exactly one possible outcome, such as heads in a coin flip, a roll of 4 in dice, or 21 minutes to get home by the new route.

Now that we have those definitions, we can outline the formal features of a probability, which were first defined by the Russian mathematician Andrei Kolmogorov. If  $P(X_i)$  is the probability of event  $X_i$ :

- Probability cannot be negative:  $P(X_i) \geq 0$
- The total probability of all outcomes in the sample space is 1. We can express this using the summation symbol  $\sum$ :

$$\sum_{i=1}^N P(X_i) = P(X_1) + P(X_2) + \dots + P(X_N) = 1$$

This is interpreted as saying “Take all of the  $N$  elementary events, which we have labeled from 1 to  $N$ , and add up their probabilities. These must sum to one.” An implication of this is that the probability of any individual event cannot be greater than one:  $P(X_i) \leq 1$

## 3.2 How do we determine probabilities?

Now that we know what a probability is, how do we actually figure out what the probability is for any particular event?

### 3.2.1 Personal opinion

Let’s say that I asked you what the probability was that Bernie Sanders would have won the US Presidential Election in 2016 if he had gained the Democratic nomination instead of Hillary Clinton. Here the sample space is {Sanders wins, Sanders loses}, but we can’t actually do the experiment to find the outcome. However, most people with knowledge of the election would be willing to offer a guess at the probability of this event. In many cases personal knowledge and/or opinion is the only guide we have determining the probability of an event, but this is not very scientifically satisfying.

### 3.2.2 Empirical frequency

Another way to determine the probability of an event is to do the experiment many times and count how often each event happens. From the relative frequency of the different outcomes, we can compute the probability of each. For example, let’s say that we are interested in knowing the probability of rain in San Francisco. We first have to define the experiment — let’s say that we will look at the National Weather Service data for each day in 2017 (which can be downloaded from <https://www.ncdc.noaa.gov/>) and determine whether there was any rain at the downtown San Francisco weather station.

```
# load data on rain in San Francisco and compute probability
SFrain <- read_csv("data/SanFranciscoRain/1329219.csv")

# create a new variable indicating whether it rained on each day
SFrain <-
  SFrain %>%
  mutate(rainToday = as.integer(PRCP > 0))

SFrain_summary <-
  SFrain %>%
  summarize(
    nRainyDays = sum(rainToday),
    nDaysMeasured = n(),
    pRainInSF = nRainyDays / nDaysMeasured
  )

pander(SFrain_summary)
```

| nRainyDays | nDaysMeasured | pRainInSF |
|------------|---------------|-----------|
| 73         | 365           | 0.2       |

According to these data, in 2017 there were 73 rainy days. To compute the probability of rain in San Francisco, we simply divide the number of rainy days by the number of days counted (365), giving  $P(\text{rain in SF in } 2017) = 0.2$ .



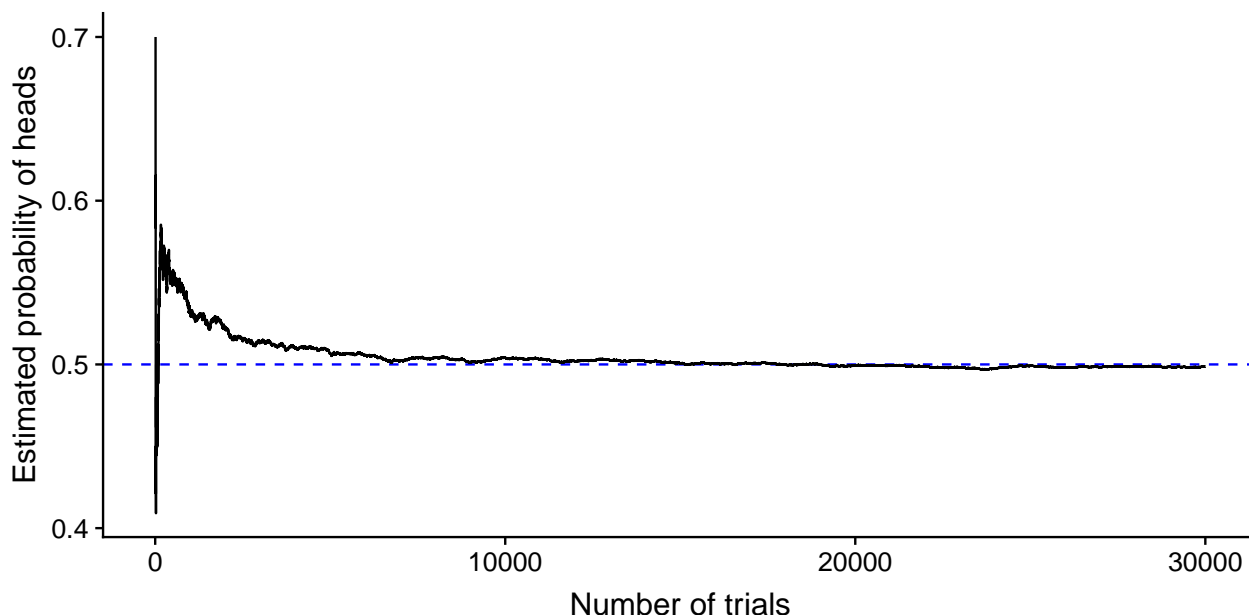


Figure 3.1: A demonstration of the law of large numbers. A coin was flipped 30,000 times, and after each flip the probability of heads was computed based on the number of heads and tail collected up to that point. It takes about 15,000 flips for the probability to settle at the true probability of 0.5.

2017)=0.2.

How do we know that empirical probability gives us the right number? The answer to this question comes from the *law of large numbers*, which shows that the empirical probability will approach the true probability as the sample size increases. We can see this by simulating a large number of coin flips, and looking at our estimate of the probability of heads after each flip. We will spend much more time discussing simulation in a later chapter; for now, just assume that we have a computational way to generate a random outcome for each coin flip.

Figure 3.1 shows that as the number of samples (i.e., coin flip trials) increases, the estimated probability of heads converges onto the true value of 0.5. However, note that the estimates can be very far off from the true value when the sample sizes are small. A real-world example of this was seen in the 2017 special election for the US Senate in Georgia, which pitted the Republican Roy Moore against Democrat Doug Jones. Figure 3.2 shows the relative amount of the vote reported for each of the candidates over the course of the evening, as an increasing number of ballots were counted. Early in the evening the vote counts were especially volatile, swinging from a large initial lead for Jones to a long period where Moore had the lead, until finally Jones took the lead to win the race.

These two examples show that while large samples will ultimately converge on the true probability, the results with small samples can be far off. Unfortunately, many people forget this and overinterpret results from small samples. This was referred to as the *law of small numbers* by the psychologists Danny Kahneman and Amos Tversky, who showed that people (even trained researchers) often behave as if the law of large numbers applies even to small samples, giving too much credence to results from small datasets. We will see examples throughout the course of just how unstable statistical results can be when they are generated on the basis of small samples.

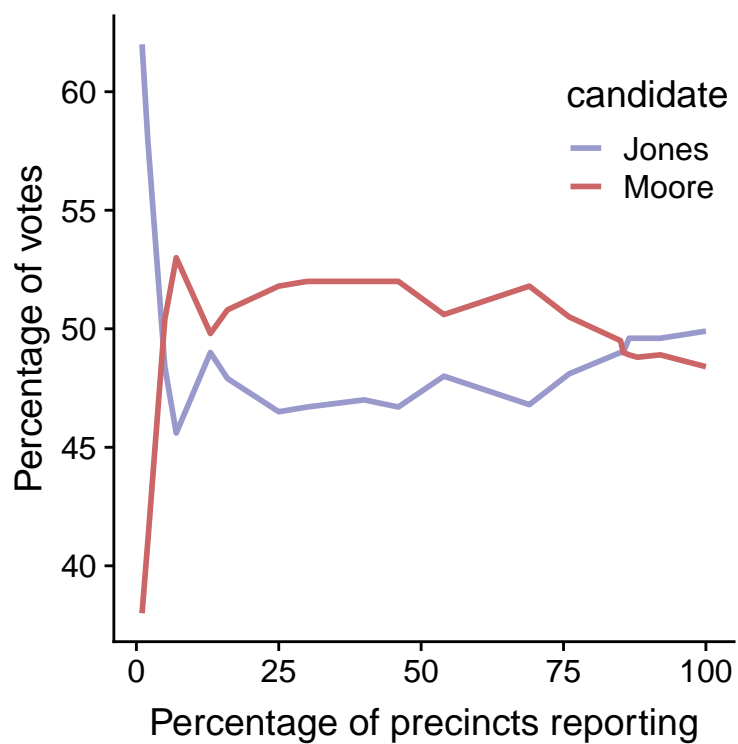


Figure 3.2: Relative proportion of the vote in the Dec 12, 2017 special election for the US Senate seat in Georgia, as a function of the percentage of precincts reporting. These data were transcribed from <https://www.ajc.com/news/national/alabama-senate-race-live-updates-roy-moore-doug-jones/KPRfkdaewoiXICW3FHjXqI/>

### 3.2.3 Classical probability

It's unlikely that any of us has ever flipped a coin tens of thousands of times, but we are nonetheless willing to believe that the probability of flipping heads is 0.5. This reflects the use of yet another approach to computing probabilities, which we refer to as *classical probability*. In this approach, we compute the probability directly based on our knowledge of the situation.

Classical probability arose from the study of games of chance such as dice and cards. A famous example arose from a problem encountered by a French gambler who went by the name of Chevalier de Méré. de Méré played two different dice games: In the first he bet on the chance of at least one six on four rolls of a six-sided die, while in the second he bet on the chance of at least one double-six on 24 rolls of two dice. He expected to win money on both of these gambles, but he found that while on average he won money on the first gamble, he actually lost money on average when he played the second gamble many times. To understand this he turned to his friend, the mathematician Blaise Pascal, who is now recognized as one of the founders of probability theory.

How can we understand this question using probability theory? In classical probability, we start with the assumption that all of the elementary events in the sample space are equally likely; that is, when you roll a die, all of the possible outcomes ( $\{1,2,3,4,5,6\}$ ) are equally likely to occur. (No loaded dice allowed!) Given this, we can compute the probability of any individual outcome as:

$$P(\text{outcome}_i) = \frac{1}{\text{number of possible outcomes}}$$

For the six-sided die, the probability of each individual outcome is  $1/6$ .

This is nice, but de Méré was interested in more complex events, like what happens on multiple dice throws. How do we compute the probability of a complex event (which is a union of single events), like rolling a one on the first *or* the second throw? de Méré thought (incorrectly, as we will see below) that he could simply add together the probabilities of the individual events to compute the probability of the combined event, meaning that the probability of rolling a one on the first or second roll would be computed as follows:

$$P(\text{Roll1}_{\text{throw1}} \cup \text{Roll1}_{\text{throw2}}) = P(\text{Roll1}_{\text{throw1}}) + P(\text{Roll1}_{\text{throw2}}) = 1/6 + 1/6 = 1/3$$

De Méré reasoned based on this that the probability of at least one six in four rolls was the sum of the probabilities on each of the individual throws:  $4 * \frac{1}{6} = \frac{2}{3}$ . Similarly, he reasoned that since the probability of a double-six in throws of dice is  $1/36$ , then the probability of at least one double-six on 24 rolls of two dice would be  $24 * \frac{1}{36} = \frac{2}{3}$ . Yet, while he consistently won money on the first bet, he lost money on the second bet. What gives?

To understand de Méré's error, we need to introduce some of the rules of probability theory. The first is the *rule of subtraction*, which says that:

$$P(\bar{A}) = 1 - P(A)$$

where  $\bar{A}$  means "not A". This rule derives directly from the axioms that we discussed above; since A and  $\bar{A}$  are the only possible outcomes, then their total probability must sum to 1. For example, if the probability of rolling a one in a single throw is  $\frac{1}{6}$ , then the probability of rolling anything other than a one is  $\frac{5}{6}$ .

A second rule tells us how to compute the probability of a conjoint event – that is, the probability of both of two events occurring. This version of the rule tells us how to compute this quantity in the special case when the two events are independent from one another; we will learn later exactly what the concept of *independence* means, but for now we can just take it for granted that the two die throws are independent events.

$$P(A \cap B) = P(A) * P(B) \text{ iff } A \text{ and } B \text{ are independent}$$



### 3.2.4 Solving de Méré's problem

Blaise Pascal used the rules of probability to come up with a solution to de Méré's problem. First, he realized that computing the probability of at least one event out of a combination was tricky, whereas computing the probability that something does not occur across several events is relatively easy – it's just the product of the probabilities of the individual events. Thus, rather than computing the probability of at least one six in four rolls, he instead computed the probability of no sixes across all rolls:

$$P(\text{no sixes in four rolls}) = \frac{5}{6} * \frac{5}{6} * \frac{5}{6} * \frac{5}{6} = \left(\frac{5}{6}\right)^4 = 0.482$$

He then used the fact that the probability of no sixes in four rolls is the complement of at least one six in four rolls (thus they must sum to one), and used the rule of subtraction to compute the probability of interest:

$$P(\text{at least one six in four rolls}) = 1 - \left(\frac{5}{6}\right)^4 = 0.517$$

de Méré's gamble that he would throw at least one six in four rolls has a probability of greater than 0.5, explaining why de Méré made money on this bet on average.

But what about de Méré's second bet? Pascal used the same trick:

$$P(\text{no double six in 24 rolls}) = \left(\frac{35}{36}\right)^{24} = 0.509$$

$$P(\text{at least one double six in 24 rolls}) = 1 - \left(\frac{35}{36}\right)^{24} = 0.491$$

The probability of this outcome was slightly below 0.5, showing why de Méré lost money on average on this bet.

## 3.3 Probability distributions

We often want to be able to quantify the probability of any possible value in an experiment. For example, on Jan 20 2018, the basketball player Steph Curry hit only 2 out of 4 free throws in a game against the Houston Rockets. We know that Curry's overall probability of hitting free throws across the entire season was 0.91, so it seems pretty unlikely that he would hit only 50% of his free throws in a game, but exactly how unlikely is it? We can determine this using a theoretical probability distribution; during this course we will encounter a number of these probability distributions, each of which is appropriate to describe different types of data. In this case, we use the *binomial* distribution, which provides a way to compute the probability of some number of successes out of a number of "Bernoulli trials" (i.e. trials on which there is either success or failure and nothing in between) given some known probability of success on each trial. This distribution is defined as:

$$P(k; n, p) = P(X = k) = \binom{n}{k} p^k (1 - p)^{n-k}$$

This refers to the probability of  $k$  successes on  $n$  trials when the probability of success is  $p$ . You may not be familiar with  $\binom{n}{k}$ , which is referred to as the *binomial coefficient*. The binomial coefficient is also referred to as "n-choose-k" because it describes the number of different ways that one can choose  $k$  items out of  $n$  total items. The binomial coefficient is computed as:

$$\binom{n}{k} = \frac{n!}{k!(n-k)!}$$

where the explanation point (!) refers to the *factorial* of the number:

$$n! = \prod_{i=1}^n i = n * (n-1) * \dots * 2 * 1$$

In the example of Steph Curry's free throws:

$$P(2; 4, 0.91) = \binom{4}{2} 0.91^2 (1 - 0.91)^{4-2} = 0.040$$

This shows that given Curry's overall free throw percentage, it is very unlikely that he would hit only 2 out of 4 free throws. Which just goes to show that unlikely things do actually happen in the real world.

### 3.3.1 Cumulative probability distributions

Often we want to know not just how likely a specific value is, but how likely it is to find a value that is as extreme or more than a particular value. To answer this question, we can use a *cumulative* probability distribution; whereas a standard probability distribution tells us the probability of some specific value, the cumulative distribution tells us the probability of a value as large or larger (or as small or smaller) than some specific value.

In the free throw example, we might want to know: What is the probability that Steph Curry hits 2 *or fewer* free throws out of four, given his overall free throw probability of 0.91. To determine this, we could simply use the binomial probability equation and plug in all of the possible values of k:

$$P(k \leq 2) = P(k = 2) + P(k = 1) + P(k = 0) = 6e^{-5} + .002 + .040 = .043$$

In many cases the number of possible outcomes would be too large for us to compute the cumulative probability by enumerating all possible values; fortunately, it can be computed directly. For the binomial, we can do this in R using the `pbinom()` function:

```
# compute cumulative probability distribution for Curry's free throws

tibble(
  numSuccesses = seq(0, 4)
) %>%
  mutate(
    probability = pbinom(numSuccesses, size = 4, prob = 0.91)
  ) %>%
  pander()
```

| numSuccesses | probability |
|--------------|-------------|
| 0            | 0           |
| 1            | 0.003       |
| 2            | 0.043       |
| 3            | 0.314       |
| 4            | 1           |

From this we can see that the probability of Curry landing 2 or fewer free throws out of 4 attempts is 0.043.

## 3.4 Conditional probability

So far we have limited ourselves to simple probabilities - that is, the probability of a single event or combination of events. However, we often wish to determine the probability of some event given that some other event has occurred, which are known as *conditional probabilities*.

Let's take the 2016 US Presidential election as an example. There are two simple probabilities that we could use to describe the electorate. First, we know the probability that a voter in the US affiliated with the Republican party:  $p(\text{Republican}) = 0.44$ . We also know the probability that a voter cast their vote in favor of Donald Trump:  $p(\text{Trumpvoter}) = 0.46$ . However, let's say that we want to know the following: What is the probability that a person cast their vote for Donald Trump, *given that they are a Republican*?

To compute the conditional probability of A given B (which we write as  $P(A|B)$ , "probability of A, given B"), we need to know the *joint probability* (that is, the probability A and B) as well as the overall probability of B:

$$P(A|B) = \frac{P(A \cap B)}{P(B)}$$

That is, we want to know the probability that both things are true, given that the one being conditioned upon is true.

It can be useful to think of this is graphically. Figure 3.4 shows a flow chart depicting how the full population of voters breaks down into Republicans and Democrats, and how the conditional probability (conditioning on party) further breaks down the members of each party according to their vote.

## 3.5 Computing conditional probabilities from data

For many examples in this course we will use data obtained from the National Health and Nutrition Examination Survey (NHANES). NHANES is a large ongoing study organized by the US Centers for Disease Control that is designed to provide an overall picture of the health and nutritional status of both adults and children in the US. Every year, the survey examines a sample of about 5000 people across the US using both interviews and physical and medical tests. The NHANES data is included as a package in R, making it easy to access and work with. It also provides us with a large, realistic dataset that will serve as an example for many different statistical tools.

Let's say that we are interested in the following question: What is the probability that someone has diabetes, given that they are not physically active? - that is,  $P(\text{diabetes}|\text{inactive})$ . NHANES records two variables that address the two parts of this question. The first (**Diabetes**) asks whether the person has ever been told that they have diabetes, and the second (**PhysActive**) records whether the person engages in sports, fitness, or recreational activities that are at least of moderate intensity. Let's first compute the simple probabilities.

```
# Summarize NHANES data for diabetes and physical activity

# drop duplicated IDs within the NHANES dataset
NHANES_diabetes_activity <-
  NHANES %>%
  distinct(ID, .keep_all = TRUE) %>%
  drop_na(PhysActive, Diabetes)

pander('Summary data for diabetes')
```

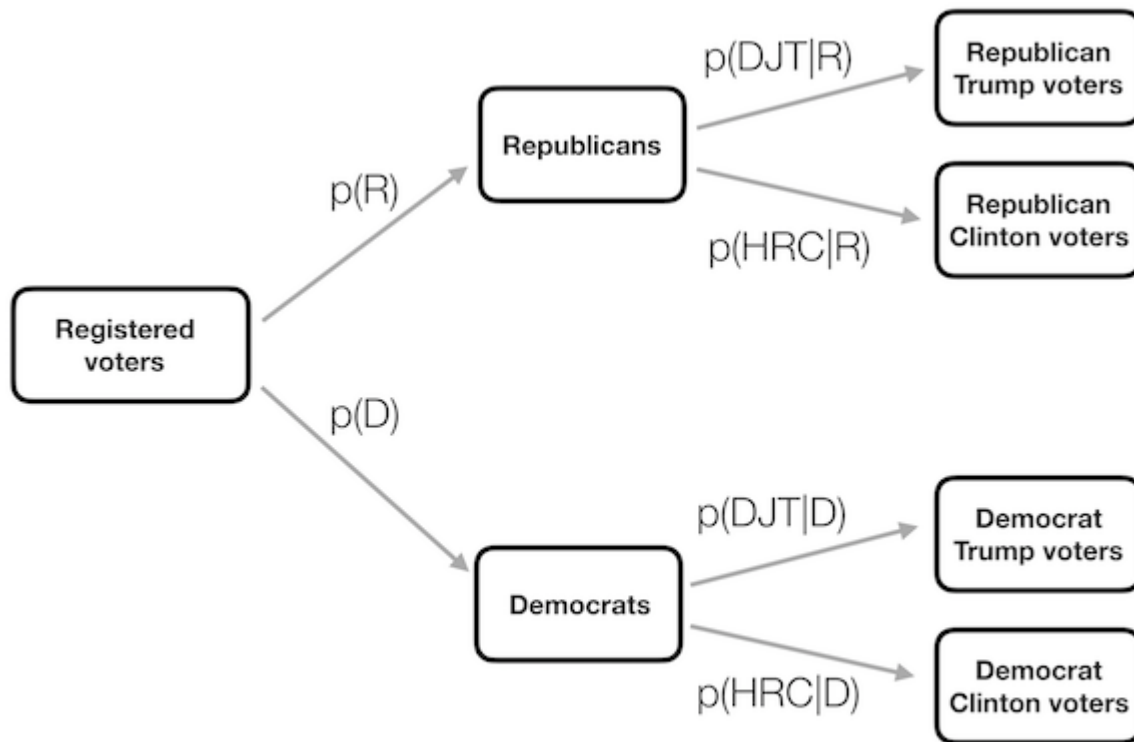


Figure 3.4: A graphical depiction of conditional probability, showing how the conditional probability limits our analysis to a subset of the data.



Summary data for diabetes

```
NHANES_diabetes_activity %>%
  count(Diabetes) %>%
  mutate(
    prob = n / sum(n)
  ) %>%
  pander()
```

| Diabetes | n    | prob  |
|----------|------|-------|
| No       | 4893 | 0.899 |
| Yes      | 550  | 0.101 |

```
pander('Summary data for physical activity')
```

Summary data for physical activity

```
NHANES_diabetes_activity %>%
  count(PhysActive) %>%
  mutate(
    prob = n / sum(n)
  ) %>%
  pander()
```

| PhysActive | n    | prob  |
|------------|------|-------|
| No         | 2472 | 0.454 |
| Yes        | 2971 | 0.546 |

This shows that the probability that someone in the NHANES dataset has diabetes is .101, and the probability that someone is inactive is .454.

To compute  $P(\text{diabetes}|\text{inactive})$  we would also need to know the joint probability of being diabetic *and* inactive, in addition to the simple probabilities of each:

```
# compute joint probabilities for diabetes and physical activity
```

```
NHANES_diabetes_stats_by_activity <-
  NHANES_diabetes_activity %>%
  count(Diabetes, PhysActive) %>%
  mutate(
    prob = n / sum(n)
  )
```

```
pander(NHANES_diabetes_stats_by_activity)
```

| Diabetes | PhysActive | n    | prob  |
|----------|------------|------|-------|
| No       | No         | 2123 | 0.39  |
| No       | Yes        | 2770 | 0.509 |
| Yes      | No         | 349  | 0.064 |
| Yes      | Yes        | 201  | 0.037 |

Based on these joint probabilities, we can compute  $P(\text{diabetes}|\text{inactive})$ :

```
# compute conditional probability p(diabetes|inactive)

P_inactive <-
  NHANES_diabetes_activity %>%
    summarise(
      mean(PhysActive == "No")
    ) %>%
    pull()

P_diabetes_and_inactive <-
  NHANES_diabetes_stats_by_activity %>%
    dplyr::filter(Diabetes == "Yes", PhysActive == "No") %>%
    pull(prob)

P_diabetes_given_inactive <-
  P_diabetes_and_inactive / P_inactive

P_diabetes_given_inactive

## [1] 0.1411812
```

The first line of code in this chunk computed  $P(\text{inactive})$  by taking the mean of a test for whether the `PhysActive` variable was equal to “No” for each individual. This trick works because TRUE/FALSE values are treated as 1/0 respectively by R; thus, if we want to know the probability of some event, we can generate a Boolean variable that tests for that event, and then simply take the mean of that variable. We then use that value to compute the conditional probability, where we find that the probability of someone having diabetes given that they are physically inactive is 0.141.

## 3.6 Independence

The term “independent” has a very specific meaning in statistics, which is somewhat different from the common usage of the term. Statistical independence between two variables means that knowing the value of one variable doesn’t tell us anything about the value of the other. This can be expressed as:

$$P(A|B) = P(A)$$

That is, the probability of A given some value of B is just the same as the overall probability of A. Looking at it this way, we see that many cases of what we would call “independence” in the world are not actually statistically independent. For example, there is currently a move by a small group of California citizens to declare a new independent state called Jefferson, which would comprise a number of counties in northern California and Oregon. If this were to happen, then the probability that a current California resident would now live in the state of Jefferson would be  $P(\text{Jefferson}) = 0.014$ , whereas the probability that they would remain a California resident would be  $P(\text{California}) = 0.986$ . The new states might be politically independent, but they would *not* be statistically independent, because  $P(\text{California}|\text{Jefferson}) = 0$ ! That is, while independence in common language often refers to sets that are exclusive, statistical independence refers to the case where one cannot predict anything about one variable from the value of another variable. For example, knowing a person’s hair color is unlikely to tell you whether they prefer chocolate or strawberry ice cream.

Let’s look at another example, using the NHANES data: Are physical health and mental health independent of one another? NHANES includes two relevant questions: *PhysActive*, which asks whether the individual is physically active, and *DaysMentHlthBad*, which asks how many days out of the last 30 that the individual

experienced bad mental health. We will define a new variable called `badMentalHealth` as having more than 7 days of bad mental health in the last month, and then determine whether they are independent by asking whether the simple probability of bad mental health is different from the conditional probability of bad mental health given that one is physically active.

```
# compute probabilities for mental health and physical activity
NHANES_adult <-
  NHANES %>%
  dplyr::filter(
    Age >= 18,
    !is.na(PhysActive),
    !is.na(DaysMentHlthBad)
  ) %>%
  mutate(badMentalHealth = DaysMentHlthBad > 7)

NHANES_MentalHealth_summary <-
  NHANES_adult %>%
  summarize(badMentalHealth = mean(badMentalHealth))

pander(NHANES_MentalHealth_summary)
```

| badMentalHealth |
|-----------------|
| 0.164           |

```
NHANES_MentalHealth_by_PhysActive <-
  NHANES_adult %>%
  group_by(PhysActive) %>%
  summarize(badMentalHealth = mean(badMentalHealth))

pander(NHANES_MentalHealth_by_PhysActive)
```

| PhysActive | badMentalHealth |
|------------|-----------------|
| No         | 0.2             |
| Yes        | 0.132           |

From this we see that  $P(\text{bad mental health})$  is 0.1640567 while  $P(\text{bad mental health}|\text{physically active})$  is 0.1320808. Thus, it seems that the conditional probability is somewhat smaller than the overall probability, suggesting that they are not independent, though we can't know for sure just by looking at the numbers. Later in the course we will encounter tools that will let us more directly quantify whether two variables are independent.

### 3.7 Reversing a conditional probability: Bayes' rule

In many cases, we know  $P(A|B)$  but we really want to know  $P(B|A)$ . This commonly occurs in medical screening, where we know  $P(\text{positive test result}|\text{disease})$  but what we want to know is  $P(\text{disease}|\text{positive test result})$ . For example, some doctors recommend that men over the age of 50 undergo screening using a test called prostate specific antigen (PSA) to screen for possible prostate cancer. Before a test is approved for use in medical practice, the manufacturer needs to test two aspects of the test's performance. First, they need to show how *sensitive* it is – that is, how likely is it to find the disease when it is present:  $\text{sensitivity} = P(\text{positive test}|\text{disease})$ . They also need to show how *specific* it is: that is, how likely is it to give a negative result when there is

no disease present: specificity =  $P(\text{negative test}|\text{no disease})$ . For the PSA test, we know that sensitivity is about 80% and specificity is about 70%. However, these don't answer the question that the physician wants to answer for any particular patient: what is the likelihood that they actually have cancer, given that the test comes back positive? This requires that we reverse the conditional probability that defines sensitivity: instead of  $P(\text{positive test}|\text{disease})$  we want to know  $P(\text{disease}|\text{positive test})$ .

In order to reverse a conditional probability, we can use *Bayes' rule*:

$$P(B|A) = \frac{P(A|B) * P(B)}{P(A)}$$

Bayes' rule is fairly easy to derive, based on the rules of probability that we learned earlier in the chapter. First, remember the rule for computing a conditional probability:

$$P(A|B) = \frac{P(A \cap B)}{P(B)}$$

We can rearrange this to get the formula to compute the joint probability using the conditional:

$$P(A \cap B) = P(A|B) * P(B)$$

Using this we can compute the inverse probability:

$$P(B|A) = \frac{P(A \cap B)}{P(A)} = \frac{P(A|B) * P(B)}{P(A)}$$

If we have only two outcomes, we can express this in a somewhat clearer way, using the sum rule to redefine  $P(A)$ :

$$P(A) = P(A|B) * P(B) + P(A|\neg B) * P(\neg B)$$

Using this, we can redefine Bayes's rule:

$$P(B|A) = \frac{P(A|B) * P(B)}{P(A|B) * P(B) + P(A|\neg B) * P(\neg B)}$$

We can plug the relevant numbers into this equation to determine the likelihood that an individual with a positive PSA result actually has cancer – but note that in order to do this, we also need to know the overall probability of cancer in the person, which we often refer to as the *base rate*. Let's take a 60 year old man, for whom the probability of prostate cancer in the next 10 years is  $P(\text{cancer}) = 0.058$ . Using the sensitivity and specificity values that we outlined above, we can compute the individual's likelihood of having cancer given a positive test:

$$\begin{aligned} P(\text{cancer}|\text{test}) &= \frac{P(\text{test}|\text{cancer}) * P(\text{cancer})}{P(\text{test}|\text{cancer}) * P(\text{cancer}) + P(\text{test}|\neg\text{cancer}) * P(\neg\text{cancer})} \\ &= \frac{0.8 * 0.058}{0.8 * 0.058 + 0.3 * 0.942} = 0.14 \end{aligned}$$

That's pretty small – do you find that surprising? Many people do, and in fact there is a substantial psychological literature showing that people systematically neglect *base rates* (i.e. overall prevalence) in their judgments.

## 3.8 Learning from data

Another way to think of Bayes' rule is as a way to update our beliefs on the basis of data – that is, learning about the world using data. Let's look at Bayes' rule again:

$$P(B|A) = \frac{P(A|B) * P(B)}{P(A)}$$

The different parts of Bayes' rule have specific names, that relate to their role in using Bayes rule to update our beliefs. We start out with an initial guess about the probability of B ( $P(B)$ ), which we refer to as the *prior* probability. In the PSA example we used the base rate for the prior, since it was our best guess before we knew the test result. We then collect some data, which in our example was the test result. The degree to which the data A are consistent with outcome B is given by  $P(A|B)$ , which we refer to as the *likelihood*. You can think of this as how likely the data are, given the particular hypothesis being tested. In our example, the hypothesis being tested was whether the individual had cancer, and the likelihood was based on our knowledge about the specificity of the test. The denominator ( $P(A)$ ) is referred to as the *marginal likelihood*, because it expresses the overall likelihood of the data, averaged across all of the possible values of A (which in our example were the positive and negative test results). The outcome to the left ( $P(B|A)$ ) is referred to as the *posterior* - because it's what comes out the back end of the computation.

There is a another way of writing Bayes rule that makes this a bit clearer:

$$P(B|A) = \frac{P(A|B)}{P(A)} * P(B)$$

The part on the left ( $\frac{P(A|B)}{P(A)}$ ) tells us how much more or less likely the data A are given B, relative to the overall (marginal) likelihood of the data, while the part on the right side ( $P(B)$ ) tells us how likely we think B is (before we know anything about the data). This makes it clearer that the role of Bayes theorem is to update our prior knowledge based on the degree to which the data are more likely given B than they would be overall.

## 3.9 Odds and odds ratios

The result in the last section showed that the likelihood that the individual has cancer based on a positive PSA test result is still fairly low, even though it's more than twice as big as it was before we knew the test result. We would often like to quantify the relation between probabilities more directly, which we can do by converting them into *odds* which express the relative likelihood of something happening or not:

$$\text{odds of A} = \frac{P(A)}{P(\neg A)}$$

In our PSA example, the odds of having cancer (given the positive test) are:

$$\text{odds of cancer} = \frac{P(\text{cancer})}{P(\neg \text{cancer})} = \frac{0.14}{1 - 0.14} = 0.16$$

This tells us that the that the odds are fairly low of having cancer, even though the test was positive. For comparison, the odds of rolling a 6 in a single dice throw are:

$$\text{odds of 6} = \frac{1}{5} = 0.2$$

As an aside, this is a reason why many medical researchers have become increasingly wary of the use of widespread screening tests for relatively uncommon conditions; most positive results will turn out to be false positives.

We can also use odds to compare different probabilities, by computing what is called an *odds ratio* - which is exactly what it sounds like. For example, let's say that we want to know how much the positive test increases the individual's odds of having cancer. We can first compute the *prior odds* - that is, the odds before we knew that the person had tested positively. These are computed using the base rate:

$$\text{prior odds} = \frac{P(\text{cancer})}{P(\neg\text{cancer})} = \frac{0.058}{1 - 0.058} = 0.061$$

We can then compare these with the posterior odds, which are computed using the posterior probability:

$$\text{odds ratio} = \frac{\text{posterior odds}}{\text{prior odds}} = \frac{0.16}{0.061} = 2.62$$

This tells us that the odds of having cancer are increased by 2.62 given the positive test result.

### 3.10 What do probabilities mean?

It might strike you that it is a bit odd to talk about the odds of a person having cancer depending on a test result; after all, the person either has cancer or they don't. Historically, there have been two different ways that probabilities have been interpreted. The first (known as the *frequentist* interpretation) interprets probabilities in terms of long-run frequencies. For example, in the case of a coin flip, it would reflect the relative frequencies of heads in the long run after a large number of flips. While this interpretation might make sense for events that can be repeated many times like a coin flip, it makes less sense for events that will only happen once, like an individual person's life or a particular presidential election; and as the economist John Maynard Keynes famously said, "In the long run, we are all dead."

The other interpretation of probabilities (known as the *Bayesian* interpretation) is as a degree of belief in a particular proposition. If I were to ask you "How likely is it that the US will return to the moon by 2026", you can provide an answer to this question based on your knowledge and beliefs, even though there are no relevant frequencies to compute a frequentist probability. One way that we often frame subjective probabilities is in terms of one's willingness to accept a particular gamble. For example, if you think that the probability of the US landing on the moon by 2026 is 0.1 (i.e. odds of 9 to 1), then that means that you should be willing to accept a gamble that would pay off with anything more than 9 to 1 odds if the event occurs.

As we will see, these two different definitions of probability are very relevant to the two different ways that statisticians think about testing statistical hypotheses, which we will encounter in later chapters.

### 3.11 Suggested readings

- *The Drunkard's Walk: How Randomness Rules Our Lives*, by Leonard Mlodinow

## Chapter 4

# Summarizing data

In this Chapter we will discuss why and how to summarize data.

### 4.1 Why summarize data?

When we summarize data, we are necessarily throwing away information, and there are many conceivable objections to this. As an example, let's go back to the PURE study that we discussed in Chapter 1. Are we not supposed to believe that all of the details about each individual matter, beyond those that are summarized in the dataset? What about the specific details of how the data were collected, such as the time of day or the mood of the participant? All of these details are lost when we summarize the data.

We summarize data in general because it provides us with a way to *generalize* - that is, to make general statements that extend beyond specific observations. The importance of generalization was highlighted by the writer Jorge Luis Borges in his short story “Funes the Memorious”, which describes an individual who loses the ability to forget. Borges focuses in on the relation between generalization (i.e. throwing away data) and thinking: “To think is to forget a difference, to generalize, to abstract. In the overly replete world of Funes, there were nothing but details.”

Psychologists have long studied all of the ways in which generalization is central to thinking. One example is categorization: We are able to easily recognize different examples of the category of “birds” even though the individual examples may be very different in their surface features (such as an ostrich, a robin, and a chicken). Importantly, generalization lets us make predictions about these individuals – in the case of birds, we can predict that they can fly and eat worms, and that they probably can't drive a car or speak English. These predictions won't always be right, but they are often good enough to be useful in the world.

### 4.2 Summarizing data using tables

A simple way to summarize data is to generate a table representing counts of various types of observations. This type of table has been used for thousands of years (see Figure 4.1).

Let's look at some examples of the use of tables, again using the NHANES dataset. Type the command `help(NHANES)` in the RStudio console, and scroll through the help page, which should open within the Help panel if you are using RStudio. This page provides some information about the dataset as well as a listing of all of the variables included in the dataset. Let's have a look at a simple variable, called “PhysActive” in the dataset. This variable contains one of three different values: “Yes” or “No” (indicating whether or not the person reports doing “moderate or vigorous-intensity sports, fitness or recreational activities”), or “NA” if the data are missing for that individual. There are different reasons that the data might be missing; for



Figure 4.1: A Sumerian tablet from the Louvre, showing a sales contract for a house and field. Public domain, via Wikimedia Commons.

example, this question was not asked of children younger than 12 years of age, while in other cases an adult may have declined to answer the question during the interview.

### 4.2.1 Frequency distributions

Let’s look at how many people fall into each of these categories. Don’t worry right now about exactly how R is doing this; we will come back to that later.

```
# summarize physical activity data

PhysActive_table <- NHANES %>%
  dplyr::select(PhysActive) %>%
  group_by(PhysActive) %>%
  summarize(AbsoluteFrequency = n())

pander(PhysActive_table)
```

| PhysActive | AbsoluteFrequency |
|------------|-------------------|
| No         | 2473              |
| Yes        | 2972              |
| NA         | 1334              |

The R code in this cell generates a table showing the frequencies of each of the different values; there were 2473 individuals who responded “No” to the question, 2972 who responded “Yes”, and 1334 for whom no response was given. We call this a *frequency distribution* because it tells us how each of the values is distributed across the sample.

Since we only want to work with people who gave an answer to the question, let’s filter the dataset to only include individuals who responded to this question.

```
# summarize physical activity data after dropping NA values using drop_na()

NHANES %>%
  drop_na(PhysActive) %>%
  dplyr::select(PhysActive) %>%
  group_by(PhysActive) %>%
  summarize(AbsoluteFrequency = n()) %>%
  pander()
```



```
# compute relative frequency of physical activity categories
```

```
NHANES %>%
  drop_na(PhysActive) %>%
  dplyr::select(PhysActive) %>%
  group_by(PhysActive) %>%
  summarize(AbsoluteFrequency = n()) %>%
  mutate(RelativeFrequency = AbsoluteFrequency / sum(AbsoluteFrequency)) %>%
  pander()
```

| PhysActive | AbsoluteFrequency | RelativeFrequency |
|------------|-------------------|-------------------|
| No         | 2473              | 0.454             |
| Yes        | 2972              | 0.546             |

The relative frequency provides a much easier way to see how big the imbalance is. We can also interpret the relative frequencies as percentages by multiplying them by 100:

```
# compute percentages for physical activity categories
```

```
PhysActive_table_filtered <- NHANES %>%
  drop_na(PhysActive) %>%
  dplyr::select(PhysActive) %>%
  group_by(PhysActive) %>%
  summarize(AbsoluteFrequency = n()) %>%
  mutate(
    RelativeFrequency = AbsoluteFrequency / sum(AbsoluteFrequency),
    Percentage = RelativeFrequency * 100
  )
pander(PhysActive_table_filtered)
```

| PhysActive | AbsoluteFrequency | RelativeFrequency | Percentage |
|------------|-------------------|-------------------|------------|
| No         | 2473              | 0.454             | 45.418     |
| Yes        | 2972              | 0.546             | 54.582     |

This lets us see that 45.42 percent of the individuals in the NHANES sample said “No” and 54.58 percent said “Yes”.

### 4.2.2 Cumulative distributions

The PhysActive variable that we examined above only had two possible values, but often we wish to summarize data that can have many more possible values. When those values are at least ordinal, then one useful way to summarize them is via what we call a *cumulative* frequency representation: rather than asking how many observations take on a specific value, we ask how many have a value of *at least* some specific value.

Let’s look at another variable in the NHANES dataset, called SleepHrsNight which records how many hours the participant reports sleeping on usual weekdays. Let’s create a frequency table as we did above, after removing anyone who didn’t provide a response to the question.

```
# create summary table for relative frequency of different
# values of SleepHrsNight
```

```

NHANES %>%
  drop_na(SleepHrsNight) %>%
  dplyr::select(SleepHrsNight) %>%
  group_by(SleepHrsNight) %>%
  summarize(AbsoluteFrequency = n()) %>%
  mutate(
    RelativeFrequency = AbsoluteFrequency / sum(AbsoluteFrequency),
    Percentage = RelativeFrequency * 100
  ) %>%
  pander()

```

| SleepHrsNight | AbsoluteFrequency | RelativeFrequency | Percentage |
|---------------|-------------------|-------------------|------------|
| 2             | 9                 | 0.002             | 0.179      |
| 3             | 49                | 0.01              | 0.973      |
| 4             | 200               | 0.04              | 3.972      |
| 5             | 406               | 0.081             | 8.064      |
| 6             | 1172              | 0.233             | 23.277     |
| 7             | 1394              | 0.277             | 27.686     |
| 8             | 1405              | 0.279             | 27.905     |
| 9             | 271               | 0.054             | 5.382      |
| 10            | 97                | 0.019             | 1.927      |
| 11            | 15                | 0.003             | 0.298      |
| 12            | 17                | 0.003             | 0.338      |

We can already begin to summarize the dataset just by looking at the table; for example, we can see that most people report sleeping between 6 and 8 hours. Let's plot the data to see this more clearly. To do this we can plot a *histogram* which shows the number of cases having each of the different values; see left panel of Figure 4.2. The `ggplot2()` library has a built in histogram function (`geom_histogram()`) which we will often use. We can also plot the relative frequencies, which we will often refer to as *densities* - see the right panel of Figure 4.2.

What if we want to know how many people report sleeping 5 hours or less? To find this, we can compute a *cumulative distribution*:

$$\text{cumulative frequency}_j = \sum_{i=1}^j \text{absolute frequency}_i$$

That is, to compute the cumulative frequency for some value  $j$ , we add up the frequencies for all of the values up to and including  $j$ . Let's do this for our sleep variable, first for the absolute frequency:

```

# create cumulative frequency distribution of SleepHrsNight data

SleepHrsNight_cumulative <-
  NHANES %>%
  drop_na(SleepHrsNight) %>%
  dplyr::select(SleepHrsNight) %>%
  group_by(SleepHrsNight) %>%
  summarize(AbsoluteFrequency = n()) %>%
  mutate(CumulativeFrequency = cumsum(AbsoluteFrequency))

pander(SleepHrsNight_cumulative)

```

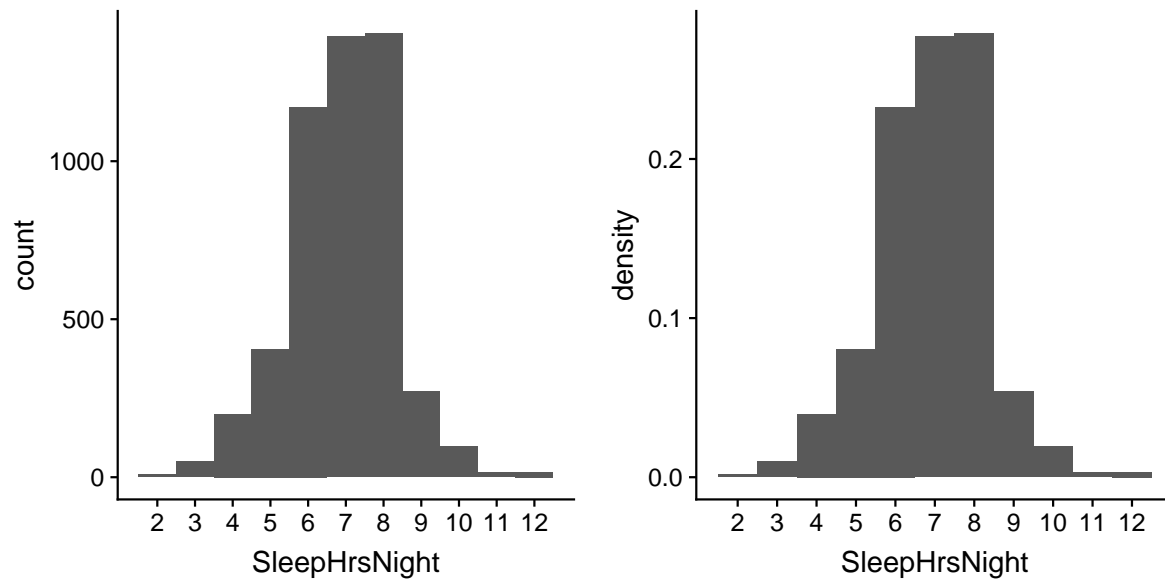


Figure 4.2: Left: Histogram showing the number (left) and proportion (right) of people reporting each possible value of the SleepHrsNight variable.

| SleepHrsNight | AbsoluteFrequency | CumulativeFrequency |
|---------------|-------------------|---------------------|
| 2             | 9                 | 9                   |
| 3             | 49                | 58                  |
| 4             | 200               | 258                 |
| 5             | 406               | 664                 |
| 6             | 1172              | 1836                |
| 7             | 1394              | 3230                |
| 8             | 1405              | 4635                |
| 9             | 271               | 4906                |
| 10            | 97                | 5003                |
| 11            | 15                | 5018                |
| 12            | 17                | 5035                |

In the left panel of Figure 4.3 we plot the data to see what these representations look like; the absolute frequency values are plotted in red, and the cumulative frequencies are plotted in blue. We see that the cumulative frequency is *monotonically increasing* – that is, it can only go up or stay constant, but it can never decrease. Again, we usually find the relative frequencies to be more useful than the absolute; those are plotted in the right panel of Figure 4.3.

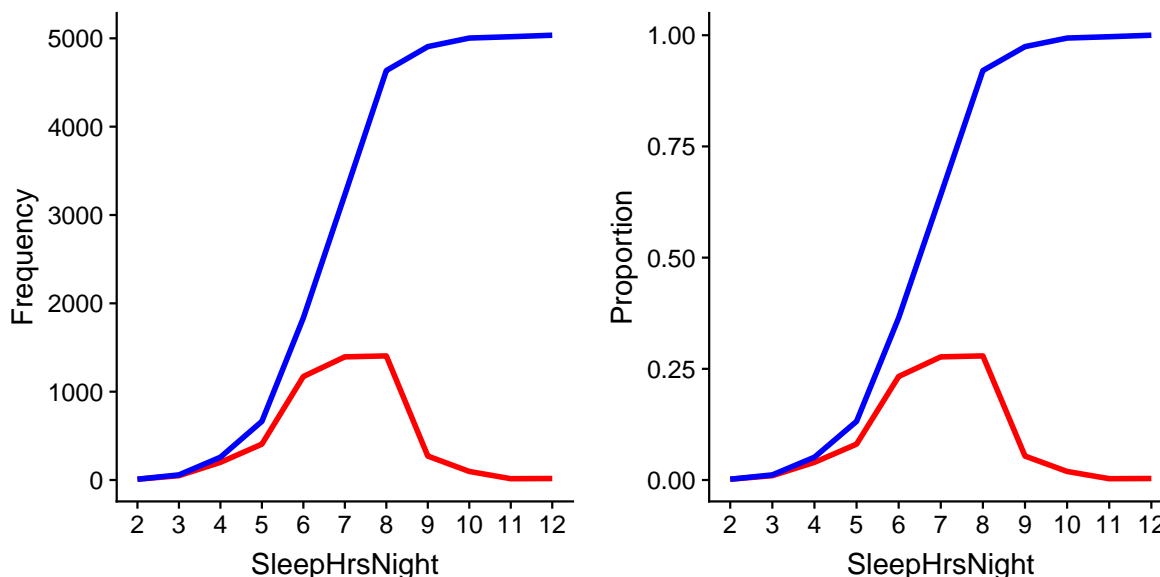


Figure 4.3: A plot of the relative (red) and cumulative relative (blue) values for frequency (left) and proportion (right) for the possible values of SleepHrsNight.

### 4.2.3 Plotting histograms

The variables that we examined above were fairly simple, having only a few possible values. Now let's look at a more complex variable: Age. First let's plot the Age variable for all of the individuals in the NHANES dataset (see left panel of Figure 4.4). What do you see there? First, you should notice that the number of individuals in each age group is declining over time. This makes sense because the population is being randomly sampled, and thus death over time leads to fewer people in the older age ranges. Second, you probably notice a large spike in the graph at age 80. What do you think that's about?

If you look at the help function for the NHANES dataset, you will see the following definition: "Age in years at screening of study participant. Note: Subjects 80 years or older were recorded as 80." The reason for this is that the relatively small number of individuals with very high ages would make it potentially easier to identify the specific person in the dataset if you knew their exact age; researchers generally promise their participants to keep their identity confidential, and this is one of the things they can do to help protect their research subjects. This also highlights the fact that it's always important to know where one's data have come from and how they have been processed; otherwise we might interpret them improperly.

Let's look at another more complex variable in the NHANES dataset: Height. The histogram of height values is plotted in the right panel of Figure 4.4. The first thing you should notice about this distribution is that most of its density is centered around about 170 cm, but the distribution has a "tail" on the left; there are a small number of individuals with much smaller heights. What do you think is going on here?

You may have intuited that the small heights are coming from the children in the dataset. One way to examine this is to plot the histogram with separate colors for children and adults (left panel of Figure 4.5). This shows that all of the very short heights were indeed coming from children in the sample. Let's create a new version of NHANES that only includes adults, and then plot the histogram just for them (right panel of Figure 4.5). In that plot that the distribution looks much more symmetric. As we will see later, this is a nice example of a *normal* (or *Gaussian*) distribution.

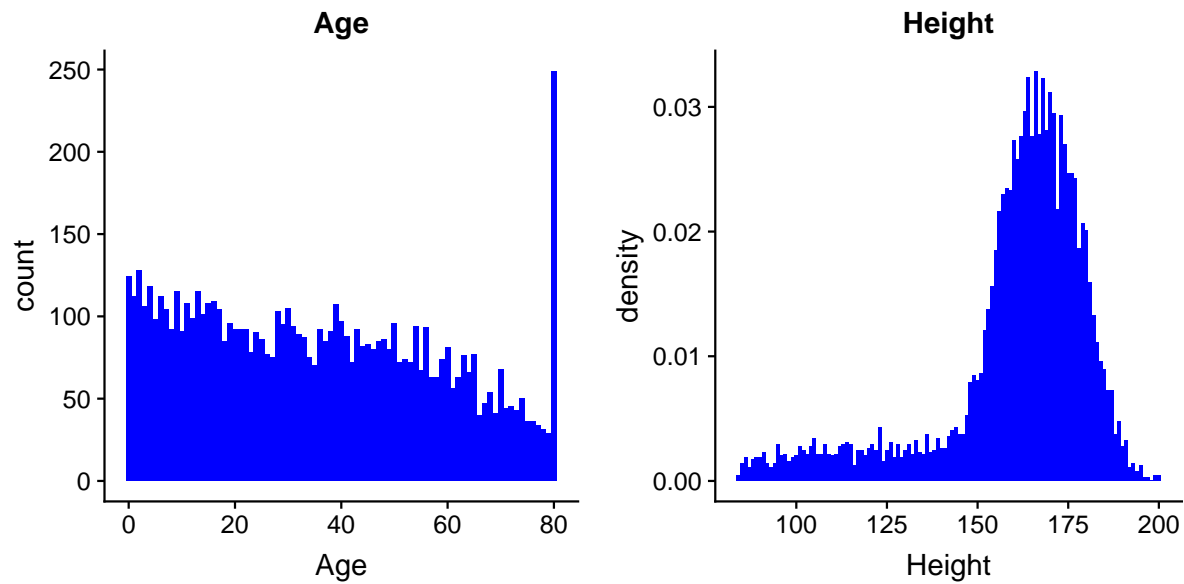


Figure 4.4: A histogram of the Age (left) and Height (right) variables in NHANES.

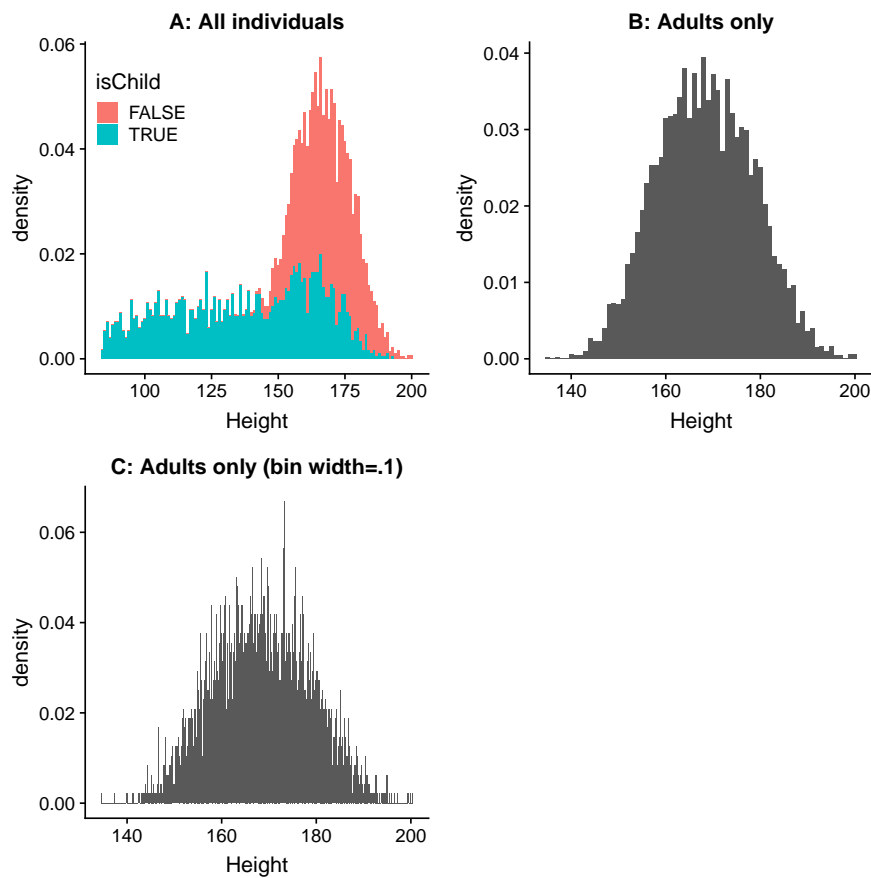


Figure 4.5: Histogram of heights for NHANES. A: values plotted separately for children (blue) and adults (red). B: values for adults only. C: Same as B, but with bin width = 0.1

### 4.2.4 Histogram bins

In our earlier example with the sleep variable, the data were reported in whole numbers, and we simply counted the number of people who reported each possible value. However, if you look at a few values of the Height variable in NHANES, you will see that it was measured in centimeters down to the first decimal place:

```
# take a slice of a few values from the full data frame
NHANES_adult %>%
  dplyr::select(Height) %>%
  slice(45:50) %>%
  pander()
```

| Height |
|--------|
| 169.6  |
| 169.8  |
| 167.5  |
| 155.2  |
| 173.8  |
| 174.5  |

Panel C of Figure 4.5 shows a histogram that counts the density of each possible value. That histogram looks really jagged, which is because of the variability in specific decimal place values. For example, the value 173.2 occurs 32 times, while the value 173.3 only occurs 15 times. We probably don’t think that there is really such a big difference between the prevalence of these two weights; more likely this is just due to random variability in our sample of people.

In general, when we create a histogram of data that are continuous or where there are many possible values, we will *bin* the values so that instead of counting and plotting the frequency of every specific value, we count and plot the frequency of values falling within a specific range. That’s why the plot looked less jagged above in Panel B of 4.5; if you look at the `geom_histogram` command you will see that we set “`binwidth = 1`” which told the command to compute the histogram by combining values within bins with a width of one; thus, the values 1.3, 1.5, and 1.6 would all count toward the frequency of the same bin, which would span from values equal to one up through values less than 2.

Note that once the bin size has been selected, then the number of bins is determined by the data:

$$\text{number of bins} = \frac{\text{range of scores}}{\text{bin width}}$$

There is no hard and fast rule for how to choose the optimal bin width. Occasionally it will be obvious (as when there are only a few possible values), but in many cases it would require trial and error. There are methods that try to find an optimal bin size, such as the Freedman-Diaconis method that is implemented within the `nclass.FD()` function in R; we will use this function in some of the examples below.

## 4.3 Idealized representations of distributions

Datasets are like snowflakes, in that every one is different, but nonetheless there are patterns that one often sees in different types of data. This allows us to use idealized representations of the data to further summarize them. Let’s take the adult height data plotted in 4.5, and plot them alongside a very different variable: pulse rate (heartbeats per minute), also measured in NHANES (see Figure 4.6).

While these plots certainly don’t look exactly the same, both have the general characteristic of being relatively symmetric around a rounded peak in the middle. This shape is in fact one of the commonly observed shapes

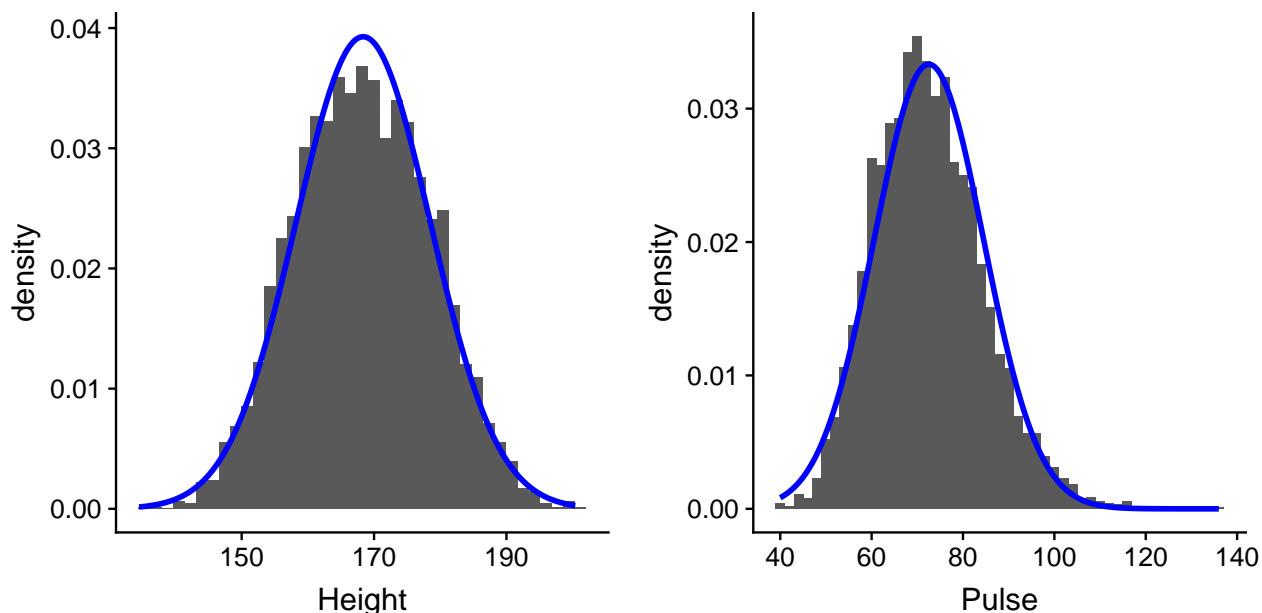


Figure 4.6: Histograms for height (left) and pulse (right) in the NHANES dataset, with the normal distribution overlaid for each dataset.

of distributions when we collect data, which we call the *normal* (or *Gaussian*) distribution. This distribution is defined in terms of two values (which we call *parameters* of the distribution): the location of the center peak (which we call the *mean*) and the width of the distribution (which is described in terms of a parameter called the *standard deviation*). Figure 4.6 shows the appropriate normal distribution plotted on top of each of the histograms. You can see that although the curves don't fit the data exactly, they do a pretty good job of characterizing the distribution – with just two numbers!

As we will see later in the course when we discuss the central limit theorem, there is a deep mathematical reason why many variables in the world exhibit the form of a normal distribution.

### 4.3.1 Skewness

The examples in Figure 4.6 followed the normal distribution fairly well, but in many cases the data will deviate in a systematic way from the normal distribution. One way in which the data can deviate is when they are asymmetric, such that one tail of the distribution is more dense than the other. We refer to this as “skewness”. Skewness commonly occurs when the measurement is constrained to be non-negative, such as when we are counting things or measuring elapsed times (and thus the variable can't take on negative values).

An example of skewness can be seen in the average waiting times at the airport security lines at San Francisco International Airport, plotted in the left panel of Figure 4.7. You can see that while most wait times are less than 20 minutes, there are a number of cases where they are much longer, over 60 minutes! This is an example of a “right-skewed” distribution, where the right tail is longer than the left; these are common when looking at counts or measured times, which can't be less than zero. It's less common to see “left-skewed” distributions, but they can occur, for example when looking at fractional values that can't take a value greater than one.

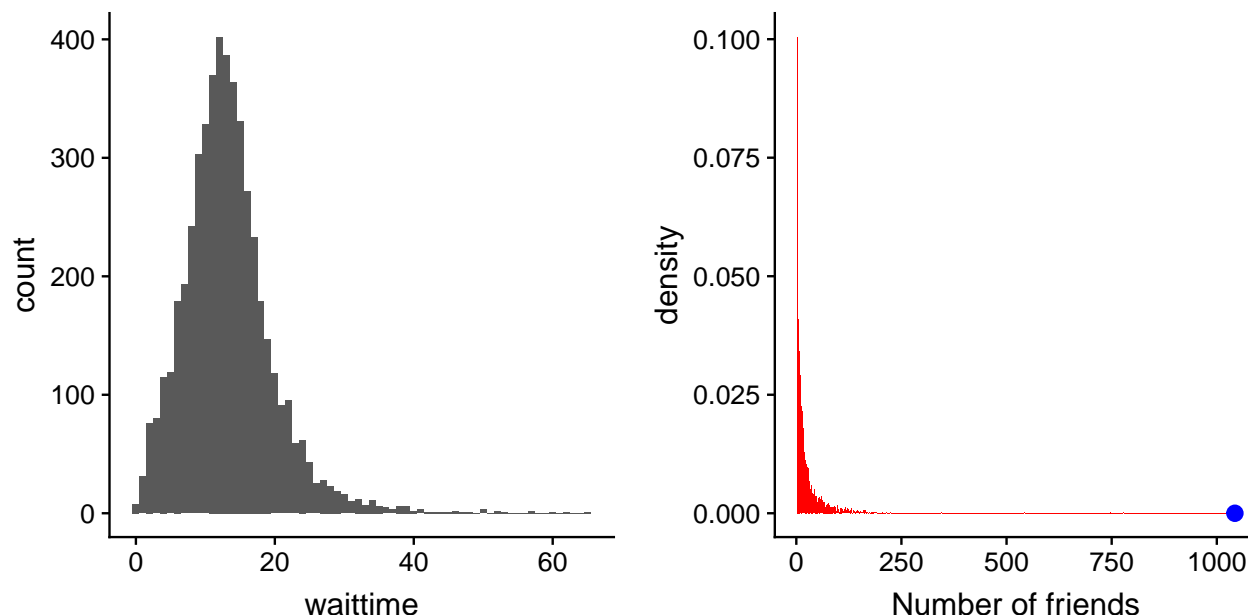


Figure 4.7: Examples of right-skewed and long-tailed distributions. Left: Average wait times for security at SFO Terminal A (Jan-Oct 2017), obtained from <https://awt.cbp.gov/> . Right: A histogram of the number of Facebook friends amongst 3,663 individuals, obtained from the Stanford Large Network Database. The person with the maximum number of friends is indicated by the blue dot.

### 4.3.2 Long-tailed distributions

Historically, statistics has focused heavily on data that are normally distributed, but there are many data types that look nothing like the normal distribution. In particular, many real-world distributions are “long-tailed”, meaning that the right tail extends far beyond the most typical members of the distribution. One of the most interesting types of data where long-tailed distributions occur arise from the analysis of social networks. For an example, let’s look at the Facebook friend data from the Stanford Large Network Database and plot the histogram of number of friends across the 3,663 people in the database (see right panel of Figure 4.7). As we can see, this distribution has a very long right tail – the average person has 24.09 friends, while the person with the most friends (denoted by the blue dot) has 1043!

Long-tailed distributions are increasingly being recognized in the real world. In particular, many features of complex systems are characterized by these distributions, from the frequency of words in text, to the number of flights in and out of airports, to the connectivity of brain networks. There are a number of different ways that long-tailed distributions can come about, but a common one occurs in cases of the so-called “Matthew effect” from the Christian Bible:

For to every one who has will more be given, and he will have abundance; but from him who has not, even what he has will be taken away. — Matthew 25:29, Revised Standard Version

often paraphrased as “the rich get richer”. In these situations, advantages compound, such that those with more friends have access to even more new friends, and those with more money have the ability do things that increase their riches even more.

As the course progresses we will see several examples of long-tailed distributions, and we should keep in mind that many of the tools in statistics can fail when faced with long-tailed data. As Nassim Nicholas Taleb pointed out in his book “The Black Swan”, such long-tailed distributions played a critical role in the 2008 financial crisis, because many of the financial models used by traders assumed that financial systems would follow the normal distribution, which they clearly did not.



## 4.4 Suggested readings

- *The Black Swan: The Impact of the Highly Improbable*, by Nassim Nicholas Taleb



## Chapter 5

# Fitting models to data

One of the fundamental activities in statistics is creating models that can summarize data using a small set of numbers, thus providing a compact description of the data. In this chapter we will discuss the concept of a statistical model and how it can be used to describe data.

### 5.1 What is a model?

In the physical world, “models” are generally simplifications of things in the real world that nonetheless convey the essence of the thing being modeled. A model of a building conveys the structure of the building while being small and light enough to pick up with one’s hands; a model of a cell in biology is much larger than the actual thing, but again conveys the major parts of the cell and their relationships.

In statistics, a model is meant to provide a similarly condensed description, but for data rather than for a physical structure. Like physical models, a statistical model is generally much simpler than the data being described; it is meant to capture the structure of the data as simply as possible. In both cases, we realize that the model is a convenient fiction that necessarily glosses over some of the details of the actual thing being modeled. As the statistician George Box famously said: “All models are wrong but some are useful.”

The basic structure of a statistical model is:

$$data = model + error$$

This expresses the idea that the data can be described by a statistical model, which describes what we expect to occur in the data, along with the difference between the model and the data, which we refer to as the *error*.

### 5.2 Statistical modeling: An example

Let’s look at an example of fitting a model to data, using the data from NHANES. In particular, we will try to build a model of the height of children in the NHANES sample. First let’s load the data and plot them (see Figure 5.1).

Remember that we want to describe the data as simply as possible while still capturing their important features. What is the simplest model we can imagine that might still capture the essence of the data? How about the most common value in the dataset (which we call the *mode*)? R doesn’t have a built-in function for the mode, so we will create one first, which we will call `getmode()`.

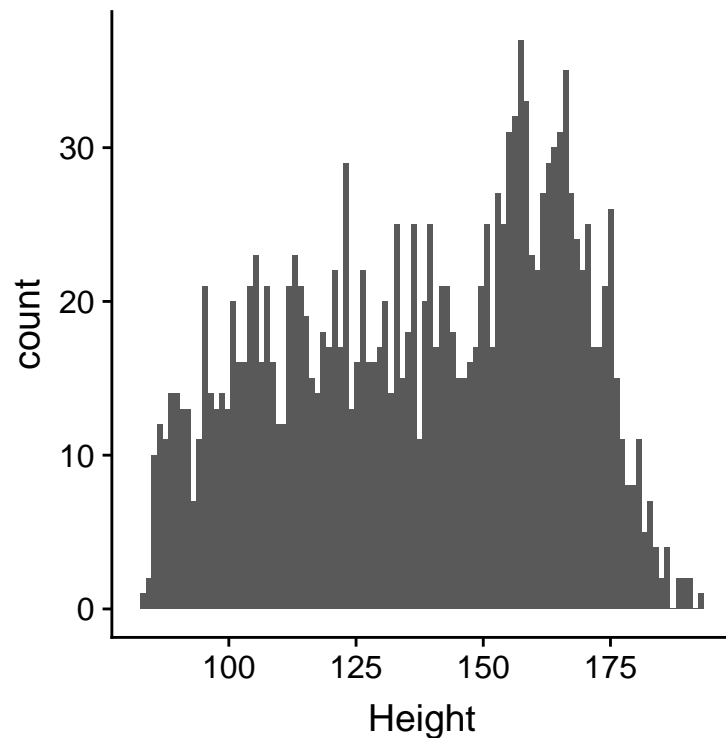


Figure 5.1: Histogram of height of children in NHANES.

```
# create function to compute mode and apply to child height data from NHANES
getmode <- function(v) {
  uniqv <- unique(v)
  return(uniqv[which.max(tabulate(match(v, uniqv)))]))
}

height_mode <- getmode(NHANES_child$Height)

paste("mode of children's height from NHANES:", height_mode)

## [1] "mode of children's height from NHANES: 166.5"
```

Given this, our model for an individual datapoint  $i$  would be:

$$height_i = 166.5 + error$$

This redescribes the entire set of 1691 children in terms of a single number, and if we wanted to predict the height of any new children, then our guess would be the same number: 166.5 centimeters.

How good of a model is this? In general we define the goodness of a model in terms of the error, which represents the difference between model and the data; all things being equal, the model that produces lower error is the better model.

```
# compute error compared to the mode and plot histogram

error_mode <- NHANES_child$Height - height_mode
sprintf("average error from mode (cm): %0.2f", mean(error_mode))

## [1] "average error from mode (cm): -28.80"
```

What we find is that the average individual has a fairly large error of -28.8 centimeters. We would like to have a model where the average error is zero, and it turns out that if we use the arithmetic mean (commonly known as the *average*) as our model then this will be the case.

The mean (often denoted by a bar over the variable, such as  $\bar{X}$ ) is defined as:

$$\bar{X} = \frac{\sum_{i=1}^n x_i}{n}$$

That is, it is the sum of all of the values, divided by the number of values. We can prove that the sum of errors from the mean (and thus the average error) is zero:

$$error = \sum_{i=1}^n (x_i - \bar{X}) = 0$$

$$\sum_{i=1}^n x_i - \sum_{i=1}^n \bar{X} = 0$$

$$\sum_{i=1}^n x_i = \sum_{i=1}^n \bar{X}$$

$$\sum_{i=1}^n x_i = n\bar{X}$$

$$\sum_{i=1}^n x_i = \sum_{i=1}^n x_i$$

Given that the average error is zero, this seems like a better model. Let's confirm that it comes out correctly.

```
# compute error from mean
```

```
error_mean <- NHANES_child$Height - mean(NHANES_child$Height)
sprintf("average error for mean (cm): %e", mean(error_mean))
```

```
## [1] "average error for mean (cm): -9.864171e-15"
```

The average error here is a very small number, though not technically zero; we will discuss later in the course why this happens (which is due to how computers represent numbers), but for now you can just treat it as being close enough to zero to call it zero.

Even though the average of errors from the mean is zero, we can see from the histogram in Figure 5.2 that each individual still has some degree of error; some are positive and some are negative, and those cancel each other out. For this reason, we generally summarize errors in terms of some kind of measure that counts both positive and negative errors as bad. We could use the absolute value of each error value, but it's more common to use the squared errors, for reasons that we will see later in the course.

There are several common ways to summarize the squared error that you will encounter at various points in this book, so it's important to understand how they relate to one another. First, we could simply add them up; this is referred to as the *sum of squared errors*. The reason we don't usually use this is that its magnitude depends on the number of data points, so it can be difficult to interpret unless we are looking at the same number of observations. Second, we could take the mean of the squared error values, which is referred to as the *mean squared error (MSE)*. However, because we squared the values before averaging, they are not on the same scale as the original data; they are in *centimeters<sup>2</sup>*. For this reason, it's also common to take the square root of the MSE, which we refer to as the *root mean squared error (RMSE)*, so that it is in the same units as the original values (in this example, centimeters).

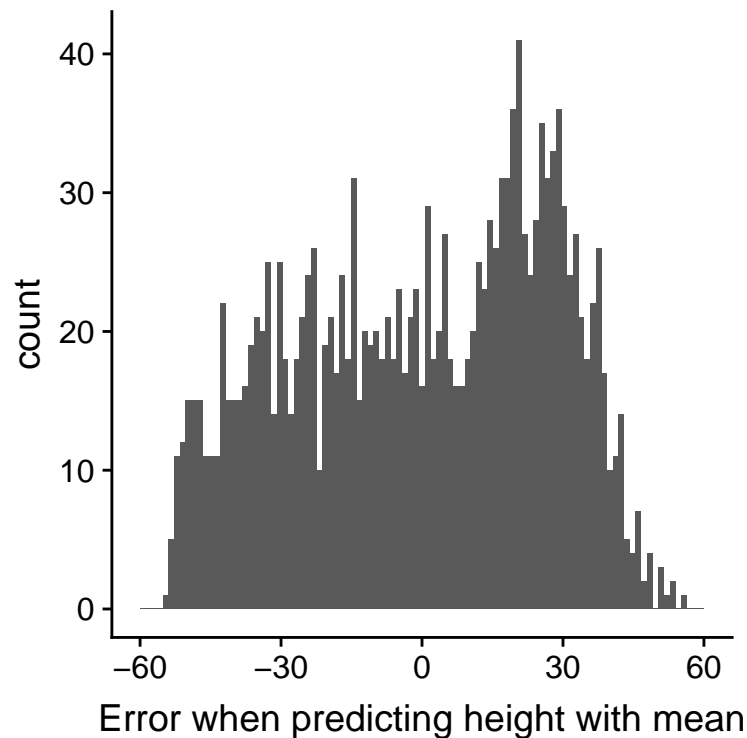


Figure 5.2: Distribution of errors from the mean.

```
# compute and print RMSE for mean and mode
rmse_mean <- sqrt(mean(error_mean**2))

rmse_mode <- sqrt(mean(error_mode**2))

print(paste("Mode: root mean squared error (centimeters):", rmse_mode))

## [1] "Mode: root mean squared error (centimeters): 39.4197926582947"
print(paste("Mean: root mean squared error (centimeters):", rmse_mean))

## [1] "Mean: root mean squared error (centimeters): 26.9116738708646"
```

This shows that the mean has a pretty substantial amount of error – any data point will be about 27 cm from the mean on average – but it’s still much better than the mode.

### 5.2.1 Improving our model

Can we imagine a better model? Remember that these data are from all children in the NHANES sample, who vary from 2 to 17 years of age. Given this wide age range, we might expect that our model of height should also include age. Let’s plot the data for height against age, to see if this relationship really exists.

The black points in Panel A of Figure 5.3 show individuals in the dataset, and there seems to be a strong relationship between height and age, as we would expect. Thus, we might build a model that relates height to age:

$$height_i = \beta * age_i + error_i$$

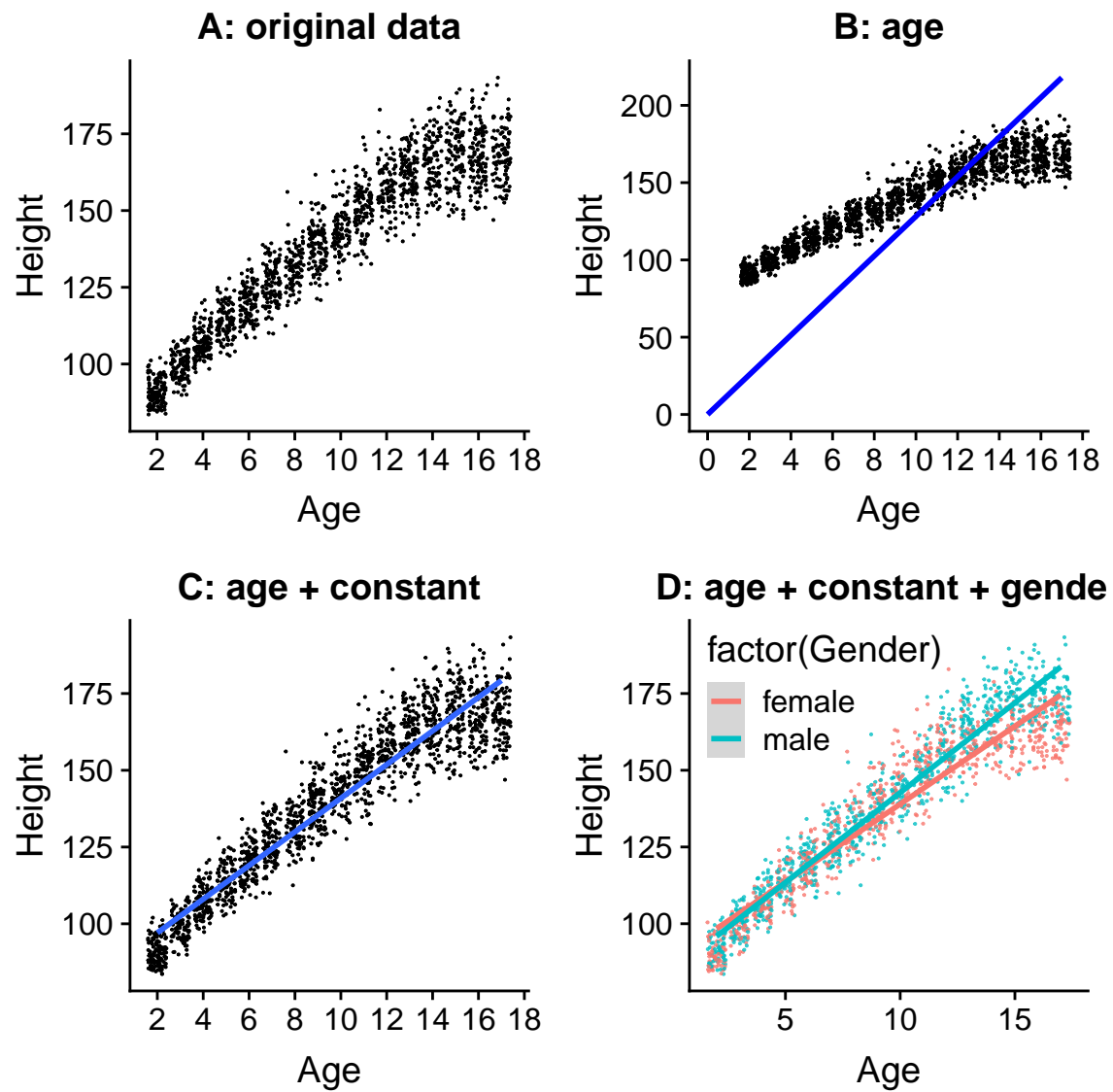


Figure 5.3: Height of children in NHANES, plotted without a model (A), with a linear model including only age (B) or age and a constant (C), and with a linear model that fits separate effects of age for males and females (D).

where  $\beta$  is a *parameter* that we multiply by age to get the smallest error. You might have noticed that this is simply a line with a slope of  $\beta$  - to see this, let's plot the best fitting line in blue on top of the data (Panel B in Figure 5.3). Something is clearly wrong with this model, as the line doesn't seem to follow the data very well. In fact, the RMSE for this model (39.16) is actually higher than the model that only includes the mean! The problem comes from the fact that our model only includes age, which means that the predicted value of height from the model must take on a value of zero when age is zero. Even though the data do not include any children with an age of zero, the line is mathematically constrained to have a y-value of zero when x is zero, which explains why the line is pulled down below the younger datapoints. We can fix this by including a constant value in our model, which basically represents the estimated value of height when age is equal to zero; even though an age of zero is not plausible in this dataset, this is a mathematical trick that will allow the model to account for the overall magnitude of the data. The model is:

$$height_i = constant + \beta * age_i + error_i$$

where *constant* is a constant value added to the prediction for all individuals (which we also call the *intercept*, since it maps onto the intercept in the equation for a line). We will also learn later how it is that we actually compute these values; for now, we will use the `lm()` function in R to compute the values of the constant and  $\beta$  that give us the smallest error. Panel C in Figure 5.3 shows this model fitted to the NHANES data, where we see that the line matches the data much better than the one without a constant.

```
## [1] "model: height = 86.11 + 5.48*Age"
```

```
## [1] "root mean squared error: 8.36"
```

Our error is much smaller using this model – only 8.36 centimeters on average. Can you think of other variables that might also be related to height? What about gender? In Panel D of Figure 5.3 we plot the data with lines fitted separately for males and females. From the plot, it seems that there is a difference between males and females, but it is relatively small and only emerges after the age of puberty. Let's estimate this model and see how the errors look:

```
# compute model fit for modeling with age and gender

model_age_gender <- lm(Height ~ Age + Gender, data = NHANES_child)

rmse_age_gender <-
  NHANES_child %>%
  add_predictions(model_age_gender, var = "predicted_age_gender") %>%
  summarise(
    sqrt(mean((Height - predicted_age_gender)**2))
  ) %>%
  pull()

sprintf(
  "model: height = %0.2f + %0.2f*Age + %0.2f*Gender",
  model_age_gender$coefficients[1],
  model_age_gender$coefficients[2],
  model_age_gender$coefficients[3]
)

## [1] "model: height = 84.37 + 5.48*Age + 3.28*Gender"
print(sprintf("root mean squared error: %0.2f", rmse_age_gender))

## [1] "root mean squared error: 8.20"
```

In Figure 5.4 we plot the root mean squared error values across the different models. From this we see that the model got a little bit better going from mode to mean, much better going from mean to mean+age, and



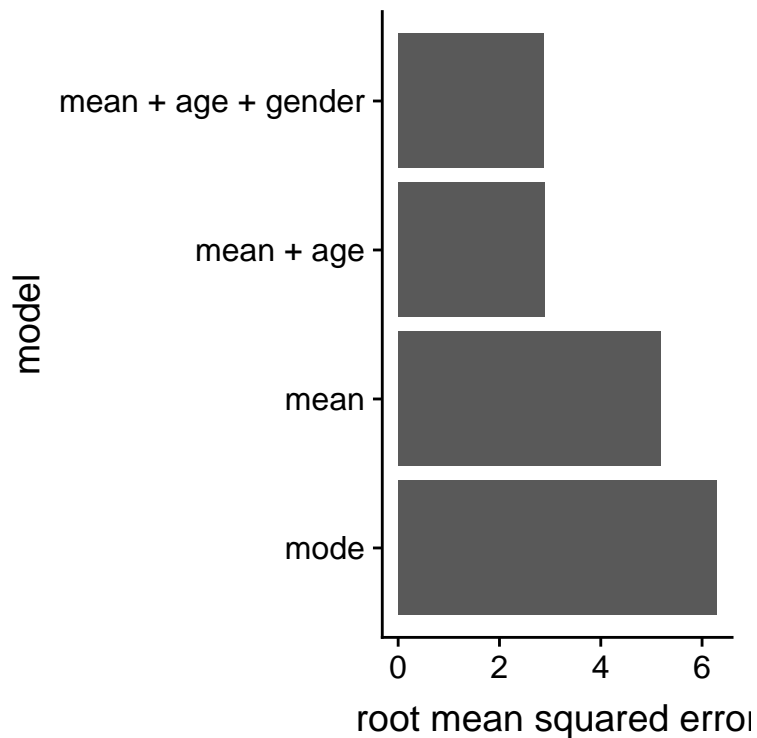


Figure 5.4: Mean squared error plotted for each of the models tested above.

only very slightly better by including gender as well.

### 5.3 What makes a model “good”?

There are generally two different things that we want from our statistical model. First, we want it to describe our data well; that is, we want it to have the lowest possible error when modeling our data. Second, we want it to generalize well to new datasets; that is, we want its error to be as low as possible when we apply it to a new dataset. It turns out that these two features can often be in conflict.

To understand this, let’s think about where error comes from. First, it can occur if our model is wrong; for example, if we inaccurately said that height goes down with age instead of going up, then our error will be higher than it would be for the correct model. Similarly, if there is an important factor that is missing from our model, that will also increase our error (as it did when we left age out of the model for height). However, error can also occur even when the model is correct, due to random variation in the data, which we often refer to as “measurement error” or “noise”. Sometimes this really is due to error in our measurement – for example, when the measurements rely on a human, such as using a stopwatch to measure elapsed time in a footrace. In other cases, our measurement device is highly accurate (like a digital scale to measure body weight), but the thing being measured is affected by many different factors that cause it to be variable. If we knew all of these factors then we could build a more accurate model, but in reality that’s rarely possible.

Let’s use an example to show this. Rather than using real data, we will generate some data for the example; we will discuss the generation of simulated data in much more detail later in the course. Let’s say that we want to understand the relationship between a person’s blood alcohol content (BAC) and their reaction time on a simulated driving test. We can generate some simulated data and plot the relationship (see Panel A of Figure 5.5).

In this example, reaction time goes up systematically with blood alcohol content – the blue line shows the

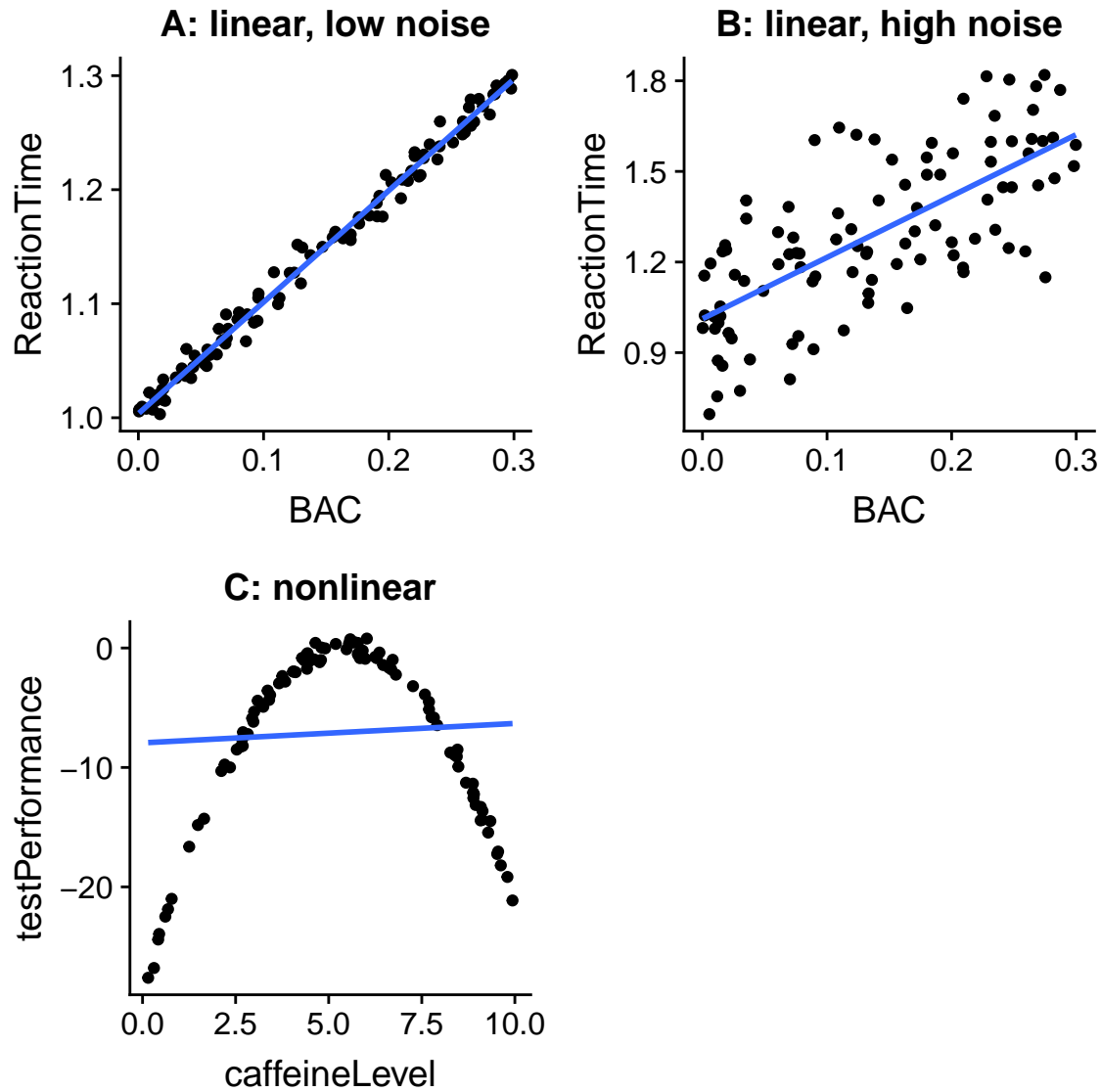


Figure 5.5: Simulated relationship between blood alcohol content and reaction time on a driving test, with best-fitting linear model. A: linear relationship with low measurement error. B: linear relationship with higher measurement error. C: Nonlinear relationship with low measurement error and (incorrect) linear model

best fitting model, and we can see that there is very little error, which is evident in the fact that all of the points are very close to the line.

We could also imagine data that show the same linear relationship, but have much more error, as in Panel B of Figure 5.5. Here we see that there is still a systematic increase of reaction time with BAC, but it's much more variable across individuals.

These were both examples where the *linear model* seems appropriate, and the error reflects noise in our measurement. The linear model specifies that the relationship between two variables follows a straight line. For example, in a linear model, change in BAC is always associated with a specific change in ReactionTime, regardless of the level of BAC.

On the other hand, there are other situations where the linear model is incorrect, and error will be increased because the model is not properly specified. Let's say that we are interested in the relationship between caffeine intake and performance on a test. The relation between stimulants like caffeine and test performance is often *nonlinear* - that is, it doesn't follow a straight line. This is because performance goes up with smaller amounts of caffeine (as the person becomes more alert), but then starts to decline with larger amounts (as the person becomes nervous and jittery). We can simulate data of this form, and then fit a linear model to the data (see Panel C of Figure 5.5). The blue line shows the straight line that bests fits these data; clearly, there is a high degree of error. Although there is a very lawful relation between test performance and caffeine intake, it follows a curve rather than a straight line. The linear model has high error because it's the wrong model for these data.

## 5.4 Can a model be too good?

Error sounds like a bad thing, and usually we will prefer a model that has lower error over one that has higher error. However, we mentioned above that there is a tension between the ability of a model to accurately fit the current dataset and its ability to generalize to new datasets, and it turns out that the model with the lowest error often is much worse at generalizing to new datasets!

To see this, let's once again generate some data so that we know the true relation between the variables. We will create two simulated datasets, which are generated in exactly the same way - they just have different random noise added to them.

The left panel in Figure 5.6 shows that the more complex model (in red) fits the data better than the simpler model (in blue). However, we see the opposite when the same model is applied to a new dataset generated in the same way - here we see that the simpler model fits the new data better than the more complex model. Intuitively, we can see that the more complex model is influenced heavily by the specific data points in the first dataset; since the exact position of these data points was driven by random noise, this leads the more complex model to fit badly on the new dataset. This is a phenomenon that we call *overfitting*, which we will discuss repeatedly over this course. Later we will learn about techniques that we can use to prevent overfitting while still being sensitive to the structure of the data. For now it's important to keep in mind that our model fit needs to be good, but not too good. As Albert Einstein (1933) said: "It can scarcely be denied that the supreme goal of all theory is to make the irreducible basic elements as simple and as few as possible without having to surrender the adequate representation of a single datum of experience." Which is often paraphrased as: "Everything should be as simple as it can be, but not simpler."

## 5.5 The simplest model: The mean

We have already encountered the mean (or average), and in fact most people know about the average even if they have never taken a statistics class. It is commonly used to describe what we call the "central tendency" of a dataset - that is, what value are the data centered around? Most people don't think of computing a mean as fitting a model to data. However, that's exactly what we are doing when we compute the mean.

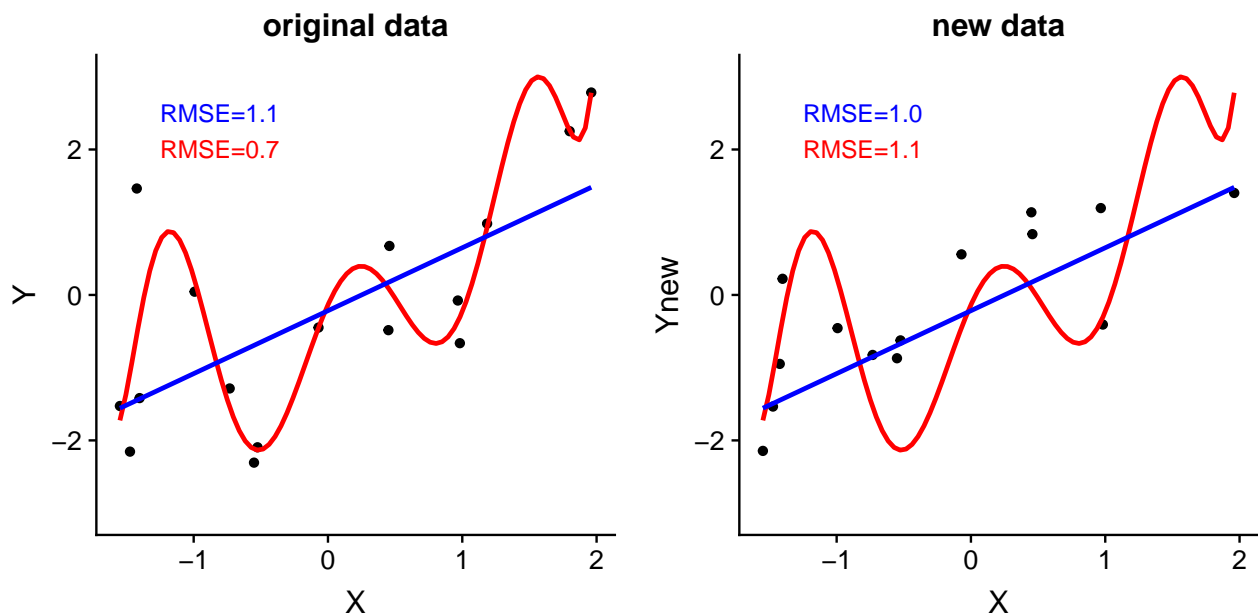


Figure 5.6: An example of overfitting. Both datasets were generated using the same model, with different random noise added to generate each set. The left panel shows the data used to fit the model, with a simple linear fit in blue and a complex (8th order polynomial) fit in red. The root mean square error values for each model are shown in the figure; in this case, the complex model has a lower RMSE than the simple model. The right panel shows the second dataset, with the same model overlaid on it and the RMSE values computed using the model obtained from the first dataset. Here we see that the simpler model actually fits the new dataset better than the more complex model, which was overfitted to the first dataset.

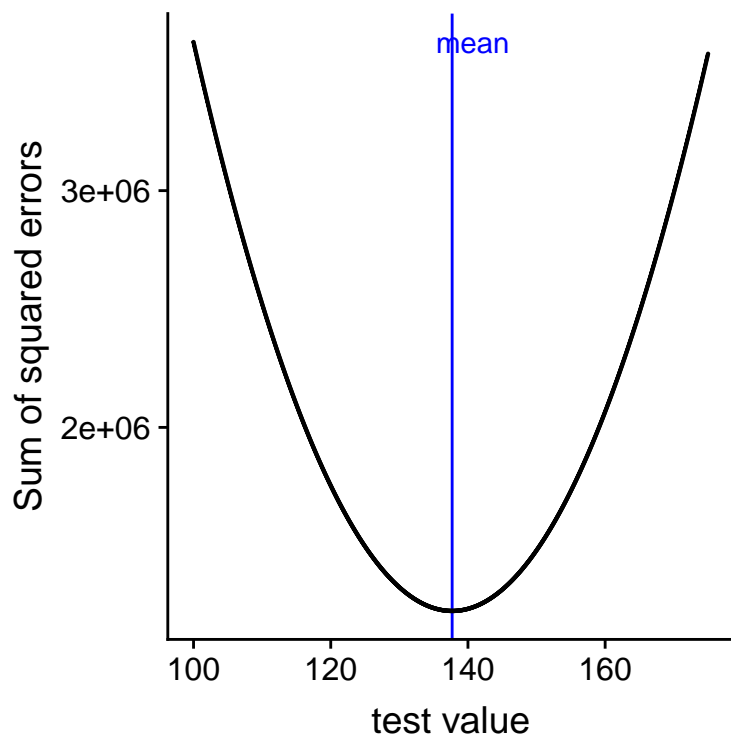


Figure 5.7: A demonstration of the mean as the statistic that minimizes the sum of squared errors. Using the NHANES child height data, we compute the mean (denoted by the blue bar). Then, we test a range of other values, and for each one we compute the sum of squared errors for each data point from that value, which are denoted by the black curve. We see that the mean falls at the minimum of the squared error plot.

We have already seen the formula for computing the mean of a sample of data:

$$\bar{X} = \frac{\sum_{i=1}^n x_i}{n}$$

Note that I said that this formula was specifically for a *sample* of data, which is a set of data points selected from a larger population. Using a sample, we wish to characterize a larger population – the full set of individuals that we are interested in. For example, if we are a political pollster our population of interest might be all registered voters, whereas our sample might just include a few thousand people sampled from this population. Later in the course we will talk in more detail about sampling, but for now the important point is that statisticians generally like to use different symbols to differentiate statistics that describe values for a sample from parameters that describe values for a population; in this case, the formula for the population mean (denoted as  $\mu$ ) is:

$$\mu = \frac{\sum_{i=1}^N x_i}{N}$$

where  $N$  is the size of the entire population.

We have already seen that the mean is the summary statistic that is guaranteed to give us a mean error of zero. The mean also has another characteristic: It is the summary statistic that minimizes the sum of squared errors (SSE). In statistics, we refer to this as being the “best” estimator. We could prove this mathematically, but instead we will demonstrate it graphically in Figure 5.7.

This minimization of SSE is a good feature, and it’s why the mean is the most commonly used statistic to summarize data. However, the mean also has a dark side. Let’s say that five people are in a bar, and we examine each person’s income:

```
# create income data frame

incomeDf <-
  tibble(
    income = c(48000, 64000, 58000, 72000, 66000),
    person = c("Joe", "Karen", "Mark", "Andrea", "Pat")
  )
# glimpse(incomeDf)

panderOptions('digits', 2)
pander(incomeDf)
```

| income | person |
|--------|--------|
| 48000  | Joe    |
| 64000  | Karen  |
| 58000  | Mark   |
| 72000  | Andrea |
| 66000  | Pat    |

```
sprintf("Mean income: %0.2f", mean(incomeDf$income))
```

```
## [1] "Mean income: 61600.00"
```

The mean seems to be a pretty good summary of the income of those five people. Now let's look at what happens if Beyoncé Knowles walks into the bar:

```
# add Beyonce to income data frame

incomeDf <-
  incomeDf %>%
  rbind(c(54000000, "Beyonce")) %>%
  mutate(income = as.double(income))

pander(incomeDf)
```

| income  | person  |
|---------|---------|
| 48000   | Joe     |
| 64000   | Karen   |
| 58000   | Mark    |
| 72000   | Andrea  |
| 66000   | Pat     |
| 5.4e+07 | Beyonce |

```
sprintf("Mean income: %0.2f", mean(incomeDf$income))
```

```
## [1] "Mean income: 9051333.33"
```

The mean is now almost 10 million dollars, which is not really representative of any of the people in the bar – in particular, it is heavily driven by the outlying value of Beyoncé. In general, the mean is highly sensitive to extreme values, which is why it's always important to ensure that there are no extreme values when using the mean to summarize data.

### 5.5.1 The median

If we want to summarize the data in a way that is less sensitive to outliers, we can use another statistic called the *median*. If we were to sort all of the values in order of their magnitude, then the median is the value in the middle. If there is an even number of values then there will be two values tied for the middle place, in which case we take the mean (i.e. the halfway point) of those two numbers.

Let's look at an example. Say we want to summarize the following values:

```
# create example data frame
dataDf <-
  tibble(
    values = c(8, 6, 3, 14, 12, 7, 6, 4, 9)
  )

pander(dataDf)
```

| values |
|--------|
| 8      |
| 6      |
| 3      |
| 14     |
| 12     |
| 7      |
| 6      |
| 4      |
| 9      |

If we sort those values:

```
# sort values and print
dataDf <-
  dataDf %>%
  arrange(values)

pander(dataDf)
```

| values |
|--------|
| 3      |
| 4      |
| 6      |
| 6      |
| 7      |
| 8      |
| 9      |
| 12     |
| 14     |

Then the median is the middle value – in this case, the 5th of the 9 values.

Whereas the mean minimizes the sum of squared errors, the median minimizes a slightly different quantity: The sum of *absolute* errors. This explains why it is less sensitive to outliers – squaring is going to exacerbate the effect of large errors compared to taking the absolute value. We can see this in the case of the income

example:

```
# print income table
pander(incomeDf)
```

| income  | person  |
|---------|---------|
| 48000   | Joe     |
| 64000   | Karen   |
| 58000   | Mark    |
| 72000   | Andrea  |
| 66000   | Pat     |
| 5.4e+07 | Beyonce |

```
sprintf('Mean income: %.2f',mean(incomeDf$income))
```

```
## [1] "Mean income: 9051333.33"
```

```
sprintf('Median income: %.2f',median(incomeDf$income))
```

```
## [1] "Median income: 65000.00"
```

The median is much more representative of the group as a whole, and less sensitive to the one large outlier.

Given this, why would we ever use the mean? As we will see in a later chapter, the mean is the “best” estimator in the sense that it will vary less from sample to sample compared to other estimators. It’s up to us to decide whether that is worth the sensitivity to potential outliers – statistics is all about tradeoffs.

## 5.6 The mode

Sometimes we wish to describe the central tendency of a dataset that is not numeric. For example, let’s say that we want to know which models of iPhone are most commonly used. Let’s say we ask a group of iPhone users which model they own, and get the following results:

```
# compute mean of iPhone model numbers
iphoneDf <-
  tribble(
    ~iPhoneModel, ~count,
    5, 325,
    6, 450,
    7, 700,
    8, 625
  )

meanPhoneNumber <-
  iphoneDf %>%
  summarize(
    sum(iPhoneModel * count) / sum(count)
  ) %>%
  pull()
```

If we were to take the average of these values, we would see that the mean iPhone model is 6.77, which is clearly nonsensical, since the iPhone model numbers are on an ordinal scale. In this case, a more appropriate measure of central tendency is the mode, which is the most common value in the dataset, as we discussed above.



## 5.7 Variability: How well does the mean fit the data?

Once we have described the central tendency of the data, we often also want to describe how variable the data are – this is sometimes also referred to as “dispersion”, reflecting the fact that it describes how widely dispersed the data are.

We have already encountered the sum of squared errors above, which is the basis for the most commonly used measures of variability: the *variance* and the *standard deviation*. The variance for a population (referred to as  $\sigma^2$ ) is simply the sum of squared errors divided by the number of observations - that is, the *mean squared error* that you encountered earlier:

$$\sigma^2 = \frac{SSE}{N} = \frac{\sum_{i=1}^n (x_i - \mu)^2}{N}$$

where  $\mu$  is the population mean. The standard deviation is simply the square root of this – that is, the *root mean squared error* that we saw before. The standard deviation is useful because the errors are in the same units as the original data (undoing the squaring that we applied to the errors).

We usually don’t have access to the entire population, so we have to compute the variance using a sample, which we refer to as  $\hat{\sigma}^2$ , with the “hat” representing the fact that this is an estimate based on a sample. The equation for  $\hat{\sigma}^2$  is similar to the one for  $\sigma^2$ :

$$\hat{\sigma}^2 = \frac{\sum_{i=1}^N (x_i - \bar{X})^2}{n - 1}$$

The only difference between the two equations is that we divide by  $n - 1$  instead of  $N$ . This relates to a fundamental statistical concept: *degrees of freedom*. Remember that in order to compute the sample variance, we first had to estimate the sample mean  $\bar{X}$ . Having estimated this, one value in the data is no longer free to vary. For example, let’s say we have the following data points:

```
# generate example data points
```

```
dfDf <-
  tibble(
    x = c(3, 5, 7, 9, 11)
  )

pander(dfDf)
```

| x  |
|----|
| 3  |
| 5  |
| 7  |
| 9  |
| 11 |

Now we compute the mean:

```
# compute mean
```

```
meanx <-
  dfDf %>%
  summarize(
    mean(x)
```

```

) %>%
pull()

sprintf('%0.2f', meanx)

## [1] "7.00"

```

Because we know that the mean of this dataset is 7, we can compute what any specific value would be if it were missing. For example, let's say we were to obscure the first value (3). Having done this, we still know that its value must be 3, because the mean of 7 implies that the sum of all of the values is  $7 * n = 35$  and  $35 - (5 + 7 + 9 + 11) = 3$ .

So when we say that we have “lost” a degree of freedom, it means that there is a value that is not free to vary after fitting the model. In the context of the sample variance, if we don't account for the lost degree of freedom, then our estimate of the sample variance will be *biased* – that is, it will be smaller than the true (population) value.

## 5.8 Using simulations to understand statistics

I am a strong believer in the use of computer simulations to understand statistical concepts, and in later sessions we will dig deeply into their use. Here we will introduce the idea by asking whether we can confirm the need to subtract 1 from the sample size in computing the sample variance.

Let's treat the entire sample of children from the NHANES data as our “population”, and see how well the calculations of sample variance using either N or N-1 in the denominator will estimate the population variance, across a large number of simulated random samples from the data. Don't worry about the details now – we will return to those later in the course.

```

# compare variance estimates using N or N-1 in denominator

population_variance <-
  NHANES_child %>%
  summarize(
    var(Height)
  ) %>%
  pull()

# take 100 samples and estimate the sample variance using both N or N-1 in the demoninator
sampsiz <- 50
nsamp <- 1000
varhat_n <- array(data = NA, dim = nsamp)
varhat_nm1 <- array(data = NA, dim = nsamp)

for (i in 1:nsamp) {
  samp <- sample_n(NHANES_child, 1000)[1:sampsiz, ]
  sampmean <- mean(samp$Height)
  sse <- sum((samp$Height - sampmean)**2)
  varhat_n[i] <- sse / sampsiz
  varhat_nm1[i] <- sse / (sampsiz - 1)
}

sprintf("population variance: %.2f", population_variance)

```

```
## [1] "population variance: 724.67"
sprintf("variance estimate(n): %.2f", mean(varhat_n))

## [1] "variance estimate(n): 709.03"
sprintf("variance estimate(n-1): %.2f", mean(varhat_nm1))

## [1] "variance estimate(n-1): 723.50"
```

This shows us that the theory outlined above was correct: The variance estimate using  $n - 1$  as the denominator is very close to the variance computed on the full data (i.e, the population), whereas the variance computed using  $n$  as the denominator is biased (smaller) compared to the true value.

## 5.9 Z-scores

```
crimeData <-
  read.table(
    "data/CrimeOneYearofData_clean.csv",
    header = TRUE,
    sep = ",",
  )

# let's drop DC since it is so small
crimeData <-
  crimeData %>%
  dplyr::filter(State != "District of Columbia")

caCrimeData <-
  crimeData %>%
  dplyr::filter(State == "California")
```

Having characterized a distribution in terms of its central tendency and variability, it is often useful to express the individual scores in terms of where they sit with respect to the overall distribution. Let's say that we are interested in characterizing the relative level of crimes across different states, in order to determine whether California is a particularly dangerous place. We can ask this question using data for 2014 from the FBI's Uniform Crime Reporting site. The left panel of Figure 5.8 shows a histogram of the number of violent crimes per state, highlighting the value for California. Looking at these data, it seems like California is terribly dangerous, with 153709 crimes in that year.

With R it's also easy to generate a map showing the distribution of a variable across states, which is presented in the right panel of Figure 5.8.

It may have occurred to you, however, that CA also has the largest population of any state in the US, so it's reasonable that it will also have a larger number of crimes. If we plot the two against one another (see left panel of Figure 5.9), we see that there is a direct relationship between population and the number of crimes.

Instead of using the raw numbers of crimes, we should instead use the per-capita violent crime rate, which we obtain by dividing the number of crimes by the population of the state. The dataset from the FBI already includes this value (expressed as rate per 100,000 people).

```
# print crime rate statistics, normalizing for population
sprintf("rate of 2014 violent crimes in CA: %.2f", caCrimeData$Violent.Crime.rate)

## [1] "rate of 2014 violent crimes in CA: 396.10"
```

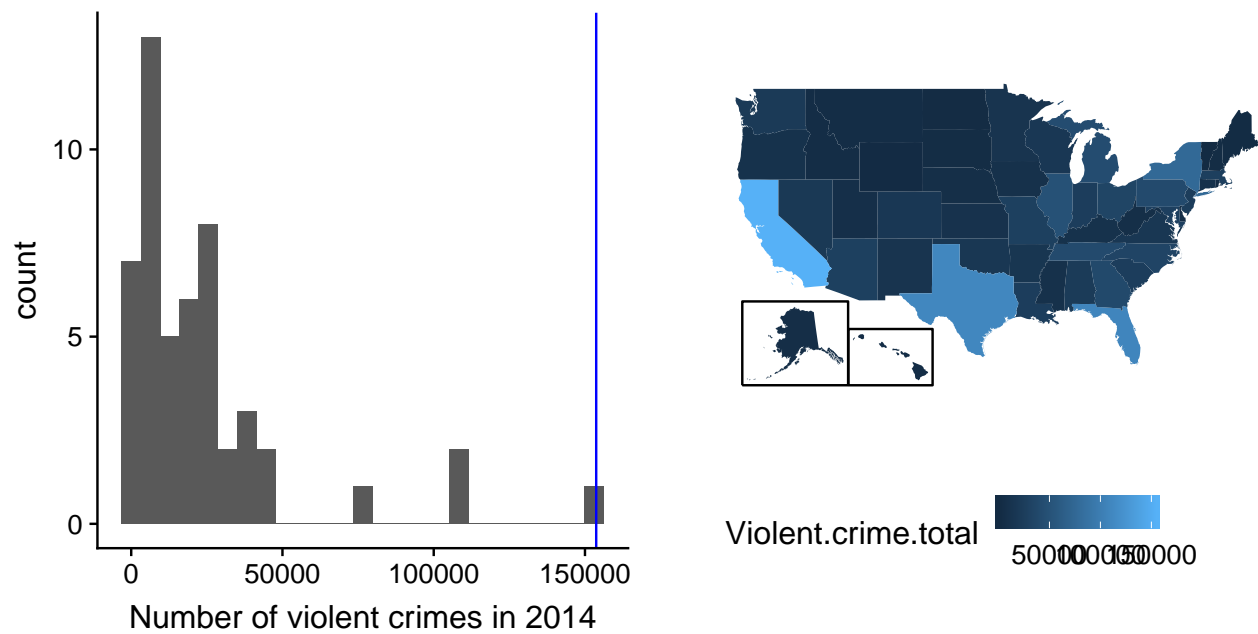


Figure 5.8: Left: Histogram of the number of violent crimes. The value for CA is plotted in blue. Right: A map of the same data, with number of crimes plotted for each state in color.

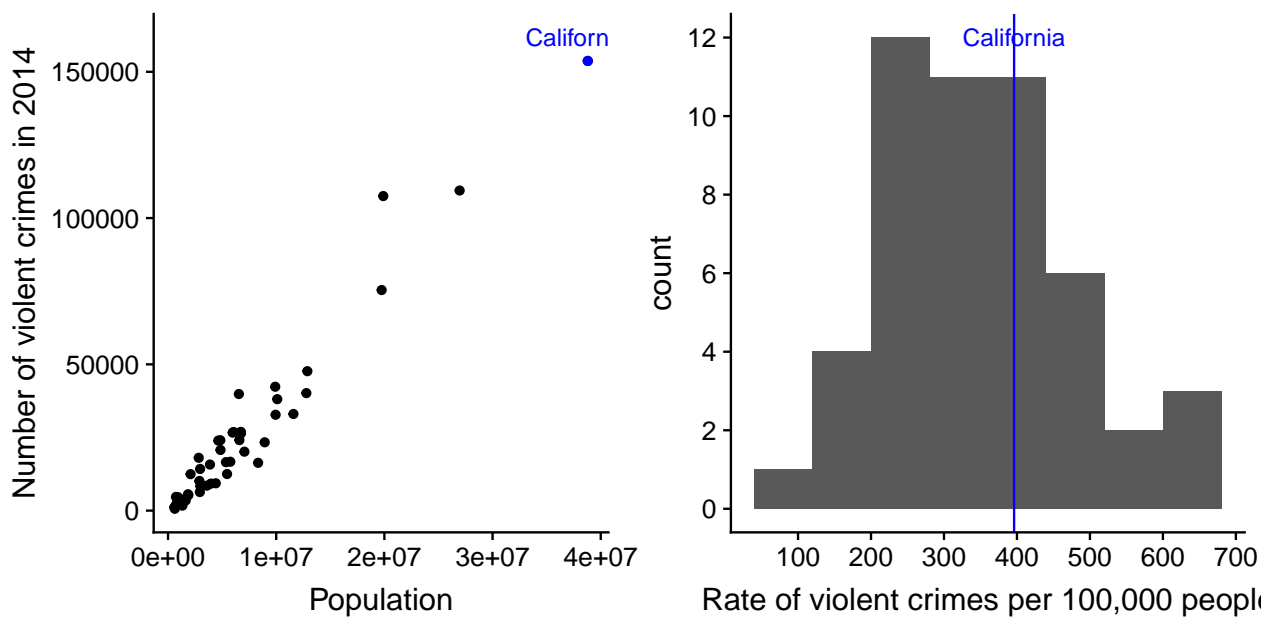


Figure 5.9: Left: A plot of number of crimes versus population by state. Right: A histogram of per capita crime rates, expressed as crimes per 100,000 people.

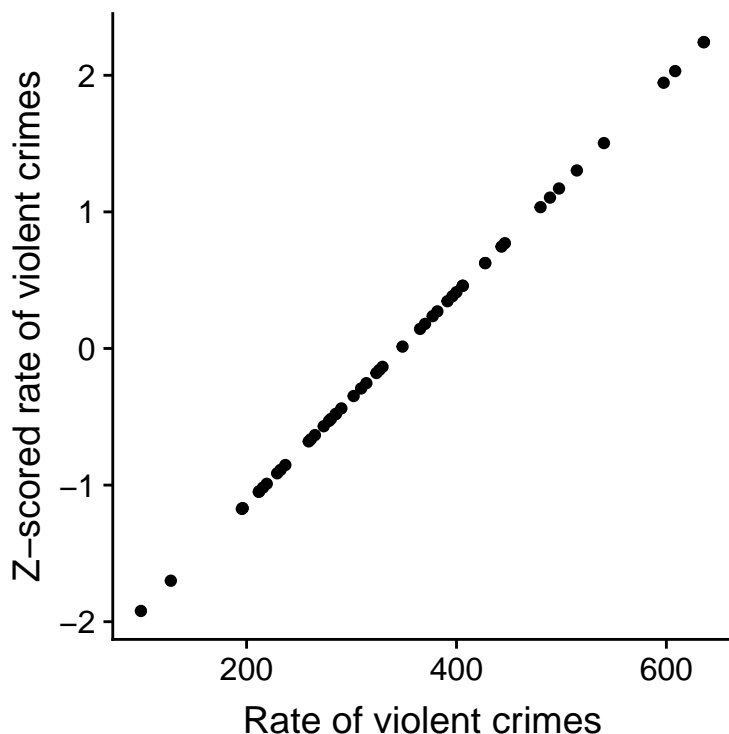


Figure 5.10: Scatterplot of original crime rate data against Z-scored data.

```
sprintf("mean rate: %.2f", mean(crimeData$Violent.Crime.rate))
```

```
## [1] "mean rate: 346.81"
```

```
sprintf("std of rate: %.2f", sd(crimeData$Violent.Crime.rate))
```

```
## [1] "std of rate: 128.82"
```

From the right panel of Figure 5.9 we see that California is not so dangerous after all – its crime rate of 396.1 per 100,000 people is a bit above the mean of 346.81, but well within the range of many other states. But what if we want to get a clearer view of how far it is from the rest of the distribution?

The *Z-score* allows us to express data in a way that provides more insight into each data point's relationship to the overall distribution. The formula to compute a Z-score for a data point given that we know the value of the population mean  $\mu$  and standard deviation  $\sigma$  is:

$$Z(x) = \frac{x - \mu}{\sigma}$$

Intuitively, you can think of a Z-score as telling you how far away from the mean any data point is, in units of standard deviation. We can compute this for the crime rate data, as shown in Figure 5.10.

```
## [1] "mean of Z-scored data: 1.4658413372004e-16"
```

```
## [1] "std deviation of Z-scored data: 1"
```

The scatterplot shows us that the process of Z-scoring doesn't change the relative distribution of the data points (visible in the fact that the original data and Z-scored data fall on a straight line when plotted against each other) – it just shifts them to have a mean of zero and a standard deviation of one. However, if you look closely, you will see that the mean isn't exactly zero – it's just very small. What is going on here is that the

computer represents numbers with a certain amount of *numerical precision* - which means that there are numbers that are not exactly zero, but are small enough that R considers them to be zero.

```
# examples of numerical precision

print(paste("smallest number such that 1+x != 1", .Machine$double.eps))

## [1] "smallest number such that 1+x != 1 2.22044604925031e-16"

# We can confirm this by showing that adding anything less than that number to
# 1 is treated as 1 by R
print((1 + .Machine$double.eps) == 1)

## [1] FALSE

print((1 + .Machine$double.eps / 2) == 1)

## [1] TRUE

# we can also look at the largest number
print(paste("largest number", .Machine$double.xmax))

## [1] "largest number 1.79769313486232e+308"

# similarly here, we can see that adding 1 to the largest possible number
# is no different from the largest possible number, in R's eyes at least.
print((1 + .Machine$double.xmax) == .Machine$double.xmax)

## [1] TRUE
```

Figure 5.11 shows the Z-scored crime data using the geographical view.

This provides us with a slightly more interpretable view of the data. For example, we can see that Nevada, Tennessee, and New Mexico all have crime rates that are roughly two standard deviations above the mean.

### 5.9.1 Interpreting Z-scores

The “Z” in “Z-score” comes from the fact that the standard normal distribution (that is, a normal distribution with a mean of zero and a standard deviation of 1) is often referred to as the “Z” distribution. We can use the standard normal distribution to help us understand what specific Z scores tell us about where a data point sits with respect to the rest of the distribution.

The upper panel in Figure 5.12 shows that we expect about 16% of values to fall in  $Z \geq 1$ , and the same proportion to fall in  $Z \leq -1$ .

Figure 5.13 shows the same plot for two standard deviations. Here we see that only about 2.3% of values fall in  $Z \leq -2$  and the same in  $Z \geq 2$ . Thus, if we know the Z-score for a particular data point, we can estimate how likely or unlikely we would be to find a value at least as extreme as that value, which lets us put values into better context.

### 5.9.2 Standardized scores

Let’s say that instead of Z-scores, we wanted to generate standardized crime scores with a mean of 100 and standard deviation of 10. This is similar to the standardization that is done with scores from intelligence tests to generate the intelligence quotient (IQ). We can do this by simply multiplying the Z-scores by 10 and then adding 100.

```
## [1] "mean of standardized score data: 100"
```

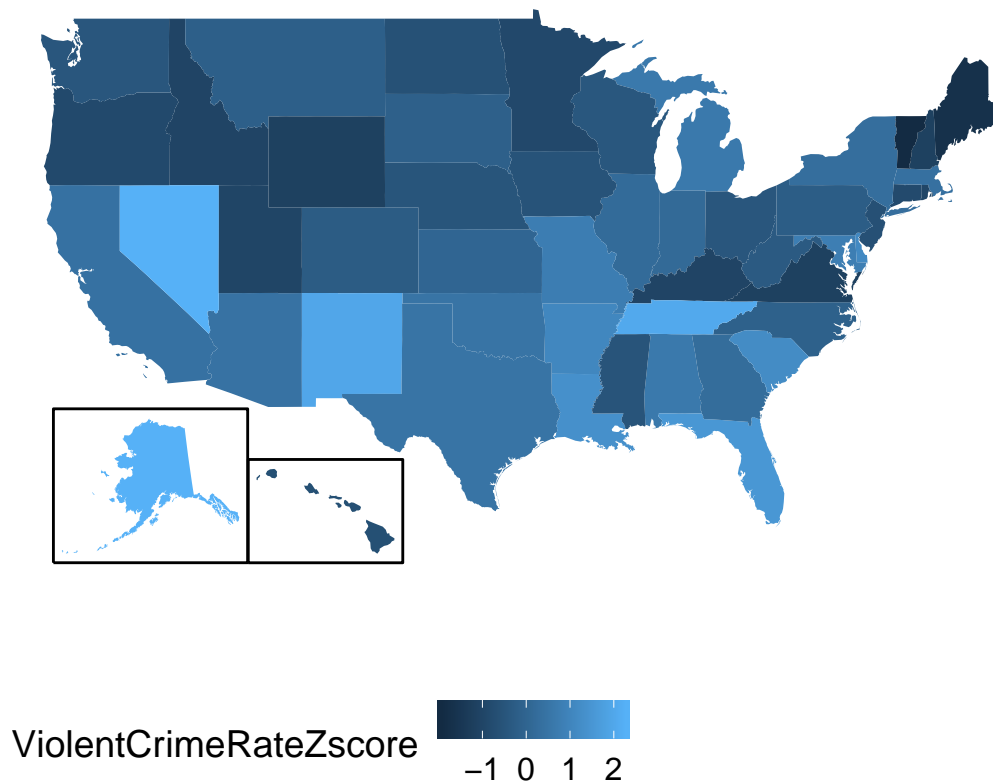


Figure 5.11: Crime data rendered onto a US map, presented as Z-scores.

```
## [1] "std deviation of standardized score data: 10"
```

### 5.9.2.1 Using Z-scores to compare distributions

One useful application of Z-scores is to compare distributions of different variables. Let's say that we want to compare the distributions of violent crimes and property crimes across states. In the left panel of Figure 5.15 we plot those against one another, with CA plotted in blue. As you can see the raw rates of property crimes are far higher than the raw rates of violent crimes, so we can't just compare the numbers directly. However, we can plot the Z-scores for these data against one another (right panel of Figure 5.15)– here again we see that the distribution of the data does not change. Having put the data into Z-scores for each variable makes them comparable, and lets us see that California is actually right in the middle of the distribution in terms of both violent crime and property crime.

Let's add one more factor to the plot: Population. In the left panel of Figure 5.16 we show this using the size of the plotting symbol, which is often a useful way to add information to a plot.

Because Z-scores are directly comparable, we can also compute a "Violence difference" score that expresses the relative rate of violent to non-violent (property) crimes across states. We can then plot those scores against population (see right panel of Figure 5.16). This shows how we can use Z-scores to bring different variables together on a common scale.

It is worth noting that the smallest states appear to have the largest differences in both directions. While it might be tempting to look at each state and try to determine why it has a high or low difference score, this probably reflects the fact that the estimates obtained from smaller samples are necessarily going to be more variable, as we will discuss in more detail in a couple of chapters.

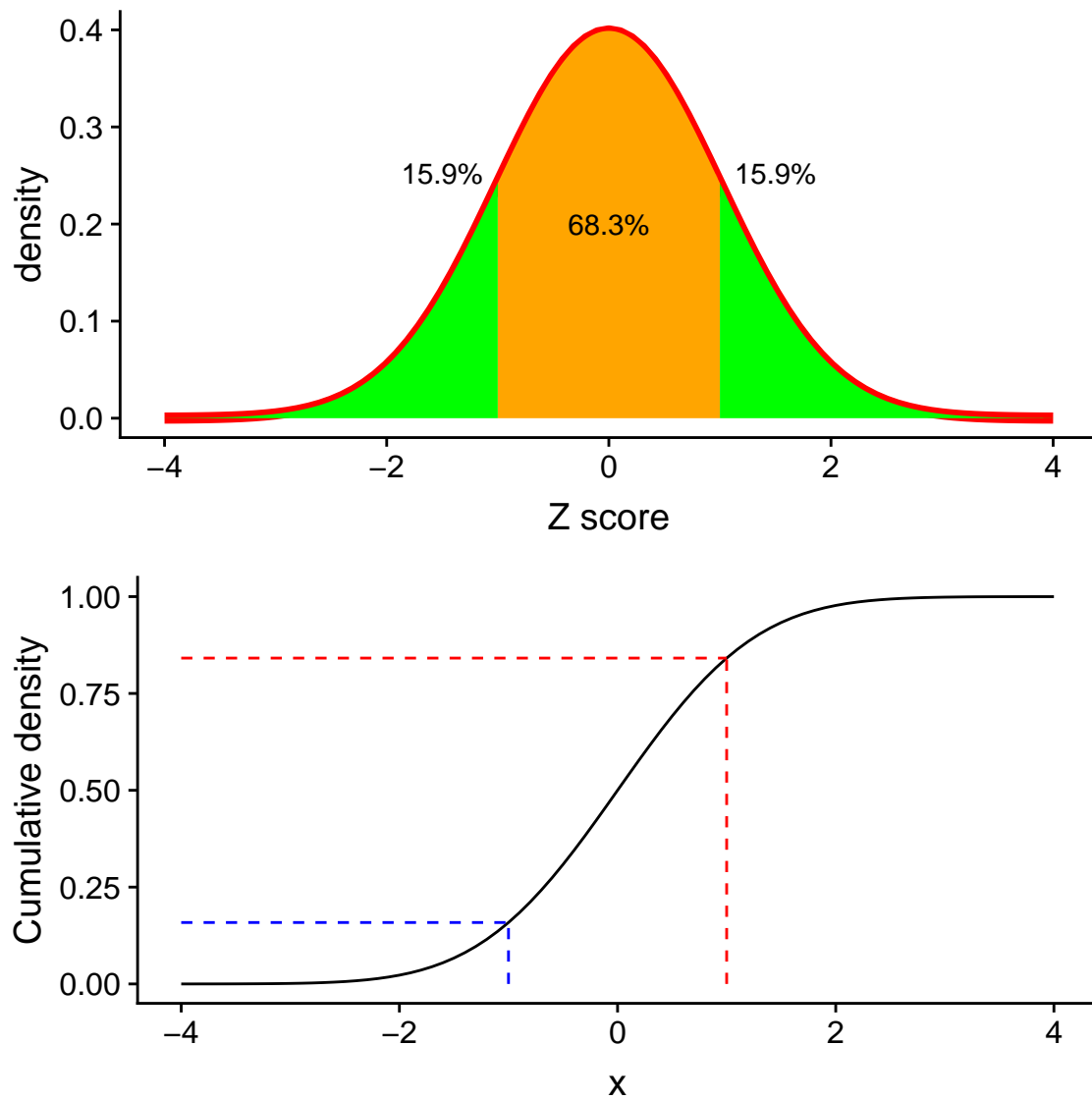


Figure 5.12: Density (top) and cumulative distribution (bottom) of a standard normal distribution, with cutoffs at one standard deviation above/below the mean.



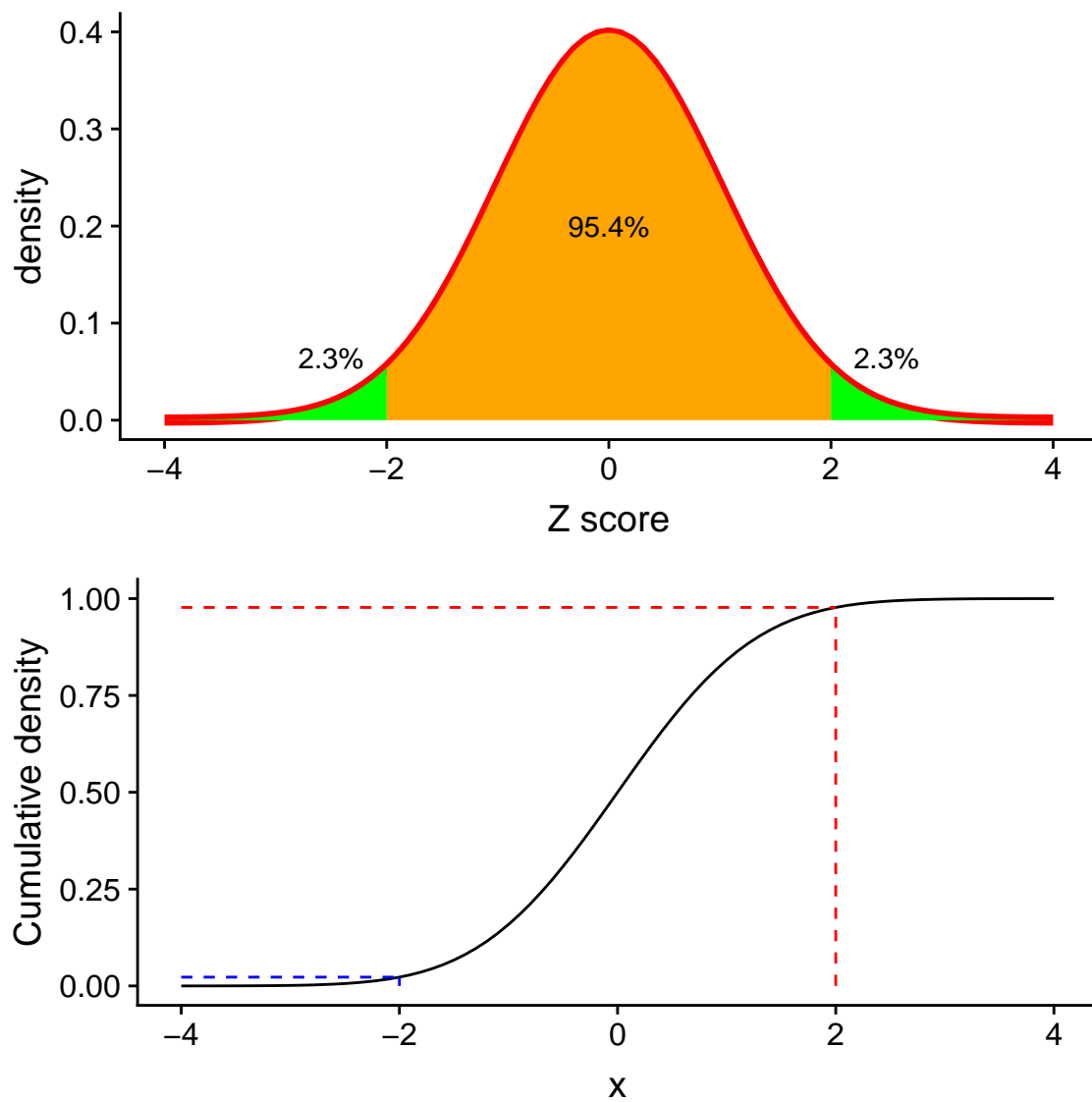


Figure 5.13: Density (top) and cumulative distribution (bottom) of a standard normal distribution, with cutoffs at two standard deviations above/below the mean

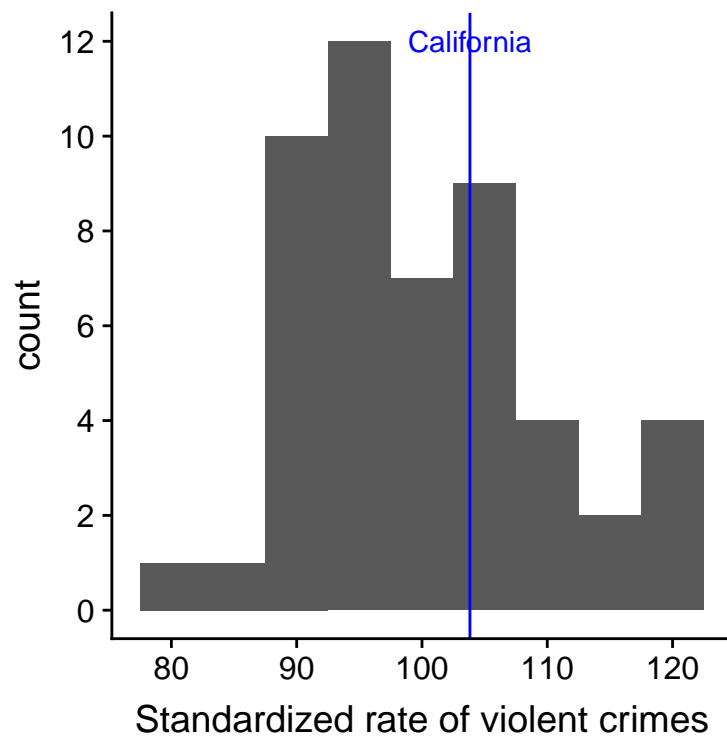


Figure 5.14: Crime data presented as standardized scores with mean of 100 and standard deviation of 10.

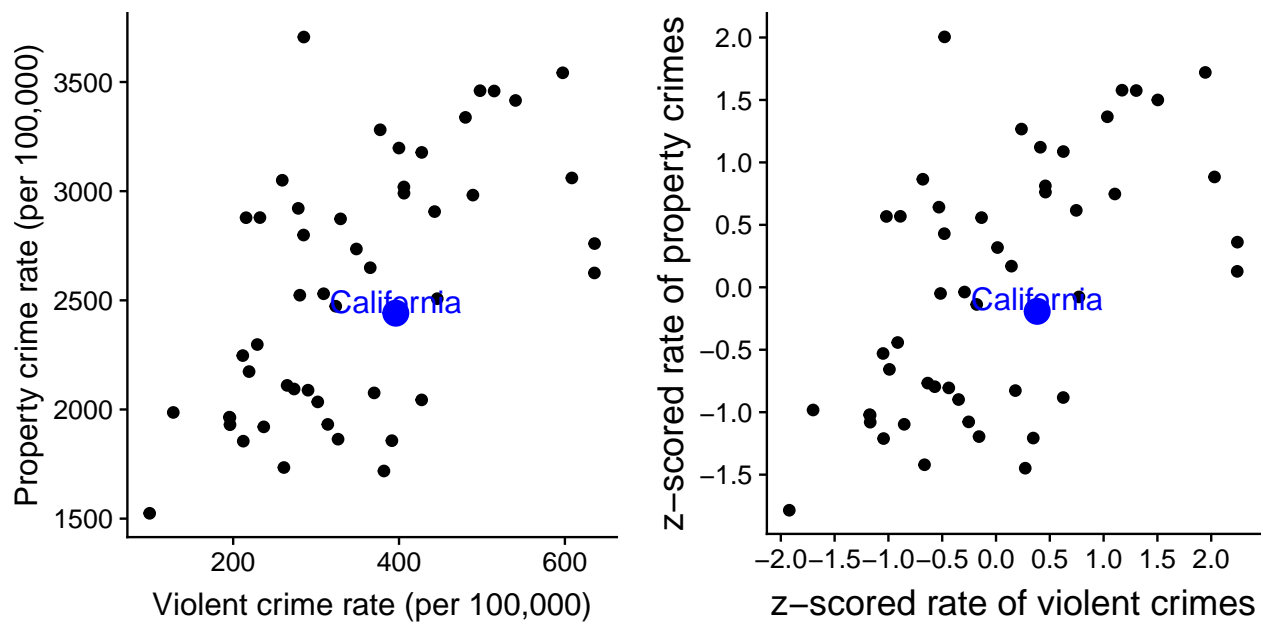


Figure 5.15: Plot of violent vs. property crime rates (left) and Z-scored rates (right).

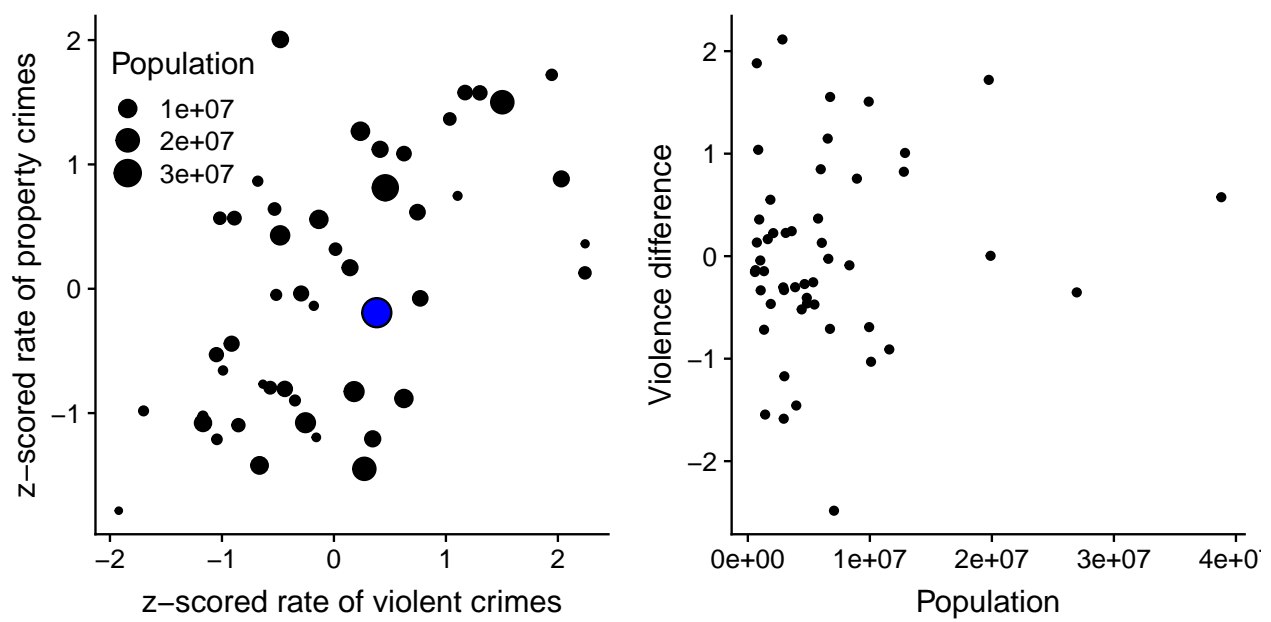


Figure 5.16: Left: Plot of violent vs. property crime rates, with population size presented through the size of the plotting symbol; California is presented in blue. Right: Difference scores for violent vs. property crime, plotted against population.



## Chapter 6

# Data Visualization

One of the most important things that we can do with a dataset is to look at it, but there are many ways to look at data, and some are much more effective than others. In this chapter we will discuss how to effectively visualize data.

### 6.1 How data visualization can save lives

On January 28, 1986, the Space Shuttle Challenger exploded 73 seconds after takeoff, killing all 7 of the astronauts on board. As when any such disaster occurs, there was an official investigation into the cause of the accident, which found that an O-ring connecting two sections of the solid rocket booster had leaked, resulting in failure of the joint and explosion of the large liquid fuel tank (see figure 6.1).

The investigation found that many aspects of the NASA decision making process were flawed, and focused in particular on a meeting that was had between NASA staff and engineers from Morton Thiokol, a contractor who had built the solid rocket boosters. These engineers were particularly concerned because the temperatures were forecast to be very cold on the morning of the launch, and they had data from previous launches showing that performance of the O-rings was compromised at lower temperatures. In a meeting on the evening before the launch, the engineers presented their data to the NASA managers, but were unable to convince them to postpone the launch.

The visualization expert Edward Tufte has argued that with a proper presentation of all of the data, the engineers could have been much more persuasive. In particular, they could have shown a figure like the one in



Figure 6.1: An image of the solid rocket booster leaking fuel, seconds before the explosion. By NASA (Great Images in NASA Description) [Public domain], via Wikimedia Commons

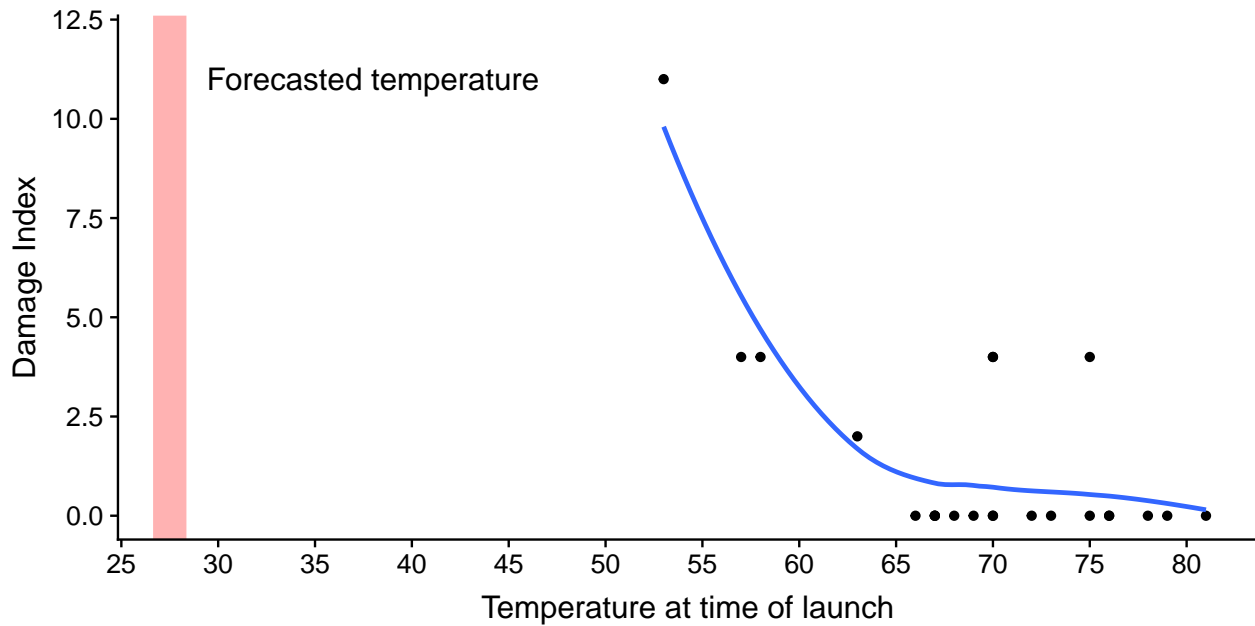


Figure 6.2: A replotting of Tufte’s damage index data. The blue line shows the trend in the data, and the red patch shows the projected temperatures for the morning of the launch.

Figure 6.2, which highlights two important facts. First, it shows that the amount of O-ring damage (defined by the amount of erosion and soot found outside the rings after the solid rocket boosters were retrieved from the ocean in previous flights) was closely related to the temperature at takeoff. Second, it shows that the range of forecasted temperatures for the morning of January 28 (shown in the shaded red area) was well outside of the range of all previous launches. While we can’t know for sure, it seems at least plausible that this could have been more persuasive.

## 6.2 Anatomy of a plot

The goal of plotting data is to present a summary of a dataset in a two-dimensional (or occasionally three-dimensional) presentation. We refer to the dimensions as *axes* – the horizontal axis is called the *X-axis* and the vertical axis is called the *Y-axis*. We can arrange the data along the axes in a way that highlights the data values. These values may be either continuous or categorical.

There are many different types of plots that we can use, which have different advantages and disadvantages. Let’s say that we are interested in characterizing the difference in height between men and women in the NHANES dataset. Figure ?? shows four different ways to plot these data.

1. The bar graph in panel A shows the difference in means, but doesn’t show us how much spread there is in the data around these means – and as we will see later, knowing this is essential to determine whether we think the difference between the groups is large enough to be important.
2. The second plot shows the bars with all of the data points overlaid - this makes it a bit clearer that the distributions of height for men and women are overlapping, but it’s still hard to see due to the large number of data points.

In general we prefer using a plotting technique that provides a clearly view of the distribution of the data points.

3. In panel C, we see one example of clearly showing the data points, known as a *violin plot*, which plots the distribution of data in each condition (after smoothing it out a bit).
4. Another option is the *box plot* shown in panel D, which shows the median (central line), a measure of variability (the width of the box, which is based on a measure called the interquartile range), and any outliers (noted by the points at the ends of the lines). These are both effective ways to show data that provide a good feel for the distribution of the data.





## Chapter 7

# plot height by Gender

```
dfmean=NHANES_adult %>% group_by(Gender) %>% summarise(Height=mean(Height))

p1 = ggplot(dfmean,aes(x=Gender,y=Height)) + geom_bar(stat="identity",color='gray') + coord_cartesian(ylim=c(0,210)) + ggtitle('Bar graph') + theme(aspect.ratio=1)

p2 = ggplot(dfmean,aes(x=Gender,y=Height)) + geom_bar(stat="identity",color='gray') + coord_cartesian(ylim=c(0,210)) + ggtitle('Bar graph with points') + theme(aspect.ratio=1) + geom_jitter(data=NHANES_adult)

p3 = ggplot(NHANES_adult,aes(x=Gender,y=Height)) + geom_violin() + ggtitle('Violin plot') + theme(aspect.ratio=1)

p4 = ggplot(NHANES_adult,aes(x=Gender,y=Height)) + geom_boxplot() + ggtitle('Box plot') + theme(aspect.ratio=1)

plot_grid(p1,p2,p3,p4,nrow=2,labels='AUTO')
```

““

## 7.1 Plotting in R using ggplot

There are many different tools for plotting data in R, but we will focus on the `ggplot()` function provided by a package called `ggplot2`. `ggplot` is very powerful, but using it requires getting one's head around how it works.

Let's say that we want to create a *scatterplot* that plots height against weight for each adult in a sample of 150 people from the NHANES dataset, with different markers used to denote men and women. First we create our sample:

```
NHANES_sample <-
  NHANES_adult %>%
  drop_na(Weight, Gender) %>% #remove rows (individuals) with missing values for Weight and Gender
  sample_n(150) #take a random sample of n = 150 rows (individuals)
```

Now let's set up the `ggplot()` command. This requires us to specify two things. First, we need to tell it which data frame to obtain the data from (in this case, `NHANES_sample`). Second, we need to tell it which variables from the data frame to use, which we do via the *aesthetics* function `aes()`. In this case, we want to plot height on the X axis and weight on the Y axis. The result is shown in Figure 7.1: The command generates a set of plot axes but doesn't actually show any data.

```
NHANES_sample %>%
  ggplot(aes(x = Height, y = Weight))
```

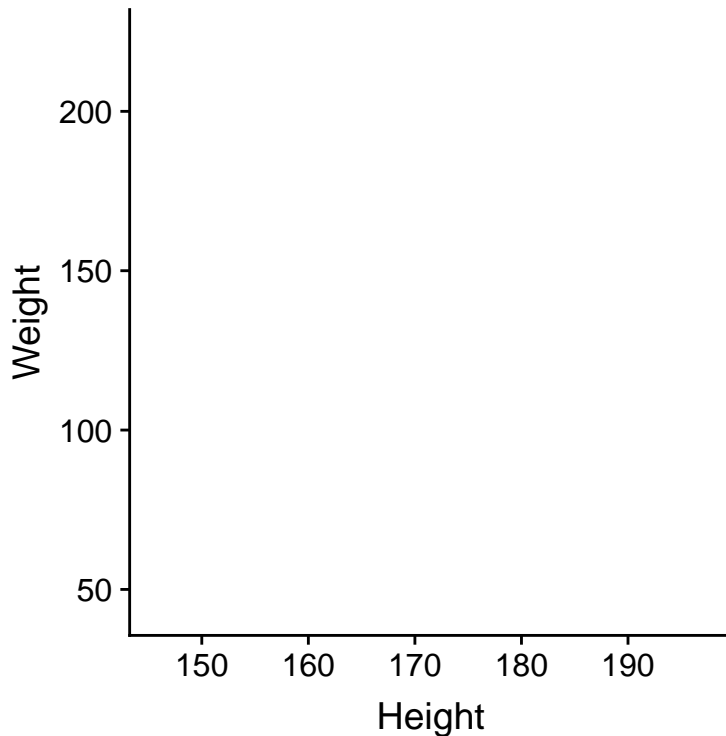


Figure 7.1: Empty plot frame generated by `ggplot()`

We next need to add a presentation of the data. The way that we tell `ggplot` what to show is by adding various commands to the main `ggplot()` command. In particular, we generally need to add a *geometry* or “geom”, which specifies how the data will be arranged in the plot. For example, to show each data point we can use the `geom_point()` geometry, as shown in Figure 7.2. Each data point represents an individual row in our `NHANES_sample` dataset with each row corresponding to an individual person in this dataset.

```
NHANES_sample %>%  
  ggplot(aes(x = Height, y = Weight)) +  
  geom_point()
```

Finally, we want to plot the points in separate colors depending on their gender. We do this by simply adding a *color* keyword to the aesthetics, which tells the `geom_point()` function to separately color points by Gender. This is shown in Figure 7.3. This figure also shows an example of how we can include multiple geometry layers in a single figure – in this case, we use `geom_smooth()` to plot the lines that best describe the relation between height and weight, separately by gender. The shading around the lines reflects our confidence in the estimate at that point.

```
NHANES_sample %>%  
  ggplot(aes(x = Height, y = Weight, color = Gender)) +  
  geom_point() +  
  geom_smooth(method = "lm")
```

## 7.2 Principles of good visualization

Many books have been written on effective visualization of data. There are some principles that most of these authors agree on, while others are more contentious. Here we summarize some of the major principles; if you want to learn more, then some good resources are listed in the *Suggested Readings* section at the end

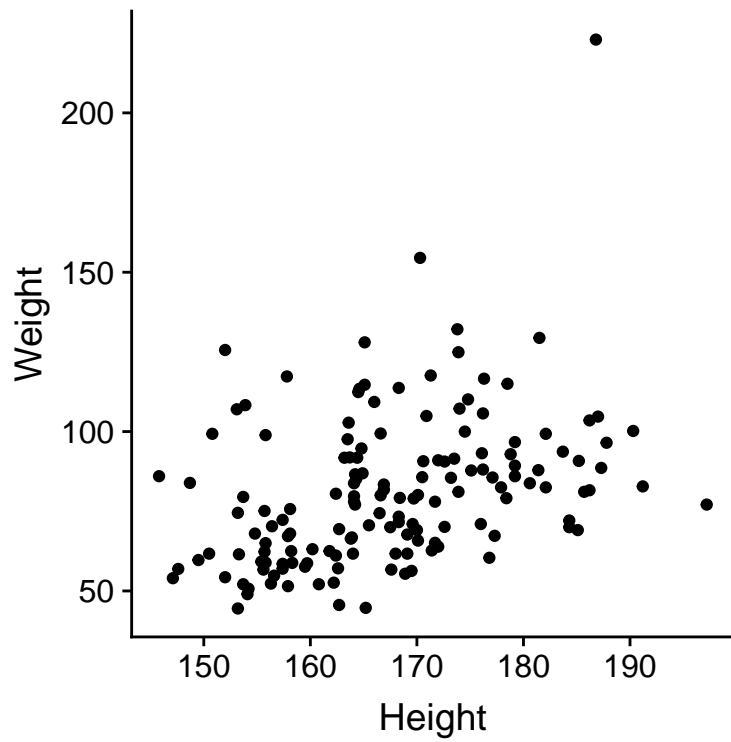


Figure 7.2: Simple scatter plot

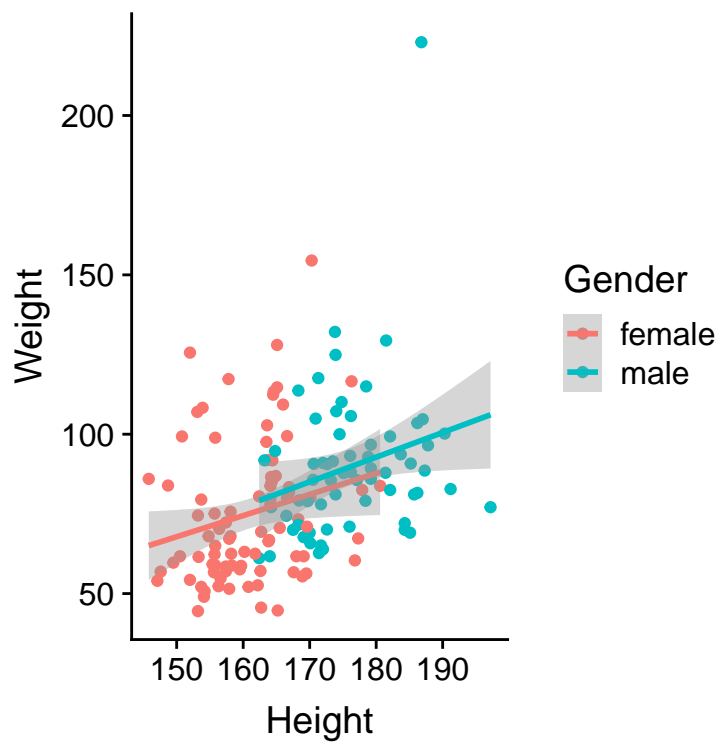


Figure 7.3: Scatterplot with points separately colored by Gender.

of this chapter.

Here is our distillation of some important principles for data visualization.

### 7.2.1 Show the data and make them stand out

Let's say that I had performed a study that examined the relationship between dental health and time spent flossing, and I would like to visualize my data. Figure 7.4 shows four possible presentations of these data.

1. In panel A, we don't actually show the data, just a line expressing the relationship between the data. This is clearly not optimal, because we can't actually see what the underlying data look like.

Panels B-D show three possible outcomes from plotting the actual data, where each plot shows a different way that the data could have been generated.

2. If we saw the plot in Panel B, we would probably be suspicious – rarely would real data follow such a precise pattern.
3. The data in Panel C, on the other hand, look like real data – they show a general trend, but they are messy, as data in the world usually are.
4. The data in Panel D show us that the apparent relationship between the two variables is solely caused by one individual, who we would refer to as an *outlier* because they fall so far outside of the pattern of the rest of the group. It should be clear that we probably don't want to conclude very much from an effect that is driven by one data point. This figure highlights why it is *always* important to look at the raw data before putting too much faith in any summary of the data.

## 7.3 Maximize the data/ink ratio

Edward Tufte has proposed an idea called the data/ink ratio:

$$\text{data/ink ratio} = \frac{\text{amount of ink used on data}}{\text{total amount of ink}}$$

The point of this is to minimize visual clutter and let the data show through. For example, take the two presentations of the dental health data in Figure 7.5. Both panels show the same data, but panel A is much easier to apprehend, because of its relatively higher data/ink ratio.

## 7.4 Avoid chartjunk

It's especially common to see presentations of data in the popular media that are adorned with lots of visual elements that are thematically related to the content but unrelated to the actual data. This is known as *chartjunk*, and should be avoided at all costs.

One good way to avoid chartjunk is to avoid using popular spreadsheet programs to plot one's data. For example, the chart in Figure 7.6 (created using Microsoft Excel) plots the relative popularity of different religions in the United States. There are at least three things wrong with this figure:

- it has graphics overlaid on each of the bars which have nothing to do with the actual data.
- it has a distracting background texture.
- it uses three-dimensional bars

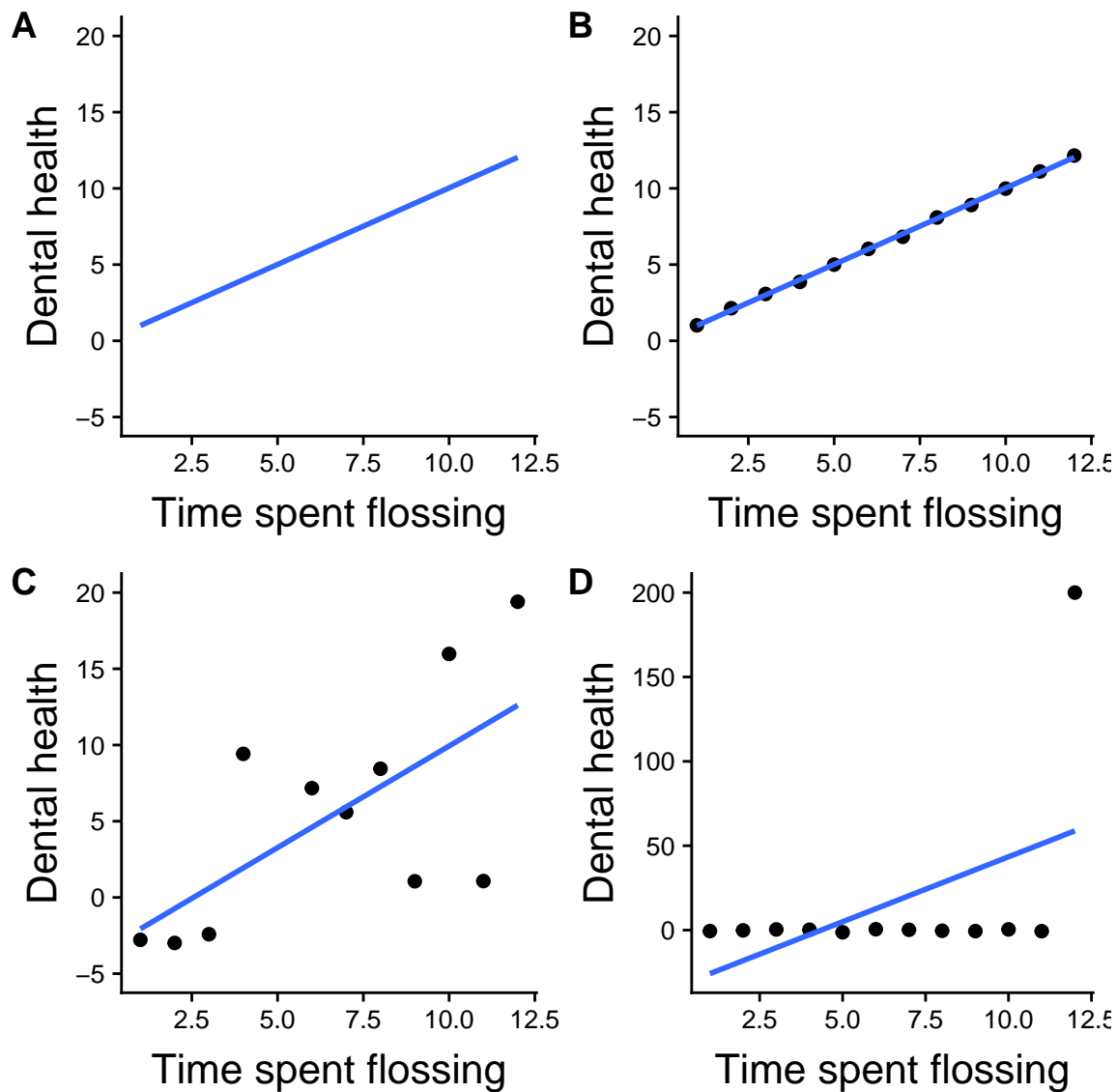


Figure 7.4: Four different possible presentations of data for the dental health example. Each point in the scatter plot represents one data point in the dataset, and the line in each plot represents the linear trend in the data.

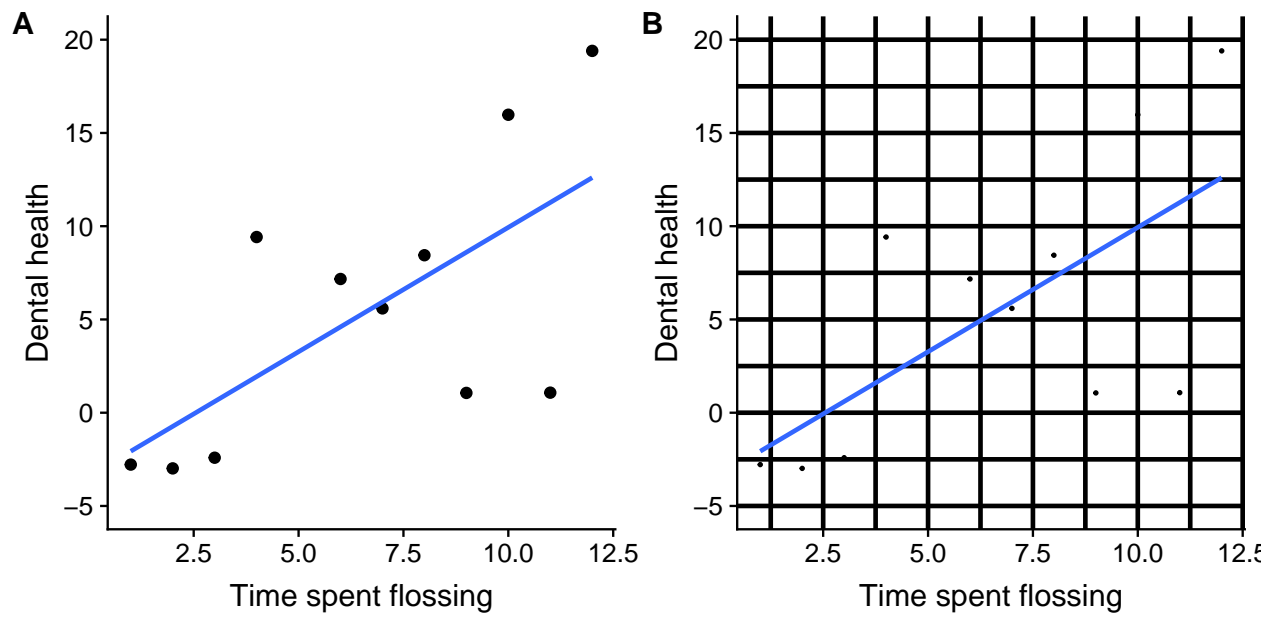


Figure 7.5: An example of the same data plotted with two different data/ink ratios.

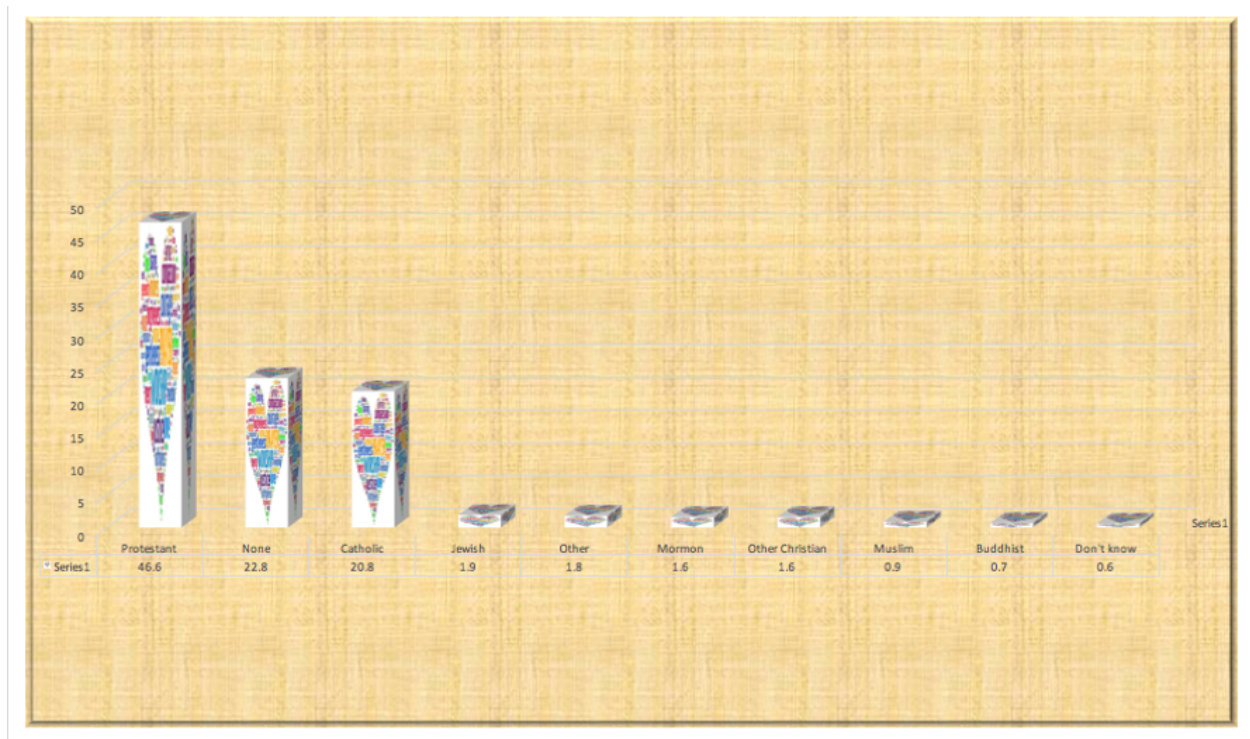


Figure 7.6: An example of chart junk.

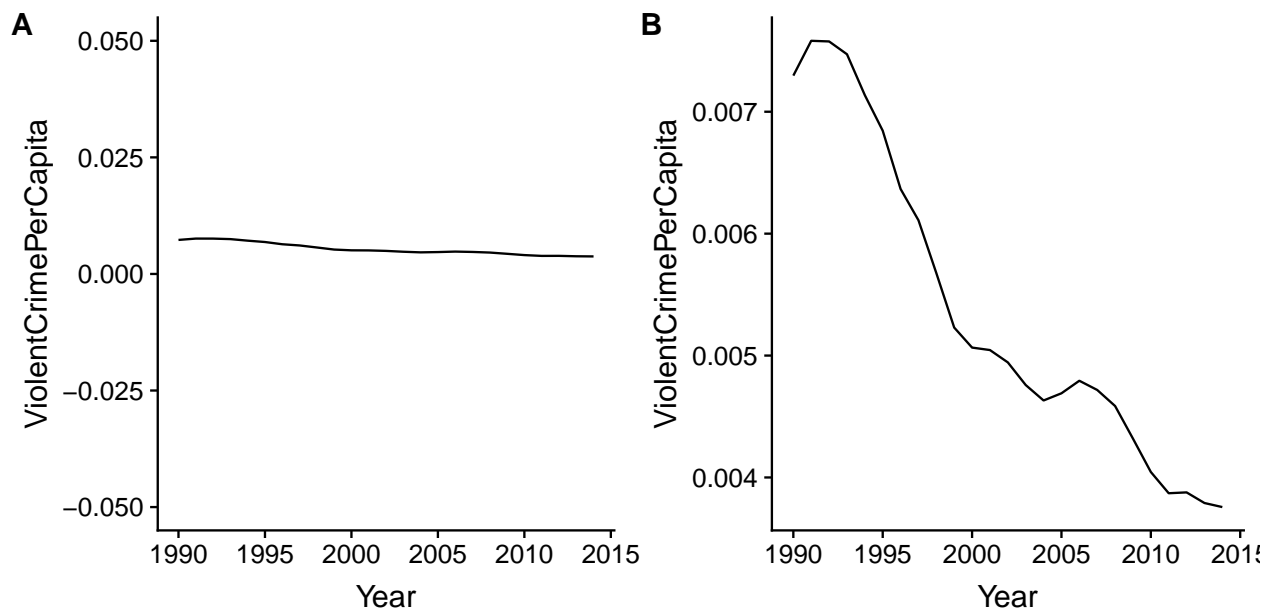


Figure 7.7: Crime data from 1990 to 2014 plotted over time. Panels A and B show the same data, but with different axis ranges. Data obtained from <https://www.ucrdatatool.gov/Search/Crime/State/RunCrimeStatebyState.cfm>

## 7.5 Avoid distorting the data

It's often possible to use visualization to distort the message of a dataset. A very common one is use of different axis scaling to either exaggerate or hide a pattern of data. For example, let's say that we are interested in seeing whether rates of violent crime have changed in the US. In Figure 7.7, we can see these data plotted in ways that either make it look like crime has remained constant, or that it has plummeted. The same data can tell two very different stories!

One of the major controversies in statistical data visualization is how to choose the Y axis, and in particular whether it should always include zero. In his famous book "How to lie with statistics", Darrell Huff argued strongly that one should always include the zero point in the Y axis. On the other hand, Edward Tufte has argued against this:

"In general, in a time-series, use a baseline that shows the data not the zero point; don't spend a lot of empty vertical space trying to reach down to the zero point at the cost of hiding what is going on in the data line itself." (from <https://qz.com/418083/its-ok-not-to-start-your-y-axis-at-zero/>)

There are certainly cases where using the zero point makes no sense at all. Let's say that we are interested in plotting body temperature for an individual over time. In Figure 7.8 we plot the same (simulated) data with or without zero in the Y axis. It should be obvious that by plotting these data with zero in the Y axis (Panel A) we are wasting a lot of space in the figure, given that body temperature of a living person could never go to zero! By including zero, we are also making the apparent jump in temperature during days 21-30 much less evident. In general, my inclination for line plots and scatterplots is to use all of the space in the graph, unless the zero point is truly important to highlight.

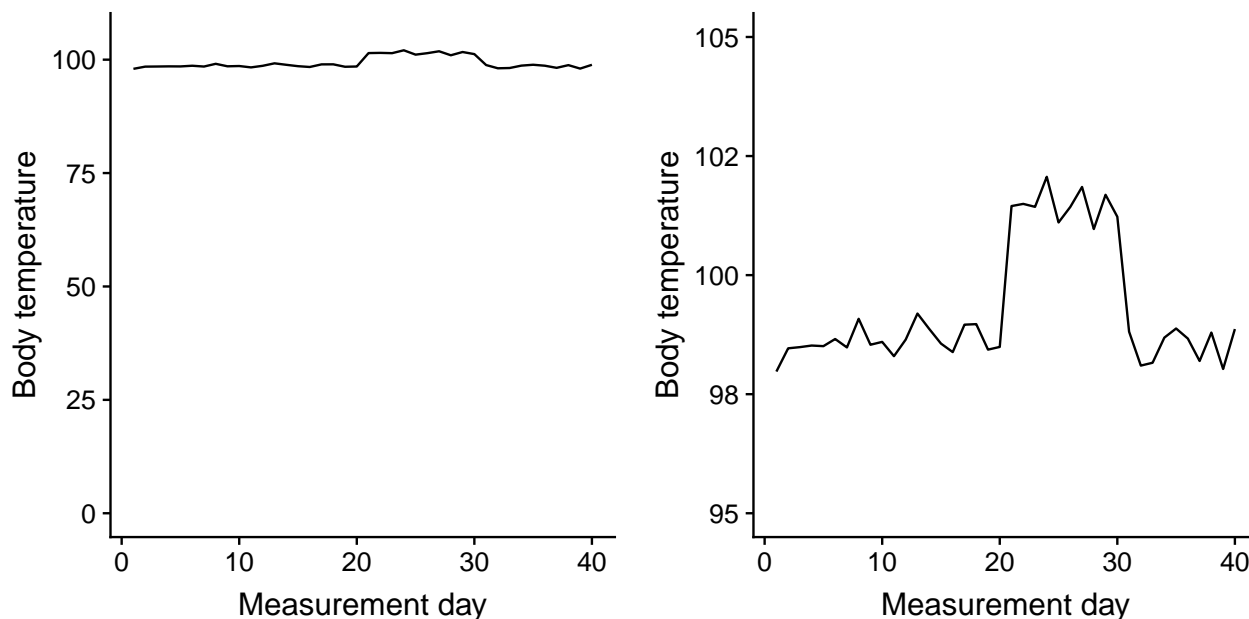


Figure 7.8: Body temperature over time, plotted with or without the zero point in the Y axis.

## 7.6 The lie factor

Edward Tufte introduced the concept of the “lie factor” to describe the degree to which physical differences in a visualization correspond to the magnitude of the differences in the data. If a graphic has a lie factor near 1, then it is appropriately representing the data, whereas lie factors far from one reflect a distortion of the underlying data.

The lie factor supports the argument that one should always include the zero point in a bar chart in many cases. In Figure 7.9 we plot the same data with and without zero in the Y axis. In panel A, the proportional difference in area between the two bars is exactly the same as the proportional difference between the values (i.e. lie factor = 1), whereas in Panel B (where zero is not included) the proportional difference in area between the two bars is roughly 2.8 times bigger than the proportional difference in the values, and thus it visually exaggerates the size of the difference.

## 7.7 Remember human limitations

Humans have both perceptual and cognitive limitations that can make some visualizations very difficult to understand. It’s always important to keep these in mind when building a visualization.

### 7.7.1 Perceptual limitations

One important perceptual limitation that many people (including myself) suffer from is color blindness. This can make it very difficult to perceive the information in a figure (like the one in Figure 7.10) where there is only color contrast between the elements but no brightness contrast. It is always helpful to use graph elements that differ substantially in brightness and/or texture, in addition to color. There are also “colorblind-friendly” palettes available for use in R.

Even for people with perfect color vision, there are perceptual limitations that can make some plots ineffective.



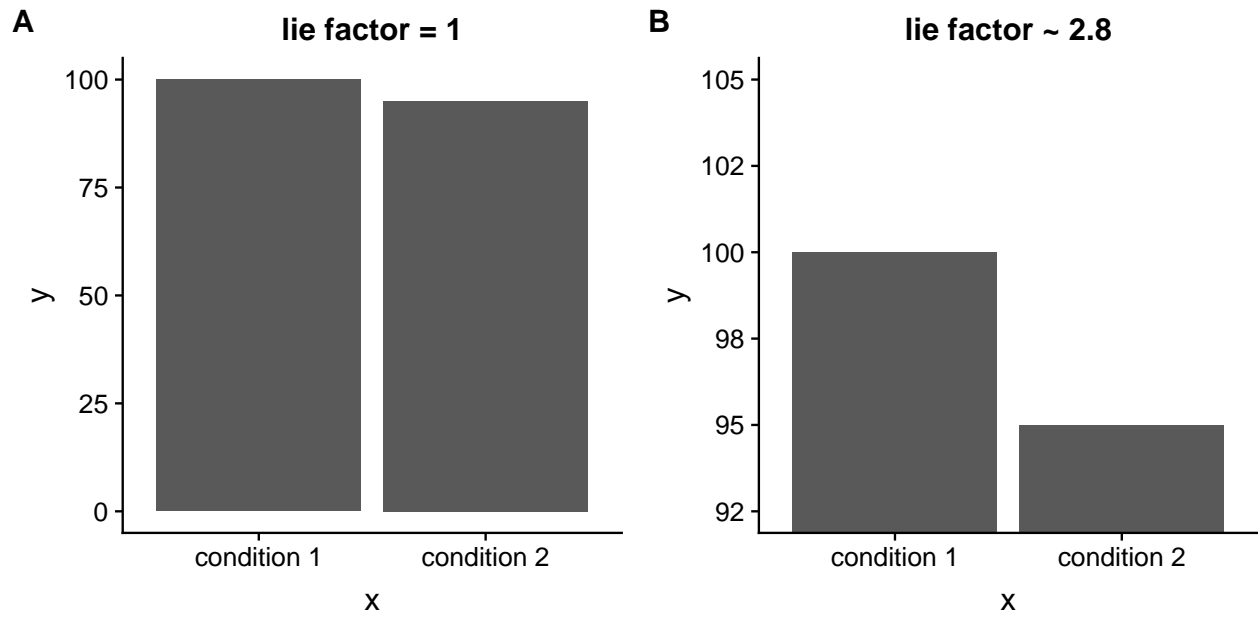


Figure 7.9: Two bar charts with associated lie factors.

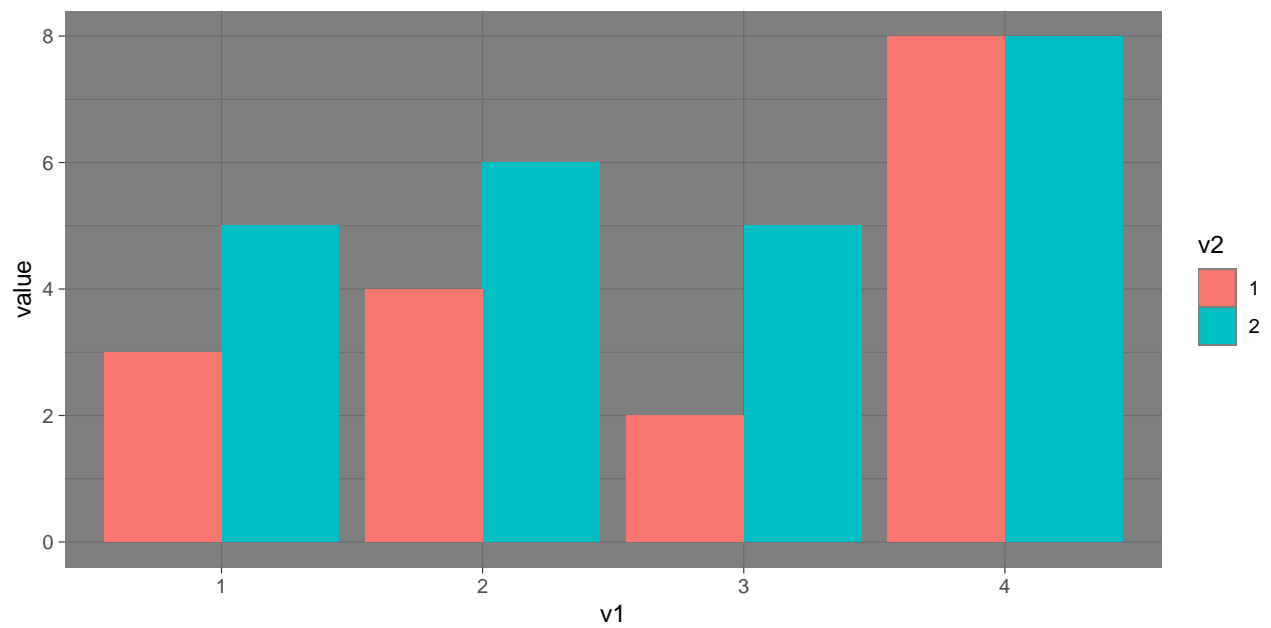


Figure 7.10: Example of a bad figure that relies solely on color contrast.

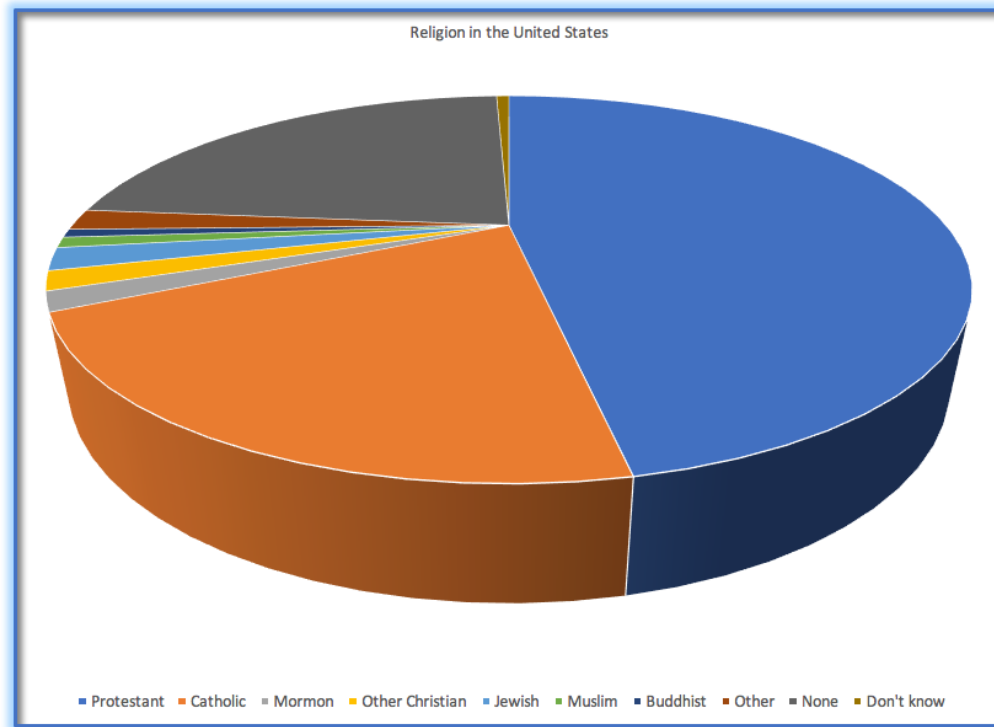


Figure 7.11: An example of a pie chart, highlighting the difficult in apprehending the relative volume of the different pie slices.

This is one reason why statisticians never use pie charts: It can be very difficult for humans to apprehend differences in the volume of shapes. The pie chart in Figure 7.11 (presenting the same data on religious affiliation that we showed above) shows how tricky this can be.

This plot is terrible for several reasons. First, it requires distinguishing a large number of colors from very small patches at the bottom of the figure. Second, the visual perspective distorts the relative numbers, such that the pie wedge for Catholic appears much larger than the pie wedge for None, when in fact the number for None is slightly larger (22.8 vs 20.8 percent), as was evident in Figure 7.6. Third, by separating the legend from the graphic, it requires the viewer to hold information in their working memory in order to map between the graphic and legend and to conduct many “table look-ups” in order to continuously match the legend labels to the visualization. And finally, it uses text that is far too small, making it impossible to read without zooming in.

Plotting the data using a more reasonable approach (Figure 7.12), we can see the pattern much more clearly. This plot may not look as flashy as the pie chart generated using Excel, but it’s a much more effective and accurate representation of the data.

This plot allows the viewer to make comparisons based on the the **length** of the bars **along a common scale** (the y-axis). Humans tend to be more accurate when decoding differences based on these perceptual elements than based on area or color.

## 7.8 Correcting for other factors

Often we are interested in plotting data where the variable of interest is affected by other factors than the one we are interested in. For example, let’s say that we want to understand how the price of gasoline has

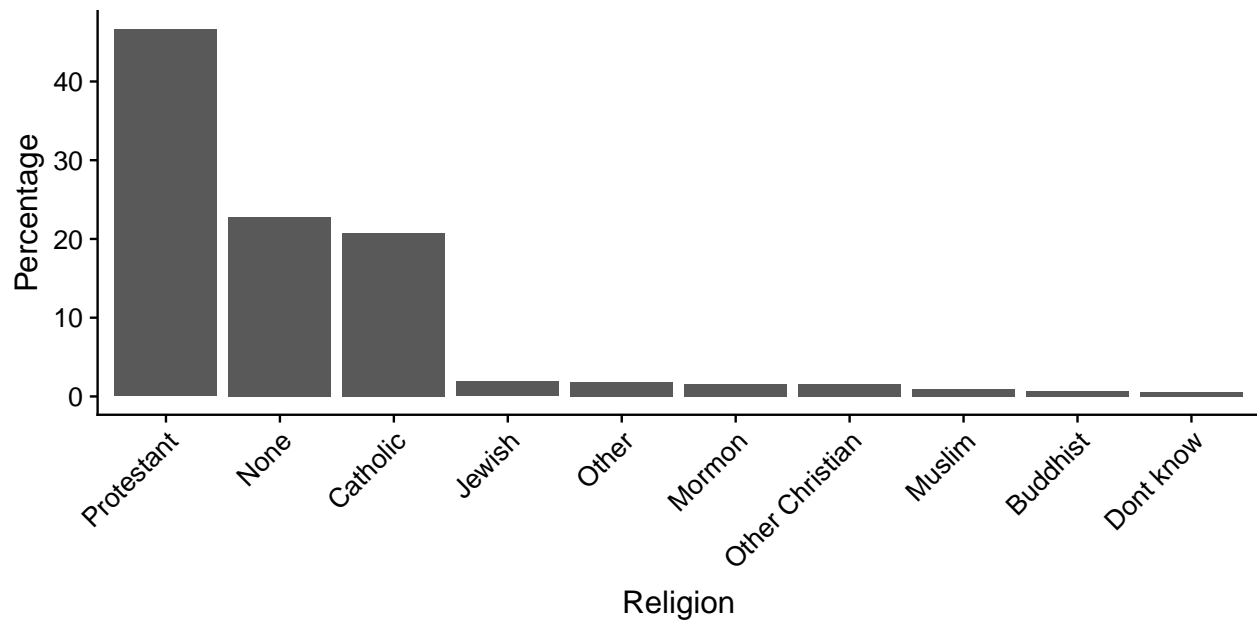


Figure 7.12: A clearer presentation of the religious affiliation data (obtained from <http://www.pewforum.org/religious-landscape-study/>).

changed over time. Figure 7.13 shows historical gas price data, plotted either with or without adjustment for inflation. Whereas the unadjusted data show a huge increase, the adjusted data show that this is mostly just reflective of inflation. Other examples where one needs to adjust data for other factors include population size (as we saw in the crime rate examples in an earlier chapter) and data collected across different seasons.

## 7.9 Suggested readings and videos

- *Fundamentals of data visualization*, by Claus Wilke
- *Visual Explanations*, by Edward Tufte
- *Visualizing Data*, by William S. Cleveland
- *Graph Design for the Eye and Mind*, by Stephen M. Kosslyn
- *How Humans See Data*, by John Rauser

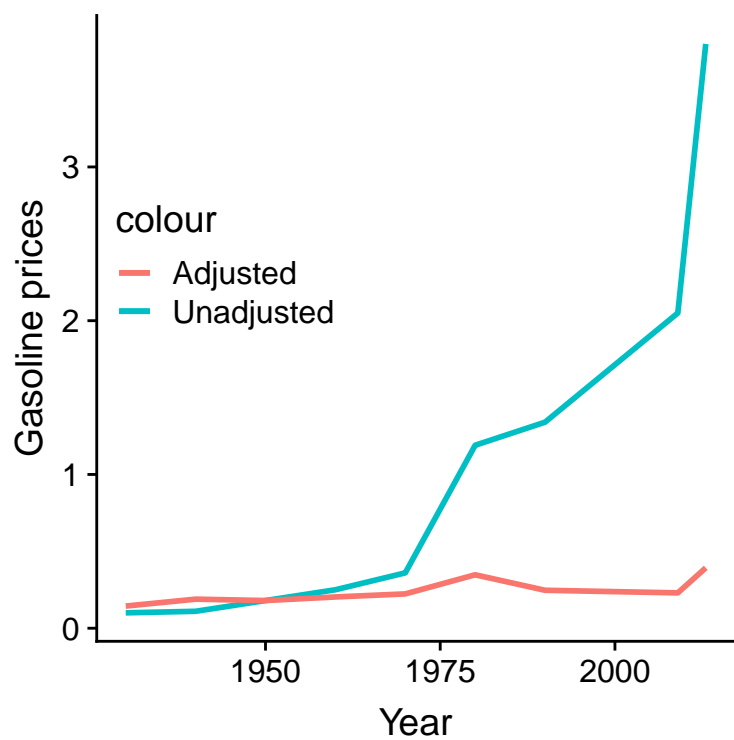


Figure 7.13: The price of gasoline in the US from 1930 to 201 (obtained from <http://www.thepeoplehistory.com/70yearsofpricechange.html>) with or without correction for inflation (based on Consumer Price Index).

## Chapter 8

# Sampling

One of the foundational ideas in statistics is that we can make inferences about an entire population based on a relatively small sample of individuals from that population. In this chapter we will introduce the concept of statistical sampling and discuss why it works.

Anyone living in the United States will be familiar with the concept of sampling from the political polls that have become a central part of our electoral process. In some cases, these polls can be incredibly accurate at predicting the outcomes of elections. The best known example comes from the 2008 and 2012 US Presidential elections, when the pollster Nate Silver correctly predicted electoral outcomes for 49/50 states in 2008 and for all 50 states in 2012. Silver did this by combining data from 21 different polls, which vary in the degree to which they tend to lean towards either the Republican or Democratic side. Each of these polls included data from about 1000 likely voters – meaning that Silver was able to almost perfectly predict the pattern of votes of more than 125 million voters using data from only 21,000 people, along with other knowledge (such as how those states have voted in the past).

### 8.1 How do we sample?

Our goal in sampling is to determine some feature of the full population of interest, using just a small subset of the population. We do this primarily to save time and effort – why go to the trouble of measuring every individual in the population when just a small sample is sufficient to accurately estimate the variable of interest?

In the election example, the population is all voters, and the sample is the set of 1000 individuals selected by the polling organization. The way in which we select the sample is critical to ensuring that the sample is *representative* of the entire population, which is a main goal of statistical sampling. It's easy to imagine a non-representative sample; if a pollster only called individuals whose names they had received from the local Democratic party, then it would be unlikely that the results of the poll would be representative of the population as a whole. In general, we would define a representative poll as being one in which every member of the population has an equal chance of being selected. When this fails, then we have to worry about whether the statistic that we compute on the sample is *biased* - that is, whether its value is systematically different from the population value (which we refer to as a *parameter*). Keep in mind that we generally don't know this population parameter, because if we did then we wouldn't need to sample! But we will use examples where we have access to the entire population, in order to explain some of the key ideas.

It's important to also distinguish between two different ways of sampling: with replacement versus without replacement. In sampling *with replacement*, after a member of the population has been sampled, they are put back into the pool so that they can potentially be sampled again. In *sampling without replacement*, once a member has been sampled they are not eligible to be sampled again. It's most common to use sampling

without replacement, but there will be some contexts in which we will use sampling with replacement, as when we discuss a technique called *bootstrapping* in Chapter 9.

## 8.2 Sampling error

Regardless of how representative our sample is, it's likely that the statistic that we compute from the sample is going to differ at least slightly from the population parameter. We refer to this as *sampling error*. The value of our statistical estimate will also vary from sample to sample; we refer to this distribution of our statistic across samples as the *sampling distribution*.

Sampling error is directly related to the quality of our measurement of the population. Clearly we want the estimates obtained from our sample to be as close as possible to the true value of the population parameter. However, even if our statistic is unbiased (that is, in the long run we expect it to have the same value as the population parameter), the value for any particular estimate will differ from the population estimate, and those differences will be greater when the sampling error is greater. Thus, reducing sampling error is an important step towards better measurement.

We will use the NHANES dataset as an example; we are going to assume that NHANES is the entire population, and then we will draw random samples from the population. We will have more to say in the next chapter about exactly how the generation of “random” samples works in a computer.

```
# load the NHANES data library
library(NHANES)

# create a NHANES dataset without duplicated IDs
NHANES <-
  NHANES %>%
    distinct(ID, .keep_all = TRUE)

#create a dataset of only adults
NHANES_adult <-
  NHANES %>%
    filter(
      !is.na(Height),
      Age >= 18
    )

#print the NHANES population mean and standard deviation of adult height
sprintf(
  "Population height: mean = %.2f",
  mean(NHANES_adult$Height)
)

## [1] "Population height: mean = 168.35"

sprintf(
  "Population height: std deviation = %.2f",
  sd(NHANES_adult$Height)
)

## [1] "Population height: std deviation = 10.16"
```

In this example, we know the adult population mean and standard deviation for height because we are assuming that the NHANES dataset contains the entire population of adults. Now let's take a single sample of 50 individuals from the NHANES population, and compare the resulting statistics to the population parameters.

```
# sample 50 individuals from NHANES dataset
exampleSample <-
  NHANES_adult %>%
  sample_n(50)

#print the sample mean and standard deviation of adult height
sprintf(
  'Sample height: mean = %.2f',
  mean(exampleSample$Height)
)
```

```
## [1] "Sample height: mean = 169.46"
```

```
sprintf(
  'Sample height: std deviation = %.2f',
  sd(exampleSample$Height)
)
```

```
## [1] "Sample height: std deviation = 10.07"
```

The sample mean and standard deviation are similar but not exactly equal to the population values. Now let's take a large number of samples of 50 individuals, compute the mean for each sample, and look at the resulting sampling distribution of means. We have to decide how many samples to take in order to do a good job of estimating the sampling distribution – in this case, let's take 5000 samples so that we are really confident in the answer. Note that simulations like this one can sometimes take a few minutes to run, and might make your computer huff and puff. The histogram in Figure 8.1 shows that the means estimated for each of the samples of 50 individuals vary somewhat, but that overall they are centered around the population mean.

```
# compute sample means across 5000 samples from NHANES data
sampSize <- 50 # size of sample
nsamps <- 5000 # number of samples we will take

# set up variable to store all of the results
sampMeans <- array(NA, nsamps)

# Loop through and repeatedly sample and compute the mean
for (i in 1:nsamps) {
  NHANES_sample <- sample_n(NHANES_adult, sampSize)
  sampMeans[i] <- mean(NHANES_sample$Height)
}

sampdataDf <- tibble(mean = sampMeans)

sprintf(
  "Average sample mean = %.2f",
  mean(sampMeans)
)
```

```
## [1] "Average sample mean = 168.33"
```

```
sampMeans_df <- tibble(sampMeans = sampMeans)
```

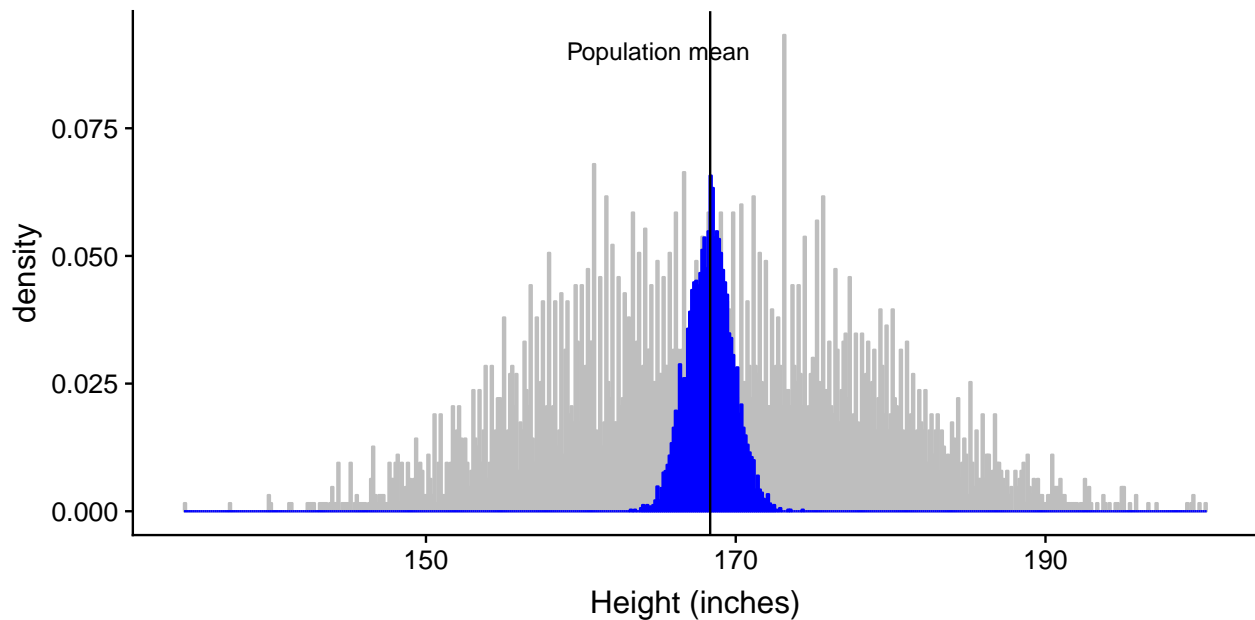


Figure 8.1: The blue histogram shows the sampling distribution of the mean over 5000 random samples from the NHANES dataset. The histogram for the full dataset is shown in gray for reference.

### 8.3 Standard error of the mean

Later in the course it will become essential to be able to characterize how variable our samples are, in order to make inferences about the sample statistics. For the mean, we do this using a quantity called the *standard error* of the mean (SEM), which one can think of as the standard deviation of the sampling distribution. If we know the population standard deviation, then we can compute the standard error using:

$$SEM = \frac{\sigma}{\sqrt{n}}$$

where  $n$  is the size of the sample. We don't usually know  $\sigma$  (the population standard deviation), so instead we would usually plug in our estimate of  $\sigma$ , which is the standard deviation computed on the sample ( $\hat{\sigma}$ ):

$$SEM = \frac{\hat{\sigma}}{\sqrt{n}}$$

However, we have to be careful about computing SEM using the estimated standard deviation if our sample is small (less than about 30).

Because we have many samples from the NHANES population and we actually know the population parameter, we can confirm that the SEM estimated using the population parameter is very close to the observed standard deviation of the samples that we took from the NHANES dataset.

```
# compare standard error based on population to standard deviation
# of sample means

sprintf(
  'Estimated standard error based on population SD: %.2f',
  sd(NHANES_adult$Height)/sqrt(sampSize)
)
```



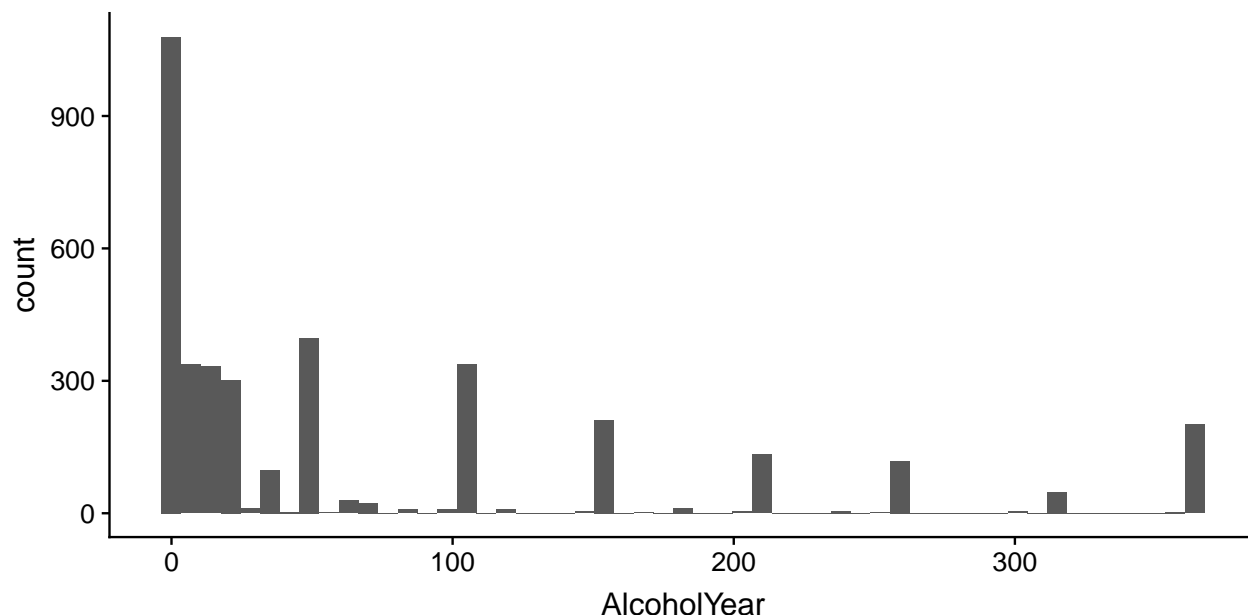


Figure 8.2: Distribution of the variable AlcoholYear in the NHANES dataset, which reflects the number of days that the individual drank in a year.

```
## [1] "Estimated standard error based on population SD: 1.44"
```

```
sprintf(
  'Standard deviation of sample means = %.2f',
  sd(sampMeans)
)
```

```
## [1] "Standard deviation of sample means = 1.43"
```

The formula for the standard error of the mean says that the quality of our measurement involves two quantities: the population variability, and the size of our sample. Of course, because the sample size is the denominator in the formula for SEM, a larger sample size will yield a smaller SEM when holding the population variability constant. We have no control over the population variability, but we *do* have control over the sample size. Thus, if we wish to improve our sample statistics (by reducing their sampling variability) then we should use larger samples. However, the formula also tells us something very fundamental about statistical sampling – namely, that the utility of larger samples diminishes with the square root of the sample size. This means that doubling the sample size will *not* double the quality of the statistics; rather, it will improve it by a factor of  $\sqrt{2}$ . In Section 10.3.6 (statistical-power) we will discuss statistical power, which is intimately tied to this idea.

## 8.4 The Central Limit Theorem

The Central Limit Theorem tells us that as sample sizes get larger, the sampling distribution of the mean will become normally distributed, *even if the data within each sample are not normally distributed*.

We can also see this in real data. Let's work with the variable AlcoholYear in the NHANES distribution, which is highly skewed, as shown in Figure 8.2.

This distribution is, for lack of a better word, funky – and definitely not normally distributed. Now let's look at the sampling distribution of the mean for this variable. Figure 8.3 shows the sampling distribution for this

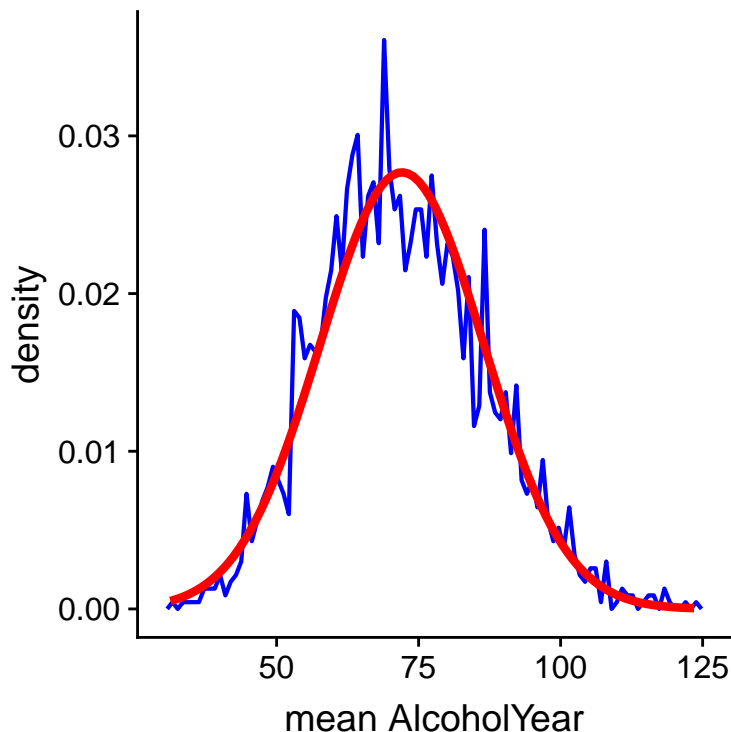


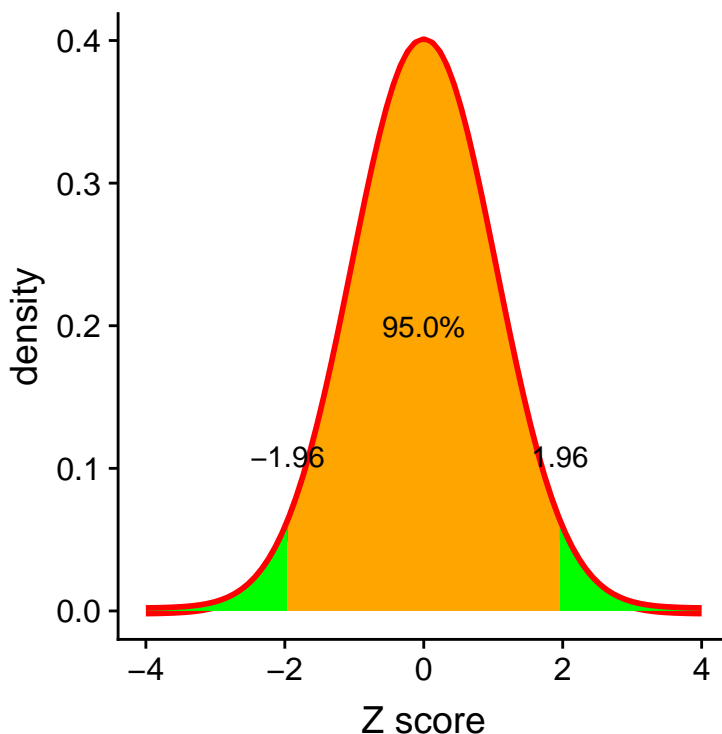
Figure 8.3: The sampling distribution of the mean for AlcoholYear in the NHANES dataset, obtained by drawing repeated samples of size 50, in blue. The normal distribution with the same mean and standard deviation is shown in red.

variable, which is obtained by repeatedly drawing samples of size 50 from the NHANES dataset and taking the mean. Despite the clear non-normality of the original data, the sampling distribution is remarkably close to the normal.

## 8.5 Confidence intervals

Most people are familiar with the idea of a “margin of error” for political polls. These polls usually try to provide an answer that is accurate within  $\pm 3$  percent. For example, when a candidate is estimated to win an election by 9 percentage points with a margin of error of 3, the percentage by which they will win is estimated to fall within 6-12 percentage points. In statistics we refer to this range of values as the *confidence interval*, which provides a measure of our degree of uncertainty about how close our estimate is to the population parameter. The larger the confidence interval, the greater our uncertainty.

We saw in the previous section that with sufficient sample size, the sampling distribution of the mean is normally distributed, and that the standard error describes the standard deviation of this sampling distribution. Using this knowledge, we can ask: What is the range of values within which we would expect to capture 95% of all estimates of the mean? To answer this, we can use the normal distribution, for which we know the values between which we expect 95% of all sample means to fall. Specifically, we use the *quantile* function for the normal distribution (`qnorm()` in R) to determine the values of the normal distribution that fall at the 2.5% and 97.5% points in the distribution. We choose these points because we want to find the 95% of values in the center of the distribution, so we need to cut off 2.5% on each end in order to end up with 95% in the middle. Figure 8.5 shows that this occurs for  $Z \pm 1.96$ .



`\begin{figure}` `\caption{Normal distribution,`  
 with the orange section in the center denoting the range in which we expect 95% of all values to fall. The  
 green sections show the portions of the distribution that are more extreme, which we would expect to occur  
 less than 5% of the time. `\end{figure}`

Using these cutoffs, we can create a confidence interval for the estimate of the mean:

$$CI_{95\%} = \bar{X} \pm 1.96 * SEM$$

Let's compute the confidence interval for the NHANES height data,

```
# compute confidence intervals

NHANES_sample <- sample_n(NHANES_adult, 250)

sample_summary <- NHANES_sample %>%
  summarize(mean=mean(Height),
             sem=sd(Height)/sqrt(sampSize)) %>%
  mutate(CI_lower=mean-1.96*sem,
         CI_upper=mean+1.96*sem)
pander(sample_summary)
```

| mean    | sem   | CI_lower | CI_upper |
|---------|-------|----------|----------|
| 166.869 | 1.446 | 164.036  | 169.702  |

Confidence intervals are notoriously confusing, primarily because they don't mean what we would hope they mean. It seems natural to think that the 95% confidence interval tells us that there is a 95% chance that the population mean falls within the interval. However, as we will see throughout the course, concepts in statistics often don't mean what we think they should mean. In the case of confidence intervals, we can't interpret them in this way because the population parameter has a fixed value – it either is or isn't in the interval. The proper interpretation of the 95% confidence interval is that it is the interval that will capture

the true population mean 95% of the time. We can confirm this by resampling the NHANES data repeatedly and counting how often the interval contains the true population mean.

```
# compute how often the confidence interval contains the true population mean
nsamples <- 2500
sampSize <- 100

ci_contains_mean <- array(NA, nsamples)

for (i in 1:nsamples) {
  NHANES_sample <- sample_n(NHANES_adult, sampSize)
  sample_summary <-
    NHANES_sample %>%
    summarize(
      mean = mean(Height),
      sem = sd(Height) / sqrt(sampSize)
    ) %>%
    mutate(
      CI_upper = mean + 1.96 * sem,
      CI_lower = mean - 1.96 * sem
    )
  ci_contains_mean[i] <-
    (sample_summary$CI_upper > mean(NHANES_adult$Height)) &
    (sample_summary$CI_lower < mean(NHANES_adult$Height))
}

sprintf(
  'proportion of confidence intervals containing population mean: %.3f',
  mean(ci_contains_mean)
)
```

```
## [1] "proportion of confidence intervals containing population mean: 0.953"
```

This confirms that the confidence interval does indeed capture the population mean about 95% of the time.

## 8.6 Suggested readings

- *The Signal and the Noise: Why So Many Predictions Fail - But Some Don't*, by Nate Silver

## Chapter 9

# Resampling and simulation

The use of computer simulations has become an essential aspect of modern statistics. For example, one of the most important books in practical computer science, called *Numerical Recipes*, says the following:

“Offered the choice between mastery of a five-foot shelf of analytical statistics books and middling ability at performing statistical Monte Carlo simulations, we would surely choose to have the latter skill.”

In this chapter we will introduce the concept of a Monte Carlo simulation and discuss how they can be used to perform statistical analyses.

### 9.1 Monte Carlo simulation

The concept of Monte Carlo simulation was devised by the mathematicians Stan Ulam and Nicholas Metropolis, who were working to develop an atomic weapon as part of the Manhattan Project ([https://en.wikipedia.org/wiki/Manhattan\\_Project](https://en.wikipedia.org/wiki/Manhattan_Project)). They needed to compute the average distance that a neutron would travel in a substance before it collided with an atomic nucleus, but they could not compute this using standard mathematics. Ulam realized that these computations could be simulated using random numbers, just like a casino game. In a casino game, numbers are drawn at random; to estimate the probability of a specific outcome, you could play the game hundreds of times. Ulam’s uncle had gambled at the Monte Carlo casino in Monaco, which is apparently where the name came from for this new technique.

There are four steps to performing a Monte Carlo simulation:

1. Define a domain of possible values
2. Generate random numbers within that domain from a probability distribution
3. Perform a computation using the random numbers
4. Combine the results across many repetitions

As an example, let’s say that I want to figure out how much time to allow for an in-class quiz. Say that we know that the distribution of quiz completion times is normal, with mean of 5 mins and standard deviation of 1 min. Given this, how long does the test period need to be so that we expect everyone to finish 99% of the time? There are two ways to solve this problem. The first is to calculate the answer using a mathematical theory known as the statistics of extreme values. However, this is quite complicated mathematically. Alternatively, we could use Monte Carlo simulation. To do this, we need to generate random samples from a normal distribution.

## 9.2 Randomness in statistics

The term “random” is often used colloquially to refer to things that are bizarre or unexpected, but in statistics the term has a very specific meaning: A process is *random* if it is unpredictable. For example, if I flip a fair coin 10 times, the value of the outcome on one flip does not provide me with any information that lets me predict the outcome on the next flip. It’s important to note that the fact that something is unpredictable doesn’t necessarily mean that it is not deterministic. For example, when we flip a coin, the outcome of the flip is determined by the laws of physics; if we knew all of the conditions in enough detail, we should be able to predict the outcome of the flip. However, many factors combine to make the outcome of the coin flip unpredictable in practice.

Psychologists have shown that humans actually have a fairly bad sense of randomness. First, we tend to see patterns when they don’t exist. In the extreme, this leads to the phenomenon of *pareidolia*, in which people will perceive familiar objects within random patterns (such as perceiving a cloud as a human face or seeing the Virgin Mary in a piece of toast). Second, humans tend to think of random processes as self-correcting, which leads us to expect that we are “due for a win” after losing many rounds in a game, a phenomenon known as the “gambler’s fallacy”.

## 9.3 Generating random numbers

Running a Monte Carlo simulation requires that we generate random numbers. Generating truly random numbers (i.e. numbers that are completely unpredictable) is only possible through physical processes, such as the decay of atoms or the rolling of dice, which are difficult to obtain and/or too slow to be useful for computer simulation (though they can be obtained from the NIST Randomness Beacon).

In general, instead of truly random numbers we use *pseudo-random* numbers generated using a computer algorithm; these numbers will seem random in the sense that they are difficult to predict, but the series of numbers will actually repeat at some point. For example, the random number generator used in R will repeat after  $2^{19937} - 1$  numbers. That’s far more than the number of seconds in the history of the universe, and we generally think that this is fine for most purposes in statistical analysis.

In R, there is a function to generate random numbers for each of the major probability distributions, such as:

- `runif()` - uniform distribution (all values between 0 and 1 equally)
- `rnorm()` - normal distribution
- `rbinom()` - binomial distribution (e.g. rolling the dice, coin flips)

Figure 9.1 shows examples of numbers generated using the `runif()` and `rnorm()` functions, generated using the following code:

```
p1 <-  
  tibble(  
    x = runif(10000)  
  ) %>%  
  ggplot(aes(x)) +  
  geom_histogram(bins = 100) +  
  labs(title = "Uniform")  
  
p2 <-  
  tibble(  
    x = rnorm(10000)  
  ) %>%  
  ggplot(aes(x)) +  
  geom_histogram(bins = 100) +  
  labs(title = "Normal")
```

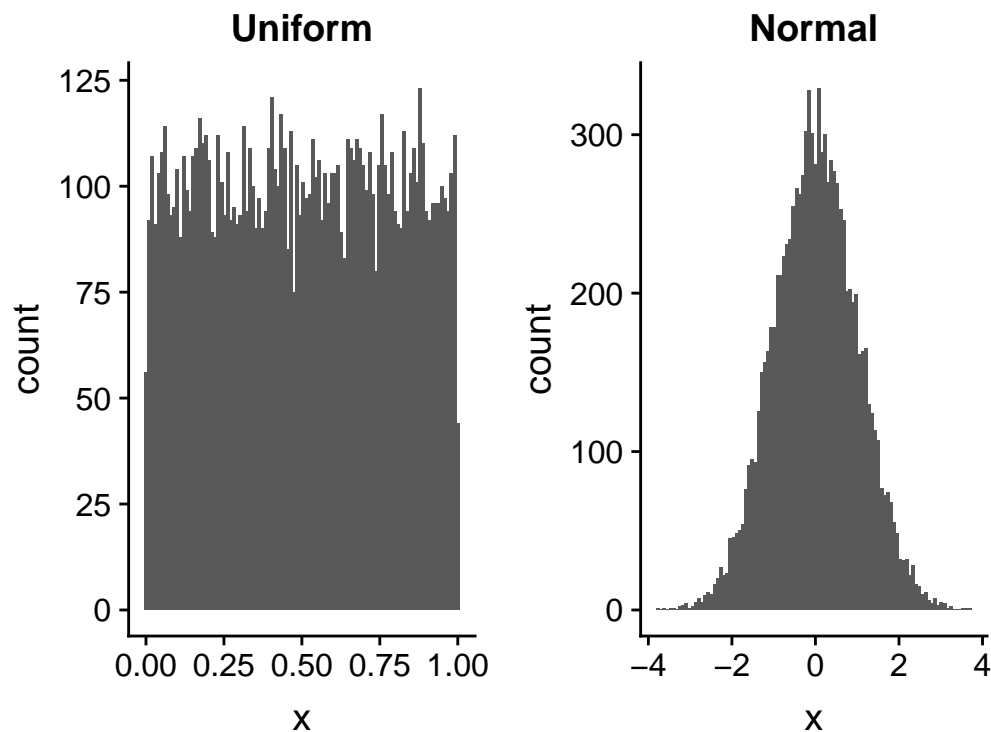


Figure 9.1: Examples of random numbers generated from a uniform (left) or normal (right) distribution.

```
plot_grid(p1, p2, ncol = 3)
```

You can also generate random numbers for any distribution if you have a *quantile* function for the distribution. This is the inverse of the cumulative distribution function; instead of identifying the cumulative probabilities for a set of values, the quantile function identifies the values for a set of cumulative probabilities. Using the quantile function, we can generate random numbers from a uniform distribution, and then map those into the distribution of interest via its quantile function.

By default, R will generate a different set of random numbers every time you run one of the random number generator functions described above. However, it is also possible to generate exactly the same set of random numbers, by setting what is called the *random seed* to a specific value. We will do this in many of the examples in this book, in order to make sure that the examples are reproducible.

*# if we run the rnorm() command twice, it will give us different sets of pseudorandom numbers each time*

```
print(rnorm(n = 5))
```

```
## [1]  1.48  0.18  0.21 -0.15 -1.72
```

```
print(rnorm(n = 5))
```

```
## [1] -0.691 -2.231  0.391  0.029 -0.647
```

*# if we set the random seed to the same value each time, then it will give us the same series of pseudorandom numbers*

```
set.seed(12345)
```

```
print(rnorm(n = 5))
```

```
## [1]  0.59  0.71 -0.11 -0.45  0.61
```

```
set.seed(12345)
```

```
print(rnorm(n = 5))
```

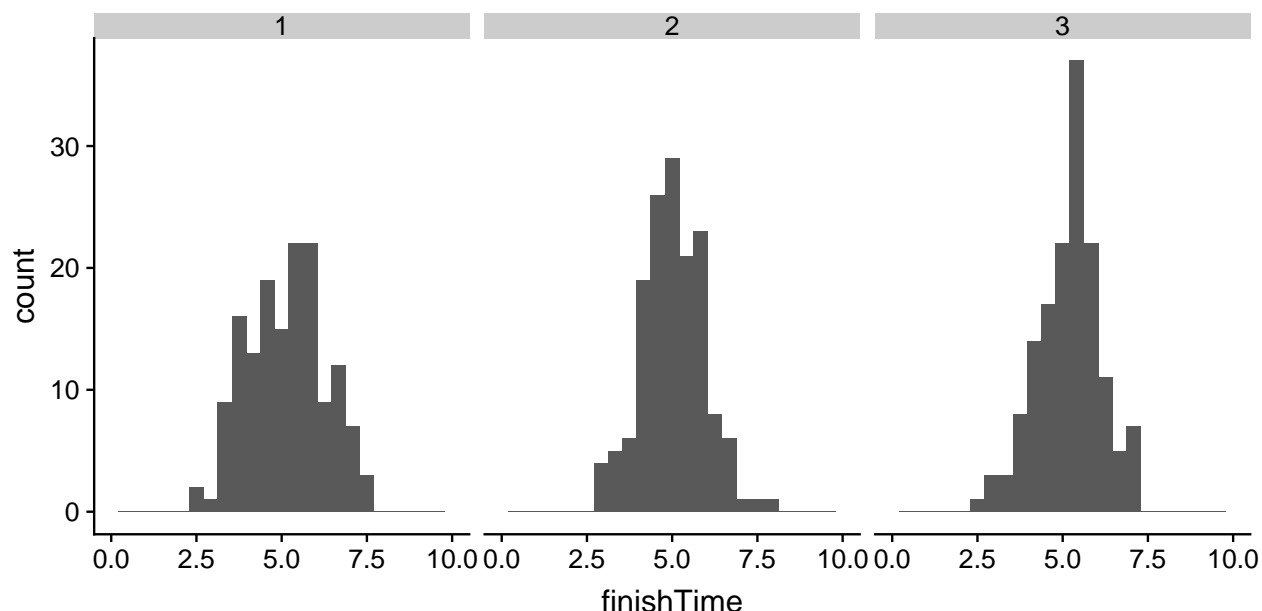


Figure 9.2: Simulated finishing time distributions.

```
## [1] 0.59 0.71 -0.11 -0.45 0.61
```

## 9.4 Using Monte Carlo simulation

Let's go back to our example of exam finishing times. Let's say that I administer three quizzes and record the finishing times for each student for each exam, which might look like the distributions presented in Figure 9.2.

However, what we really want to know is not what the distribution of finishing times looks like, but rather what the distribution of the *longest* finishing time for each quiz looks like. To do this, we can simulate a large number of quizzes (using the assumption that the finishing times are distributed normally, as stated above); for each of these simulated quizzes, we can record the longest finishing time. To do this, we create a new function in R called `sampleMax()` which simulates a sample of the appropriate size (i.e. the number of students in the class) from the appropriate distribution (i.e., normal), and returns the maximum value in the sample. We then repeat this simulation a large number of times (5000 should be enough) using the `replicate()` function, which will store all of the outputs into a single variable. The distribution of finishing times is shown in Figure 9.3.

```
# sample maximum value 5000 times and compute 99th percentile
nRuns <- 5000
sampSize <- 150

sampleMax <- function(sampSize = 150) {
  samp <- rnorm(sampSize, mean = 5, sd = 1)
  return(max(samp))
}

maxTime <- replicate(nRuns, sampleMax())

cutoff <- quantile(maxTime, 0.99)
sprintf("99th percentile of maxTime distribution: %.2f", cutoff)
```



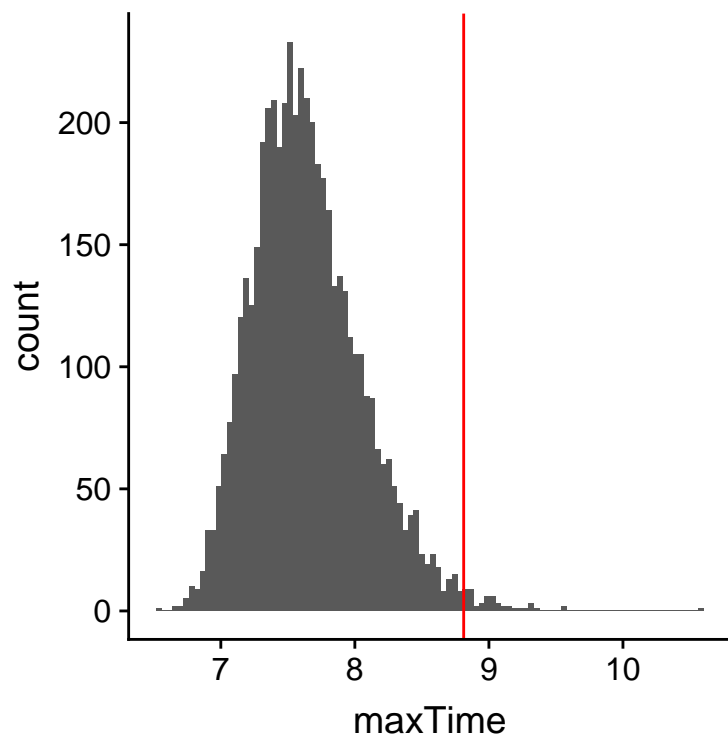


Figure 9.3: Distribution of maximum finishing times across simulations.

```
## [1] "99th percentile of maxTime distribution: 8.81"
```

This shows that the 99th percentile of the finishing time distribution falls at 8.81, meaning that if we were to give that much time for the quiz, then everyone should finish 99% of the time. It's always important to remember that our assumptions matter – if they are wrong, then the results of the simulation are useless. In this case, we assumed that the finishing time distribution was normally distributed with a particular mean and standard deviation; if these assumptions are incorrect (and they almost certainly are), then the true answer could be very different.

## 9.5 Using simulation for statistics: The bootstrap

So far we have used simulation to demonstrate statistical principles, but we can also use simulation to answer real statistical questions. In this section we will introduce a concept known as the *bootstrap* that lets us use simulation to quantify our uncertainty about statistical estimates. Later in the course, we will see other examples of how simulation can often be used to answer statistical questions, especially when theoretical statistical methods are not available or when their assumptions are too stifling.

### 9.5.1 Computing the bootstrap

In the section above, we used our knowledge of the sampling distribution of the mean to compute the standard error of the mean and confidence intervals. But what if we can't assume that the estimates are normally distributed, or we don't know their distribution? The idea of the bootstrap is to use the data themselves to estimate an answer. The name comes from the idea of pulling one's self up by one's own bootstraps, expressing the idea that we don't have any external source of leverage so we have to rely upon the data themselves. The bootstrap method was conceived by Bradley Efron of the Stanford Department of Statistics, who is one of the world's most influential statisticians.

The idea behind the bootstrap is that we repeatedly sample from the actual dataset; importantly, we sample *with replacement*, such that the same data point will often end up being represented multiple times within one of the samples. We then compute our statistic of interest on each of the bootstrap samples, and use the distribution of those estimates

Let's start by using the bootstrap to estimate the sampling distribution of the mean, so that we can compare the result to the standard error of the mean (SEM) that we discussed earlier.

```
# perform the bootstrap to compute SEM and compare to parametric method
```

```
nRuns <- 2500
sampleSize <- 32
```

```
heightSample <-
  NHANES_adult %>%
  sample_n(sampleSize)
```

```
bootMeanHeight <- function(df) {
  bootSample <- sample_n(df, dim(df)[1], replace = TRUE)
  return(mean(bootSample$Height))
}
```

```
bootMeans <- replicate(nRuns, bootMeanHeight(heightSample))
```

```
SEM_standard <- sd(heightSample$Height) / sqrt(sampleSize)
sprintf("SEM computed using sample SD: %f", SEM_standard)
```

```
## [1] "SEM computed using sample SD: 1.595789"
```

```
SEM_bootstrap <- sd(bootMeans)
sprintf("SEM computed using SD of bootstrap estimates: %f", SEM_bootstrap)
```

```
## [1] "SEM computed using SD of bootstrap estimates: 1.586913"
```

Figure 9.4 shows that the distribution of means across bootstrap samples is fairly close to the theoretical estimate based on the assumption of normality. We can also use the bootstrap samples to compute a confidence interval for the mean, simply by computing the quantiles of interest from the distribution of bootstrap samples.

```
# compute bootstrap confidence interval
```

```
bootCI <- quantile(bootMeans, c(0.025, 0.975))
pander("bootstrap confidence limits:")
```

```
bootstrap confidence limits:
```

```
pander(bootCI)
```

| 2.5%    | 98%     |
|---------|---------|
| 164.634 | 170.883 |

```
# now let's compute the confidence intervals using the sample mean and SD
```

```
sampleMean <- mean(heightSample$Height)
```

```
normalCI <-
  tibble(
```

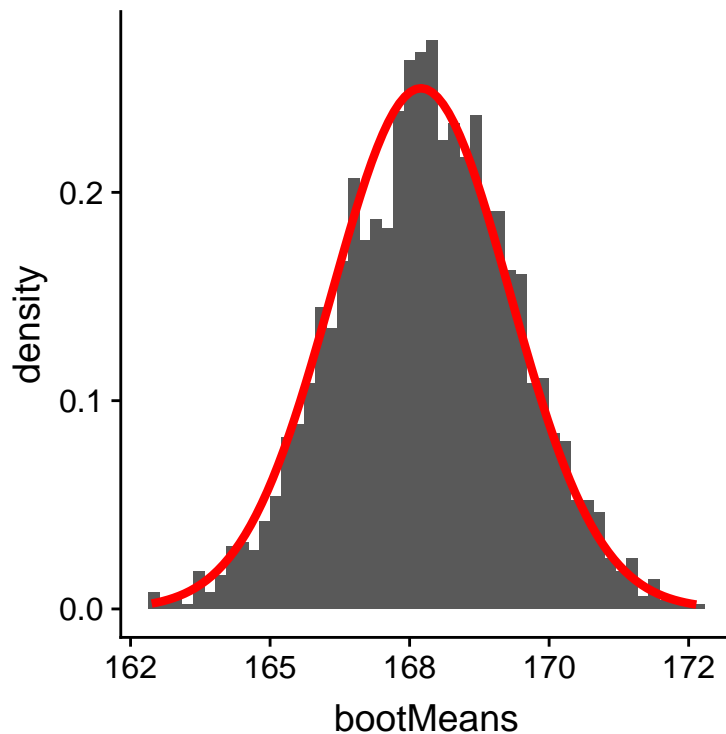


Figure 9.4: An example of bootstrapping to compute the standard error of the mean. The histogram shows the distribution of means across bootstrap samples, while the red line shows the normal distribution based on the sample mean and standard deviation.

```
"2.5%" = sampleMean - 1.96 * SEM_standard,
"97.5%" = sampleMean + 1.96 * SEM_standard
)

print("confidence limits based on sample SD and normal distribution:")

## [1] "confidence limits based on sample SD and normal distribution:"
pander(normalCI)
```

| 2.5%    | 97.5%   |
|---------|---------|
| 164.575 | 170.831 |

We would not usually employ the bootstrap to compute confidence intervals for the mean (since we can generally assume that the normal distribution is appropriate for the sampling distribution of the mean, as long as our sample is large enough), but this example shows how the method gives us roughly the same result as the standard method based on the normal distribution. The bootstrap would more often be used to generate standard errors for estimates of other statistics where we know or suspect that the normal distribution is not appropriate.

## 9.6 Suggested readings

- *Computer Age Statistical Inference: Algorithms, Evidence and Data Science*, by Bradley Efron and Trevor Hastie



# Chapter 10

## Hypothesis testing

In the first chapter we discussed the three major goals of statistics:

- Describe
- Decide
- Predict

In this chapter we will introduce the ideas behind the use of statistics to make decisions – in particular, decisions about whether a particular hypothesis is supported by the data.

### 10.1 Null Hypothesis Statistical Testing (NHST)

The specific type of hypothesis testing that we will discuss is known (for reasons that will become clear) as *null hypothesis statistical testing* (NHST). If you pick up almost any scientific or biomedical research publication, you will see NHST being used to test hypotheses, and in their introductory psychology textbook, Gerrig & Zimbardo (2002) referred to NHST as the “backbone of psychological research”. Thus, learning how to use and interpret the results from hypothesis testing is essential to understand the results from this research.

It is also important for you to know, however, that NHST is deeply flawed, and that many statisticians and researchers (including myself) think that it has been the cause of serious problems in science, which we will discuss in Chapter 18. For more than 50 years, there have been calls to abandon NHST in favor of other approaches (like those that we will discuss in the following chapters):

- “The test of statistical significance in psychological research may be taken as an instance of a kind of essential mindlessness in the conduct of research” (Bakan, 1966)
- Hypothesis testing is “a wrongheaded view about what constitutes scientific progress” (Luce, 1988)

NHST is also widely misunderstood, largely because it violates our intuitions about how statistical hypothesis testing should work. Let’s look at an example to see.

### 10.2 Null hypothesis statistical testing: An example

There is great interest in the use of body-worn cameras by police officers, which are thought to reduce the use of force and improve officer behavior. However, in order to establish this we need experimental evidence, and it has become increasingly common for governments to use randomized controlled trials to test such ideas. A randomized controlled trial of the effectiveness of body-worn cameras was performed by the Washington, DC government and DC Metropolitan Police Department in 2015/2016 in order to test the hypothesis that body-worn cameras are effective. Officers were randomly assigned to wear a body-worn camera or not, and

their behavior was then tracked over time to determine whether the cameras resulted in less use of force and fewer civilian complaints about officer behavior.

Before we get to the results, let's ask how you would think the statistical analysis might work. Let's say we want to specifically test the hypothesis of whether the use of force is decreased by the wearing of cameras. The randomized controlled trial provides us with the data to test the hypothesis – namely, the rates of use of force by officers assigned to either the camera or control groups. The next obvious step is to look at the data and determine whether they provide convincing evidence for or against this hypothesis. That is: What is the likelihood that body-worn cameras reduce the use of force, given the data and everything else we know?

It turns out that this is *not* how null hypothesis testing works. Instead, we first take our hypothesis of interest (i.e. whether body-worn cameras reduce use of force), and flip it on its head, creating a *null hypothesis* – in this case, the null hypothesis would be that cameras do not reduce use of force. Importantly, we then assume that the null hypothesis is true. We then look at the data, and determine whether the data are sufficiently unlikely under the null hypothesis that we can reject the null in favor of the *alternative hypothesis* which is our hypothesis of interest. If there is not sufficient evidence to reject the null, then we say that we “failed to reject” the null.

Understanding some of the concepts of NHST, particularly the notorious “p-value”, is invariably challenging the first time one encounters them, because they are so counter-intuitive. As we will see later, there are other approaches that provide a much more intuitive way to address hypothesis testing (but have their own complexities). However, before we get to those, it's important for you to have a deep understanding of how hypothesis testing works, because it's clearly not going to go away any time soon.

### 10.3 The process of null hypothesis testing

We can break the process of null hypothesis testing down into a number of steps:

1. Formulate a hypothesis that embodies our prediction (*before seeing the data*)
2. Collect some data relevant to the hypothesis
3. Specify null and alternative hypotheses
4. Fit a model to the data that represents the alternative hypothesis and compute a test statistic
5. Compute the probability of the observed value of that statistic assuming that the null hypothesis is true
6. Assess the “statistical significance” of the result

For a hands-on example, let's use the NHANES data to ask the following question: Is physical activity related to body mass index? In the NHANES dataset, participants were asked whether they engage regularly in moderate or vigorous-intensity sports, fitness or recreational activities (stored in the variable *PhysActive*). They also measured height and weight and computed Body Mass Index:

$$BMI = \frac{weight(kg)}{height(m)^2}$$

#### 10.3.1 Step 1: Formulate a hypothesis

For step 1, we hypothesize that BMI should be greater for people who do not engage in physical activity, compared to those who do.

#### 10.3.2 Step 2: Collect some data

For step 2, we collect some data. In this case, we will sample 250 individuals from the NHANES dataset. Figure 10.1 shows an example of such a sample, with BMI shown separately for active and inactive individuals.

```

# sample 250 adults from NHANES and compute mean BMI separately for active
# and inactive individuals

sampSize <- 250

NHANES_sample <-
  NHANES_adult %>%
  sample_n(sampSize)

sampleSummary <-
  NHANES_sample %>%
  group_by(PhysActive) %>%
  summarize(
    N = length(BMI),
    mean = mean(BMI),
    sd = sd(BMI)
  )

# calculate the mean difference in BMI between active
# and inactive individuals; we'll use this later to calculate the t-statistic
meanDiff <-
  sampleSummary %>%
  select(
    PhysActive,
    mean
  ) %>%
  spread(PhysActive, mean) %>%
  mutate(
    meanDiff = No - Yes
  ) %>%
  pull(meanDiff)

# calculate the summed variances in BMI for active
# and inactive individuals; we'll use this later to calculate the t-statistic
sumVariance <-
  sampleSummary %>%
  select(
    PhysActive,
    N,
    sd
  ) %>%
  gather(column, stat, N:sd) %>%
  unite(temp, PhysActive, column) %>%
  spread(temp, stat) %>%
  mutate(
    sumVariance = No_sd**2 / No_N + Yes_sd**2 / Yes_N
  ) %>%
  pull(sumVariance)

# print sampleSummary table
pander(sampleSummary)

```

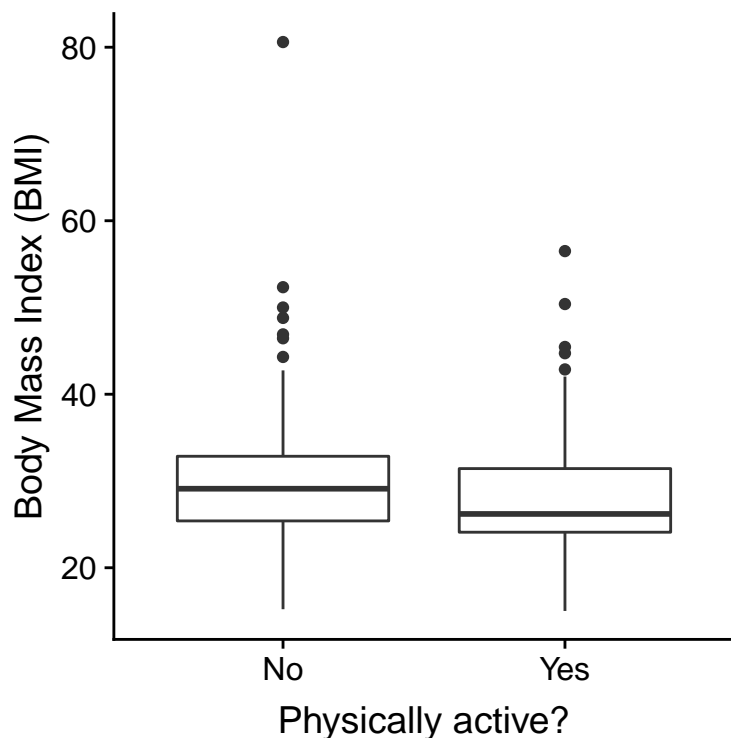


Figure 10.1: Box plot of BMI data from a sample of adults from the NHANES dataset, split by whether they reported engaging in regular physical activity.

| PhysActive | N   | mean  | sd   |
|------------|-----|-------|------|
| No         | 135 | 30.25 | 8.2  |
| Yes        | 115 | 28.6  | 6.88 |

### 10.3.3 Step 3: Specify the null and alternative hypotheses

For step 3, we need to specify our null hypothesis (which we call  $H_0$ ) and our alternative hypothesis (which we call  $H_A$ ).  $H_0$  is the baseline against which we test our hypothesis of interest: that is, what would we expect the data to look like if there was no effect? The null hypothesis always involves some kind of equality ( $=$ ,  $\leq$ , or  $\geq$ ).  $H_A$  describes what we expect if there actually is an effect. The alternative hypothesis always involves some kind of inequality ( $\neq$ ,  $>$ , or  $<$ ). Importantly, null hypothesis testing operates under the assumption that the null hypothesis is true unless the evidence shows otherwise.

We also have to decide whether to use *directional* or *non-directional* hypotheses. A non-directional hypothesis simply predicts that there will be a difference, without predicting which direction it will go. For the BMI/activity example, a non-directional null hypothesis would be:

$$H_0 : BMI_{active} = BMI_{inactive}$$

and the corresponding non-directional alternative hypothesis would be:

$$H_A : BMI_{active} \neq BMI_{inactive}$$

A directional hypothesis, on the other hand, predicts which direction the difference would go. For example, we have strong prior knowledge to predict that people who engage in physical activity should weigh less than those who do not, so we would propose the following directional null hypothesis:



$$H_0 : BMI_{active} \geq BMI_{inactive}$$

and directional alternative:

$$H_0 : BMI_{active} < BMI_{inactive}$$

### 10.3.4 Step 4: Fit a model to the data and compute a test statistic

For step 4, we want to use the data to compute a statistic that will ultimately let us decide whether the null hypothesis is rejected or not. To do this, the model needs to quantify the amount of evidence in favor of the alternative hypothesis, relative to the variability in the data. Thus we can think of the test statistic as providing a measure of the size of the effect compared to the variability in the data. In general, this test statistic will have a probability distribution associated with it, because that allows us to determine how likely our observed value of the statistic is under the null hypothesis.

For the BMI example, we need a test statistic that allows us to test for a difference between two means, since the hypotheses are stated in terms of mean BMI for each group. One statistic that is often used to compare two means is the *t-statistic*, first developed by the statistician William Sealy Gossett, who worked for the Guinness Brewery in Dublin and wrote under the pen name “Student” - hence, it is often called “Student’s t-statistic”. The t-statistic is appropriate for comparing the means of two groups when the sample sizes are relatively small and the population standard deviation is unknown. The t-statistic for comparison of two independent groups is computed as:

$$t = \frac{\bar{X}_1 - \bar{X}_2}{\sqrt{\frac{S_1^2}{n_1} + \frac{S_2^2}{n_2}}}$$

where  $\bar{X}_1$  and  $\bar{X}_2$  are the means of the two groups,  $S_1^2$  and  $S_2^2$  are the estimated variances of the groups, and  $n_1$  and  $n_2$  are the sizes of the two groups. The t-statistic is distributed according to a probability distribution known as a *t* distribution. The *t* distribution looks quite similar to a normal distribution, but it differs depending on the number of degrees of freedom, which for this example is the number of observations minus 2, since we have computed two means and thus given up two degrees of freedom. When the degrees of freedom are large (say 1000), then the *t* distribution looks essentially like the normal distribution, but when they are small then the *t* distribution has longer tails than the normal (see Figure 10.2).

### 10.3.5 Step 5: Determine the probability of the data under the null hypothesis

This is the step where NHST starts to violate our intuition – rather than determining the likelihood that the null hypothesis is true given the data, we instead determine the likelihood of the data under the null hypothesis - because we started out by assuming that the null hypothesis is true! To do this, we need to know the probability distribution for the statistic under the null hypothesis, so that we can ask how likely the data are under that distribution. Before we move to our BMI data, let’s start with some simpler examples.

#### 10.3.5.0.1 Randomization: A very simple example

Let’s say that we wish to determine whether a coin is fair. To collect data, we flip the coin 100 times, and we count 70 heads. In this example,  $H_0 : P(heads) = 0.5$  and  $H_A : P(heads) \neq 0.5$ , and our test statistic is simply the number of heads that we counted. The question that we then want to ask is: How likely is it that we would observe 70 heads if the true probability of heads is 0.5. We can imagine that this might happen very occasionally just by chance, but doesn’t seem very likely. To quantify this probability, we can use the *binomial distribution*:

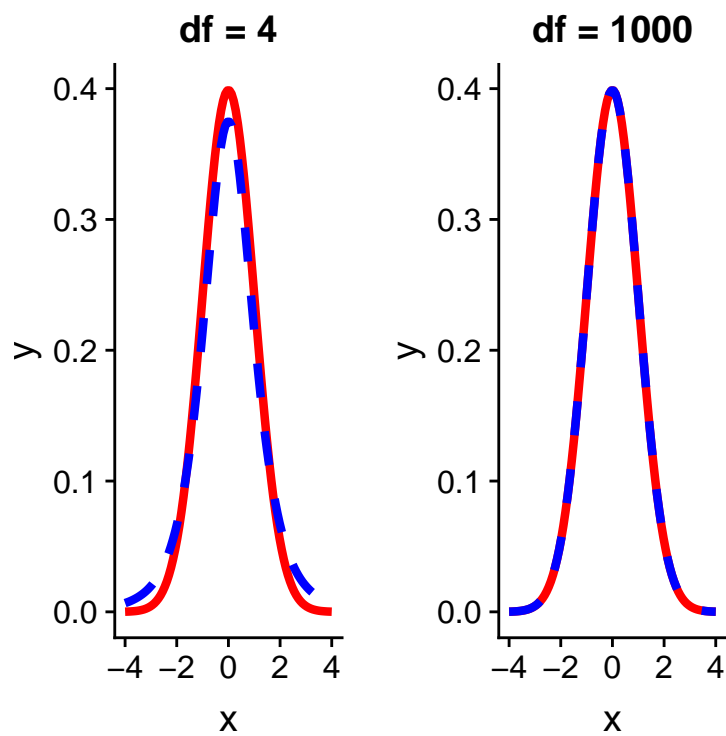


Figure 10.2: Each panel shows the  $t$  distribution (in blue dashed line) overlaid on the normal distribution (in solid red line). The left panel shows a  $t$  distribution with 4 degrees of freedom, in which case the distribution is similar but has slightly wider tails. The right panel shows a  $t$  distribution with 1000 degrees of freedom, in which case it is virtually identical to the normal.

$$P(X < k) = \sum_{i=0}^k \binom{N}{i} p^i (1-p)^{(n-i)}$$

This equation will tell us the likelihood of a certain number of heads or fewer, given a particular probability of heads. However, what we really want to know is the probability of a certain number or more, which we can obtain by subtracting from one:

$$P(X \geq k) = 1 - P(X < k)$$

We can compute the probability for our example using the `pbinom()` function in R as follows:

```
# compute the probability of 69 or fewer heads, when P(heads)=0.5
p_lt_70 <- pbinom(69, 100, 0.5)
sprintf("probability of 69 or fewer heads given P(heads)=0.5: %0.6f", p_lt_70)
```

```
## [1] "probability of 69 or fewer heads given P(heads)=0.5: 0.999961"
```

```
# the probability of 70 or more heads is simply the complement of p_lt_70
p_ge_70 <- 1 - p_lt_70
sprintf("probability of 70 or more heads given P(heads)=0.5: %0.6f", p_ge_70)
```

```
## [1] "probability of 70 or more heads given P(heads)=0.5: 0.000039"
```

This computation shows us that the likelihood of getting 70 heads if the coin is indeed fair is very small. Now, what if we didn't have the `pbinom()` function to tell us the probability of that number of heads? We could instead determine it by simulation – we repeatedly flip a coin 100 times using a true probability of 0.5, and then compute the distribution of the number of heads across those simulation runs. Figure 10.3 shows the result from this simulation.

```
# simulate tossing of 100,000 flips of 100 coins to identify empirical
# probability of 70 or more heads out of 100 flips
```

```
# create function to toss coins
```

```
tossCoins <- function() {
  flips <- runif(100) > 0.5
  return(sum(flips))
}
```

```
# use a large number of replications since this is fast
coinFlips <- replicate(100000, tossCoins())
```

```
p_ge_70_sim <- mean(coinFlips >= 70)
sprintf(
  "empirical probability of 70 or more heads given P(heads)=0.5: %0.6f",
  p_ge_70_sim
)
```

```
## [1] "empirical probability of 70 or more heads given P(heads)=0.5: 0.000020"
```

Here we can see that the probability computed via simulation (0.000020) is very close to the theoretical probability (.00004).

Let's do the analogous computation for our BMI example. First we compute the t statistic using the values from our sample that we calculated above:

```
tStat <-
  meanDiff / sqrt(sumVariance)
```

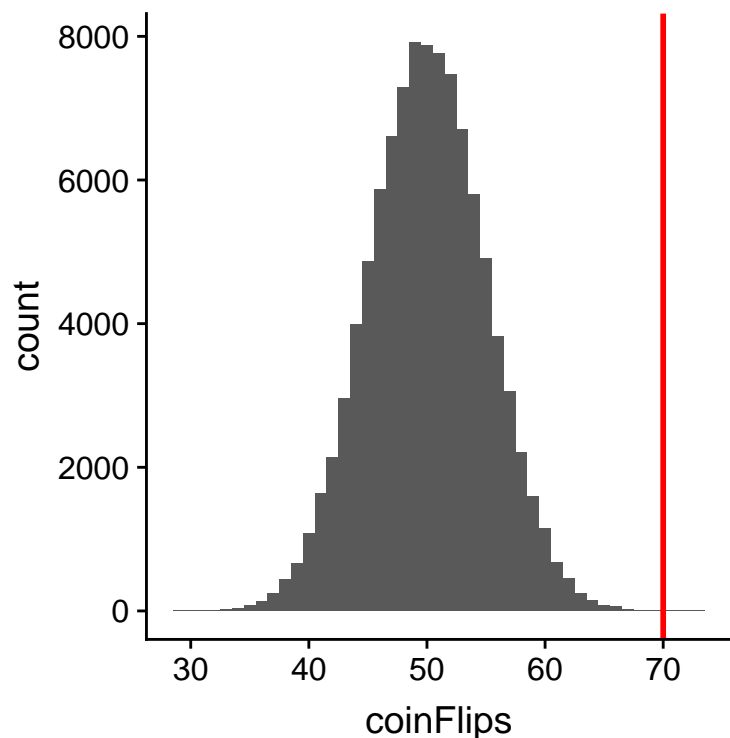


Figure 10.3: Distribution of numbers of heads (out of 100 flips) across 100,000 simulated runs.

```
sprintf("t statistic = %0.3f", tStat)
```

```
## [1] "t statistic = 1.735"
```

The question that we then want to ask is: What is the likelihood that we would find a  $t$  statistic of this size, if the true difference between groups is zero or less (i.e. the directional null hypothesis)?

We can use the  $t$  distribution to determine this probability. Our sample size is 250, so the appropriate  $t$  distribution has 248 degrees of freedom. We can use the `pt()` function in R to determine the probability of finding a value of the  $t$ -statistic greater than or equal to our observed value. Note that we want to know the probability of a value greater than our observed value, but by default `pt()` gives us the probability of a value less than the one that we provide it, so we have to tell it explicitly to provide us with the “upper tail” probability (by setting `lower.tail = FALSE`).

```
pvalue_tdist <-
```

```
  pt(tStat, df = 248, lower.tail = FALSE)
```

```
sprintf("p(t > %0.2f, df = 248) = %0.3f", tStat, pvalue_tdist)
```

```
## [1] "p(t > 1.74, df = 248) = 0.042"
```

This tells us that our observed  $t$ -statistic value of 1.74 is relatively unlikely if the null hypothesis really is true.

In this case, we used a directional hypothesis, so we only had to look at one end of the null distribution. If we wanted to test a non-directional hypothesis, then we would need to be able to identify how unexpected the size of the effect is, regardless of its direction. In the context of the  $t$ -test, this means that we need to know how likely it is that the statistic would be as extreme in either the positive or negative direction. To do this, we multiply the observed  $t$  value by -1, since the  $t$  distribution is centered around zero, and then add together the two tail probabilities to get a *two-tailed*  $p$ -value:

```
pvalue_tdist_twotailed <-
  pt(tStat, df = 248, lower.tail = FALSE) +
  pt(-1 * tStat, df = 248, lower.tail = TRUE)

sprintf(
  "p(t > %0.2f or t< %0.2f, df = 248) = %0.3f",
  tStat,
  -1 * tStat, pvalue_tdist_twotailed
)
```

```
## [1] "p(t > 1.74 or t< -1.74, df = 248) = 0.084"
```

Here we see that the p value for the two-tailed test is twice as large as that for the one-tailed test, which reflects the fact that an extreme value is less surprising since it could have occurred in either direction.

How do you choose whether to use a one-tailed versus a two-tailed test? The two-tailed test is always going to be more conservative, so it's always a good bet to use that one, unless you had a very strong prior reason for using a one-tailed test. In that case, you should have written down the hypothesis before you ever looked at the data. In Chapter doing-reproducible-research) we will discuss the idea of pre-registration of hypotheses, which formalizes the idea of writing down your hypotheses before you ever see the actual data. You should *never* make a decision about how to perform a hypothesis test once you have looked at the data, as this can introduce serious bias into the results.

### 10.3.5.1 Computing p-values using randomization

So far we have seen how we can use the t-distribution to compute the probability of the data under the null hypothesis, but we can also do this using simulation. The basic idea is that we generate simulated data like those that we would expect under the null hypothesis, and then ask how extreme the observed data are in comparison to those simulated data. The key question is: How can we generate data for which the null hypothesis is true? The general answer is that we can randomly rearrange the data in a specific way that makes the data look like they would if the null was really true. This is similar to the idea of bootstrapping, in the sense that it uses our own data to come up with an answer, but it does it in a different way.

#### 10.3.5.1.1 Randomization: a simple example

Let's start with a simple example. Let's say that we want to compare the mean squatting ability of football players with cross-country runners, with  $H_0 : \mu_{FB} \leq \mu_{XC}$  and  $H_A : \mu_{FB} > \mu_{XC}$ . We measure the maximum squatting ability of 5 football players and 5 cross-country runners (which we will generate randomly, assuming that  $\mu_{FB} = 300$ ,  $\mu_{XC} = 140$ , and  $\sigma = 30$ ).

```
# generate simulated data for squatting ability across football players
# and cross country runners

# reset random seed for this example
set.seed(12345678)

# create a function to round values to nearest product of 5,
# to keep example simple
roundToNearest5 <- function(x, base = 5) {
  return(base * round(x / base))
}

# create and show data frame containing simulated data
squatDf <- tibble(
```

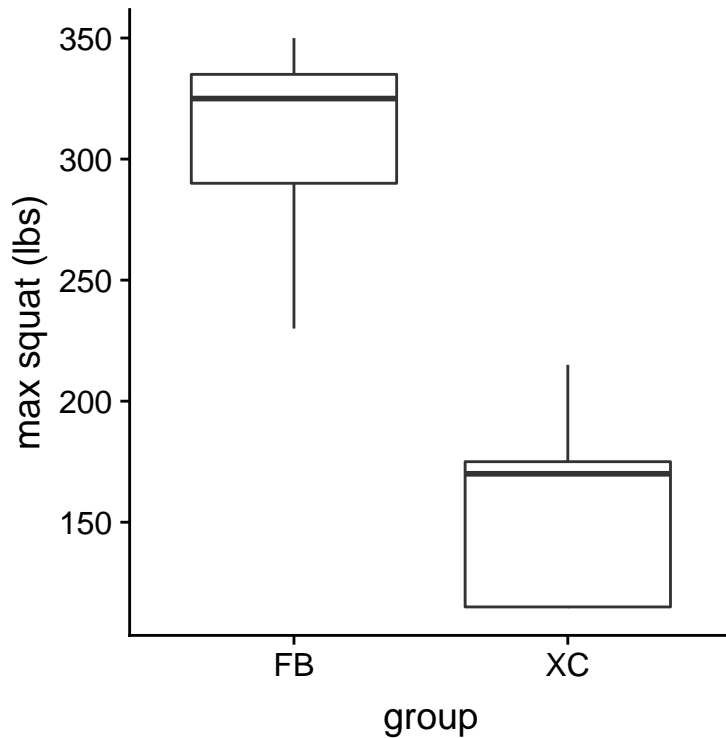


Figure 10.4: Box plots of simulated squatting ability for football players and cross-country runners.

```
group = as.factor(c(rep("FB", 5), rep("XC", 5))),
squat = roundToNearest5(c(rnorm(5) * 30 + 300, rnorm(5) * 30 + 140))
)

pander(squatDf)
```

| group | squat |
|-------|-------|
| FB    | 335   |
| FB    | 350   |
| FB    | 230   |
| FB    | 290   |
| FB    | 325   |
| XC    | 115   |
| XC    | 115   |
| XC    | 170   |
| XC    | 175   |
| XC    | 215   |

From the plot in Figure 10.4 it's clear that there is a large difference between the two groups. We can do a standard t-test to test our hypothesis, using the `t.test()` command in R:

```
# compute and print t statistic comparing two groups

tt <-
  t.test(
    squat ~ group,
```

```

data = squatDf,
alternative = "greater",
var.equal = TRUE
)

sprintf("p(t > %0.2f, df = 8) = %0.5f", tt$statistic, tt$p.value)

## [1] "p(t > 5.14, df = 8) = 0.00044"

```

This shows that the likelihood of such a difference under the null hypothesis is very small, using the  $t$  distribution to define the null. Now let's see how we could answer the same question using randomization. The basic idea is that if the null hypothesis of no difference between groups is true, then it shouldn't matter which group one comes from (football players versus cross-country runners) – thus, to create data that are like our actual data but also conform to the null hypothesis, we can randomly reorder the group labels for the individuals in the dataset, and then recompute the difference between the groups. The results of such a shuffle are shown in Figure 10.5.

```

# create a scrambled version of the group membership variable

dfScram <-
  squatDf %>%
  mutate(
    scrambledGroup = sample(group)
  ) %>%
  select(-group)

pander(dfScram)

```

| squat | scrambledGroup |
|-------|----------------|
| 335   | FB             |
| 350   | XC             |
| 230   | FB             |
| 290   | XC             |
| 325   | XC             |
| 115   | FB             |
| 115   | FB             |
| 170   | XC             |
| 175   | FB             |
| 215   | XC             |

After scrambling the labels, we see that the two groups are now much more similar, and in fact the cross-country group now has a slightly higher mean. Now let's do that 10000 times and store the  $t$  statistic for each iteration; this may take a moment to complete.

```

# shuffle data 10,000 times and compute distribution of t values

nRuns <- 10000

shuffleAndMeasure <- function(df) {
  dfScram <-
    df %>%
    mutate(
      scrambledGroup = sample(group)
    )
}

```

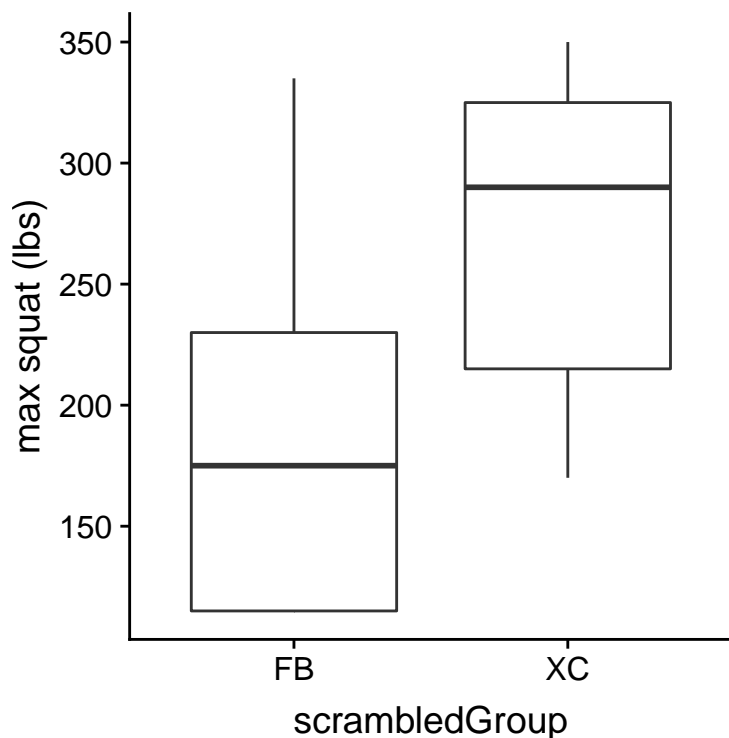


Figure 10.5: Box plots for subjects assigned to each group after scrambling group labels.

```
tt <- t.test(
  squat ~ scrambledGroup,
  data = dfScram,
  alternative = "greater",
  var.equal = TRUE
)
return(tt$statistic)
}

shuffleDiff <- replicate(nRuns, shuffleAndMeasure(squatDf))

sprintf("mean t value across shuffles = %0.3f", mean(shuffleDiff))

## [1] "mean t value across shuffles = -0.004"
```

We can now look at the distribution of mean differences across the shuffled datasets. Figure 10.6 shows the histogram of the group differences across all of the random shuffles. As expected under the null hypothesis, this distribution is centered at zero.

We can see that the distribution of  $t$  values after shuffling roughly follows the theoretical  $t$  distribution under the null hypothesis (with  $\text{mean}=0$ ), showing that randomization worked to generate null data. We also see something interesting if we compare the shuffled  $t$  values to the actual  $t$  value:

```
# compute number of runs on which t statistic for shuffle data was
# equal to observed t statistic

equalSum <- sum(shuffleDiff == tt$statistic)
sprintf("Number of runs on which shuffled t == observed t: %d", equalSum)
```



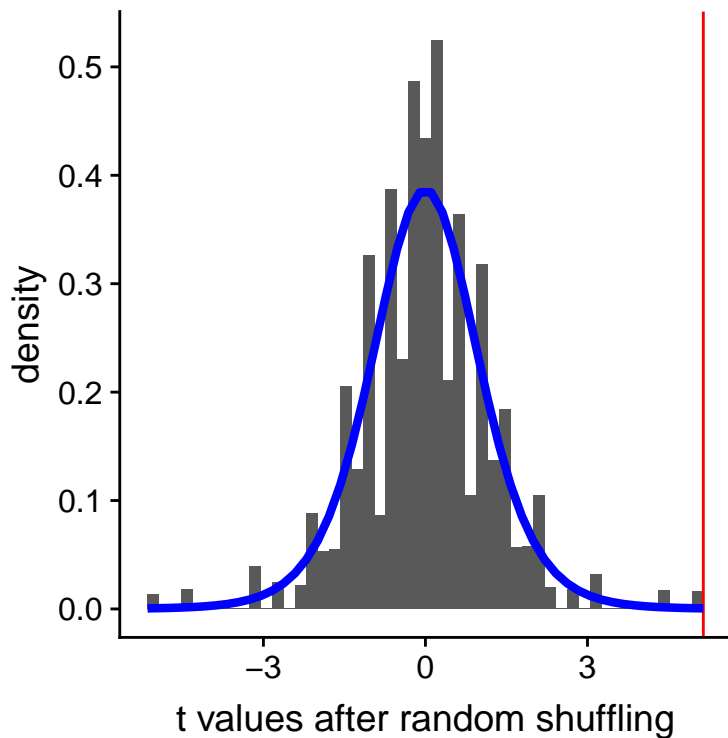


Figure 10.6: Histogram of differences between the football and cross-country groups after randomly shuffling group membership. The red line denotes the actual difference observed between the two groups, and the blue line shows the theoretical  $t$  distribution for this analysis.

```
## [1] "Number of runs on which shuffled t == observed t: 33"
# compute number of runs on which t statistic for shuffle data was
# equal to observed t statistic times -1

equalSumMinus <- sum(shuffleDiff == tt$statistic * -1)
sprintf("Number of runs on which shuffled t == observed t*-1: %d", equalSumMinus)

## [1] "Number of runs on which shuffled t == observed t*-1: 28"
```

There are 33 shuffle runs on which the  $t$  statistic for the shuffled data was exactly the same as the observed data – which means that shuffling resulted in the same labeling as the actual data! This is unlikely, but not *that* unlikely, and we can actually compute its likelihood using a bit of probability theory. The number of possible permutations of 10 items is  $10!$  which comes out to 3628800. The number of possible rearrangements of each set of 5 is  $5!$  which comes out to 120, so the number of possible rearrangements of two sets of five is  $5! * 5!$  or 14400. Thus, we expect that 0.0039 of the random labelings should come out exactly the same as the original, which is fairly close to the 0.0033 that we see in our simulation. We have a similar expectation for the number of times that the labeling will be exactly opposite of the true labeling, giving us the negative of the observed  $t$  value.

We can compute the  $p$ -value from the randomized data by measuring how many of the shuffled values are at least as extreme as the observed value:

```
# compute p value using randomization
pvalRandomization <- mean(shuffleDiff >= tt$statistic)

sprintf(
  'p(t > %0.2f, df = 8) using randomization = %0.5f',
```

```
tt$statistic,
pvalRandomization
)
```

```
## [1] "p(t > 5.14, df = 8) using randomization = 0.00330"
```

This p-value is very similar to the p-value that we obtained using the t distribution, and both are quite extreme, suggesting that the observed data are very unlikely to have arisen if the null hypothesis is true - and in this case we *know* that it's not true, because we generated the data.

### 10.3.5.1.2 Randomization: BMI/activity example

Now let's use randomization to compute the p-value for the BMI/activity example. In this case, we will randomly shuffle the `PhysActive` variable and compute the difference between groups after each shuffle, and then compare our observed t statistic to the distribution of t statistics from the shuffled datasets.

```
# create function to shuffle BMI data

shuffleBMiStat <- function() {
  bmiDataShuffled <-
    NHANES_sample %>%
    select(BMI, PhysActive) %>%
    mutate(
      PhysActive = sample(PhysActive)
    )
  # compute the difference
  simResult <- t.test(
    BMI ~ PhysActive,
    data = bmiDataShuffled,
    var.equal = TRUE
  )
  return(simResult$statistic)
}

# run function 5000 times and save output

nRuns <- 5000
meanDiffSimDf <-
  data.frame(
    meanDiffSim = replicate(nRuns, shuffleBMiStat())
  )
```

Let's look at the results. Figure 10.7 shows the distribution of t values from the shuffled samples, and we can also compute the probability of finding a value as large or larger than the observed value:

```
# compute the empirical probability of t values larger than observed
# value under the randomization null
bmtTTest <-
  t.test(
    BMI ~ PhysActive,
    data = NHANES_sample,
    var.equal = TRUE,
    alternative = "greater"
  )

bmiPvalRand <-
```

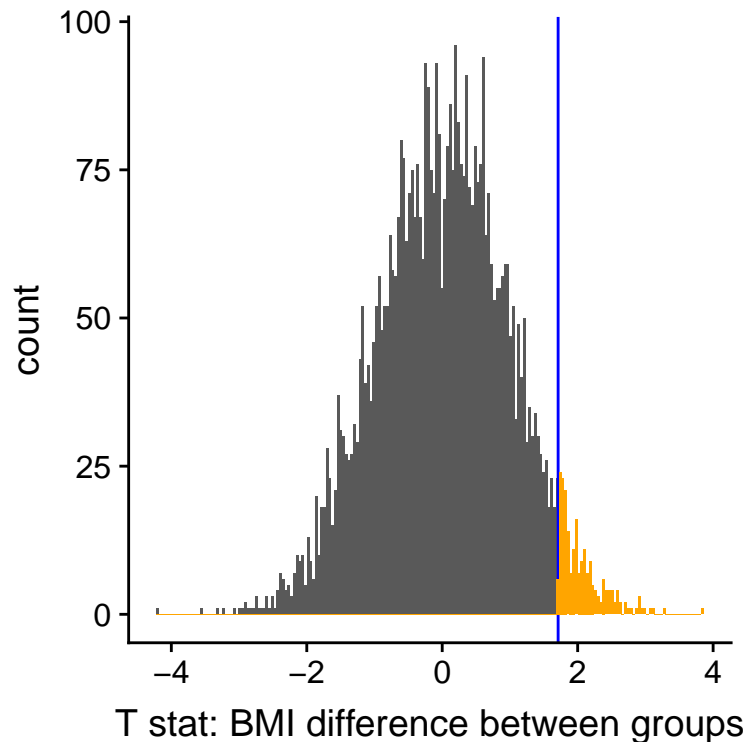


Figure 10.7: Histogram of  $t$  statistics after shuffling of group labels, with the observed value of the  $t$  statistic shown in the blue line, and values more extreme than the observed value shown in orange.

```
mean(meanDiffSimDf$meanDiffSim >= bmtTTest$statistic)

sprintf(
  "p(mean > %0.2f, df = 248) using randomization = %0.5f",
  bmtTTest$statistic,
  bmiPvalRand
)

## [1] "p(mean > 1.71, df = 248) using randomization = 0.04380"

sprintf(
  "p(mean > %0.2f, df = 248) using parametric t-test = %0.5f",
  bmtTTest$statistic,
  bmtTTest$p.value
)

## [1] "p(mean > 1.71, df = 248) using parametric t-test = 0.04413"
```

Again, the  $p$ -value obtained from randomization (0.044) is very similar to the one obtained using the  $t$  distribution (0.044). The advantage of the randomization test is that it doesn't require that we assume that the data from each of the groups are normally distributed, though the  $t$ -test is generally quite robust to violations of that assumption. In addition, the randomization test can allow us to compute  $p$ -values for statistics when we don't have a theoretical distribution like we do for the  $t$ -test.

We do have to make one main assumption when we use the randomization test, which we refer to as *exchangeability*. This means that all of the observations are distributed in the same way, such that we can interchange them without changing the overall distribution. The main place where this can break down is when there are related observations in the data; for example, if we had data from individuals in 4 different

families, then we couldn't assume that individuals were exchangeable, because siblings would be closer to each other than they are to individuals from other families. In general, if the data were obtained by random sampling, then the assumption of exchangeability should hold.

### 10.3.6 Step 6: Assess the “statistical significance” of the result

The next step is to determine whether the p-value that results from the previous step is small enough that we are willing to reject the null hypothesis and conclude instead that the alternative is true. How much evidence do we require? This is one of the most controversial questions in statistics, in part because it requires a subjective judgment – there is no “correct” answer.

Historically, the most common answer to this question has been that we should reject the null hypothesis if the p-value is less than 0.05. This comes from the writings of Ronald Fisher, who has been referred to as “the single most important figure in 20th century statistics” (Efron 1998):

“If  $P$  is between .1 and .9 there is certainly no reason to suspect the hypothesis tested. If it is below .02 it is strongly indicated that the hypothesis fails to account for the whole of the facts. We shall not often be astray if we draw a conventional line at .05 ... it is convenient to draw the line at about the level at which we can say: Either there is something in the treatment, or a coincidence has occurred such as does not occur more than once in twenty trials” (Fisher 1925)

However, Fisher never intended  $p < 0.05$  to be a fixed rule:

“no scientific worker has a fixed level of significance at which from year to year, and in all circumstances, he rejects hypotheses; he rather gives his mind to each particular case in the light of his evidence and his ideas” [fish:1956]

Instead, it is likely that it became a ritual due to the reliance upon tables of p-values that were used before computing made it easy to compute p values for arbitrary values of a statistic. All of the tables had an entry for 0.05, making it easy to determine whether one's statistic exceeded the value needed to reach that level of significance.

The choice of statistical thresholds remains deeply controversial, and recently (Benjamin et al., 2018) it has been proposed that the standard threshold be changed from .05 to .005, making it substantially more stringent and thus more difficult to reject the null hypothesis. In large part this move is due to growing concerns that the evidence obtained from a significant result at  $p < .05$  is relatively weak; we will discuss this in much more detail in our later discussion of reproducibility in Chapter doing-reproducible-research).

#### 10.3.6.1 Hypothesis testing as decision-making: The Neyman-Pearson approach

Whereas Fisher thought that the p-value could provide evidence regarding a specific hypothesis, the statisticians Jerzy Neyman and Egon Pearson disagreed vehemently. Instead, they proposed that we think of hypothesis testing in terms of its error rate in the long run:

“no test based upon a theory of probability can by itself provide any valuable evidence of the truth or falsehood of a hypothesis. But we may look at the purpose of tests from another viewpoint. Without hoping to know whether each separate hypothesis is true or false, we may search for rules to govern our behaviour with regard to them, in following which we insure that, in the long run of experience, we shall not often be wrong” (J. Neyman and Pearson 1933)

That is: We can't know which specific decisions are right or wrong, but if we follow the rules, we can at least know how often our decisions will be wrong.

To understand the decision making framework that Neyman and Pearson developed, we first need to discuss statistical decision making in terms of the kinds of outcomes that can occur. There are two possible states of reality ( $H_0$  is true, or  $H_0$  is false), and two possible decisions (reject  $H_0$ , or fail to reject  $H_0$ ). There are two ways in which we can make a correct decision:

- We can decide to reject  $H_0$  when it is false (in the language of decision theory, we call this a *hit*)
- We can fail to reject  $H_0$  when it is true (we call this a *correct rejection*)

There are also two kinds of errors we can make:

- We can decide to reject  $H_0$  when it is actually true (we call this a *false alarm*, or *Type I error*)
- We can fail to reject  $H_0$  when it is actually false (we call this a *miss*, or *Type II error*)

Neyman and Pearson coined two terms to describe the probability of these two types of errors in the long run:

- $P(\text{Type I error}) = \alpha$
- $P(\text{Type II error}) = \beta$

That is, if we set  $\alpha$  to .05, then in the long run we should make a Type I error 5% of the time. Whereas it's common to set  $\alpha$  as .05, the standard value for  $\beta$  is .2 - that is, we are willing to accept that 20% of the time we will fail to detect a true effect. We will return to this below when we discuss statistical power in Section 11.3, which is the complement of Type II error.

### 10.3.7 What does a significant result mean?

There is a great deal of confusion about what p-values actually mean (Gigerenzer, 2004). Let's say that we do an experiment comparing the means between conditions, and we find a difference with a p-value of .01. There are a number of possible interpretations.

#### 10.3.7.1 Does it mean that the probability of the null hypothesis being true is .01?

No. Remember that in null hypothesis testing, the p-value is the probability of the data given the null hypothesis ( $P(\text{data}|H_0)$ ). It does not warrant conclusions about the probability of the null hypothesis given the data ( $P(H_0|\text{data})$ ). We will return to this question when we discuss Bayesian inference in a later chapter, as Bayes theorem lets us invert the conditional probability in a way that allows us to determine the latter probability.

#### 10.3.7.2 Does it mean that the probability that you are making the wrong decision is .01?

No. This would be  $P(H_0|\text{data})$ , but remember as above that p-values are probabilities of data under  $H_0$ , not probabilities of hypotheses.

#### 10.3.7.3 Does it mean that if you ran the study again, you would obtain the same result 99% of the time?

No. The p-value is a statement about the likelihood of a particular dataset under the null; it does not allow us to make inferences about the likelihood of future events such as replication.

#### 10.3.7.4 Does it mean that you have found a meaningful effect?

No. There is an important distinction between *statistical significance* and *practical significance*. As an example, let's say that we performed a randomized controlled trial to examine the effect of a particular diet on body weight, and we find a statistically significant effect at  $p < .05$ . What this doesn't tell us is how much weight was actually lost, which we refer to as the *effect size* (to be discussed in more detail in Chapter 11). If we think about a study of weight loss, then we probably don't think that the loss of ten ounces (i.e. the weight of a bag of potato chips) is practically significant. Let's look at our ability to detect a significant difference of 1 ounce as the sample size increases.

```

# create simulated data for weight loss trial

weightLossTrial <- function(nPerGroup, weightLossOz = 1) {
  # mean and SD in Kg based on NHANES adult dataset
  kgToOz <- 35.27396195 # conversion constant for Kg to Oz
  meanOz <- 81.78 * kgToOz
  sdOz <- 21.29 * kgToOz
  # create data
  controlGroup <- rnorm(nPerGroup) * sdOz + meanOz
  expGroup <- rnorm(nPerGroup) * sdOz + meanOz - weightLossOz
  ttResult <- t.test(expGroup, controlGroup)
  return(c(
    nPerGroup, weightLossOz, ttResult$p.value,
    diff(ttResult$estimate)
  ))
}

nRuns <- 1000
sampSizes <- 2**seq(5,17) # powers of 2

simResults <- c() ## create an empty list to add results onto
for (i in 1:length(sampSizes)) {
  tmpResults <- replicate(
    nRuns,
    weightLossTrial(sampSizes[i], weightLossOz = 10)
  )
  summaryResults <- c(
    tmpResults[1, 1], tmpResults[2, 1],
    sum(tmpResults[3, ] < 0.05),
    mean(tmpResults[4, ])
  )
  simResults <- rbind(simResults, summaryResults)
}

simResultsDf <-
  as.tibble(simResults) %>%
  rename(
    sampleSize = V1,
    effectSizeLbs = V2,
    nSigResults = V3,
    meanEffect = V4
  ) %>%
  mutate(pSigResult = nSigResults / nRuns)

```

Figure 10.8 shows how the proportion of significant results increases as the sample size increases, such that with a very large sample size (about 262,000 total subjects), we will find a significant result in more than 90% of studies when there is a 1 ounce weight loss. While these are statistically significant, most physicians would not consider a weight loss of one ounce to be practically or clinically significant. We will explore this relationship in more detail when we return to the concept of *statistical power* in Section 11.3, but it should already be clear from this example that statistical significance is not necessarily indicative of practical significance.

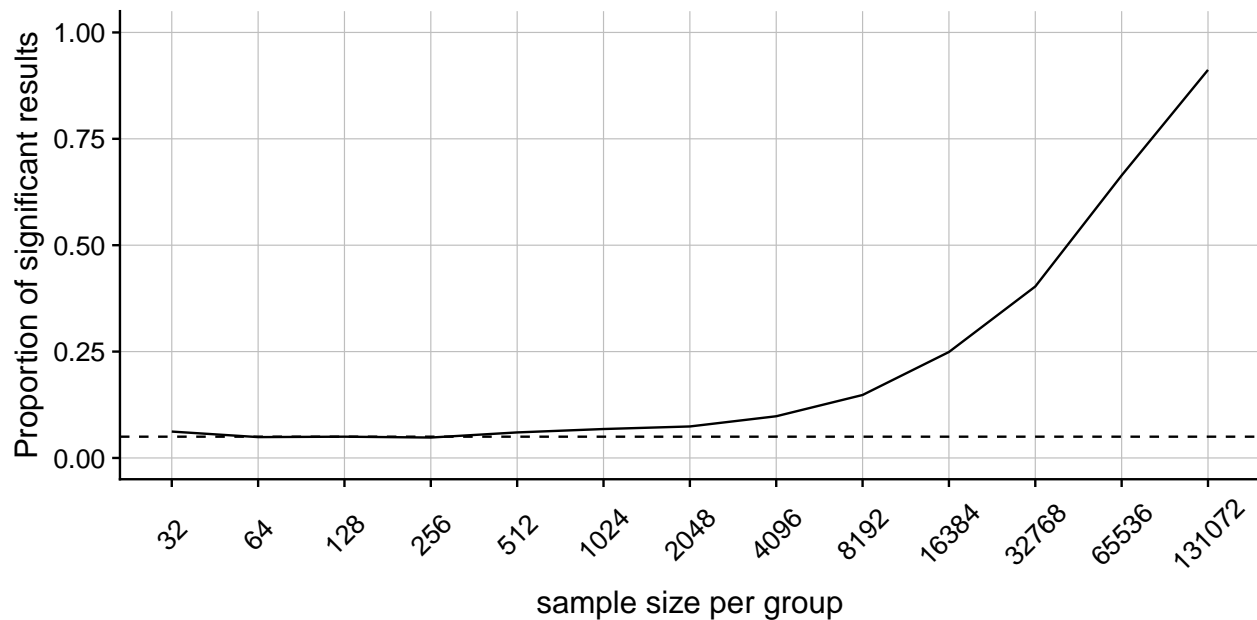


Figure 10.8: The proportion of significant results for a very small change (1 ounce, which is about .001 standard deviations) as a function of sample size.

## 10.4 NHST in a modern context: Multiple testing

So far we have discussed examples where we are interested in testing a single statistical hypothesis, and this is consistent with traditional science which often measured only a few variables at a time. However, in modern science we can often measure millions of variables per individual. For example, in genetic studies that quantify the entire genome, there may be many millions of measures per individual, and in brain imaging we often collect data from more than 100,000 locations in the brain at once. When standard hypothesis testing is applied in these contexts, bad things can happen unless we take appropriate care.

Let's look at an example to see how this might work. There is great interest in understanding the genetic factors that can predispose individuals to major mental illnesses such as schizophrenia, because we know that about 80% of the variation between individuals in the presence of schizophrenia is due to genetic differences. The Human Genome Project and the ensuing revolution in genome science has provided tools to examine the many ways in which humans differ from one another in their genomes. One approach that has been used in recent years is known as a *genome-wide association study* (GWAS), in which the genome of each individual is characterized at one million or more places in their genome to determine which letters of the genetic code (which we call “variants”) they have at that location. After these have been determined, the researchers perform a statistical test at each location in the genome to determine whether people diagnosed with schizophrenia are more or less likely to have one specific variant at that location.

Let's imagine what would happen if the researchers simply asked whether the test was significant at  $p < .05$  at each location, when in fact there is no true effect at any of the locations. To do this, we generate a large number of simulated  $t$  values from a null distribution, and ask how many of them are significant at  $p < .05$ . Let's do this many times, and each time count up how many of the tests come out as significant (see Figure 10.9).

```
# simulate 1500 studies with 10,000 tests each, thresholded at  $p < .05$ 
```

```
nRuns <- 1500 # number of simulated studies to run
```

```
nTests <- 10000 # number of simulated genes to test in each run
```

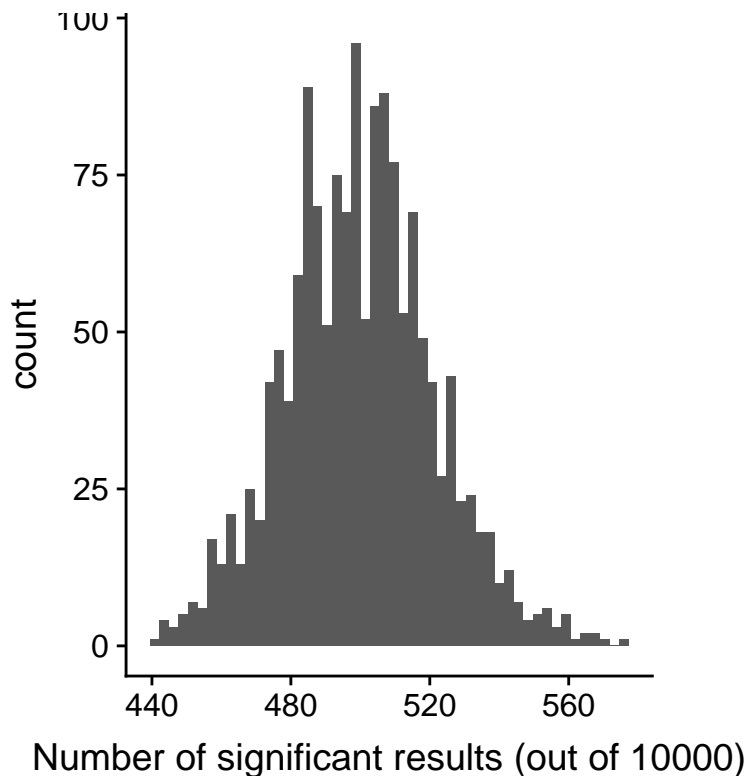


Figure 10.9: A histogram of the number of significant results in each set of 1 million statistical tests, when there is in fact no true effect.

```
uncAlpha <- 0.05 # alpha level

uncOutcome <- replicate(nRuns, sum(rnorm(nTests) < qnorm(uncAlpha)))

sprintf("mean proportion of significant tests per run: %0.2f", mean(uncOutcome) / nTests)

## [1] "mean proportion of significant tests per run: 0.05"

# compute proportion of studies with at least one false positive result,
# known as the familywise error rate
sprintf("familywise error rate: %0.3f", mean(uncOutcome > 0))

## [1] "familywise error rate: 1.000"
```

This shows that about 5% of all of the tests were significant in each run, meaning that if we were to use  $p < .05$  as our threshold for statistical significance, then even if there were no truly significant relationships present, we would still “find” about 500 genes that were seemingly significant (the expected number of significant results is simply  $n * \alpha$ ). That is because while we controlled for the error per test, we didn’t control the *familywise error*, or the error across all of the tests, which is what we really want to control if we are going to be looking at the results from a large number of tests. Using  $p < .05$ , our familywise error rate in the above example is one – that is, we are pretty much guaranteed to make at least one error in any particular study.

A simple way to control for the familywise error is to divide the alpha level by the number of tests; this is known as the *Bonferroni* correction, named after the Italian statistician Carlo Bonferroni. Using the data from our example above, we see in Figure 10.10 that only about 5 percent of studies show any significant results using the corrected alpha level of 0.000005 instead of the nominal level of .05. We have effectively



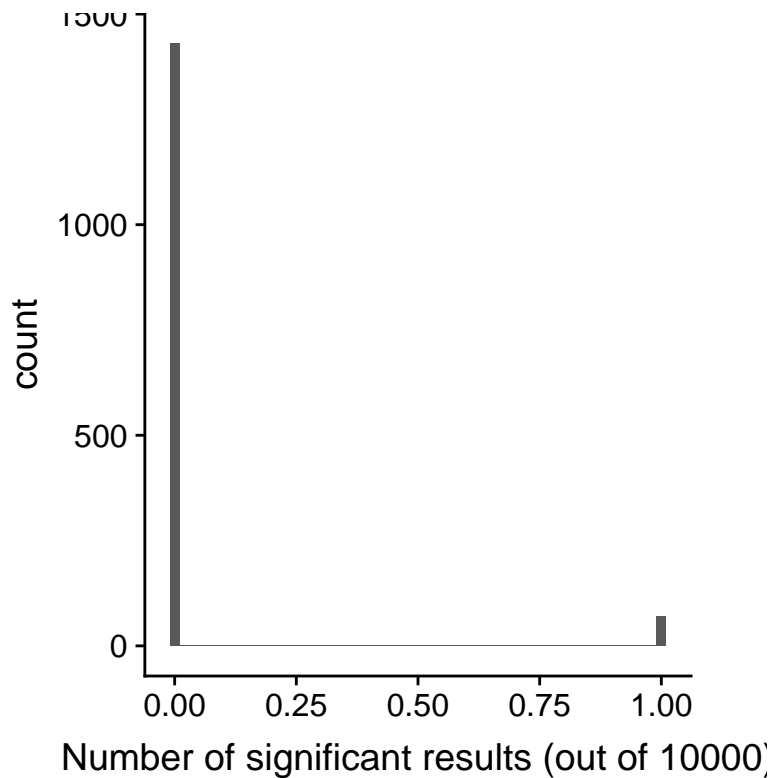


Figure 10.10: A histogram of the number of significant results across all simulation runs after applying the Bonferroni correction for multiple tests.

controlled the familywise error, such that the probability of making *any* errors in our study is controlled at right around .05.

```
# compute Bonferroni-corrected alpha
corAlpha <- 0.05 / nTests

corOutcome <- replicate(nRuns, sum(rnorm(nTests) < (qnorm(corAlpha))))

sprintf("corrected familywise error rate: %0.3f", mean(corOutcome > 0))

## [1] "corrected familywise error rate: 0.046"
```

## 10.5 Suggested readings

- Mindless Statistics, by Gerd Gigerenzer



## Chapter 11

# Confidence intervals, effect sizes, and statistical power

In the previous chapter we discussed how we can use data to test hypotheses. Those methods provided a binary answer: we either reject or fail to reject the null hypothesis. However, this kind of decision overlooks a couple of important questions. First, we would like to know how much uncertainty we have about the answer (regardless of which way it goes). In addition, sometimes we don't have a clear null hypothesis, so we would like to see what range of estimates are consistent with the data. Second, we would like to know how large the effect actually is, since as we saw in the weight loss example in the previous chapter, a statistically significant effect is not necessarily a practically important effect.

In this chapter we will discuss methods to address these two questions: confidence intervals to provide a measure of our uncertainty about our estimates, and effect sizes to provide a standardized way to understand how large the effects are. We will also discuss the concept of *statistical power* which tells us how well we can expect to find any true effects that might exist.

### 11.1 Confidence intervals

So far in the book we have focused on estimating the specific value of a statistic. For example, let's say we want to estimate the mean weight of adults in the NHANES dataset. We could take a sample from the dataset and estimate the mean:

```
# take a sample from adults in NHANES and summarize their weight
```

```
sampSize <- 250
NHANES_sample <- sample_n(NHANES_adult, sampSize)

sample_summary <-
  NHANES_sample %>%
  summarize(
    meanWeight = mean(Weight),
    sdWeight = sd(Weight)
  )
pander(sample_summary)
```

| meanWeight | sdWeight |
|------------|----------|
| 82.77      | 22.27    |

In this sample, the mean weight was 82.77 kilograms. We refer to this as a *point estimate* since it provides us with a single number to describe the difference. However, we know from our earlier discussion of sampling error that there is some uncertainty about this estimate, which is described by the standard error. You should also remember that the standard error is determined by two components: the population standard deviation (which is the numerator), and the square root of the sample size (which is in the denominator). The population standard deviation is an unknown but fixed parameter that is not under our control, whereas the sample size *is* under our control. Thus, we can decrease our uncertainty about the estimate by increasing our sample size – up to the limit of the entire population size, at which point there is no uncertainty at all because we can just calculate the population parameter directly from the data of the entire population.

You may also remember that earlier we introduced the concept of a *confidence interval*, which is a way of describing our uncertainty about a statistical estimate. Remember that a confidence interval describes an interval that will on average contain the true population parameter with a given probability; for example, the 95% confidence interval is an interval that will capture the true population parameter 95% of the time. Note again that this is not a statement about the population parameter; any particular confidence interval either does or does not contain the true parameter. As Jerzy Neyman, the inventor of the confidence interval, said:

“The parameter is an unknown constant and no probability statement concerning its value may be made.”(J Neyman 1937)

The confidence interval for the mean is computed as:

$$CI = \text{point estimate} \pm \text{critical value}$$

where the critical value is determined by the sampling distribution of the estimate. The important question, then, is what that sampling distribution is.

### 11.1.1 Confidence intervals using the normal distribution

If we know the population standard deviation, then we can use the normal distribution to compute a confidence interval. We usually don't, but for our example of the NHANES dataset we do (it's 21.3 for weight).

Let's say that we want to compute a 95% confidence interval for the mean. The critical value would then be the values of the standard normal distribution that capture 95% of the distribution; these are simply the 2.5th percentile and the 97.5th percentile of the distribution, which we can compute using the `qnorm()` function in R, and come out to  $\pm 1.96$ . Thus, the confidence interval for the mean ( $\bar{X}$ ) is:

$$CI = \bar{X} \pm 1.96 * SE$$

Using the estimated mean from our sample (82.77) and the known population standard deviation, we can compute the confidence interval of [80.13,85.41].

### 11.1.2 Confidence intervals using the t distribution

As stated above, if we knew the population standard deviation, then we could use the normal distribution to compute our confidence intervals. However, in general we don't – in which case the *t* distribution is more appropriate as a sampling distribution. Remember that the *t* distribution is slightly broader than the normal distribution, especially for smaller samples, which means that the confidence intervals will be slightly wider than they would if we were using the normal distribution. This incorporates the extra uncertainty that arises when we make conclusions based on small samples.

We can compute the 95% confidence interval in a way similar to the normal distribution example above, but the critical value is determined by the 2.5th percentile and the 97.5th percentile of the *t* distribution, which we can compute using the `qt()` function in R. Thus, the confidence interval for the mean ( $\bar{X}$ ) is:

$$CI = \bar{X} \pm t_{crit} * SE$$

where  $t_{crit}$  is the critical t value. For the NHANES weight example (with sample size of 250), the confidence interval would be:

```
# compute confidence intervals for weight in NHANES data

sample_summary <-
  sample_summary %>%
  mutate(
    cutoff_lower = qt(0.025, sampSize),
    cutoff_upper = qt(0.975, sampSize),
    CI_lower = meanWeight + cutoff_lower * sdWeight / sqrt(sampSize),
    CI_upper = meanWeight + cutoff_upper * sdWeight / sqrt(sampSize)
  )
pander(sample_summary)
```

| meanWeight | sdWeight | cutoff_lower | cutoff_upper | CI_lower | CI_upper |
|------------|----------|--------------|--------------|----------|----------|
| 82.77      | 22.27    | -1.97        | 1.97         | 80       | 85.54    |

Remember that this doesn't tell us anything about the probability of the true population value falling within this interval, since it is a fixed parameter (which we know is 81.77 because we have the entire population in this case) and it either does or does not fall within this specific interval (in this case, it does). Instead, it tells us that in the long run, if we compute the confidence interval using this procedure, 95% of the time that confidence interval will capture the true population parameter.

### 11.1.3 Confidence intervals and sample size

Because the standard error decreases with sample size, the means confidence interval should get narrower as the sample size increases, providing progressively tighter bounds on our estimate. Figure 11.1 shows an example of how the confidence interval would change as a function of sample size for the weight example. From the figure it's evident that the confidence interval becomes increasingly tighter as the sample size increases, but increasing samples provide diminishing returns, consistent with the fact that the denominator of the confidence interval term is proportional to the square root of the sample size.

### 11.1.4 Computing confidence intervals using the bootstrap

In some cases we can't assume normality, or we don't know the sampling distribution of the statistic. In these cases, we can use the bootstrap (which we introduced in Chapter 9). As a reminder, the bootstrap involves repeatedly resampling the data *with replacement*, and then using the distribution of the statistic computed on those samples as a surrogate for the sampling distribution of the statistic.

Earlier we ran the bootstrap using hand-crafted code, but R includes a package called `boot` that we can use to run the bootstrap and compute confidence intervals. Let's use it to compute the confidence interval for weight in our NHANES sample.

```
# compute bootstrap confidence intervals on NHANES weight data

meanWeight <- function(df, foo) {
  return(mean(df[foo, ]$Weight))
}
```

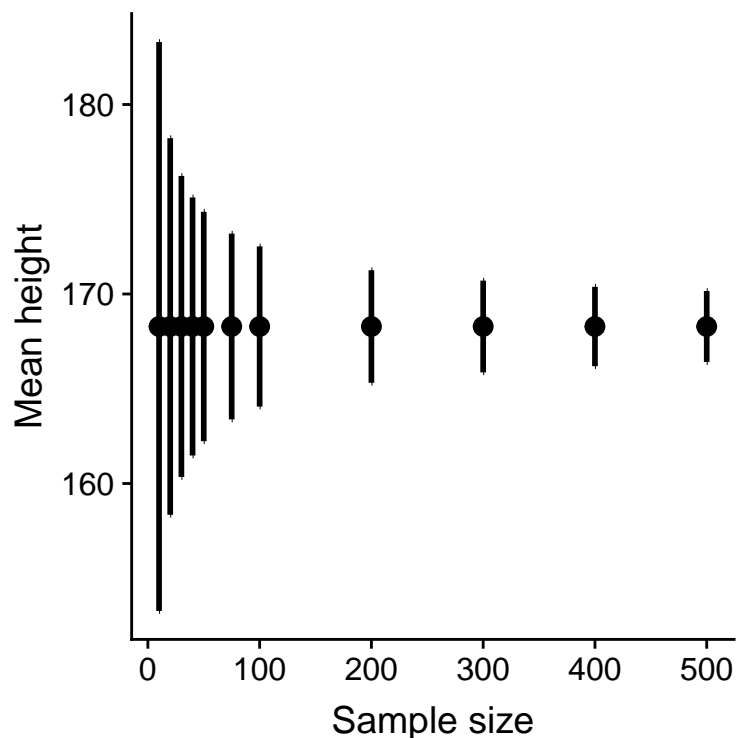


Figure 11.1: An example of the effect of sample size on the width of the confidence interval for the mean.

```
bs <- boot(NHANES_sample, meanWeight, 1000)

# use the percentile bootstrap
bootci <- boot.ci(bs, type = "perc")
print("Bootstrap confidence intervals:")

## [1] "Bootstrap confidence intervals:"

tibble(
  lower = bootci$perc[4],
  upper = bootci$perc[5]
) %>%
  pander()
```

| lower | upper |
|-------|-------|
| 80.12 | 85.71 |

These values are fairly close to the values obtained using the  $t$  distribution above, though not exactly the same.

### 11.1.5 Relation of confidence intervals to hypothesis tests

There is a close relationship between confidence intervals and hypothesis tests. In particular, if the confidence interval does not include the null hypothesis, then the associated statistical test would be statistically significant. For example, if you are testing whether the mean of a sample is greater than zero with  $\alpha = 0.05$ , you could simply check to see whether zero is contained within the 95% confidence interval for the mean.

Things get trickier if we want to compare the means of two conditions (Schenker and Gentleman 2001). There are a couple of situations that are clear. First, each mean is contained within the confidence interval for the other mean, then there is certainly no significant difference at the chosen confidence level. Second, if there is no overlap between the confidence intervals, then there is certainly a significant difference at the chosen level; in fact, this test is substantially *conservative*, such that the actual error rate will be lower than the chosen level. But what about the case where the confidence intervals overlap one another but don't contain the

### 11.2.1 Cohen's D

One of the most common measures of effect size is known as *Cohen's d*, named after the statistician Jacob Cohen (who is most famous for his 1994 paper titled “The Earth Is Round ( $p < .05$ )”). It is used to quantify the difference between two means, in terms of their standard deviation:

$$d = \frac{\bar{X}_1 - \bar{X}_2}{s}$$

where  $\bar{X}_1$  and  $\bar{X}_2$  are the means of the two groups, and  $s$  is the pooled standard deviation (which is a combination of the standard deviations for the two samples, weighted by their sample sizes):

$$s = \sqrt{\frac{(n_1 - 1)s_1^2 + (n_2 - 1)s_2^2}{n_1 + n_2 - 2}}$$

where  $n_1$  and  $n_2$  are the sample sizes and  $s_1^2$  and  $s_2^2$  are the standard deviations for the two groups respectively.

There is a commonly used scale for interpreting the size of an effect in terms of Cohen's  $d$ :

| D   | Interpretation |
|-----|----------------|
| 0.2 | small          |
| 0.5 | medium         |
| 0.8 | large          |

It can be useful to look at some commonly understood effects to help understand these interpretations.

*# compute effect size for gender difference in NHANES*

```
NHANES_sample <-
  NHANES_adult %>%
  drop_na(Height) %>%
  sample_n(250)

hsum <-
  NHANES_sample %>%
  group_by(Gender) %>%
  summarize(
    meanHeight = mean(Height),
    varHeight = var(Height),
    n = n()
  )

#pooled SD
s_height_gender <- sqrt(
  ((hsum$n[1] - 1) * hsum$varHeight[1] + (hsum$n[2] - 1) * hsum$varHeight[2]) /
  (hsum$n[1] + hsum$n[2] - 2)
)

#cohen's d
d_height_gender <- (hsum$meanHeight[2] - hsum$meanHeight[1]) / s_height_gender

sprintf("Cohens d for male vs. female height = %0.2f", d_height_gender)
```

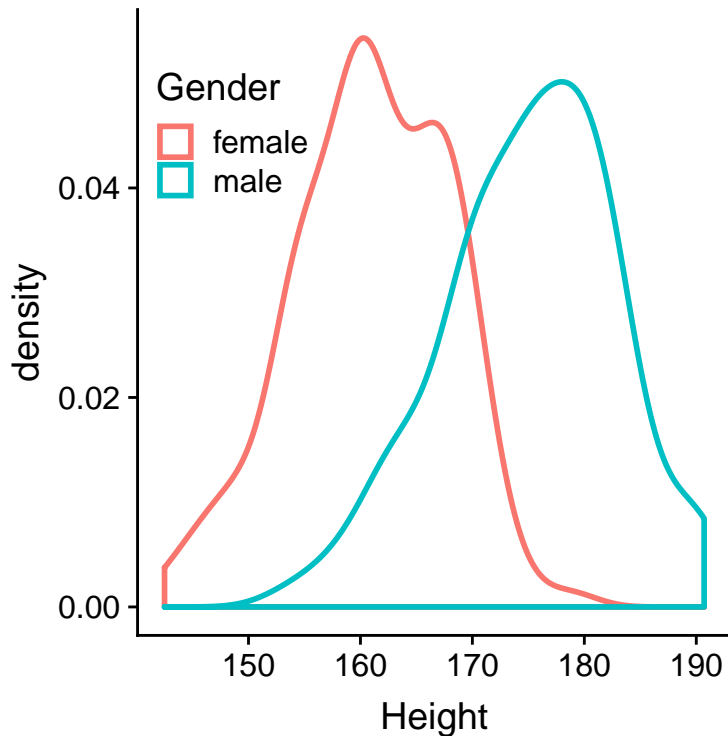


Figure 11.2: Smoothed histogram plots for male and female heights in the NHANES dataset, showing clearly distinct but also clearly overlapping distributions.

```
## [1] "Cohens d for male vs. female height = 1.95"
```

The effect size for gender differences in height ( $d = 1.95$ ) is huge by reference to our table above. We can also see this by looking at the distributions of male and female heights in our sample. Figure 11.2 shows that the two distributions are quite well separated, though still overlapping, highlighting the fact that even when there is a very large effect size for the difference between two groups, there will be individuals from each group that are more like the other group.

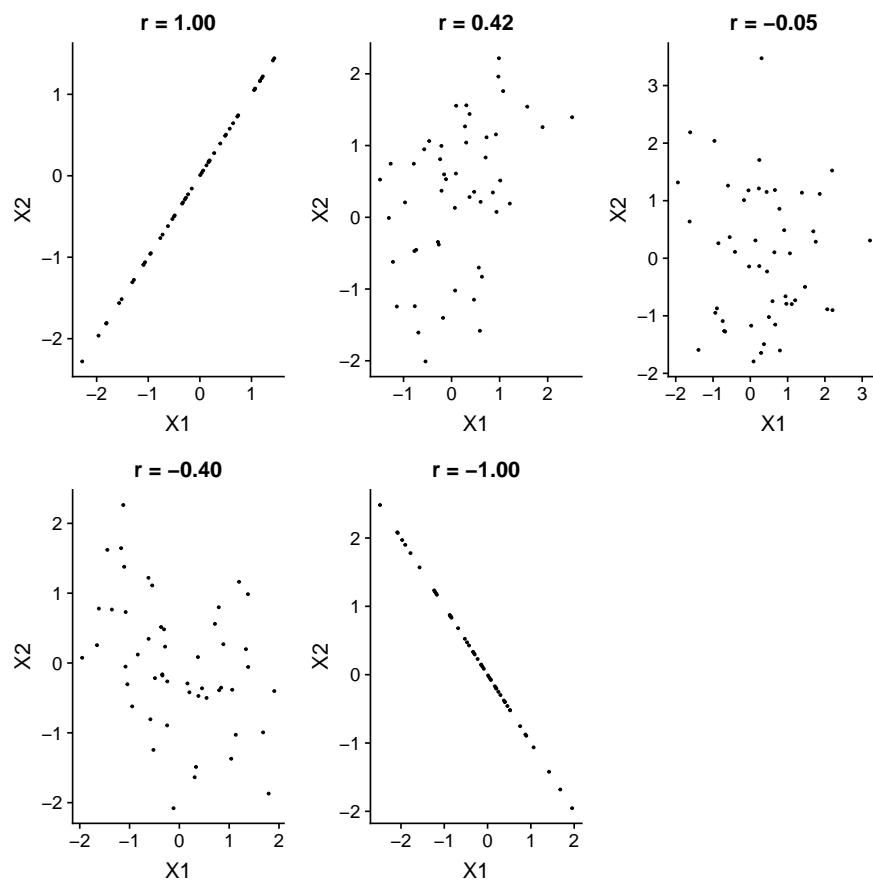
It is also worth noting that we rarely encounter effects of this magnitude in science, in part because they are such obvious effects that we don't need scientific research to find them. As we will see in Chapter 18 on reproducibility, very large reported effects in scientific research often reflect the use of questionable research practices rather than truly huge effects in nature. It is also worth noting that even for such a huge effect, the two distributions still overlap - there will be some females who are taller than the average male, and vice versa. For most interesting scientific effects, the degree of overlap will be much greater, so we shouldn't immediately jump to strong conclusions about different populations based on even a large effect size.

### 11.2.2 Pearson's $r$

Pearson's  $r$ , also known as the *correlation coefficient*, is a measure of the strength of the linear relationship between two continuous variables. We will discuss correlation in much more detail in Chapter 14, so we will save the details for that chapter; here, we simply introduce  $r$  as a way to quantify the relation between two variables.

$r$  is a measure that varies from -1 to 1, where a value of 1 represents a perfect positive relationship between the variables, 0 represents no relationship, and -1 represents a perfect negative relationship. Figure 11.3 shows examples of various levels of correlation using randomly generated data.



Figure 11.3: Examples of various levels of Pearson's  $r$ .

### 11.2.3 Odds ratio

In our earlier discussion of probability we discussed the concept of odds – that is, the relative likelihood of some event happening versus not happening:

$$\text{odds of } A = \frac{P(A)}{P(\neg A)}$$

The odds ratio is simply the ratio of two odds. For example, let's take the case of smoking and lung cancer. A study published in the International Journal of Cancer in 2012 (Pesch et al. 2012) combined data regarding the occurrence of lung cancer in smokers and individuals who have never smoked across a number of different studies. Note that these data come from case-control studies, which means that participants in the studies were recruited because they either did or did not have cancer; their smoking status was then examined. These numbers thus do not represent the prevalence of cancer amongst smokers in the general population – but they can tell us about the relationship between cancer and smoking.

```
# create table for cancer occurrence depending on smoking status
smokingDf <- tibble(
  NeverSmoked = c(2883, 220),
  CurrentSmoker = c(3829, 6784),
  row.names = c("NoCancer", "Cancer")
)
pander(smokingDf)
```

| NeverSmoked | CurrentSmoker | row.names |
|-------------|---------------|-----------|
| 2883        | 3829          | NoCancer  |
| 220         | 6784          | Cancer    |

We can convert these numbers to odds ratios for each of the groups:

```
# convert smoking data to odds

smokingDf <-
  smokingDf %>%
  mutate(
    pNeverSmoked = NeverSmoked / sum(NeverSmoked),
    pCurrentSmoker = CurrentSmoker / sum(CurrentSmoker)
  )

oddsCancerNeverSmoked <- smokingDf$NeverSmoked[2] / smokingDf$NeverSmoked[1]
oddsCancerCurrentSmoker <- smokingDf$CurrentSmoker[2] / smokingDf$CurrentSmoker[1]
```

The odds of someone having lung cancer who has never smoked is 0.08 whereas the odds of a current smoker having lung cancer is 1.77. The ratio of these odds tells us about the relative likelihood of cancer between the two groups:

```
#compute odds ratio

oddsRatio <- oddsCancerCurrentSmoker/oddsCancerNeverSmoked
sprintf('odds ratio of cancer for smokers vs. nonsmokers: %0.3f',oddsRatio)

## [1] "odds ratio of cancer for smokers vs. nonsmokers: 23.218"
```

The odds ratio of 23.22 tells us that the odds of cancer in smokers are roughly 23 times higher than never-smokers.

## 11.3 Statistical power

Remember from the previous chapter that under the Neyman-Pearson hypothesis testing approach, we have to specify our level of tolerance for two kinds of errors: False positives (which they called *Type I error*) and false negatives (which they called *Type II error*). People often focus heavily on Type I error, because making a false positive claim is generally viewed as a very bad thing; for example, the now discredited claims by Wakefield (1999) that autism was associated with vaccination led to anti-vaccine sentiment that has resulted in substantial increases in childhood diseases such as measles. Similarly, we don't want to claim that a drug cures a disease if it really doesn't. That's why the tolerance for Type I errors is generally set fairly low, usually at  $\alpha = 0.05$ . But what about Type II errors?

The concept of *statistical power* is the complement of Type II error – that is, it is the likelihood of finding a positive result given that it exists:

$$\text{power} = 1 - \beta$$

Another important aspect of the Neyman-Pearson model that we didn't discuss above is the fact that in addition to specifying the acceptable levels of Type I and Type II errors, we also have to describe a specific alternative hypothesis – that is, what is the size of the effect that we wish to detect? Otherwise, we can't interpret  $\beta$  – the likelihood of finding a large effect is always going to be higher than finding a small effect, so  $\beta$  will be different depending on the size of effect we are trying to detect.

There are three factors that can affect power:

- Sample size: Larger samples provide greater statistical power
- Effect size: A given design will always have greater power to find a large effect than a small effect (because finding large effects is easier)
- Type I error rate: There is a relationship between Type I error and power such that (all else being equal) decreasing Type I error will also decrease power.

We can see this through simulation. First let's simulate a single experiment, in which we compare the means of two groups using a standard t-test. We will vary the size of the effect (specified in terms of Cohen's d), the Type I error rate, and the sample size, and for each of these we will examine how the proportion of significant results (i.e. power) is affected. Figure 11.3 shows an example of how power changes as a function of these factors.

```
# Simulate power as a function of sample size, effect size, and alpha
```

```
# create a set of functions to generate simulated results
```

```
powerDf <-
```

```
  expand.grid(
    sampSizePerGroup = c(12, 24, 48, 96),
    effectSize = c(.2, .5, .8),
    alpha = c(0.005, 0.05)
  ) %>%
  tidyr::expand(effectSize, sampSizePerGroup, alpha) %>%
  group_by(effectSize, sampSizePerGroup, alpha)
```

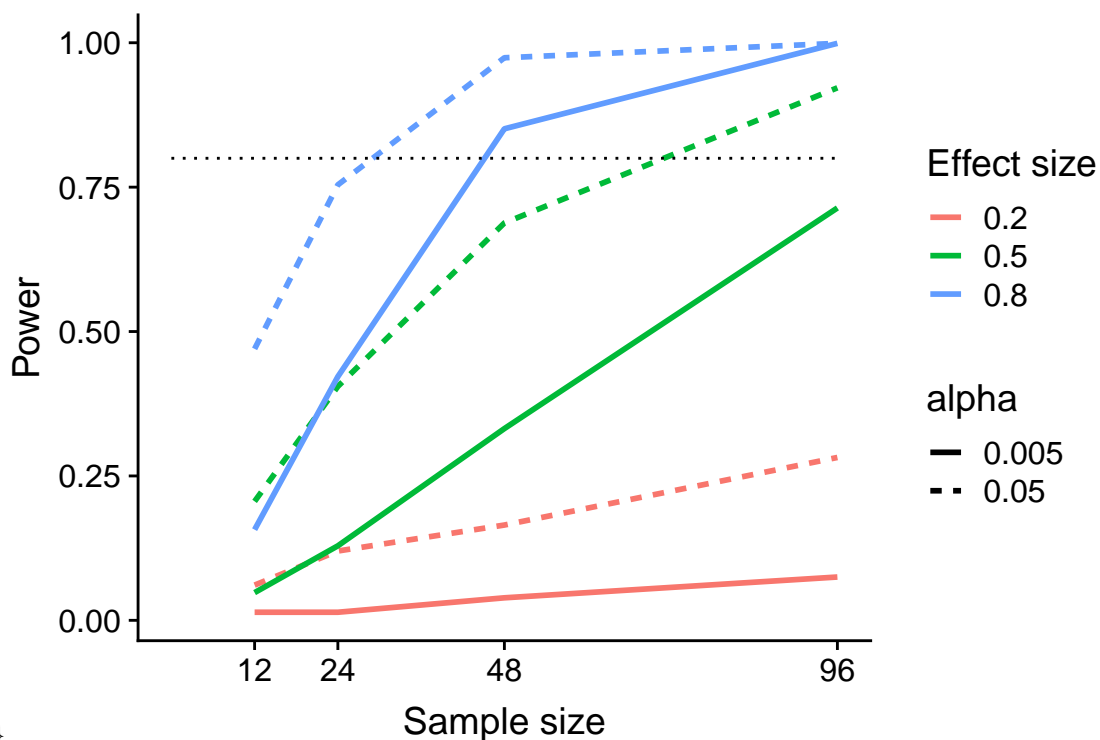
```
runPowerSim <- function(df, nsims = 1000) {
  p <- array(NA, dim = nsims)
  for (s in 1:nsims) {
    data <- data.frame(
      y = rnorm(df$sampSizePerGroup * 2),
      group = array(0, dim = df$sampSizePerGroup * 2)
    )
```

```

data$group[1:df$sampSizePerGroup] <- 1
data$y[data$group == 1] <- data$y[data$group == 1] + df$effectSize
tt <- t.test(y ~ group, data = data)
p[s] <- tt$p.value
}
return(data.frame(power = mean(p < df$alpha)))
}

# run the simulation
powerSimResults <- powerDf %>%
  do(runPowerSim(.))

```



```

\begin{figure}
\caption{Results from power simulation, showing power as a function of sample size, with effect sizes shown as different colors, and alpha shown as line type. The standard criterion of 80% power is shown by the dotted black line.} \end{figure}

```

This simulation shows us that even with a sample size of 96, we will have relatively little power to find a small effect ( $d = 0.2$ ) with  $\alpha = 0.005$ . This means that a study designed to do this would be *futile* – that is, it is almost guaranteed to find nothing even if a true effect of that size exists.

There are at least two important reasons to care about statistical power, one of which we discuss here and the other of which we will return to in Chapter ?? . If you are a researcher, you probably don't want to spend your time doing futile experiments. Running an underpowered study is essentially futile, because it means that there is a very low likelihood that one will find an effect, even if it exists.

### 11.3.1 Power analysis

Fortunately, there are tools available that allow us to determine the statistical power of an experiment. The most common use of these tools is in planning an experiment, when we would like to determine how large our sample needs to be in order to have sufficient power to find our effect of interest.

Let's say that we are interested in running a study of how a particular personality trait differs between users of iOS versus Android devices. Our plan is collect two groups of individuals and measure them on the personality trait, and then compare the two groups using a t-test. In order to determine the necessary sample size, we can use the `pwr.t.test()` function from the `pwr` library.

```
# power analysis for Cohen's d = 0.5, for 80% power with alpha = 0.05
pwr.t.test(d = 0.5, power = 0.8, sig.level = 0.05)
```

```
##
##      Two-sample t test power calculation
##
##              n = 64
##              d = 0.5
##      sig.level = 0.05
##              power = 0.8
##      alternative = two.sided
##
## NOTE: n is number in each group
```

This tells us that we would need at least 64 subjects in each group in order to have sufficient power to find a medium-sized effect. It's always important to run a power analysis before one starts a new study, to make sure that the study won't be futile due to a sample that is too small.

It might have occurred to you that if the effect size is large enough, then the necessary sample will be very small. For example, if we run the same power analysis with an effect size of  $d=3$ , then we will see that we only need about 3 subjects in each group to have sufficient power to find the difference.

```
##
##      Two-sample t test power calculation
##
##              n = 3.1
##              d = 3
##      sig.level = 0.05
##              power = 0.8
##      alternative = two.sided
##
## NOTE: n is number in each group
```

However, it's rare in science to be doing an experiment where we expect to find such a large effect – just as we don't need statistics to tell us that 16-year-olds are taller than 6-year-olds. When we run a power analysis, we need to specify an effect size that is plausible for our study, which would usually come from previous research. However, in Chapter ?? we will discuss a phenomenon known as the “winner's curse” that likely results in published effect sizes being larger than the true effect size, so this should also be kept in mind.

## 11.4 Suggested readings

- Robust misinterpretation of confidence intervals, by Hoekstra et al.



# Chapter 12

## Bayesian statistics

In this chapter we will take up the approach to statistical modeling and inference that stands in contrast to the null hypothesis testing framework that you encountered in Chapter 10. This is known as “Bayesian statistics” after the Reverend Thomas Bayes, whose theorem you have already encountered in Chapter 3. In this chapter you will learn how Bayes’ theorem provides a way of understanding data that solves many of the conceptual problems that we discussed regarding null hypothesis testing.

### 12.1 Generative models

Say you are walking down the street and a friend of yours walks right by but doesn’t say hello. You would probably try to decide why this happened – Did they not see you? Are they mad at you? Are you suddenly cloaked in a magic invisibility shield? One of the basic ideas behind Bayesian statistics is that we want to infer the details of how the data are being generated, based on the data themselves. In this case, you want to use the data (i.e. the fact that your friend did not say hello) to infer the process that generated the data (e.g. whether or not they actually saw you, how they feel about you, etc).

The idea behind a generative model is that we observe data that are generated by a *latent* (unseen) process, usually with some amount of randomness in the process. In fact, when we take a sample of data from a population and estimate a parameter from the sample, what we are doing in essence is trying to learn the value of a latent variable (the population mean) that gives rise through sampling to the observed data (the sample mean).

If we know the value of the latent variable, then it’s easy to reconstruct what the observed data should look like. For example, let’s say that we are flipping a coin that we know to be fair. We can describe the coin by a binomial distribution with a value of  $p=0.5$ , and then we could generate random samples from such a distribution in order to see what the observed data should look like. However, in general we are in the opposite situation: We don’t know the value of the latent variable of interest, but we have some data that we would like to use to estimate it.

### 12.2 Bayes’ theorem and inverse inference

The reason that Bayesian statistics has its name is because it takes advantage of Bayes’ theorem to make inferences from data back to some features of the (latent) model that generated the data. Let’s say that we want to know whether a coin is fair. To test this, we flip the coin 10 times and come up with 7 heads. Before this test we were pretty sure that the coin was fair (i.e., that  $p_{heads} = 0.5$ ), but these data certainly give us pause. We already know how to compute the conditional probability that we would flip 7 or more heads out of 10 if the coin is really fair ( $P(n \geq 7 | p_{heads} = 0.5)$ ), using the binomial distribution:

```
# compute the conditional probability of 7 or more heads when p(heads)=0.5
sprintf(
  "p(7 or more heads | p(heads) = 0.5) = %.3f",
  pbinom(7, 10, .5, lower.tail = FALSE)
)
```

```
## [1] "p(7 or more heads | p(heads) = 0.5) = 0.055"
```

That is an fairly small number, but this number doesn't really answer the question that we are asking – it is telling us about the likelihood of 7 or more heads given some particular probability of heads, whereas what we really want to know is the probability of heads. This should sound familiar, as it's exactly the situation that we were in with null hypothesis testing, which told us about the likelihood of data rather than the likelihood of hypotheses.

Remember that Bayes' theorem provides us with the tool that we need to invert a conditional probability:

$$P(H|D) = \frac{P(D|H) * P(H)}{P(D)}$$

We can think of this theorem as having four parts:

- prior ( $P(H)$ ): Our degree of belief about hypothesis H before seeing the data D
- likelihood ( $P(D|H)$ ): How likely are the observed data D under hypothesis H?
- marginal likelihood ( $P(D)$ ): How likely are the observed data, combining over all possible hypotheses?
- posterior ( $P(H|D)$ ): Our updated belief about hypothesis H, given the data D

Here we see one of the primary differences between frequentist and Bayesian statistics. Frequentists do not believe in the idea of a probability of a hypothesis (i.e., our degree of belief about a hypothesis) – for them, a hypothesis is either true or it isn't. Another way to say this is that for the frequentist, the hypothesis is fixed and the data are random, which is why frequentist inference focuses on describing the probability of data given a hypothesis (i.e. the p-value). Bayesians, on the other hand, are comfortable making probability statements about both data and hypotheses.

## 12.3 Doing Bayesian estimation

We ultimately want to use Bayesian statistics to test hypotheses, but before we do that we need to estimate the parameters that are necessary to test the hypothesis. Here we will walk through the process of Bayesian estimation. Let's use another screening example: Airport security screening. If you fly a lot like I do, it's just a matter of time until one of the random explosive screenings comes back positive; I had the particularly unfortunate experience of this happening soon after September 11, 2001, when airport security staff were especially on edge.

What the security staff want to know is what is the likelihood that a person is carrying an explosive, given that the machine has given a positive test. Let's walk through how to calculate this value using Bayesian analysis.

### 12.3.1 Specifying the prior

To use Bayes' theorem, we first need to specify the prior probability for the hypothesis. In this case, we don't know the real number but we can assume that it's quite small – for this example, let's say that one out of every 5 million travelers is expected to have an explosive device.

```
prior <- 1/5000000
```



### 12.3.2 Collect some data

The data are composed of the results of the explosive screening test. Let's say that the security staff runs the bag through their testing apparatus 10 times, and it gives a positive reading on 9 of the 10 tests.

```
nTests <- 10
nPositives <- 9
```

### 12.3.3 Computing the likelihood

We want to compute the likelihood of the data under the hypothesis that there is an explosive in the bag. Let's say that we know that the sensitivity of the test is 0.99 – that is, when a device is present, it will detect it 99% of the time. To determine the likelihood of our data under the hypothesis that a device is present, we can treat each test as a Bernoulli trial (that is, a trial with an outcome of true or false) with a probability of success of 0.99, which we can model using a binomial distribution.

```
likelihood <- dbinom(nPositives, nTests, 0.99)
likelihood
```

```
## [1] 0.091
```

### 12.3.4 Computing the marginal likelihood

We also need to know the overall likelihood of the data – that is, finding 9 positives out of 10 tests. Computing the marginal likelihood is often one of the most difficult aspects of Bayesian analysis, but for our example it's simple because we can take advantage of the specific form of Bayes' theorem that we introduced in Section 3.7:

$$P(B|A) = \frac{P(A|B) * P(B)}{P(A|B) * P(B) + P(A|\neg B) * P(\neg B)}$$

The marginal likelihood in this case is a weighted average of the likelihood of the data under either presence or absence of the explosive, multiplied by the probability of the explosive being present (i.e. the prior). In this case, let's say that we know that the specificity of the test is 0.9, such that the likelihood of a positive result when there is no explosive is 0.1.

We can compute this in R as follows:

```
marginal_likelihood <-
  dbinom(
    x = nPositives,
    size = nTests,
    prob = 0.99
  ) * prior +
  dbinom(
    x = nPositives,
    size = nTests,
    prob = .1
  ) *
  (1 - prior)

sprintf("marginal likelihood = %.3e", marginal_likelihood)
```

```
## [1] "marginal likelihood = 2.727e-08"
```

### 12.3.5 Computing the posterior

We now have all of the parts that we need to compute the posterior probability of an explosive being present, given the observed 9 positive outcomes out of 10 tests.

```
posterior <- (likelihood * prior) / marginal_likelihood
posterior
```

```
## [1] 0.67
```

This result shows us that the probability of an explosive in the bag is much higher than the prior, but nowhere near certainty, again highlighting the fact that testing for rare events is almost always liable to produce high numbers of false positives.

## 12.4 Estimating posterior distributions

In the previous example there were only two possible outcomes – the explosive is either there or it’s not – and we wanted to know which outcome was most likely given the data. However, in other cases we want to use Bayesian estimation to estimate the numeric value of a parameter. Let’s say that we want to know about the effectiveness of a new drug for pain; to test this, we can administer the drug to a group of patients and then ask them whether their pain improved or not after taking the drug. We can use Bayesian analysis to estimate the proportion of people for whom the drug will be effective using these data.

### 12.4.1 Specifying the prior

In this case, we don’t have any prior information about the effectiveness of the drug, so we will use a *uniform distribution* as our prior, since all values are equally likely under a uniform distribution. In order to simplify the example, we will only look at a subset of 99 possible values of effectiveness (from .01 to .99, in steps of .01). Therefore, each possible value has a prior probability of 1/99.

### 12.4.2 Collect some data

We need some data in order to estimate the effect of the drug. Let’s say that we administer the drug to 100 individuals, and get the following results:

```
# create a table with results
nResponders <- 64
nTested <- 100

drugDf <- tibble(
  outcome = c("improved", "not improved"),
  number = c(nResponders, nTested - nResponders)
)
pander(drugDf)
```

| outcome      | number |
|--------------|--------|
| improved     | 64     |
| not improved | 36     |

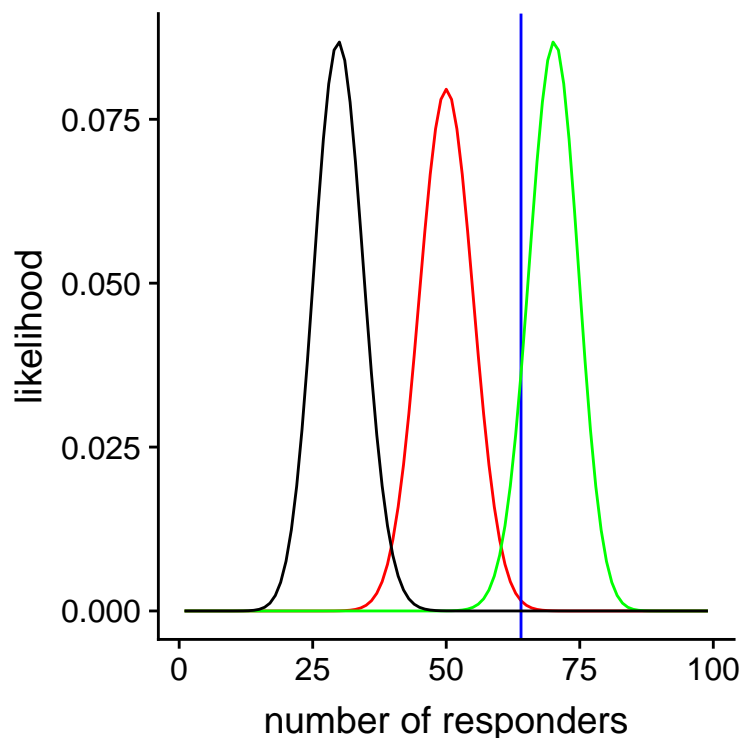


Figure 12.1: Likelihood of each possible number of responders under several different hypotheses ( $p(\text{respond})=0.5$  (red),  $0.7$  (green),  $0.3$  (black). Observed value shown in blue.

### 12.4.3 Computing the likelihood

We can compute the likelihood of the data under any particular value of the effectiveness parameter using the `dbinom()` function in R. In Figure 12.1 you can see the likelihood curves over numbers of responders for several different values of  $p_{\text{respond}}$ . Looking at this, it seems that our observed data are relatively more likely under the hypothesis of  $p_{\text{respond}} = 0.7$ , somewhat less likely under the hypothesis of  $p_{\text{respond}} = 0.5$ , and quite unlikely under the hypothesis of  $p_{\text{respond}} = 0.3$ . One of the fundamental ideas of Bayesian inference is that we will try to find the value of our parameter of interest that makes the data most likely, while also taking into account our prior knowledge.

### 12.4.4 Computing the marginal likelihood

In addition to the likelihood of the data under different hypotheses, we need to know the overall likelihood of the data, combining across all hypotheses (i.e., the marginal likelihood). This marginal likelihood is primarily important because it helps to ensure that the posterior values are true probabilities. In this case, our use of a set of discrete possible parameter values makes it easy to compute the marginal likelihood, because we can just compute the likelihood of each parameter value under each hypothesis and add them up.

```
# compute marginal likelihood
likeDf <-
  likeDf %>%
  mutate(uniform_prior = array(1 / n()))

# multiply each likelihood by prior and add them up
marginal_likelihood <-
  sum(
```

```

dbinom(
  x = nResponders, # the number who responded to the drug
  size = 100, # the number tested
  likeDf$presp # the likelihood of each response
) * likeDf$uniform_prior
)

sprintf("marginal likelihood = %0.4f", marginal_likelihood)

## [1] "marginal likelihood = 0.0100"

```

### 12.4.5 Computing the posterior

We now have all of the parts that we need to compute the posterior probability distribution across all possible values of  $p_{respond}$ , as shown in Figure 12.2.

```

# Create data for use in figure
bayesDf <-
  tibble(
    steps = seq(from = 0.01, to = 0.99, by = 0.01)
  ) %>%
  mutate(
    likelihoods = dbinom(
      x = nResponders,
      size = 100,
      prob = steps
    ),
    priors = dunif(steps) / length(steps),
    posteriors = (likelihoods * priors) / marginal_likelihood
  )

```

### 12.4.6 Maximum a posteriori (MAP) estimation

Given our data we would like to obtain an estimate of  $p_{respond}$  for our sample. One way to do this is to find the value of  $p_{respond}$  for which the posterior probability is the highest, which we refer to as the *maximum a posteriori* (MAP) estimate. We can find this from the data in 12.2:

```

# compute MAP estimate
MAP_estimate <-
  bayesDf %>%
  arrange(desc(posteriors)) %>%
  slice(1) %>%
  pull(steps)

sprintf("MAP estimate = %0.4f", MAP_estimate)

## [1] "MAP estimate = 0.6400"

```

Note that this is simply the proportion of responders from our sample – this occurs because the prior was uniform and thus didn't bias our response.

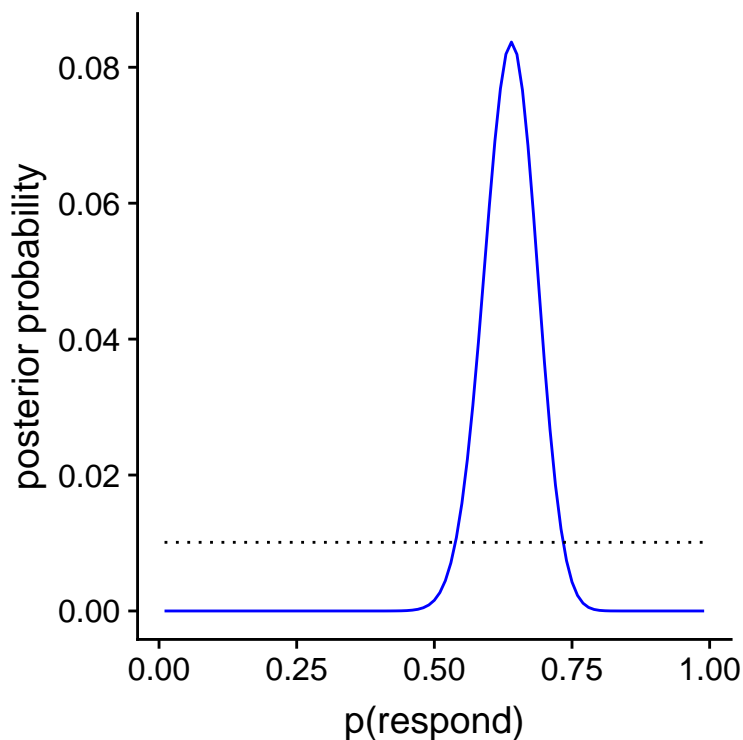


Figure 12.2: Posterior probability distribution plotted in blue against uniform prior distribution (dotted black line).

### 12.4.7 Credible intervals

Often we would like to know not just a single estimate for the posterior, but an interval in which we are confident that the posterior falls. We previously discussed the concept of confidence intervals in the context of frequentist inference, and you may remember that the interpretation of confidence intervals was particularly convoluted. What we really want is an interval in which we are confident that the true parameter falls, and Bayesian statistics can give us such an interval, which we call a *credible interval*.

In some cases the credible interval can be computed *numerically* based on a known distribution, but it's more common to generate a credible interval by sampling from the posterior distribution and then to compute quantiles of the samples. This is particularly useful when we don't have an easy way to express the posterior distribution numerically, which is often the case in real Bayesian data analysis.

We will generate samples from our posterior distribution using a simple algorithm known as *rejection sampling*. The idea is that we choose a random value of  $x$  (in this case  $p_{\text{respond}}$ ) and a random value of  $y$  (in this case, the posterior probability of  $p_{\text{respond}}$ ) each from a uniform distribution. We then only accept the sample if  $y < f(x)$  - in this case, if the randomly selected value of  $y$  is less than the actual posterior probability of  $y$ . Figure 12.4.7 shows an example of a histogram of samples using rejection sampling, along with the 95% credible intervals obtained using this method.

```
# Compute credible intervals for example

nsamples <- 100000

# create random uniform variates for x and y
x <- runif(nsamples)
y <- runif(nsamples)
```

```

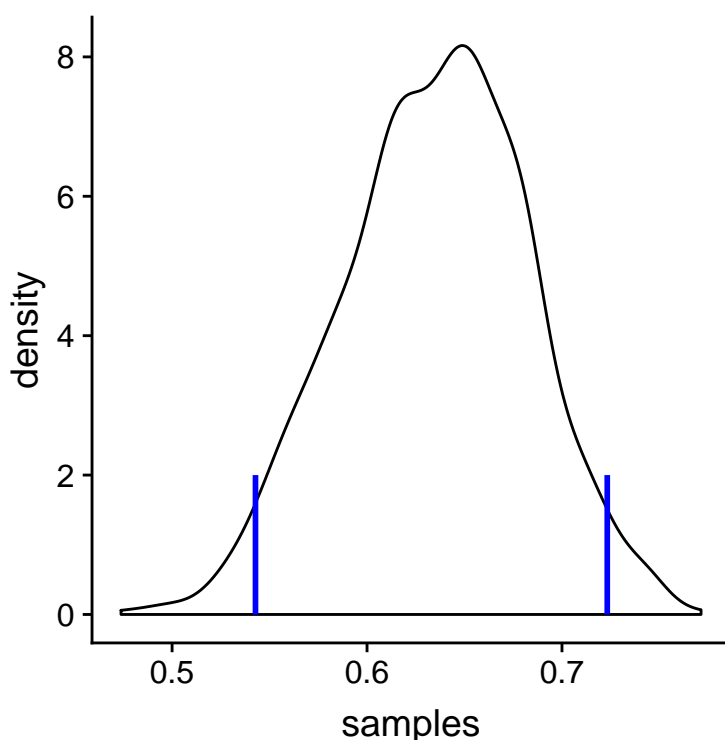
# create f(x)
fx <- dbinom(x = nResponders, size = 100, prob = x)

# accept samples where y < f(x)
accept <- which(y < fx)
accepted_samples <- x[accept]

credible_interval <- quantile(x = accepted_samples, probs = c(0.025, 0.975))
pander(credible_interval)

```

| 2.5% | 98%  |
|------|------|
| 0.54 | 0.72 |



\begin{figure} \caption{Rejection sampling example. The black line shows the density of all possible values of  $p(\text{respond})$ ; the blue lines show the 2.5th and 97.5th percentiles of the distribution, which represent the 95% credible interval for the estimate of  $p(\text{respond})$ .} \end{figure}

The interpretation of this credible interval is much closer to what we had hoped we could get from a confidence interval (but could not): It tells us that there is a 95% probability that the value of  $p_{\text{respond}}$  falls between these two values. Importantly, it shows that we have high confidence that  $p_{\text{respond}} > 0.0$ , meaning that the drug seems to have a positive effect.

### 12.4.8 Effects of different priors

In the previous example we used a *flat prior*, meaning that we didn't have any reason to believe that any particular value of  $p_{\text{respond}}$  was more or less likely. However, let's say that we had instead started with some previous data: In a previous study, researchers had tested 20 people and found that 10 of them had responded positively. This would have lead us to start with a prior belief that the treatment has an effect in 50% of

people. We can do the same computation as above, but using the information from our previous study to inform our prior (see Figure 12.3).

*# compute likelihoods for data under all values of  $p(\text{heads})$  using a flat or empirical prior. here we u*

```
df <-
  tibble(
    steps = seq(from = 0.01, to = 0.99, by = 0.01)
  ) %>%
  mutate(
    likelihoods = dbinom(nResponders, 100, steps),
    priors_flat = dunif(steps) / sum(dunif(steps)),
    priors_empirical = dbinom(10, 20, steps) / sum(dbinom(10, 20, steps))
  )

marginal_likelihood_flat <-
  sum(dbinom(nResponders, 100, df$steps) * df$priors_flat)

marginal_likelihood_empirical <-
  sum(dbinom(nResponders, 100, df$steps) * df$priors_empirical)

df <-
  df %>%
  mutate(
    posteriors_flat =
      (likelihoods * priors_flat) / marginal_likelihood_flat,
    posteriors_empirical =
      (likelihoods * priors_empirical) / marginal_likelihood_empirical
  )
```

Note that the likelihood and marginal likelihood did not change - only the prior changed. The effect of the change in prior to was to pull the posterior closer to the mass of the new prior, which is centered at 0.5.

Now let's see what happens if we come to the analysis with an even stronger prior belief. Let's say that instead of having previously observed 10 responders out of 20 people, the prior study had instead tested 500 people and found 250 responders. This should in principle give us a much stronger prior, and as we see in Figure 12.4, that's what happens: The prior is much more concentrated around 0.5, and the posterior is also much closer to the prior. The general idea is that Bayesian inference combines the information from the prior and the likelihood, weighting the relative strength of each.

*# compute likelihoods for data under all values of  $p(\text{heads})$  using strong prior.*

```
df <-
  df %>%
  mutate(
    priors_strong = dbinom(250, 500, steps) / sum(dbinom(250, 500, steps))
  )

marginal_likelihood_strong <-
  sum(dbinom(nResponders, 100, df$steps) * df$priors_strong)

df <-
  df %>%
  mutate(
    posteriors_strongprior = (likelihoods * priors_strong) / marginal_likelihood_strong
  )
```

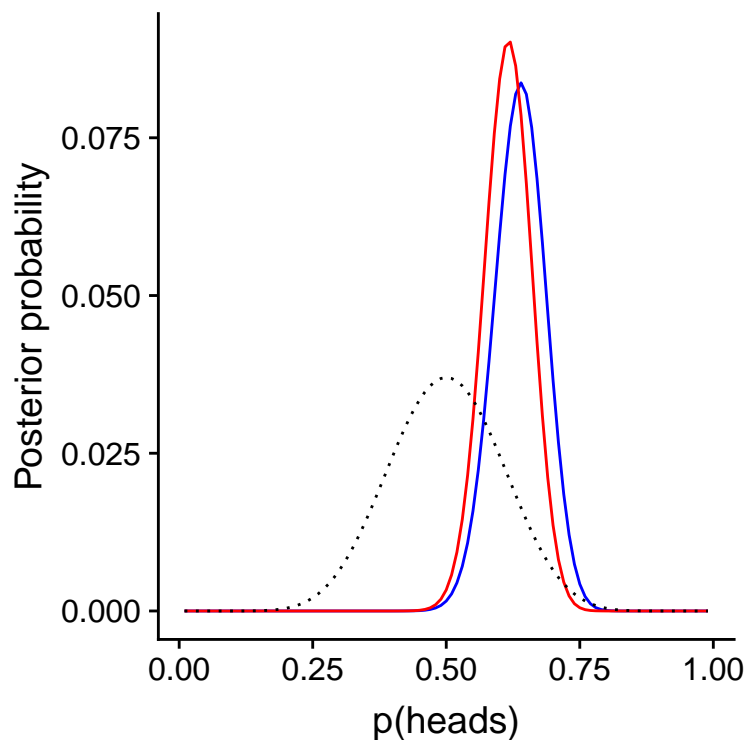


Figure 12.3: Effects of priors on the posterior distribution. The original posterior distribution based on a flat prior is plotted in blue. The prior based on the observation of 10 responders out of 20 people is plotted in the dotted black line, and the posterior using this prior is plotted in red.

This example also highlights the sequential nature of Bayesian analysis – the posterior from one analysis can become the prior for the next analysis.

Finally, it is important to realize that if the priors are strong enough, they can completely overwhelm the data. Let's say that you have an absolute prior that  $p_{respond}$  is 0.8 or greater, such that you set the prior likelihood of all other values to zero. What happens if we then compute the posterior?

```
# compute likelihoods for data under all values of p(respond) using absolute prior.
df <-
  df %>%
  mutate(
    priors_absolute = array(data = 0, dim = length(steps)),
    priors_absolute = if_else(
      steps >= 0.8,
      1, priors_absolute
    ),
    priors_absolute = priors_absolute / sum(priors_absolute)
  )

marginal_likelihood_absolute <-
  sum(dbinom(nResponders, 100, df$steps) * df$priors_absolute)

df <-
  df %>%
  mutate(
    posteriors_absolute =
```



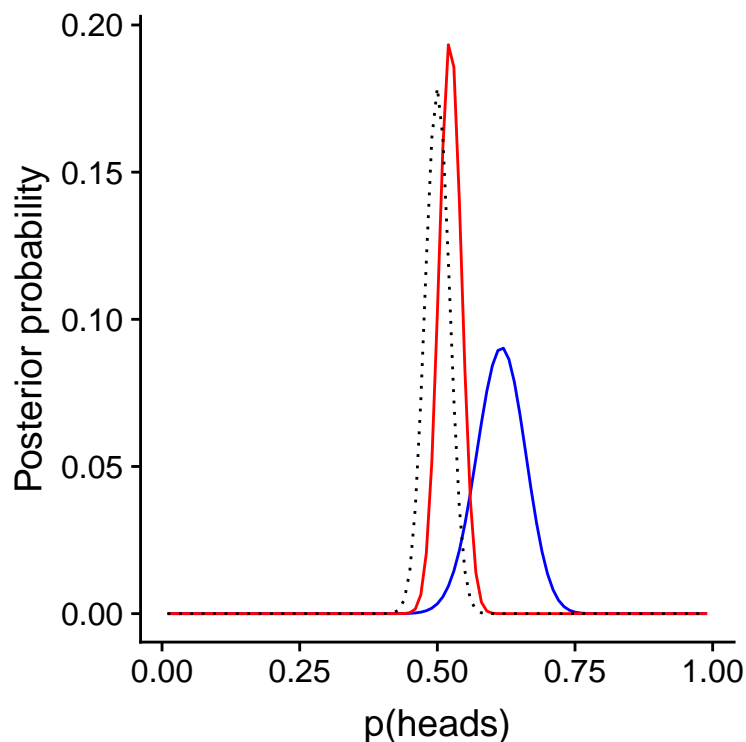


Figure 12.4: Effects of the strength of the prior on the posterior distribution. The blue line shows the posterior obtained using the prior based on 50 heads out of 100 people. The dotted black line shows the prior based on 550 heads out of 500 flips, and the red line shows the posterior based on that prior.

```
(likelihoods * priors_absolute) / marginal_likelihood_absolute
)
```

In Figure 12.5 we see that there is zero density in the posterior for any of the values where the prior was set to zero - the data are overwhelmed by the absolute prior.

## 12.5 Choosing a prior

The impact of priors on the resulting inferences are the most controversial aspect of Bayesian statistics. There are various ways to choose one's priors, which (as we saw above) can impact the resulting inferences. *Uninformative priors* attempt to bias the resulting posterior as little as possible, as we saw in the example of the uniform prior above. It's also common to use *weakly informative priors* (or *default priors*), which bias the result only very slightly. For example, if we had used a binomial distribution based on one heads out of two coin flips, the prior would have been centered around 0.5 but fairly flat, biasing the posterior only slightly.

It is also possible to use priors based on the scientific literature or pre-existing data, which we would call *empirical priors*. In general, however, we will stick to the use of uninformative/weakly informative priors, since they raise the least concern about biasing our results. In general it is a good idea to try any Bayesian analysis using multiple reasonable priors, and make sure that the results don't change in an important way based on the prior.

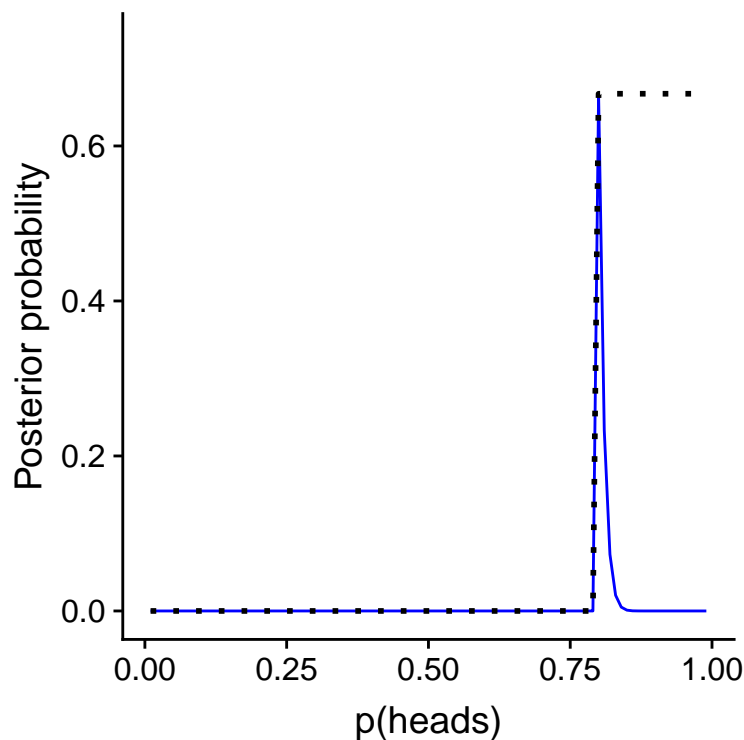


Figure 12.5: Effects of the strength of the prior on the posterior distribution. The blue line shows the posterior obtained using the prior based on 50 responders out of 100 people, using an absolute prior which states that  $p(\text{respond})$  is 0.8 or greater. The prior is shown in the dotted red line.

## 12.6 Bayesian hypothesis testing

Having learned how to perform Bayesian estimation, we now turn to the use of Bayesian methods for hypothesis testing. Let's say that there are two politicians who differ in their beliefs about whether the public supports the death penalty. Senator Smith thinks that only 40% of people support the death penalty, whereas Senator Jones thinks that 60% of people support the death penalty. They arrange to have a poll done to test this, which asks 1000 randomly selected people whether they support the death penalty. The results are that 490 of the people in the polled sample support the death penalty. Based on these data, we would like to know: Do the data support the claims of one senator over the other? We can test this using a concept known as the Bayes factor.

### 12.6.1 Bayes factors

The Bayes factor characterizes the relative likelihood of the data under two different hypotheses. It is defined as:

$$BF = \frac{p(\text{data}|H_1)}{p(\text{data}|H_2)}$$

for two hypotheses  $H_1$  and  $H_2$ . In the case of our two senators, we know how to compute the likelihood of the data under each hypothesis using the binomial distribution. We will put Senator Smith in the numerator and Senator Jones in the denominator, so that a value greater than one will reflect greater evidence for Senator Smith, and a value less than one will reflect greater evidence for Senator Jones.

```
# compute Bayes factor for Smith vs. Jones
```

```
bf <-
  dbinom(
    x = 490,
    size = 1000,
    prob = 0.4 #Smith's hypothesis
  ) / dbinom(
    x = 490,
    size = 1000,
    prob = 0.6 #Jones' hypothesis
  )

sprintf("Bayes factor = %0.2f", bf)
```

```
## [1] "Bayes factor = 3325.26"
```

This number provides a measure of the evidence that the data provides regarding the two hypotheses - in this case, it tells us the data support Senator Smith more than 3000 times more strongly than they support Senator Jones.

## 12.6.2 Bayes factors for statistical hypotheses

In the previous example we had specific predictions from each senator, whose likelihood we could quantify using the binomial distribution. However, in real data analysis we generally must deal with uncertainty about our parameters, which complicates the Bayes factor. However, in exchange we gain the ability to quantify the relative amount of evidence in favor of the null versus alternative hypotheses.

Let's say that we are a medical researcher performing a clinical trial for the treatment of diabetes, and we wish to know whether a particular drug reduces blood glucose compared to placebo. We recruit a set of volunteers and randomly assign them to either drug or placebo group, and we measure the change in hemoglobin A1C (a marker for blood glucose levels) in each group over the period in which the drug or placebo was administered. What we want to know is: Is there a difference between the drug and placebo?

First, let's generate some data and analyze them using null hypothesis testing (see Figure 12.6).

```
# create simulated data for drug trial example
```

```
set.seed(123456)
nsubs <- 40
effect_size <- 0.1

# randomize individuals to drug (1) or placebo (0)
drugDf <-
  tibble(
    group = as.integer(runif(nsubs) > 0.5)
  ) %>%
  mutate(
    hbchange = rnorm(nsubs) - group * effect_size
  )
```

Let's perform an independent-samples t-test, which shows that there is a significant difference between the groups:

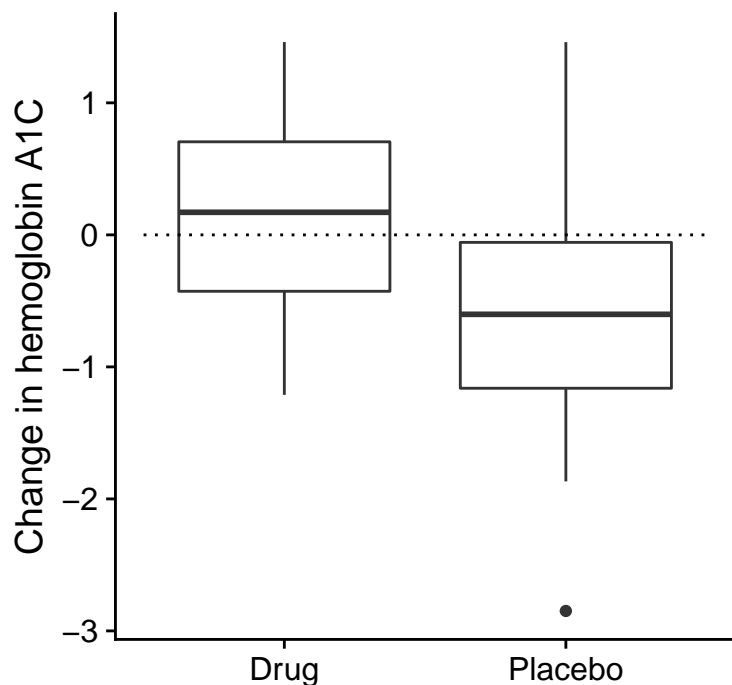


Figure 12.6: Box plots showing data for drug and placebo groups.

```
# compute t-test for drug example
drugTT <- t.test(hbchange ~ group, alternative = "greater", data = drugDf)
print(drugTT)
```

```
##
## Welch Two Sample t-test
##
## data: hbchange by group
## t = 2, df = 40, p-value = 0.03
## alternative hypothesis: true difference in means is greater than 0
## 95 percent confidence interval:
##  0.096      Inf
## sample estimates:
## mean in group 0 mean in group 1
##      0.12      -0.48
```

This test tells us that there is a significant difference between the groups, but it doesn't quantify how strongly the evidence supports the null versus alternative hypotheses. To measure that, we can compute a Bayes factor using `ttestBF` function from the `BayesFactor` package in R:

```
# compute Bayes factor for drug data
bf_drug <- ttestBF(
  formula = hbchange ~ group, data = drugDf,
  nullInterval = c(0, Inf)
)

bf_drug
```

```
## Bayes factor analysis
## -----
```

```
## [1] Alt., r=0.707 0<d<Inf      : 2.4  ±0%
## [2] Alt., r=0.707 !(0<d<Inf) : 0.12 ±0%
##
## Against denominator:
##   Null, mu1-mu2 = 0
## ---
## Bayes factor type: BFindepSample, JZS
```

The Bayes factor here tells us that the alternative hypothesis (i.e. that the difference is greater than zero) is about 2.4 times more likely than the null hypothesis given the data. This doesn't seem that strong, but how can we determine that? There is a general guideline for interpretation of Bayes factors suggested by Kass & Raftery (1995):

| BF        | Strength of evidence               |
|-----------|------------------------------------|
| 1 to 3    | not worth more than a bare mention |
| 3 to 20   | positive                           |
| 20 to 150 | strong                             |
| >150      | very strong                        |

Based on this, even though the statistical result is significant, the amount of evidence in favor of the alternative vs. the null hypothesis is weak enough that it's not worth even mentioning.

Because the Bayes factor is comparing evidence for two hypotheses, it also allows us to assess whether there is evidence in favor of the null hypothesis, which we couldn't do with standard null hypothesis testing (because it starts with the assumption that the null is true). This can be very useful for determining whether a non-significant result really provides strong evidence that there is no effect, or instead just reflects weak evidence overall.

## 12.7 Suggested readings

- *The Theory That Would Not Die: How Bayes' Rule Cracked the Enigma Code, Hunted Down Russian Submarines, and Emerged Triumphant from Two Centuries of Controversy*, by Sharon Bertsch McGrayne
- *Doing Bayesian Data Analysis: A Tutorial Introduction with R*, by John K. Kruschke



## Chapter 13

# Modeling categorical relationships

So far we have discussed the general concept of statistical modeling and hypothesis testing, and applied them to some simple analyses. In this chapter we will focus on the modeling of *categorical* relationships, by which we mean relationships between variables that are measured on a nominal (and sometimes ordinal) scale. These data are usually expressed in terms of counts; that is, for each value of the variable (or combination of values of multiple variables), how many observations take that value? For example, when we count how many people from each major are in our class, we are fitting a categorical model to the data.

### 13.1 Example: Candy colors

Let's say that I have purchased a bag of 100 candies, which are labeled as having 1/3 chocolates, 1/3 licorices, and 1/3 gumballs. When I count the candies in the bag, we get the following numbers:

```
candyDf <-  
  tibble(  
    candyType = c("chocolate", "licorice", "gumball"),  
    count = c(30, 33, 37)  
  )  
pander(candyDf)
```

| candyType | count |
|-----------|-------|
| chocolate | 30    |
| licorice  | 33    |
| gumball   | 37    |

Because I like chocolate much more than licorice or gumballs, I feel slightly ripped off. What I would like to know is: What is the likelihood that the count would come out this way if the true probability of each candy type is the averaged proportion of 1/3 each?

### 13.2 Pearson's chi-squared test

The Pearson chi-squared test provides us with a way to test whether observed count data differs from some specific expected values that define the null hypothesis:

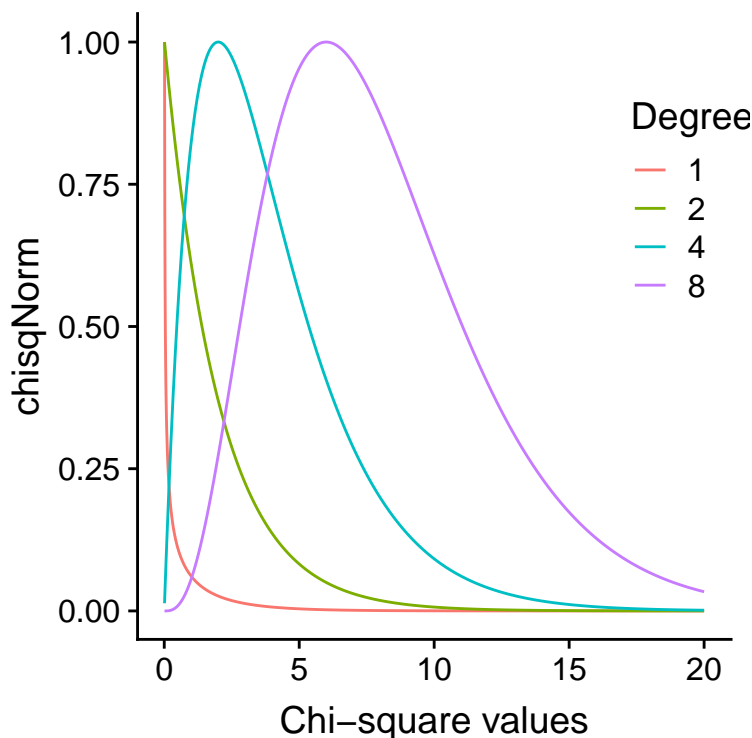


Figure 13.1: Examples of the chi-squared distribution for various degrees of freedom.

$$\chi^2 = \sum_i \frac{(\text{observed}_i - \text{expected}_i)^2}{\text{expected}_i}$$

In the case of our candy example, the null hypothesis is that the proportion of each type of candies is equal. We can compute the chi-squared statistic for our observed counts of candy as follows:

```
# compute chi-squared statistic

nullExpectation <- c(1 / 3, 1 / 3, 1 / 3) * sum(candyDf$count)

chisqVal <-
  sum(
    ((candyDf$count - nullExpectation)**2) / nullExpectation
  )
```

The chi-squared statistic for this analysis comes out to 0.74, which on its own is not interpretable, since it depends on the number of different values that were added together. However, we can take advantage of the fact that the chi-squared statistic is distributed according to a specific distribution under the null hypothesis, which is known as the *chi-squared* distribution. This distribution is defined as the sum of squares of a set of standard normal random variables; it has a number of degrees of freedom that is equal to the number of variables being added together. The shape of the distribution depends on the number of degrees of freedom. Figure 13.1 shows examples of the distribution for several different degrees of freedom.

Let's verify that the chi-squared distribution accurately describes the sum of squares of a set of standard normal random variables, using simulation.

```
# simulate 50,000 sums of 8 standard normal random variables and compare
# to theoretical chi-squared distribution
```



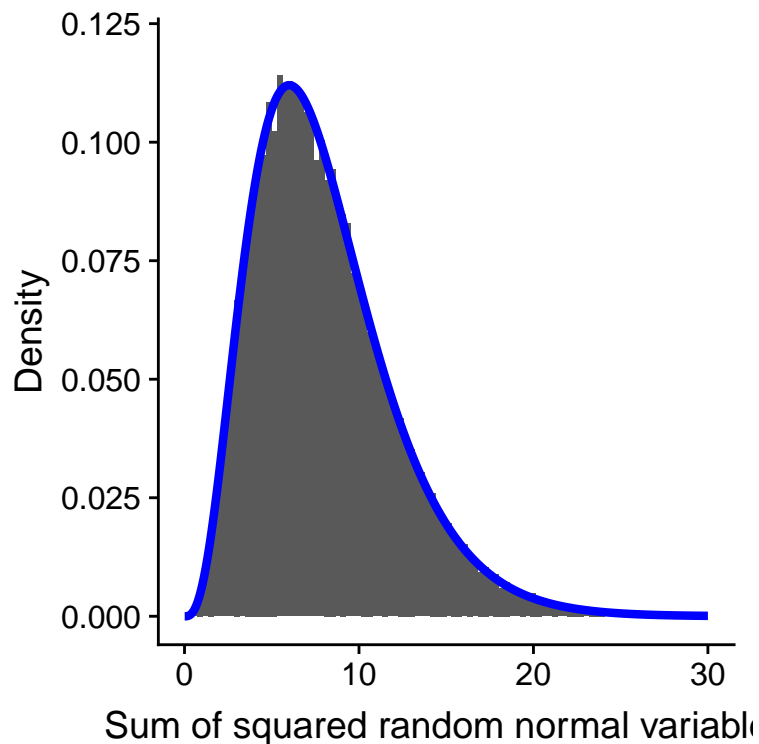


Figure 13.2: Simulation of sum of squared random normal variables. The histogram is based on the sum of squares of 50,000 sets of 8 random normal variables; the blue line shows the values of the theoretical chi-squared distribution with 8 degrees of freedom.

```
# create a matrix with 50k columns of 8 rows of squared normal random variables
d <- replicate(50000, rnorm(n = 8, mean = 0, sd = 1)**2)
# sum each column of 8 variables
dMean <- apply(d, 2, sum)

# create a data frame of the theoretical chi-square distribution
# with 8 degrees of freedom
csDf <-
  data.frame(x = seq(0.01, 30, 0.01)) %>%
  mutate(chisq = dchisq(x, 8))
```

Figure 13.2 shows that the theoretical distribution matches closely with the results of a simulation that repeatedly added

For the candy example, we can compute the likelihood of our observed chi-squared value of 0.74 under the null hypothesis of equal frequency across all candies. We use a chi-squared distribution with degrees of freedom equal to  $n - 1$ , since we lost one degree of freedom when we computed the mean in order to generate the expected values.

```
pval <- pchisq(chisqVal, df = 2, lower.tail = FALSE) #df = degrees of freedom
sprintf("p-value = %0.3f", pval)
```

```
## [1] "p-value = 0.691"
```

This shows that the observed counts of candies are not particularly surprising based on the proportions printed on the bag of candy, and we would not reject the null hypothesis of equal proportions.

### 13.3 Contingency tables and the two-way test

Another way that we often use the chi-squared test is to ask whether two categorical variables are related to one another. As a more realistic example, let's take the question of whether a black driver is more likely to be searched when they are pulled over by a police officer, compared to a white driver. The Stanford Open Policing Project (<https://openpolicing.stanford.edu/>) has studied this, and provides data that we can use to analyze the question. We will use the data from the State of Connecticut since they are fairly small. These data were first cleaned up to remove all unnecessary data (see `code/process_CT_data.py`).

```
# load police stop data
stopData <-
  read_csv("data/CT_data_cleaned.csv") %>%
  rename(searched = search_conducted)
```

The standard way to represent data from a categorical analysis is through a *contingency table*, which presents the number or proportion of observations falling into each possible combination of values for each of the variables.

Let's compute the contingency table for the police search data:

```
# compute and print two-way contingency table
summaryDf2way <-
  stopData %>%
  count(searched, driver_race) %>%
  arrange(driver_race, searched)

summaryContingencyTable <-
  summaryDf2way %>%
  spread(driver_race, n)

pander(summaryContingencyTable)
```

| searched | Black | White  |
|----------|-------|--------|
| FALSE    | 36244 | 239241 |
| TRUE     | 1219  | 3108   |

It can also be useful to look at the contingency table using proportions rather than raw numbers, since they are easier to compare visually.

```
# Compute and print contingency table using proportions
# rather than raw frequencies
summaryContingencyTableProportion <-
  summaryContingencyTable %>%
  mutate(
    Black = Black / nrow(stopData), #count of Black individuals searched / total searched
    White = White / nrow(stopData)
  )
pander(summaryContingencyTableProportion, round = 4)
```

| searched | Black  | White  |
|----------|--------|--------|
| FALSE    | 0.1295 | 0.855  |
| TRUE     | 0.0044 | 0.0111 |

The Pearson chi-squared test allows us to test whether observed frequencies are different from expected frequencies, so we need to determine what frequencies we would expect in each cell if searches and race were unrelated – which we can define as being *independent*. Remember from the chapter on probability that if X and Y are independent, then:

$$P(X \cap Y) = P(X) * P(Y)$$

That is, the joint probability under the null hypothesis of independence is simply the product of the *marginal* probabilities of each individual variable. The marginal probabilities are simply the probabilities of each event occurring regardless of other events. We can compute those marginal probabilities, and then multiply them together to get the expected proportions under independence.

|              | Black        | White        |         |
|--------------|--------------|--------------|---------|
| Not searched | $P(NS)*P(B)$ | $P(NS)*P(W)$ | $P(NS)$ |
| Searched     | $P(S)*P(B)$  | $P(S)*P(W)$  | $P(S)$  |
|              | $P(B)$       | $P(W)$       |         |

We can use a linear algebra trick known as the “outer product” (via the `outer()` function) to compute this easily.

```
# first, compute the marginal probabilities

# probability of being each race
summaryDfRace <-
  stopData %>%
    count(driver_race) %>% #count the number of drivers of each race
    mutate(
      prop = n / sum(n) #compute the proportion of each race out of all drivers
    )

# probability of being searched
summaryDfStop <-
  stopData %>%
    count(searched) %>% #count the number of searched vs. not searched
    mutate(
      prop = n / sum(n) # compute proportion of each outcome out all traffic stops
    )

# second, multiply outer product by n (all stops) to compute expected frequencies
expected <- outer(summaryDfRace$prop, summaryDfStop$prop) * nrow(stopData)

# create a data frame of expected frequencies for each race
expectedDf <-
  data.frame(expected, driverRace = c("Black", "White")) %>%
  rename(
    NotSearched = X1,
    Searched = X2
  )

# tidy the data frame
expectedDfTidy <-
  gather(expectedDf, searched, n, -driverRace) %>%
  arrange(driverRace, searched)
```

```
# third, add expected frequencies to the original summary table
# and fourth, compute the standardized squared difference between
# the observed and expected frequencies
```

```
summaryDf2way <-
  summaryDf2way %>%
  mutate(expected = expectedDfTidy$n)

summaryDf2way <-
  summaryDf2way %>%
  mutate(stdSqDiff = (n - expected)**2 / expected)

pander(summaryDf2way)
```

| searched | driver_race | n      | expected | stdSqDiff |
|----------|-------------|--------|----------|-----------|
| FALSE    | Black       | 36244  | 36883.67 | 11.09     |
| TRUE     | Black       | 1219   | 579.33   | 706.31    |
| FALSE    | White       | 239241 | 238601.3 | 1.71      |
| TRUE     | White       | 3108   | 3747.67  | 109.18    |

```
# finally, compute chi-squared statistic by
# summing the standarized squared differences
chisq <- sum(summaryDf2way$stdSqDiff)
sprintf("Chi-squared value = %0.2f", chisq)
```

```
## [1] "Chi-squared value = 828.30"
```

Having computed the chi-squared statistic, we now need to compare it to the chi-squared distribution in order to determine how extreme it is compared to our expectation under the null hypothesis. The degrees of freedom for this distribution are  $df = (nRows - 1) * (nColumns - 1)$  - thus, for a 2X2 table like the one here,  $df = (2 - 1) * (2 - 1) = 1$ . The intuition here is that computing the expected frequencies requires us to use three values: the total number of observations and the marginal probability for each of the two variables. Thus, once those values are computed, there is only one number that is free to vary, and thus there is one degree of freedom. Given this, we can compute the p-value for the chi-squared statistic:

```
pval <- pchisq(chisq, df = 1, lower.tail = FALSE)
sprintf("p-value = %e", pval)
```

```
## [1] "p-value = 3.795669e-182"
```

The p value of  $3.79e^{-182}$  is exceedingly small, showing that the observed data would be highly unlikely if there was truly no relationship between race and police searches, and thus we should reject the null hypothesis of independence.

We can also perform this test easily using the `chisq.test()` function in R:

```
# first need to rearrange the data into a 2x2 table
summaryDf2wayTable <-
  summaryDf2way %>%
  dplyr::select(-expected, -stdSqDiff) %>%
  spread(searched, n) %>%
  dplyr::select(-driver_race)

chisqTestResult <- chisq.test(summaryDf2wayTable, 1, correct = FALSE)
chisqTestResult
```

```
##
## Pearson's Chi-squared test
##
## data: summaryDf2wayTable
## X-squared = 800, df = 1, p-value <2e-16
```

## 13.4 Standardized residuals

When we find a significant effect with the chi-squared test, this tells us that the data are unlikely under the null hypothesis, but it doesn't tell us *how* the data differ. To get a deeper insight into how the data differ from what we would expect under the null hypothesis, we can examine the residuals from a model, which reflects the deviation of the data (i.e., the observed frequencies) from the model in each cell (i.e., the expected frequencies). Rather than looking at the raw residuals (which will vary simply depending on the number of observations in the data), it's more common to look at their *standardized residuals*, which are computed as:

$$\text{standardized residual}_{ij} = \frac{\text{observed}_{ij} - \text{expected}_{ij}}{\sqrt{\text{expected}_{ij}}}$$

where  $i$  and  $j$  are the indices for the rows and columns respectively. We can compute these for the police stop data:

```
# compute standardized residuals
summaryDf2way <-
  summaryDf2way %>%
  mutate(stdRes = (n - expected)/sqrt(expected))

pander(summaryDf2way)
```

| searched | driver_race | n      | expected | stdSqDiff | stdRes |
|----------|-------------|--------|----------|-----------|--------|
| FALSE    | Black       | 36244  | 36883.67 | 11.09     | -3.33  |
| TRUE     | Black       | 1219   | 579.33   | 706.31    | 26.58  |
| FALSE    | White       | 239241 | 238601.3 | 1.71      | 1.31   |
| TRUE     | White       | 3108   | 3747.67  | 109.18    | -10.45 |

These standardized residuals can be interpreted as Z scores – in this case, we see that the number of searches for black individuals are substantially higher than expected based on independence, and the number of searches for white individuals are substantially lower than expected. This provides us with the context that we need to interpret the significant chi-squared result.

## 13.5 Odds ratios

We can also represent the relative likelihood of different outcomes in the contingency table using the odds ratio that we introduced earlier, in order to better understand the size of the effect. First, we represent the odds of being stopped for each race:

$$\text{odds}_{\text{searched}|\text{black}} = \frac{N_{\text{searched} \cap \text{black}}}{N_{\text{not searched} \cap \text{black}}} = \frac{1219}{36244} = 0.034$$

$$\text{odds}_{\text{searched}|\text{white}} = \frac{N_{\text{searched} \cap \text{white}}}{N_{\text{not searched} \cap \text{white}}} = \frac{3108}{239241} = 0.013$$

$$\text{odds ratio} = \frac{\text{odds}_{\text{searched}|\text{black}}}{\text{odds}_{\text{searched}|\text{white}}} = 2.59$$

The odds ratio shows that the odds of being searched are 2.59 times higher for black versus white drivers, based on this dataset.

## 13.6 Bayes factor

We discussed Bayes factors in the earlier chapter on Bayesian statistics – you may remember that it represents the ratio of the likelihood of the data under each of the two hypotheses:

$$K = \frac{P(\text{data}|H_A)}{P(\text{data}|H_0)} = \frac{P(H_A|\text{data}) * P(H_A)}{P(H_0|\text{data}) * P(H_0)}$$

Bayes factors are similar to p-values and effect sizes in one way, which is that their interpretation is somewhat subjective. There are various guidelines for their interpretation – here is one from Kass and Raftery (1995) :

| BF            | Interpretation       |
|---------------|----------------------|
| 1 to 3        | barely worth mention |
| 3 to 20       | positive             |
| 20 to 150     | strong               |
| 150 and above | very strong          |

We can compute the Bayes factor for the police search data using the `contingencyTableBF()` function from the `BayesFactor` package:

```
# compute Bayes factor
# using independent multinomial sampling plan in which row totals (driver race)
# are fixed

bf <-
  contingencyTableBF(as.matrix(summaryDf2wayTable),
    sampleType = "indepMulti",
    fixedMargin = "cols"
  )
bf
```

```
## Bayes factor analysis
## -----
## [1] Non-indep. (a=1) : 1.8e+142 ±0%
##
## Against denominator:
##   Null, independence, a = 1
## ---
## Bayes factor type: BFcontingencyTable, independent multinomial
```

This shows that the evidence in favor of a relationship between driver race and police searches in this dataset is exceedingly strong.

## 13.7 Categorical analysis beyond the 2 X 2 table

Categorical analysis can also be applied to contingency tables where there are more than two categories for each variable.

For example, let's look at the NHANES data and compare the variable *Depressed* which denotes the “self-reported number of days where participant felt down, depressed or hopeless”. This variable is coded as *None*, *Several*, or *Most*. Let's test whether this variable is related to the *SleepTrouble* variable which reports whether the individual has reported sleeping problems to a doctor.

```
# summarize depression as a function of sleep trouble
```

```
depressedSleepTrouble <-
  NHANES_adult %>%
  drop_na(SleepTrouble, Depressed) %>%
  count(SleepTrouble, Depressed) %>%
  arrange(SleepTrouble, Depressed)
```

```
depressedSleepTroubleTable <-
  depressedSleepTrouble %>%
  spread(SleepTrouble, n) %>%
  rename(
    NoSleepTrouble = No,
    YesSleepTrouble = Yes
  )
```

```
pander(depressedSleepTroubleTable)
```

| Depressed | NoSleepTrouble | YesSleepTrouble |
|-----------|----------------|-----------------|
| None      | 2614           | 676             |
| Several   | 418            | 249             |
| Most      | 138            | 145             |

Simply by looking at these data, we can tell that it is likely that there is a relationship between the two variables; notably, while the total number of people with sleep trouble is much less than those without, for people who report being depressed most days the number with sleep problems is greater than those without. We can quantify this directly using the chi-squared test:

```
# need to remove the column with the label names
```

```
depressedSleepTroubleTable <-
  depressedSleepTroubleTable %>%
  dplyr::select(-Depressed)
```

```
depressedSleepChisq <- chisq.test(depressedSleepTroubleTable)
depressedSleepChisq
```

```
##
## Pearson's Chi-squared test
##
## data:  depressedSleepTroubleTable
## X-squared = 200, df = 2, p-value <2e-16
```

This test shows that there is a strong relationship between depression and sleep trouble. We can also compute the Bayes factor to quantify the strength of the evidence in favor the alternative hypothesis:

```
# compute bayes factor, using a joint multinomial sampling plan
bf <-
  contingencyTableBF(
    as.matrix(depressedSleepTroubleTable),
    sampleType = "jointMulti"
  )
bf

## Bayes factor analysis
## -----
## [1] Non-indep. (a=1) : 1.8e+35 ±0%
##
## Against denominator:
##   Null, independence, a = 1
## ---
## Bayes factor type: BFcontingencyTable, joint multinomial
```

Here see that the Bayes factor is exceedingly large, showing that the evidence in favor of a relation between depression and sleep problems is very strong.

## 13.8 Beware of Simpson's paradox

The contingency tables presented above represent summaries of large numbers of observations, but summaries can sometimes be misleading. Let's take an example from baseball. The table below shows the batting data (hits/at bats and batting average) for Derek Jeter and David Justice over the years 1995-1997:

| Player        | 1995    |             | 1996    |             | 1997    |             | Combined |             |
|---------------|---------|-------------|---------|-------------|---------|-------------|----------|-------------|
| Derek Jeter   | 12/48   | .250        | 183/582 | .314        | 190/654 | .291        | 385/1284 | <b>.300</b> |
| David Justice | 104/411 | <b>.253</b> | 45/140  | <b>.321</b> | 163/495 | <b>.329</b> | 312/1046 | .298        |

If you look closely, you will see that something odd is going on: In each individual year Justice had a higher batting average than Jeter, but when we combine the data across all three years, Jeter's average is actually higher than Justice's! This is an example of a phenomenon known as *Simpson's paradox*, in which a pattern that is present in a combined dataset may not be present in any of the subsets of the data. This occurs when there is another variable that may be changing across the different subsets – in this case, the number of at-bats varies across years, with Justice batting many more times in 1995 (when batting averages were low). We refer to this as a *lurking variable*, and it's always important to be attentive to such variables whenever one examines categorical data.



## Chapter 14

# Modeling continuous relationships

Most people are familiar with the concept of *correlation*, and in this chapter we will provide a more formal understanding for this commonly used and misunderstood concept.

### 14.1 An example: Hate crimes and income inequality

In 2017, the web site Fivethirtyeight.com published a story titled Higher Rates Of Hate Crimes Are Tied To Income Inequality which discussed the relationship between the prevalence of hate crimes and income inequality in the wake of the 2016 Presidential election. The story reported an analysis of hate crime data from the FBI and the Southern Poverty Law Center, on the basis of which they report:

“we found that income inequality was the most significant determinant of population-adjusted hate crimes and hate incidents across the United States”.

The data for this analysis are included in the `fivethirtyeight` R package, which makes it easy for us to access them. The analysis reported in the story focused on the relationship between income inequality (defined by a quantity called the *Gini index*) and the prevalence of hate crimes in each state.

#### 14.1.1 Quantifying inequality: The Gini index

Before we look at the analysis reported in the story, it's first useful to understand how the Gini index is used to quantify inequality. The Gini index is usually defined in terms of a curve that describes the relation between income and the proportion of the population that has income at or less than that level, known as a *Lorenz curve*. However, another way to think of it is more intuitive: It is the relative mean absolute difference between incomes, divided by two (from [https://en.wikipedia.org/wiki/Gini\\_coefficient](https://en.wikipedia.org/wiki/Gini_coefficient)):

$$G = \frac{\sum_{i=1}^n \sum_{j=1}^n |x_i - x_j|}{2n \sum_{i=1}^n x_i}$$

Figure 14.1 shows the Lorenz curves for several different income distributions. The top left panel (A) shows an example with 10 people where everyone has exactly the same income. The length of the intervals between points are equal, indicating each person earns an identical share of the total income in the population. The top right panel (B) shows an example where income is normally distributed. The bottom left panel shows an example with high inequality; everyone has equal income (\$40,000) except for one person, who has income

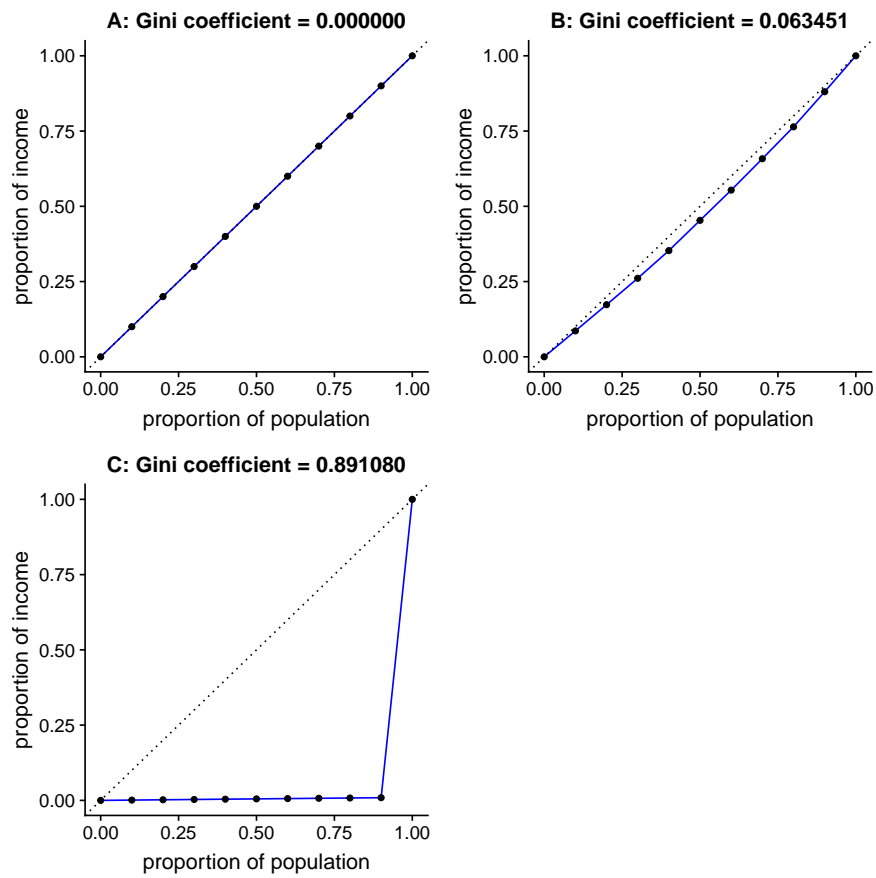


Figure 14.1: Lorenz curves for A) perfect equality, B) normally distributed income, and C) high inequality (equal income except for one very wealthy individual).



### 14.3 Covariance and correlation

One way to quantify the relationship between two variables is the *covariance*. Remember that variance for a single variable is computed as:

$$s^2 = \frac{\sum_{i=1}^n (x_i - \bar{x})^2}{N - 1}$$

This tells us how far each observation is from the mean. Covariance tells us whether there is a relation between the deviations of two different variables across observations. It is defined as:

$$covariance = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{N - 1}$$

This value will be far from zero when x and y are both highly deviant from the mean; if they are deviant in the same direction then the covariance is positive, whereas if they are deviant in opposite directions the covariance is negative. Let's look at a toy example first.

```
# create data for toy example of covariance
df <-
  tibble(x = c(3, 5, 8, 10, 12)) %>%
  mutate(y = x + round(rnorm(n = 5, mean = 0, sd = 2))) %>%
  mutate(
    y_dev = y - mean(y),
    x_dev = x - mean(x)
  ) %>%
  mutate(crossproduct = y_dev * x_dev)

pander(df)
```

| x  | y  | y_dev | x_dev | crossproduct |
|----|----|-------|-------|--------------|
| 3  | 1  | -6.6  | -4.6  | 30.36        |
| 5  | 3  | -4.6  | -2.6  | 11.96        |
| 8  | 8  | 0.4   | 0.4   | 0.16         |
| 10 | 12 | 4.4   | 2.4   | 10.56        |
| 12 | 14 | 6.4   | 4.4   | 28.16        |

```
# compute covariance

sprintf("sum of cross products = %.2f", sum(df$crossproduct))

## [1] "sum of cross products = 81.20"

covXY <- sum(df$crossproduct) / (nrow(df) - 1)
sprintf("covariance: %.2f", covXY)

## [1] "covariance: 20.30"
```

We don't usually use the covariance to describe relationships between variables, because it varies with the overall level of variance in the data. Instead, we would usually use the *correlation coefficient* (often referred to as *Pearson's correlation* after the statistician Karl Pearson). The correlation is computed by scaling the covariance by the standard deviations of the two variables:

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

```
# compute the correlation coefficient

corXY <- sum(df$crossproduct) / ((nrow(df) - 1) * sd(df$x) * sd(df$y))
sprintf("correlation coefficient = %.2f", corXY)

## [1] "correlation coefficient = 0.99"
```

We can also compute the correlation value easily using the `cor()` function in R:

```
# compute r using built-in function

c <- cor(df$x, df$y)
sprintf("correlation coefficient = %.2f", c)

## [1] "correlation coefficient = 0.99"
```

The correlation coefficient is useful because it varies between -1 and 1 regardless of the nature of the data - in fact, we already discussed the correlation coefficient earlier in the discussion of effect sizes. As we saw in the previous chapter on effect sizes, a correlation of 1 indicates a perfect linear relationship, a correlation of -1 indicates a perfect negative relationship, and a correlation of zero indicates no linear relationship.

We can compute the correlation coefficient for the hate crime data:

```
corGiniHC <-
  cor(
    hateCrimes$gini_index,
    hateCrimes$avg_hatecrimes_per_100k_fbi
  )
sprintf('correlation coefficient = %.2f', corGiniHC)

## [1] "correlation coefficient = 0.42"
```

### 14.3.1 Hypothesis testing for correlations

A correlation value of 0.42 seems to indicate a reasonably strong relationship between the two variables, but we can also imagine that this could occur by chance even if there is no relationship. We can test the null hypothesis that the correlation is zero, using a simple equation that lets us convert a correlation value into a  $t$  statistic:

$$t_r = \frac{r\sqrt{N-2}}{\sqrt{1-r^2}}$$

Under the null hypothesis  $H_0 : r = 0$ , this statistic is distributed as a  $t$  distribution with  $N - 2$  degrees of freedom. We can compute this using the `cor.test()` function in R:

```
# perform correlation test on hate crime data
cor.test(
  hateCrimes$avg_hatecrimes_per_100k_fbi,
  hateCrimes$gini_index
)

##
## Pearson's product-moment correlation
##
```

```
## data:  hateCrimes$avg_hatecrimes_per_100k_fbi and hateCrimes$gini_index
## t = 3, df = 50, p-value = 0.002
## alternative hypothesis: true correlation is not equal to 0
## 95 percent confidence interval:
##  0.16 0.63
## sample estimates:
##   cor
## 0.42
```

This test shows that the likelihood of an  $r$  value this extreme or more is quite low, so we would reject the null hypothesis of  $r = 0$ . Note that this test assumes that both variables are normally distributed.

We could also test this by randomization, in which we repeatedly shuffle the values of one of the variables and compute the correlation, and then compare our observed correlation value to this null distribution to determine how likely our observed value would be under the null hypothesis. The results are shown in Figure 14.3. The p-value computed using randomization is reasonably similar to the answer give by the t-test.

```
# compute null distribution by shuffling order of variable values

# create a function to compute the correlation on the shuffled values
shuffleCorr <- function(x, y) {
  xShuffled <- sample(x)
  return(cor(xShuffled, y))
}

# run this function 2500 times
shuffleDist <-
  replicate(
    2500,
    shuffleCorr(hateCrimes$avg_hatecrimes_per_100k_fbi, hateCrimes$gini_index)
  )
```

### 14.3.2 Robust correlations

You may have noticed something a bit odd in Figure 14.2 – one of the datapoints (the one for the District of Columbia) seemed to be quite separate from the others. We refer to this as an *outlier*, and the standard correlation coefficient is very sensitive to outliers. For example, in Figure 14.4 we can see how a single outlying data point can cause a very high positive correlation value, even when the actual relationship between the other data points is perfectly negative.

One way to address outliers is to compute the correlation on the ranks of the data after ordering them, rather than on the data themselves; this is known as *Spearman's correlation*. Whereas the Pearson correlation for the example in Figure 14.4 was 0.83, the Spearman correlation is -0.45, showing that the rank correlation reduces the effect of the outlier.

We can compute the rank correlation on the hate crime data using the `cor.test` function:

```
corTestSpearman <- cor.test(dfOutlier$x, dfOutlier$y, method = "spearman")
corTestSpearman

##
## Spearman's rank correlation rho
##
## data:  dfOutlier$x and dfOutlier$y
## S = 200, p-value = 0.2
## alternative hypothesis: true rho is not equal to 0
```

$p(\text{shuffled } r \geq \text{observed}) = 0.00$

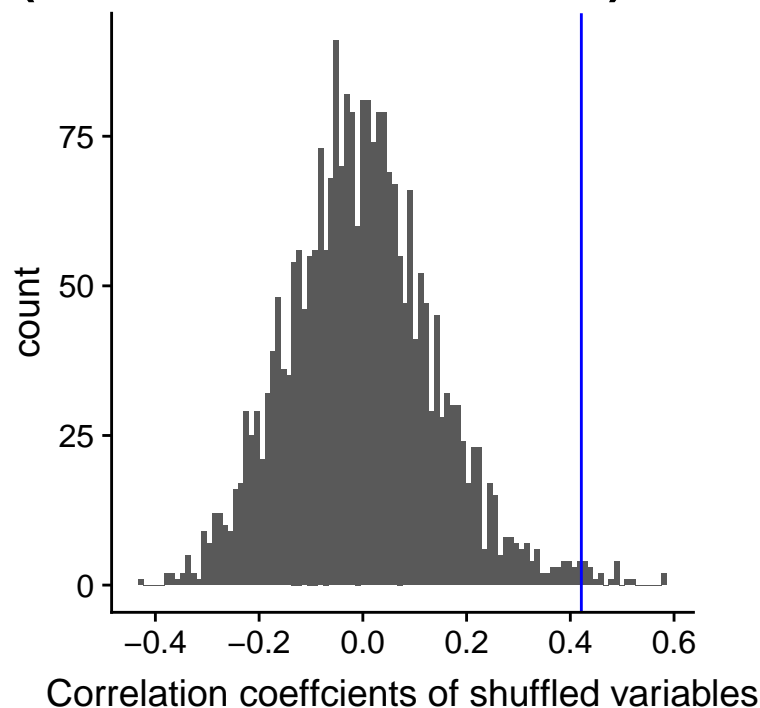


Figure 14.3: Histogram of correlation values under the null hypothesis, obtained by shuffling values. Observed value is denoted by blue line.

```
## sample estimates:
##   rho
## -0.45
```

Now we see that the correlation is no longer significant (and in fact the estimate is negative!), suggesting that the claims of the FiveThirtyEight blog post may have been incorrect due to the effect of the outlier.

### 14.3.3 Bayesian correlation analysis

We can also analyze the FiveThirtyEight data using Bayesian analysis, which has two advantages. First, it provides us with a posterior probability – in this case, the probability that the correlation value exceeds zero. Second, the Bayesian estimate combines the observed evidence with a *prior*, which has the effect of *regularizing* the correlation estimate, effectively pulling it towards zero. Here we can compute it using the `jzs_cor` function from the BayesMed package.

```
bayesCor <- jzs_cor(
  hateCrimes$avg_hatecrimes_per_100k_fbi,
  hateCrimes$gini_index
)
```

```
## Compiling model graph
##   Resolving undeclared variables
##   Allocating nodes
## Graph information:
##   Observed stochastic nodes: 50
##   Unobserved stochastic nodes: 4
```

**$r = 0.83$  (without outlier:  $r = -1.0$ )**

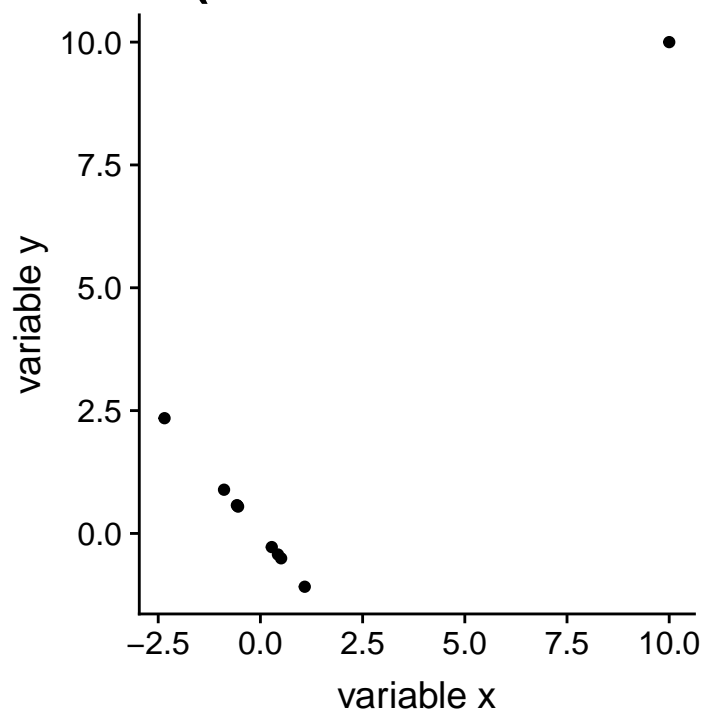


Figure 14.4: An example of the effects of outliers on correlation. Without the outlier the remainder of the datapoints have a perfect negative correlation, but the single outlier changes the correlation value to highly positive.



```
## Total graph size: 230
##
## Initializing model
bayesCor

## $Correlation
## [1] 0.41
##
## $BayesFactor
## [1] 11
##
## $PosteriorProbability
## [1] 0.92
```

Notice that the correlation estimated using the Bayesian method is slightly smaller than the one estimated using the standard correlation coefficient, which is due to the fact that the estimate is based on a combination of the evidence and the prior, which effectively shrinks the estimate toward zero. However, notice that the Bayesian analysis is not robust to the outlier, and it still says that there is fairly strong evidence that the correlation is greater than zero.

## 14.4 Correlation and causation

When we say that one thing *causes* another, what do we mean? There is a long history in philosophy of discussion about the meaning of causality, but in statistics one way that we commonly think of causation is in terms of experimental control. That is, if we think that factor X causes factor Y, then manipulating the value of X should also manipulate the value of Y.

In medicine, there is a set of ideas known as *Koch's postulates* which have historically been used to determine whether a particular organism causes a disease. The basic idea is that the organism should be present in people with the disease, and not present in those without it – thus, a treatment that eliminates the organism should also eliminate the disease. Further, infecting someone with the organism should cause them to contract the disease. An example of this was seen in the work of Dr. Barry Marshall, who had a hypothesis that stomach ulcers were caused by a bacterium (*Helicobacter pylori*). To demonstrate this, he infected himself with the bacterium, and soon thereafter developed severe inflammation in his stomach. He then treated himself with an antibiotic, and his stomach soon recovered. He later won the Nobel Prize in Medicine for this work.

Often we would like to test causal hypotheses but we can't actually do an experiment, either because it's impossible ("What is the relationship between human carbon emissions and the earth's climate?") or unethical ("What are the effects of severe abuse on child brain development?"). However, we can still collect data that might be relevant to those questions. For example, in the latter example, we can potentially collect data from children who have been abused as well as those who have not, and we can then ask whether their brain development differs.

Let's say that we did such an analysis, and we found that abused children had poorer brain development than non-abused children. Would this demonstrate that abuse *causes* poorer brain development? No. Whenever we observe a statistical association between two variables, it is certainly possible that one of those two variables causes the other. However, it is also possible that both of the variables are being influenced by a third variable; in this example, it could be that child abuse is associated with family stress, which could also cause poorer brain development through less intellectual engagement, food stress, or many other possible avenues. The point is that a correlation between two variables generally tells us that something is causing something else, but it doesn't tell us what is causing what. As the statistician Edward Tufte says, "Correlation does not imply causation, but it's a pretty good hint."

### 14.4.1 Causal graphs

One useful way to describe causal relations between variables is through a *causal graph*, which shows variables as circles and causal relations between them as arrows. For example, Figure 14.4.1 shows the causal relationships between study time and two variables that we think should be affected by it: exam grades and exam finishing times.

A graph showing causal relationships between three variables: study time, exam grades, and exam finishing time. A green arrow represents a positive relationship (i.e. more study time causes exam grades to increase), and a red arrow represents a negative relationship (i.e. more study time causes faster completion of the exam).

However, in reality the effects on finishing time and grades are not due directly to the amount of time spent studying, but rather to the amount of knowledge that the student gains by studying. We would usually say that knowledge is a *latent* variable – that is, we can’t measure it directly but we can see it reflected in variables that we can measure (like grades and finishing times). Figure 14.4.1 shows this.

A graph showing the same causal relationships as above, but now also showing the latent variable (knowledge) using a square box.

Here we would say that knowledge *mediates* the relationship between study time and grades/finishing times. That means that if we were able to hold knowledge constant (for example, by administering a drug that causes immediate forgetting), then the amount of study time should no longer have an effect on grades and finishing times.

Note that if we simply measured exam grades and finishing times we would generally see negative relationship between them, because people who finish exams the fastest in general get the highest grades. However, if we were to interpret this correlation as a causal relation, this would tell us that in order to get better grades, we should actually finish the exam more quickly! This example shows how tricky the inference of causality from non-experimental data can be.

Within statistics and machine learning, there is a very active research community that is currently studying the question of when and how we can infer causal relationships from non-experimental data. However, these methods often require strong assumptions, and must generally be used with great caution.

## 14.5 Suggested readings

- The Book of Why by Judea Pearl - an excellent introduction to the ideas behind causal inference.

## Chapter 15

# The General Linear Model

Remember that early in the book we described the basic model of statistics:

$$\text{outcome} = \text{model} + \text{error}$$

where our general goal is to find the model that minimizes the error, subject to some other constraints (such as keeping the model relatively simple so that we can generalize beyond our specific dataset). In this chapter we will focus on a particular implementation of this approach, which is known as the *general linear model* (or GLM). You have already seen the general linear model in the earlier chapter on Fitting Models to Data, where we modeled height in the NHANES dataset as a function of age; here we will provide a more general introduction to the concept of the GLM and its many uses.

Before we discuss the general linear model, let's first define two terms that will be important for our discussion:

- *dependent variable*: This is the outcome variable that our model aims to explain (usually referred to as  $Y$ )
- *independent variable*: This is a variable that we wish to use in order to explain the dependent variable (usually referred to as  $X$ ).

There may be multiple independent variables, but for this course there will only be one dependent variable in our analyses.

A general linear model is one in which the model for the dependent variable is composed of a *linear combination* of independent variables that are each multiplied by a weight (which is often referred to as the Greek letter beta -  $\beta$ ), which determines the relative contribution of that independent variable to the model prediction.

As an example, let's generate some simulated data for the relationship between study time and exam grades (see Figure 15.1).

```
# create simulated data for example
set.seed(12345)

# the number of points that having a prior class increases grades
betas <- c(6, 5)

df <-
  tibble(
    studyTime = c(2, 3, 5, 6, 6, 8, 10, 12) / 3,
    priorClass = c(0, 1, 1, 0, 1, 0, 1, 0)
  ) %>%
  mutate(
    grade =
```

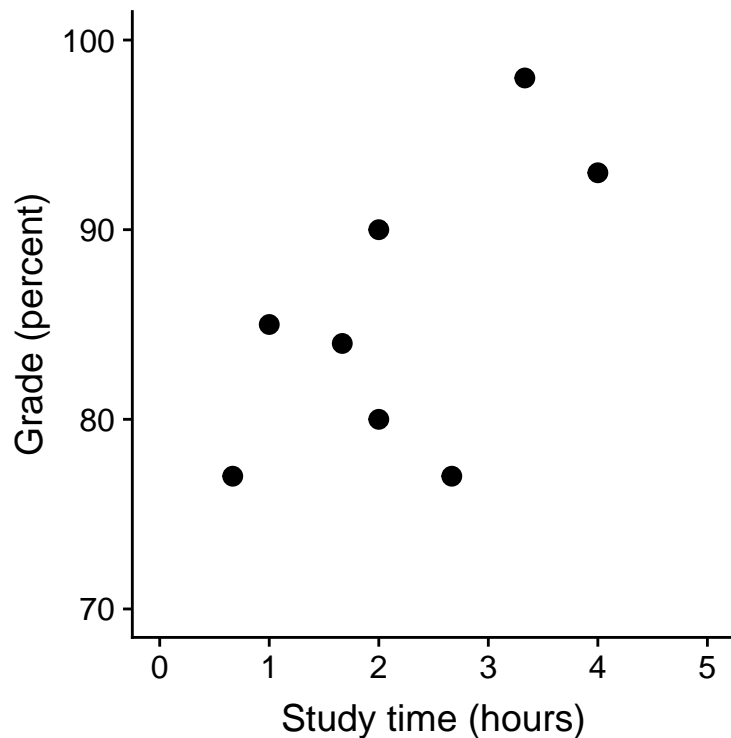


Figure 15.1: Relation between study time and grades

```

studyTime * betas[1] +
priorClass * betas[2] +
round(rnorm(8, mean = 70, sd = 5))
)

```

Given these data, we might want to engage in each of the three fundamental activities of statistics:

- *Describe*: How strong is the relationship between grade and study time?
- *Decide*: Is there a statistically significant relationship between grade and study time?
- *Predict*: Given a particular amount of study time, what grade do we expect?

In the last chapter we learned how to describe the relationship between two variables using the correlation coefficient, so we can use that to describe the relationship here, and to test whether the correlation is statistically significant:

```

# compute correlation between grades and study time
corTestResult <- cor.test(df$grade, df$studyTime, alternative = "greater")
corTestResult

```

```

##
## Pearson's product-moment correlation
##
## data: df$grade and df$studyTime
## t = 2, df = 6, p-value = 0.05
## alternative hypothesis: true correlation is greater than 0
## 95 percent confidence interval:
## 0.014 1.000
## sample estimates:
## cor

```

```
## 0.63
```

The correlation is quite high, but just barely reaches statistical significance because the sample size is so small.

## 15.1 Linear regression

We can also use the general linear model to describe the relation between two variables and to decide whether that relationship is statistically significant; in addition, the model allows us to predict the value of the dependent variable given some new value(s) of the independent variable(s). Most importantly, the general linear model will allow us to build models that incorporate multiple independent variables, whereas correlation can only tell us about the relationship between two individual variables.

The specific version of the GLM that we use for this is referred to as *linear regression*. The term *regression* was coined by Francis Galton, who had noted that when he compared parents and their children on some feature (such as height), the children of extreme parents (i.e. the very tall or very short parents) generally fell closer to the mean than their parents. This is an extremely important point that we return to below.

The simplest version of the linear regression model (with a single independent variable) can be expressed as follows:

$$y = x * \beta_x + \beta_0 + \epsilon$$

The  $\beta_x$  value tells us how much we would expect  $y$  to change given a one-unit change in  $x$ . The intercept  $\beta_0$  is an overall offset, which tells us what value we would expect  $y$  to have when  $x = 0$ ; you may remember from our early modeling discussion that this is important to model the overall magnitude of the data, even if  $x$  never actually attains a value of zero. The error term  $\epsilon$  refers to whatever is left over once the model has been fit. If we want to know how to predict  $y$  (which we call  $\hat{y}$ ), then we can drop the error term:

$$\hat{y} = x * \beta_x + \beta_0$$

Figure 15.2 shows an example of this model applied to the study time example.

### 15.1.1 Regression to the mean

The concept of *regression to the mean* was one of Galton's essential contributions to science, and it remains a critical point to understand when we interpret the results of experimental data analyses. Let's say that we want to study the effects of a reading intervention on the performance of poor readers. To test our hypothesis, we might go into a school and recruit those individuals in the bottom 25% of the distribution on some reading test, administer the intervention, and then examine their performance. Let's say that the intervention actually has no effect, and that reading scores for each individual are simply independent samples from a normal distribution. We can simulate this:

```
# create simulated data for regression to the mean example

nstudents <- 100

readingScores <- data.frame(
  #random normal distribution of scores for test 1
  test1 = rnorm(n = nstudents, mean = 0, sd = 1) * 10 + 100,
  #random normal distribution of scores for test 2
  test2 = rnorm(n = nstudents, mean = 0, sd = 1) * 10 + 100
)
```

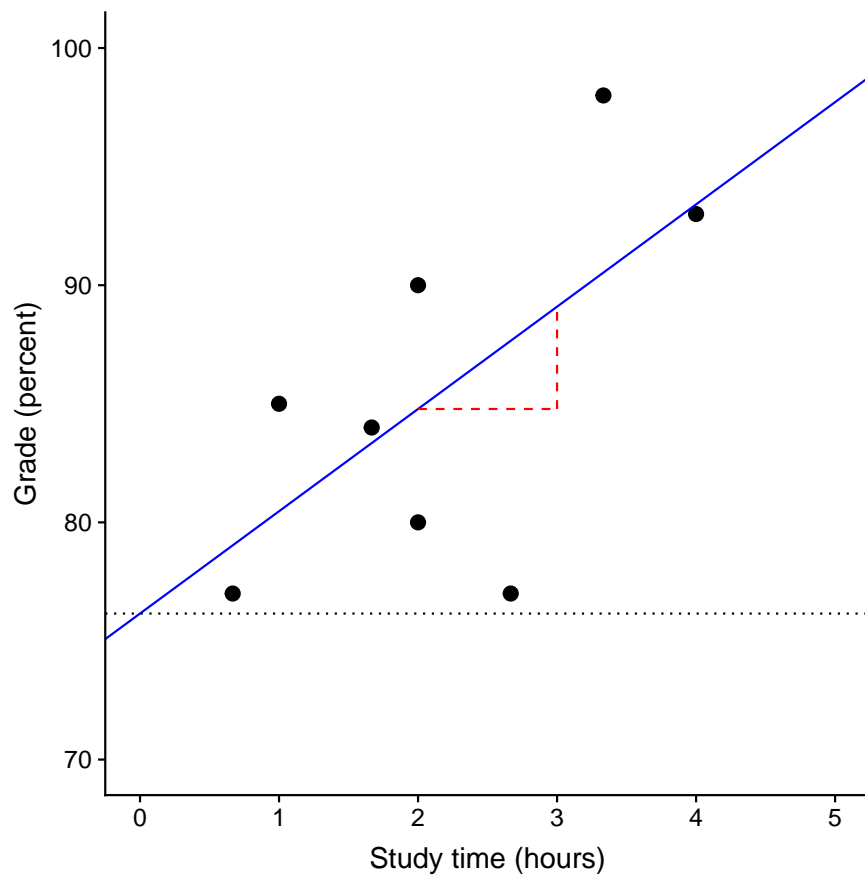


Figure 15.2: The linear regression solution for the study time data is shown in blue. The value of the intercept is equivalent to the predicted value of the  $y$  variable when the  $x$  variable is equal to zero; this is shown with a dotted black line. The value of  $\beta$  is equal to the slope of the line – that is, how much  $y$  changes for a unit change in  $x$ . This is shown schematically in the red dashed lines, which show the degree of increase in grade for a single unit increase in study time.

```
# select the students in the bottom 25% on the first test
cutoff <- quantile(readingScores$test1, 0.25)

readingScores <-
  readingScores %>%
  mutate(badTest1 = test1 < cutoff) %>%
  dplyr::filter(badTest1 == TRUE) %>%
  summarize(
    test1mean = mean(test1),
    test2mean = mean(test2)
  ) %>%
  pander()
```

If we look at the difference between the mean test performance at the first and second test, it appears that the intervention has helped these students substantially, as their scores have gone up by more than ten points on the test! However, we know that in fact the students didn't improve at all, since in both cases the scores were simply selected from a random normal distribution. What has happened is that some subjects scored badly on the first test simply due to random chance. If we select just those subjects on the basis of their first test scores, they are guaranteed to move back towards the mean of the entire group on the second test, even if there is no effect of training. This is the reason that we need an untreated *control group* in order to interpret any changes in reading over time; otherwise we are likely to be tricked by regression to the mean.

### 15.1.2 Estimating linear regression parameters

We generally estimate the parameters of a linear model from data using *linear algebra*, which is the form of algebra that is applied to vectors and matrices. If you aren't familiar with linear algebra, don't worry – you won't actually need to use it here, as R will do all the work for us. However, a brief excursion in linear algebra can provide some insight into how the model parameters are estimated in practice.

First, let's introduce the idea of vectors and matrices; you've already encountered them in the context of R, but we will review them here. A matrix is a set of numbers that are arranged in a square or rectangle, such that there are one or more *dimensions* across which the matrix varies. It is customary to place different observation units (such as people) in the rows, and different variables in the columns. Let's take our study time data from above. We could arrange these numbers in a matrix, which would have eight rows (one for each student) and two columns (one for study time, and one for grade). If you are thinking “that sounds like a data frame in R” you are exactly right! In fact, a data frame is a specialized version of a matrix, and we can convert a data frame to a matrix using the `as.matrix()` function.

```
df_matrix <-
  df %>%
  dplyr::select(studyTime, grade) %>%
  as.matrix()
```

We can write the general linear model in linear algebra as follows:

$$Y = X * \beta + E$$

This looks very much like the earlier equation that we used, except that the letters are all capitalized, which is meant to express the fact that they are vectors.

We know that the grade data go into the  $Y$  matrix, but what goes into the  $X$  matrix? Remember from our initial discussion of linear regression that we need to add a constant in addition to our independent variable of interest, so our  $X$  matrix (which we call the *design matrix*) needs to include two columns: one representing the study time variable, and one column with the same value for each individual (which we generally fill with all ones). We can view the resulting design matrix graphically (see Figure 15.3).

$$\begin{array}{rcl}
 0.67 & & 77 \quad 1 \\
 1.0 & & 85 \quad 1 \\
 1.67 & & 84 \quad 1 \\
 2.0 & = & 80 \quad 1 \\
 2.0 & & 90 \quad 1 \\
 2.67 & & 77 \quad 1 \\
 3.33 & & 98 \quad 1 \\
 4.0 & & 93 \quad 1
 \end{array} * \beta + E$$

Figure 15.3: A depiction of the linear model for the study time data in terms of matrix algebra.

The rules of matrix multiplication tell us that the dimensions of the matrices have to match with one another; in this case, the design matrix has dimensions of 8 (rows) X 2 (columns) and the Y variable has dimensions of 8 X 1. Therefore, the  $\beta$  matrix needs to have dimensions 2 X 1, since an 8 X 2 matrix multiplied by a 2 X 1 matrix results in an 8 X 1 matrix (as the matching middle dimensions drop out). The interpretation of the two values in the  $\beta$  matrix is that they are the values to be multiplied by study time and 1 respectively to obtain the estimated grade for each individual. We can also view the linear model as a set of individual equations for each individual:

$$\hat{y}_1 = \text{studyTime}_1 * \beta_1 + 1 * \beta_2$$

$$\hat{y}_2 = \text{studyTime}_2 * \beta_1 + 1 * \beta_2$$

...

$$\hat{y}_8 = \text{studyTime}_8 * \beta_1 + 1 * \beta_2$$

Remember that our goal is to determine the best fitting values of  $\beta$  given the known values of  $X$  and  $Y$ . A naive way to do this would be to solve for  $\beta$  using simple algebra – here we drop the error term  $E$  because it's out of our control:

$$\hat{\beta} = \frac{Y}{X}$$

The challenge here is that  $X$  and  $\beta$  are now matrices, not single numbers – but the rules of linear algebra tell us how to divide by a matrix, which is the same as multiplying by the *inverse* of the matrix (referred to as  $X^{-1}$ ). We can do this in R:

```
# compute beta estimates using linear algebra
```



```

Y <- as.matrix(df$grade) #create Y variable 8 x 1 matrix
X <- matrix(0, nrow = 8, ncol = 2) #create X variable 8 x 2 matrix
X[, 1] <- as.matrix(df$studyTime) #assign studyTime values to first column in X matrix
X[, 2] <- 1 #assign constant of 1 to second column in X matrix

# compute inverse of X using ginv()
# %*% is the R matrix multiplication operator

beta_hat <- ginv(X) %*% Y #multiple the inverse of X by Y
print(beta_hat)

##           [,1]
## [1,]    4.3
## [2,]   76.2

```

Anyone who is interested in serious use of statistical methods is highly encouraged to invest some time in learning linear algebra, as it provides the basis for nearly all of the tools that are used in standard statistics.

### 15.1.3 The relation between correlation and regression

There is a close relationship between correlation coefficients and regression coefficients. Remember that Pearson's correlation coefficient is computed as the ratio of the covariance and the product of the standard deviations of x and y:

$$\hat{r} = \frac{\text{covariance}_{xy}}{s_x * s_y}$$

whereas the regression beta is computed as:

$$\hat{\beta} = \frac{\text{covariance}_{xy}}{s_x * s_x}$$

Based on these two equations, we can derive the relationship between  $\hat{r}$  and  $\hat{\beta}$ :

$$\text{covariance}_{xy} = \hat{r} * s_x * s_y$$

$$\hat{\beta}_x = \frac{\hat{r} * s_x * s_y}{s_x * s_x} = \hat{r} * \frac{s_y}{s_x}$$

That is, the regression slope is equal to the correlation value multiplied by the ratio of standard deviations of y and x. One thing this tells us is that when the standard deviations of x and y are the same (e.g. when the data have been converted to Z scores), then the correlation estimate is equal to the regression slope estimate.

### 15.1.4 Standard errors for regression models

If we want to make inferences about the regression parameter estimates, then we also need an estimate of their variability. To compute this, we first need to compute the *residual variance* or *error variance* for the model – that is, how much variability in the dependent variable is not explained by the model. We can compute the model residuals as follows:

$$\text{residual} = y - \hat{y} = y - (x * \hat{\beta}_x + \hat{\beta}_0)$$

We then compute the *sum of squared errors (SSE)*:

$$SS_{error} = \sum_{i=1}^n (y_i - \hat{y}_i)^2 = \sum_{i=1}^n residuals^2$$

and from this we compute the *mean squared error*:

$$MS_{error} = \frac{SS_{error}}{df} = \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{N - p}$$

where the degrees of freedom (*df*) are determined by subtracting the number of estimated parameters (2 in this case:  $\hat{\beta}_x$  and  $\hat{\beta}_0$ ) from the number of observations (*N*). Once we have the mean squared error, we can compute the standard error for the model as:

$$SE_{model} = \sqrt{MS_{error}}$$

In order to get the standard error for a specific regression parameter estimate,  $SE_{\beta_x}$ , we need to rescale  $SE_{model}$  into the units of the particular parameter, by dividing it by the standard deviation of the X variable:

$$SE_{\beta_x} = \frac{SE_{model}}{S_x}$$

### 15.1.5 Statistical tests for regression parameters

Once we have the parameter estimates and their standard errors, we can compute a *t* statistic to tell us the likelihood of the observed parameter estimates compared to some expected value under the null hypothesis. In this case we will test against the null hypothesis of no effect (i.e.  $\beta = 0$ ):

$$\begin{aligned} t_{N-p} &= \frac{\hat{\beta} - \beta_{expected}}{SE_{\hat{\beta}}} \\ t_{N-p} &= \frac{\hat{\beta} - 0}{SE_{\hat{\beta}}} \\ t_{N-p} &= \frac{\hat{\beta}}{SE_{\hat{\beta}}} \end{aligned}$$

In R, we don't need to compute these by hand, as they are automatically returned to us by the `lm()` function:

```
summary(lmResult)

##
## Call:
## lm(formula = grade ~ studyTime, data = df)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -10.656  -2.719   0.125   4.703   7.469
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)    76.16      5.16    14.76 6.1e-06 ***
## studyTime       4.31      2.14     2.01  0.091 .
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 6.4 on 6 degrees of freedom
```

```
## Multiple R-squared:  0.403, Adjusted R-squared:  0.304
## F-statistic: 4.05 on 1 and 6 DF, p-value: 0.0907
```

In this case we see that the intercept is significantly different from zero (which is not very interesting) and that the effect of studyTime on grades is marginally significant.

### 15.1.6 Quantifying goodness of fit of the model

Sometimes it's useful to quantify how well the model fits the data overall, and one way to do this is to ask how much of the variability in the data is accounted for by the model. This is quantified using a value called  $R^2$  (also known as the *coefficient of determination*). If there is only one x variable, then this is easy to compute by simply squaring the correlation coefficient:

$$R^2 = r^2$$

In the case of our study time data,  $R^2 = 0.4$ , which means that we have accounted for about 40% of the variance in the data.

More generally we can think of  $R^2$  as a measure of the fraction of variance in the data that is accounted for by the model, which can be computed by breaking the variance into multiple components:

$$SS_{total} = SS_{model} + SS_{error}$$

where  $SS_{total}$  is the variance of the data ( $y$ ) and  $SS_{model}$  and  $SS_{error}$  are computed as shown earlier in this chapter. Using this, we can then compute the coefficient of determination as:

$$R^2 = \frac{SS_{model}}{SS_{total}} = 1 - \frac{SS_{error}}{SS_{total}}$$

A small value of  $R^2$  tells us that even if the model fit is statistically significant, it may only explain a small amount of information in the data.

## 15.2 Fitting more complex models

Often we would like to understand the effects of multiple variables on some particular outcome, and how they relate to one another. In the context of our study time example, let's say that we discovered that some of the students had previously taken a course on the topic. If we plot their grades (see Figure 15.4), we can see that those who had a prior course perform much better than those who had not, given the same amount of study time.

We would like to build a statistical model that takes this into account, which we can do by extending the model that we built above:

$$\hat{y} = \hat{\beta}_1 * studyTime + \hat{\beta}_2 * priorClass + \hat{\beta}_0$$

To model whether each individual has had a previous class or not, we use what we call *dummy coding* in which we create a new variable that has a value of one to represent having had a class before, and zero otherwise. This means that for people who have had the class before, we will simply add the value of  $\hat{\beta}_2$  to our predicted value for them – that is, using dummy coding  $\hat{\beta}_2$  simply reflects the difference in means between the two groups. Our estimate of  $\hat{\beta}_1$  reflects the regression slope over all of the data points – we are assuming that regression slope is the same regardless of whether someone has had a class before (see Figure 15.5).

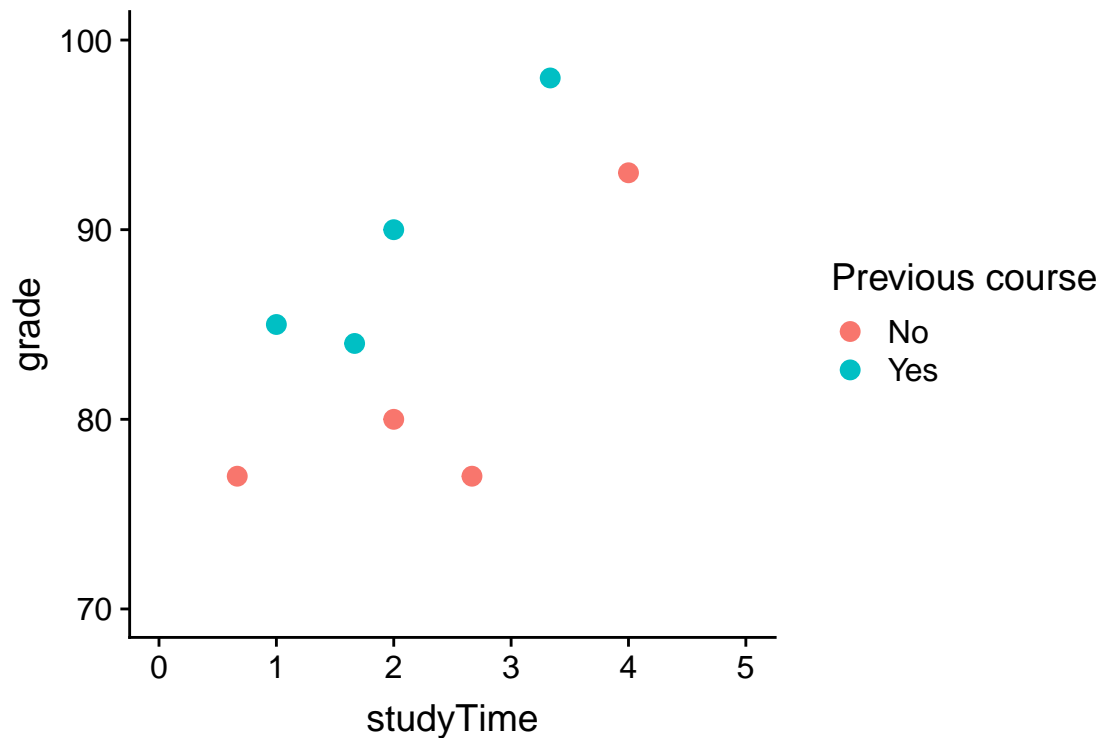


Figure 15.4: The relationship between study time and grades, with color identifying whether each student had taken a previous course on the topic

```
# perform linear regression for study time and prior class

# must change priorClass to a factor variable
df$priorClass <- as.factor(df$priorClass)

lmResultTwoVars <- lm(grade ~ studyTime + priorClass, data = df)
summary(lmResultTwoVars)

##
## Call:
## lm(formula = grade ~ studyTime + priorClass, data = df)
##
## Residuals:
##      1      2      3      4      5      6      7      8
##  3.5833  0.7500 -3.5833 -0.0833  0.7500 -6.4167  2.0833  2.9167
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)    70.08      3.77    18.60  8.3e-06 ***
## studyTime       5.00      1.37     3.66   0.015 *
## priorClass1     9.17      2.88     3.18   0.024 *
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 4 on 5 degrees of freedom
## Multiple R-squared:  0.803, Adjusted R-squared:  0.724
```

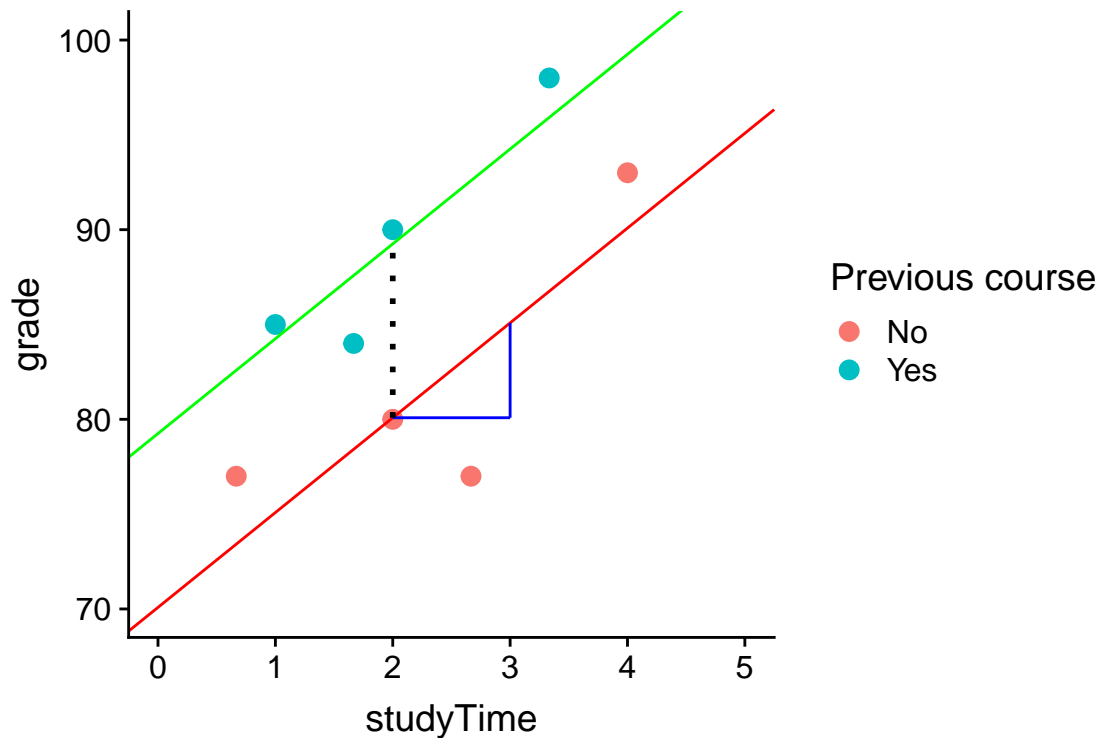


Figure 15.5: The relation between study time and grade including prior experience as an additional component in the model. The blue line shows the slope relating grades to study time, and the black dotted line corresponds to the difference in means between the two groups.

```
## F-statistic: 10.2 on 2 and 5 DF, p-value: 0.0173
```

## 15.3 Interactions between variables

In the previous model, we assumed that the effect of study time on grade (i.e., the regression slope) was the same for both groups. However, in some cases we might imagine that the effect of one variable might differ depending on the value of another variable, which we refer to as an *interaction* between variables.

Let's use a new example that asks the question: What is the effect of caffeine on public speaking? First let's generate some data and plot them. Looking at Figure 15.6, there doesn't seem to be a relationship, and we can confirm that by performing linear regression on the data:

```
# perform linear regression with caffeine as independent variable
lmResultCaffeine <- lm(speaking ~ caffeine, data = df)
summary(lmResultCaffeine)
```

```
##
## Call:
## lm(formula = speaking ~ caffeine, data = df)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -33.10 -16.02   5.01  16.45  26.98
##
## Coefficients:
```

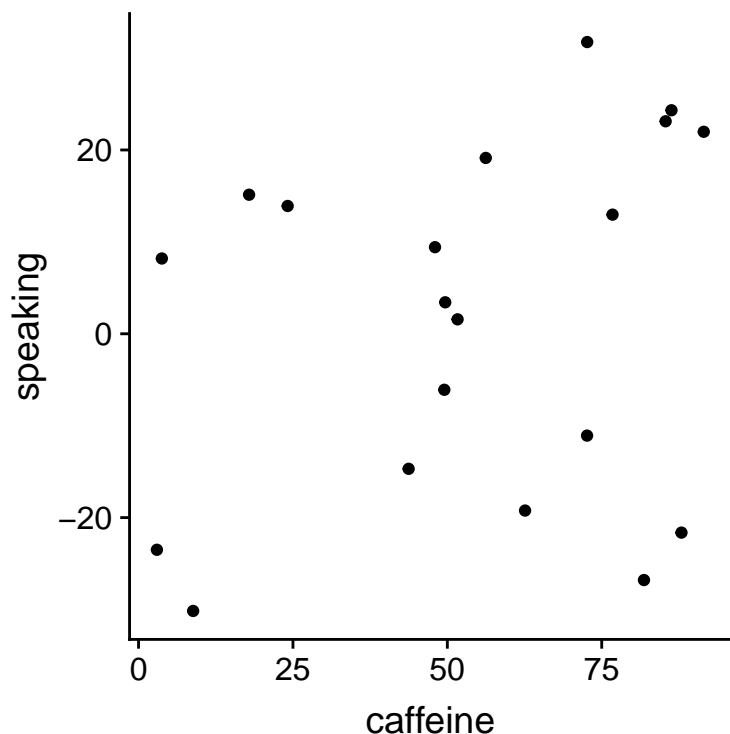


Figure 15.6: The relationship between caffeine and public speaking

```
##           Estimate Std. Error t value Pr(>|t|)
## (Intercept)  -7.413      9.165   -0.81    0.43
## caffeine      0.168      0.151    1.11    0.28
##
## Residual standard error: 19 on 18 degrees of freedom
## Multiple R-squared:  0.0642, Adjusted R-squared:  0.0122
## F-statistic: 1.23 on 1 and 18 DF,  p-value: 0.281
```

But now let's say that we find research suggesting that anxious and non-anxious people react differently to caffeine. First let's plot the data separately for anxious and non-anxious people.

As we see from Figure 15.7, it appears that the relationship between speaking and caffeine is different for the two groups, with caffeine improving performance for people without anxiety and degrading performance for those with anxiety. We'd like to create a statistical model that addresses this question. First let's see what happens if we just include anxiety in the model.

```
# compute linear regression adding anxiety to model
lmResultCafAnx <- lm(speaking ~ caffeine + anxiety, data = df)
summary(lmResultCafAnx)
```

```
##
## Call:
## lm(formula = speaking ~ caffeine + anxiety, data = df)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -32.97  -9.74   1.35  10.53  25.36
##
## Coefficients:
```

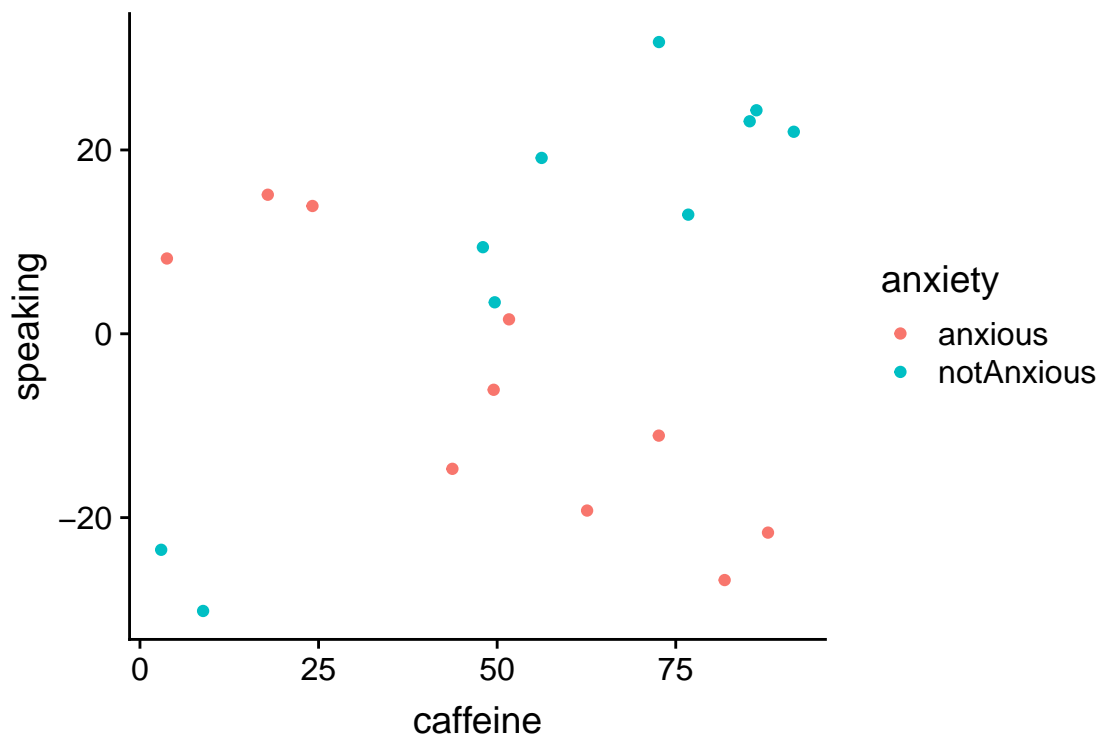


Figure 15.7: The relationship between caffeine and public speaking, with anxiety represented by the color of the data points

```
##               Estimate Std. Error t value Pr(>|t|)
## (Intercept)    -12.581      9.197   -1.37    0.19
## caffeine         0.131      0.145    0.91    0.38
## anxietynotAnxious 14.233      8.232    1.73    0.10
##
## Residual standard error: 18 on 17 degrees of freedom
## Multiple R-squared:  0.204, Adjusted R-squared:  0.11
## F-statistic: 2.18 on 2 and 17 DF, p-value: 0.144
```

Here we see there are no significant effects of either caffeine or anxiety, which might seem a bit confusing. The problem is that this model is trying to fit the same line relating speaking to caffeine for both groups. If we want to fit them using separate lines, we need to include an *interaction* in the model, which is equivalent to fitting different lines for each of the two groups; in R this is denoted by the `*` symbol.

```
# compute linear regression including caffeine X anxiety interaction
lmResultInteraction <- lm(
  speaking ~ caffeine + anxiety + caffeine * anxiety,
  data = df
)
summary(lmResultInteraction)
```

```
##
## Call:
## lm(formula = speaking ~ caffeine + anxiety + caffeine * anxiety,
##     data = df)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
```

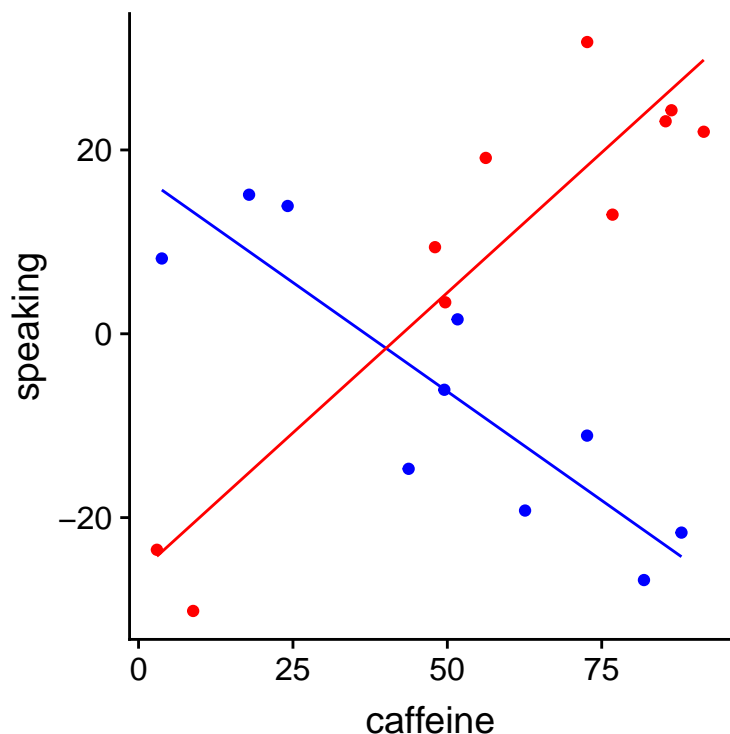


Figure 15.8: The relationship between public speaking and caffeine, including an interaction with anxiety. This results in two lines that separately model the slope for each group.

```
## -11.385 -7.103 -0.444 6.171 13.458
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)      17.4308     5.4301   3.21 0.00546 **
## caffeine          -0.4742     0.0966  -4.91 0.00016 ***
## anxietynotAnxious -43.4487     7.7914  -5.58 4.2e-05 ***
## caffeine:anxietynotAnxious 1.0839     0.1293   8.38 3.0e-07 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 8.1 on 16 degrees of freedom
## Multiple R-squared:  0.852, Adjusted R-squared:  0.825
## F-statistic: 30.8 on 3 and 16 DF, p-value: 7.01e-07
```

From these results we see that there are significant effects of both caffeine and anxiety (which we call *main effects*) and an interaction between caffeine and anxiety. Figure 15.8 shows the separate regression lines for each group.

Sometimes we want to compare the relative fit of two different models, in order to determine which is a better model; we refer to this as *model comparison*. For the models above, we can compare the goodness of fit of the model with and without the interaction, using the `anova()` command in R:

```
anova(lmResultCafAnx, lmResultInteraction)
```

```
## Analysis of Variance Table
##
## Model 1: speaking ~ caffeine + anxiety
```



```
## Model 2: speaking ~ caffeine + anxiety + caffeine * anxiety
##   Res.Df  RSS Df Sum of Sq    F Pr(>F)
## 1      17 5639
## 2      16 1046  1      4593 70.3 3e-07 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

This tells us that there is good evidence to prefer the model with the interaction over the one without an interaction. Model comparison is relatively simple in this case because the two models are *nested* – one of the models is a simplified version of the other model. Model comparison with non-nested models can get much more complicated.

## 15.4 What does “predict” really mean?

When we talk about “prediction” in daily life, we are generally referring to the ability to estimate the value of some variable in advance of seeing the data. However, the term is often used in the context of linear regression to refer to the fitting of a model to the data; the estimated values ( $\hat{y}$ ) are sometimes referred to as “predictions” and the independent variables are referred to as “predictors”. This has an unfortunate connotation, as it implies that our model should also be able to predict the values of new data points in the future. In reality, the fit of a model to the dataset used to obtain the parameters will nearly always be better than the fit of the model to a new dataset (Copas 1983).

As an example, let’s take a sample of 48 children from NHANES and fit a regression model for weight that includes several regressors (age, height, hours spent watching TV and using the computer, and household income) along with their interactions.

```
# create dataframe with children with complete data on all variables
NHANES_child <-
  NHANES %>%
  drop_na(Height, Weight, TVHrsDayChild, HHIncomeMid, CompHrsDayChild, Age) %>%
  dplyr::filter(Age < 18)

# create function to sample data and compute regression on in-sample and out-of-sample data

get_sample_predictions <- function(sample_size, shuffle = FALSE) {
  orig_sample <-
    NHANES_child %>%
    sample_n(sample_size)

  if (shuffle) {
    orig_sample$Weight <- sample(orig_sample$Weight)
  }

  heightRegressOrig <- lm(
    Weight ~ Height * TVHrsDayChild * CompHrsDayChild * HHIncomeMid * Age,
    data = orig_sample
  )

  pred_orig <- predict(heightRegressOrig)

  new_sample <-
    NHANES_child %>%
    sample_n(sample_size)
```

```

pred_new <- predict(heightRegressOrig, new_sample)
# return r-squared and rmse for original and new data
return(c(
  cor(pred_orig, orig_sample$Weight)**2,
  cor(pred_new, new_sample$Weight)**2,
  sqrt(mean((pred_orig - orig_sample$Weight)**2)),
  sqrt(mean((pred_new - new_sample$Weight)**2))
))
}

# implement the function
sim_results <-
  replicate(100, get_sample_predictions(sample_size = 48, shuffle = FALSE))

sim_results <-
  t(sim_results) %>%
  data.frame()

mean_rsquared <-
  sim_results %>%
  summarize(
    rmse_original_data = mean(X3),
    rmse_new_data = mean(X4)
  )

pander(mean_rsquared)

```

| rmse_original_data | rmse_new_data |
|--------------------|---------------|
| 2.97               | 25.72         |

Here we see that whereas the model fit on the original data showed a very good fit (only off by a few pounds per individual), the same model does a much worse job of predicting the weight values for new children sampled from the same population (off by more than 25 pounds per individual). This happens because the model that we specified is quite complex, since it includes not just each of the individual variables, but also all possible combinations of them (i.e. their *interactions*), resulting in a model with 32 parameters. Since this is almost as many coefficients as there are data points (i.e., the heights of 48 children), the model *overfits* the data, just like the complex polynomial curve in our initial example of overfitting in Section 5.4.

Another way to see the effects of overfitting is to look at what happens if we randomly shuffle the values of the weight variable. Randomly shuffling the value should make it impossible to predict weight from the other variables, because they should have no systematic relationship.

```

print("using shuffled y variable to simulate null effect")

## [1] "using shuffled y variable to simulate null effect"

sim_results <-
  replicate(100, get_sample_predictions(sample_size = 48, shuffle = TRUE))

sim_results <-
  t(sim_results) %>%
  data.frame()

mean_rsquared <-

```

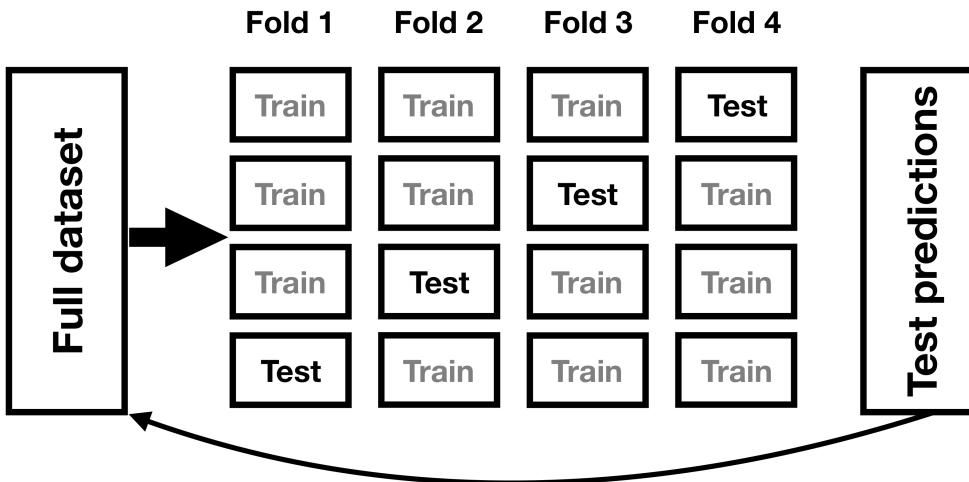


Figure 15.9: A schematic of the crossvalidation procedure.

```

sim_results %>%
  summarize(
    rmse_original_data = mean(X3),
    rmse_new_data = mean(X4)
  )
pander(mean_rsquared)

```

| rmse_original_data | rmse_new_data |
|--------------------|---------------|
| 7.56               | 60.1          |

This shows us that even when there is no true relationship to be modeled (because shuffling should have obliterated the relationship), the complex model still shows a very low error in its predictions, because it fits the noise in the specific dataset. However, when that model is applied to a new dataset, we see that the error is much larger, as it should be.

### 15.4.1 Cross-validation

One method that has been developed to help address the problem of overfitting is known as *cross-validation*. This technique is commonly used within the field of machine learning, which is focused on building models that will generalize well to new data, even when we don’t have a new dataset to test the model. The idea behind cross-validation is that we fit our model repeatedly, each time leaving out a subset of the data, and then test the ability of the model to predict the values in each held-out subset.

Let’s see how that would work for our weight prediction example. In this case we will perform 12-fold cross-validation, which means that we will break the data into 12 subsets, and then fit the model 12 times, in each case leaving out one of the subsets and then testing the model’s ability to accurately predict the value of the dependent variable for those held-out data points. The `caret` package in R provides us with the ability to easily run cross-validation across our dataset:

```

# create a function to run cross-validation
# returns the r-squared for the out-of-sample prediction

```

```

compute_cv <- function(d, nfolds = 12) {
  # based on https://quantdev.ssri.psu.edu/tutorials/cross-validation-tutorial
  train_ctrl <- trainControl(method = "cv", number = nfolds)
  model_caret <- train(
    Weight ~ Height * TVHrsDayChild * CompHrsDayChild * HHIncomeMid * Age,
    data = d,
    trControl = train_ctrl, # folds
    method = "lm"
  ) # specifying regression model

  r2_cv <- mean(model_caret$resample$Rsquared)
  rmse_cv <- mean(model_caret$resample$RMSE)
  return(c(r2_cv, rmse_cv))
}

```

Using this function we can run cross-validation on 100 samples from the NHANES dataset, and compute the RMSE for cross-validation, along with the RMSE for the original data and a new dataset, as we computed above.

```

#implement the function
sim_results <-
  replicate(100, get_sample_predictions_cv(sample_size = 48, shuffle = FALSE))

sim_results <-
  t(sim_results) %>%
  data.frame()

mean_rsquared <-
  sim_results %>%
  summarize(
    mse_original_data = mean(X4),
    mse_new_data = mean(X5),
    mse_crossvalidation = mean(X6)
  )
pander(mean_rsquared)

```

| mse_original_data | mse_new_data | mse_crossvalidation |
|-------------------|--------------|---------------------|
| 2.98              | 21.64        | 29.29               |

Here we see that crossvalidation gives us an estimate of predictive accuracy that is much closer to what we see with a completely new dataset than it is to the inflated accuracy that we see with the original dataset – in fact, it’s even slightly more pessimistic than the average for a new dataset, probably because only part of the data are being used to train each of the models. We can also confirm that cross-validation accurately estimates the predictive accuracy when the dependent variable is randomly shuffled:

| rmse_original_data | rmse_new_data | rmse_crossvalidation |
|--------------------|---------------|----------------------|
| 7.9                | 73.7          | 75.31                |

Here again we see that crossvalidation gives us an assessment of prediction accuracy that is much closer to what we expect with new data, and again even somewhat more pessimistic.

Using cross-validation properly is tricky, and it is recommended that you consult with an expert before using

it in practice. However, this section has hopefully shown you three things:

- “Prediction” doesn’t always mean what you think it means
- Complex models can overfit data very badly, such that one can see seemingly good prediction even when there is no true signal to predict
- You should view claims about prediction accuracy very skeptically unless they have been done using the appropriate methods.

## 15.5 Suggested readings

- The Elements of Statistical Learning: Data Mining, Inference, and Prediction (2nd Edition) - The bible of machine learning methods, available freely online.



## Chapter 16

# Comparing means

One of the most common questions that we want to ask in statistics is whether there is a difference between the means of two different groups. Let's say that we would like to know whether regular marijuana smokers watch more television. We can ask this question using the NHANES dataset; let's take a sample of 200 individuals from the dataset and test whether the number of hours of television watching per day is related to regular marijuana use. Figure 16.1 shows these data using a violin plot.

```
# create sample with tv watching and marijuana use
NHANES_sample <-
  NHANES_adult %>%
  drop_na(TVHrsDay, RegularMarij) %>%
  mutate(
    TVHrsNum = recode( #recode character values into numerical values
      TVHrsDay,
      "More_4_hr" = 5,
      "4_hr" = 4,
      "2_hr" = 2,
      "1_hr" = 1,
      "3_hr" = 3,
      "0_to_1_hr" = 0.5,
      "0_hrs" = 0
    )
  ) %>%
  sample_n(200)
```

### 16.1 Student's T test

We have already encountered Student's t statistic in the previous chapter on hypothesis testing. This statistic provides us with a way to test for differences between two groups of independent observations; we will turn later in the chapter to cases where the observations are not independent. As a reminder, the t-statistic for comparison of two independent groups is computed as:

$$t = \frac{\bar{X}_1 - \bar{X}_2}{\sqrt{\frac{S_1^2}{n_1} + \frac{S_2^2}{n_2}}}$$

where  $\bar{X}_1$  and  $\bar{X}_2$  are the means of the two groups,  $S_1^2$  and  $S_2^2$  are the variances for each the groups, and  $n_1$  and  $n_2$  are the sizes of the two groups. Under the null hypothesis of no difference between means, this

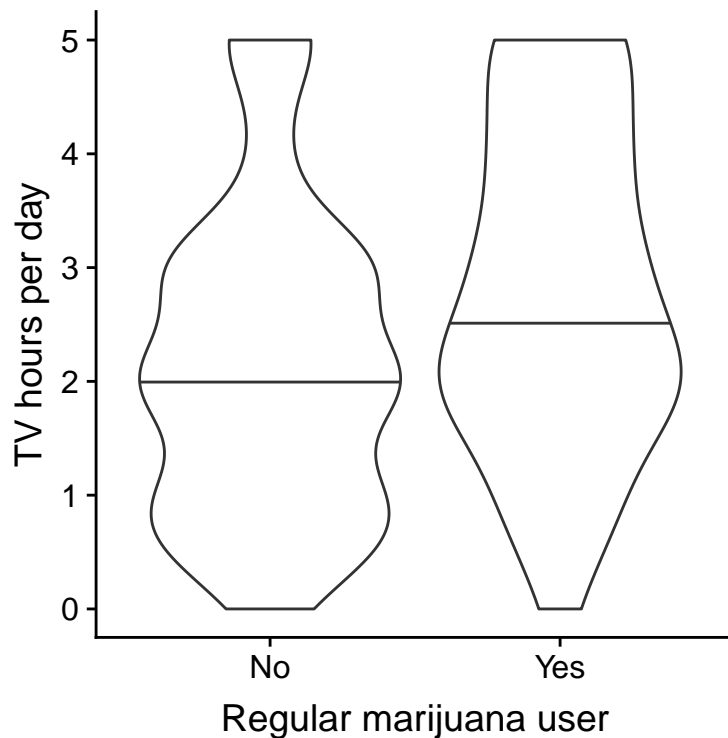


Figure 16.1: Violin plot showing distributions of TV watching separated by regular marijuana use.

statistic is distributed according to a  $t$  distribution with  $n-2$  degrees of freedom (since we have computed two parameter estimates, namely the means of the two groups). We can compute the  $t$ -test in R using the `t.test()` function:

```
# compute t test for tv watching as function of marijuana use
t.test(
  TVHrsNum ~ RegularMarij,
  data = NHANES_sample,
  var.equal = TRUE
)
```

```
##
## Two Sample t-test
##
## data: TVHrsNum by RegularMarij
## t = -3, df = 200, p-value = 0.003
## alternative hypothesis: true difference in means is not equal to 0
## 95 percent confidence interval:
## -1.07 -0.22
## sample estimates:
## mean in group No mean in group Yes
## 2.2 2.8
```

In this case we see that there is a statistically significant difference between groups, in the expected direction - regular pot smokers watch more TV.



## 16.2 The t-test as a linear model

The t-test is often presented as a specialized tool for comparing means, but it can also be viewed as an application of the general linear model. In this case, the model would look like this:

$$\hat{BP} = \hat{\beta}_1 * Smoking + \hat{\beta}_0$$

However, smoking is a binary variable, so we treat it as a *dummy variable* like we discussed in the previous chapter, setting it to a value of 1 for smokers and zero for nonsmokers. In that case,  $\hat{\beta}_1$  is simply the difference in means between the two groups, and  $\hat{\beta}_0$  is the mean for the group that was coded as zero. We can fit this model using the `lm()` function, and see that it gives the same t statistic as the t-test above:

```
# print summary of linear regression to perform t-test
s <- summary(lm(TVHrsNum ~ RegularMarij, data = NHANES_sample))
s

##
## Call:
## lm(formula = TVHrsNum ~ RegularMarij, data = NHANES_sample)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -2.810 -1.165 -0.166  0.835  2.834
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)      2.165      0.115   18.86  <2e-16 ***
## RegularMarijYes  0.645      0.213    3.02  0.0028 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 1.4 on 198 degrees of freedom
## Multiple R-squared:  0.0441, Adjusted R-squared:  0.0393
## F-statistic: 9.14 on 1 and 198 DF,  p-value: 0.00282
```

We can also view this graphically (see Figure :

In this case, the predicted value for nonsmokers is  $\hat{\beta}_0$  (2.17) and the predicted value for smokers is  $\hat{\beta}_0 + \hat{\beta}_1$  (2.81).

To compute the standard errors for this analysis, we can use exactly the same equations that we used for linear regression – since this really is just another example of linear regression. In fact, if you compare the p-value from the t-test above with the p-value in the linear regression analysis for the marijuana use variable, you will see that they are exactly the same.

### 16.2.1 Effect sizes for comparing two means

The most commonly used effect size for a comparison between two means is Cohen's d, which (as you may remember from Chapter 11) is an expression of the effect in terms of standard error units. For the t-test estimated using the general linear model outlined above, this is expressed as:

$$d = \frac{\hat{\beta}_1}{SE_{\text{residual}}}$$

We can obtain these values from the analysis output above, giving us a  $d = 0.47$ , which we would generally interpret as a medium sized effect.

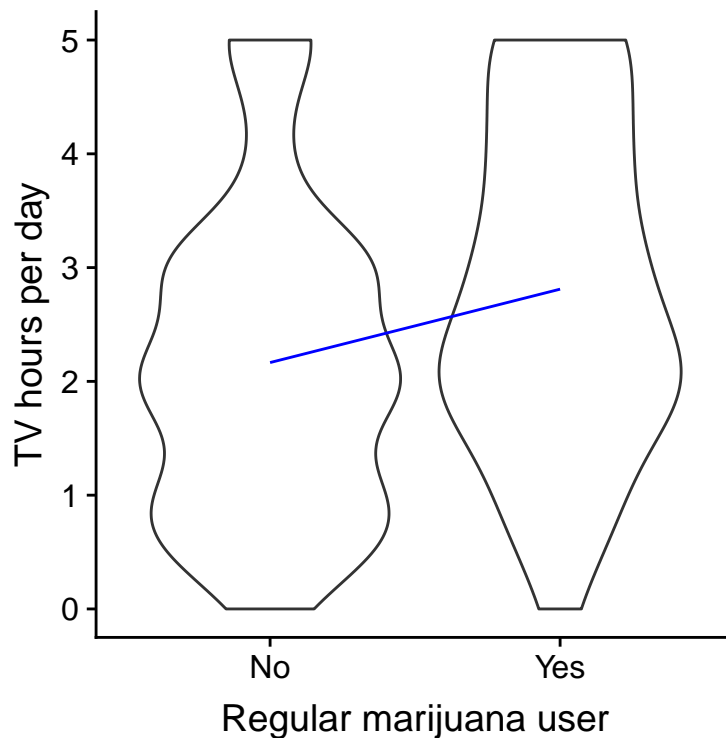


Figure 16.2: Violin plots showing data for each group, with a blue line connecting the predicted values for each group, computed on the basis of the results of the linear model.

We can also compute  $R^2$  for this analysis, which tells us how much variance in TV watching is accounted for. This value (which is reported in the summary of the `lm()` analysis) is 0.04, which tells us that while the effect may be statistically significant, it accounts for relatively little of the variance in TV watching.

### 16.3 Bayes factor for mean differences

As we discussed in the chapter on Bayesian analysis, Bayes factors provide a way to better quantify evidence in favor or against the null hypothesis of no difference.

```
# compute bayes factor for group comparison
bf <- ttestBF(
  formula = TVHrsNum ~ RegularMarij,
  data = NHANES_sample
)
bf
```

```
## Bayes factor analysis
## -----
## [1] Alt., r=0.707 : 11 ±0%
##
## Against denominator:
##   Null, mu1-mu2 = 0
## ---
## Bayes factor type: BFindepSample, JZS
```

This shows us that although the difference between groups is highly significant, the evidence against the null

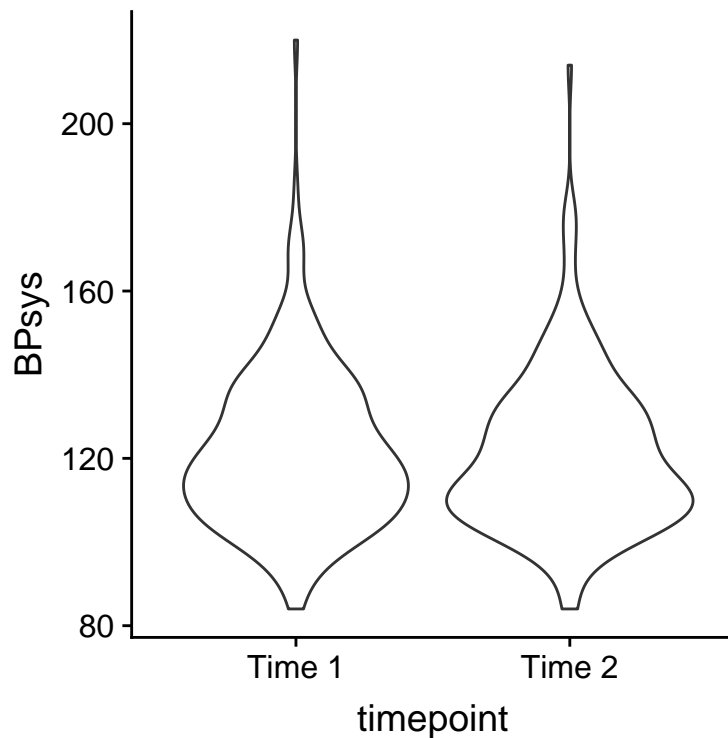


Figure 16.3: Violin plot of systolic blood pressure on first and second recording, from NHANES.

hypothesis is suggestive but not particularly strong.

## 16.4 Paired t-tests

In experimental research, we often use *within-subjects* designs, in which we compare the same person on multiple measurements. For example, in the NHANES dataset blood pressure was measured three times. Let's say that we are interested in testing whether there is a difference in mean blood pressure between the first and second measurement (Figure 16.3).

We see that there does not seem to be much of a difference in mean blood pressure between time points (about one point). First let's test for a difference using an independent samples t-test, which ignores the fact that pairs of data points come from the the same individuals.

```
t.test(
  BPsyst ~ timepoint,
  data = NHANES_sample_tidy,
  paired = FALSE,
  var.equal = TRUE
)

##
## Two Sample t-test
##
## data:  BPsyst by timepoint
## t = 0.5, df = 400, p-value = 0.6
## alternative hypothesis: true difference in means is not equal to 0
## 95 percent confidence interval:
```

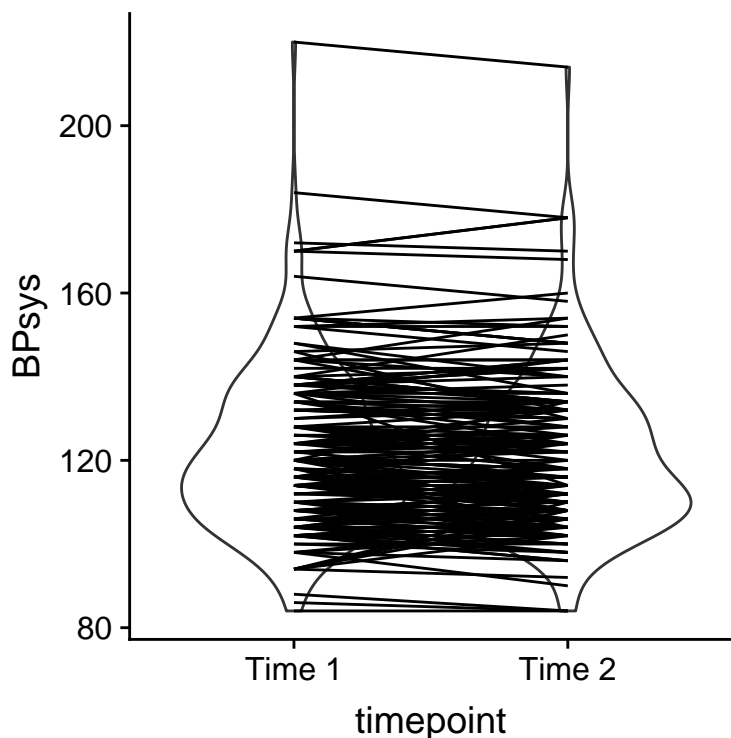


Figure 16.4: Violin plot of systolic BP on each recording, with lines connecting the two data points for each individual.

```
## -2.8 4.6
## sample estimates:
## mean in group BPSys1 mean in group BPSys2
##          122          121
```

This analysis shows no significant difference. However, this analysis is inappropriate since it assumes that the two samples are independent, when in fact they are not, since the data come from the same individuals. We can plot the data with a line for each individual to show this (see Figure 16.4).

In this analysis, what we really care about is whether the blood pressure for each person changed in a systematic way between the two measurements, so another way to represent the data is to compute the difference between the two timepoints for each individual, and then analyze these difference scores rather than analyzing the individual measurements. In Figure 16.5, we show a histogram of these difference scores, with a blue line denoting the mean difference.

### 16.4.1 Sign test

One simple way to test for differences is using a test called the *sign test*, which asks whether the proportion of positive differences (ignoring their magnitude) is different than what we would expect by chance. To do this, we take the differences and compute their sign, and then we use a binomial test to ask whether the proportion of positive signs differs from 0.5.

```
# compute sign test for differences between first and second measurement
npos <- sum(NHANES_sample$diffPos)
bt <- binom.test(npos, nrow(NHANES_sample))
bt

##
```

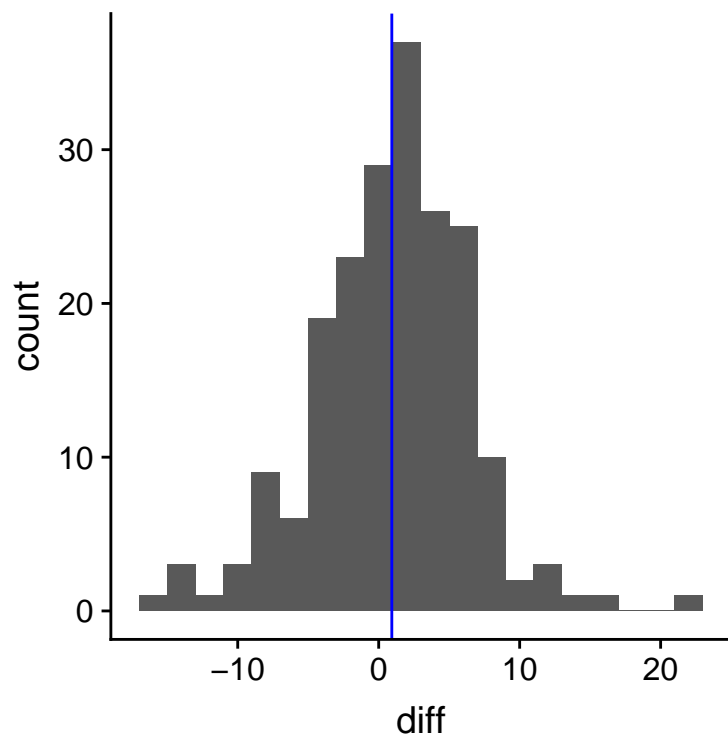


Figure 16.5: Histogram of difference scores between first and second BP measurement.

```
## Exact binomial test
##
## data:  npos and nrow(NHANES_sample)
## number of successes = 100, number of trials = 200, p-value = 0.4
## alternative hypothesis: true probability of success is not equal to 0.5
## 95 percent confidence interval:
##  0.46 0.60
## sample estimates:
## probability of success
##                0.53
```

Here we see that the proportion of individuals with positive signs (0.53) is not large enough to be surprising under the null hypothesis of  $p = 0.5$ . However, one problem with the sign test is that it is throwing away information about the magnitude of the differences, and thus might be missing something.

### 16.4.2 Paired t-test

A more common strategy is to use a *paired t-test*, which is equivalent to a one-sample t-test for whether the mean difference between the measurements is zero. We can compute this using the `t.test()` function in R and setting `paired=TRUE`.

```
# compute paired t-test
t.test(BPsys ~ timepoint, data = NHANES_sample_tidy, paired = TRUE)
```

```
##
## Paired t-test
##
## data:  BPsys by timepoint
```

```
## t = 2, df = 200, p-value = 0.02
## alternative hypothesis: true difference in means is not equal to 0
## 95 percent confidence interval:
##  0.17 1.69
## sample estimates:
## mean of the differences
##                0.93
```

With this analyses we see that there is in fact a significant difference between the two measurements. Let's compute the Bayes factor to see how strong this effect is:

```
# compute Bayes factor for paired t-test
ttestBF(x = NHANES_sample$BPSys1, y = NHANES_sample$BPSys2, paired = TRUE)

## Bayes factor analysis
## -----
## [1] Alt., r=0.707 : 1.3 ±0%
##
## Against denominator:
##   Null, mu = 0
## ---
## Bayes factor type: BFoneSample, JZS
```

This shows us that although the effect was significant in a paired t-test, it actually provides very little evidence in favor of the alternative hypothesis.

### 16.4.3 The paired t-test as a linear model

We can also define the paired t-test in terms of a general linear model. To do this, we include all of the measurements for each subject as data points (within a tidy data frame). We then include in the model a variable that codes for the identity of each individual (in this case, the ID variable that contains a subject ID for each person). This is known as a *mixed model*, since it includes effects of independent variables as well as effects of individuals. The standard model fitting procedure `lm()` can't do this, but we can do it using the `lmer()` function from a popular R package called *lme4*, which is specialized for estimating mixed models. The `(1|ID)` in the formula tells `lmer()` to estimate a separate intercept (which is what the 1 refers to) for each value of the ID variable (i.e. for each individual in the dataset), and then estimate a common slope relating timepoint to BP.

```
# compute mixed model for paired test

lmrResult <- lmer(BPSys ~ timepoint + (1 | ID), data = NHANES_sample_tidy)
summary(lmrResult)

## Linear mixed model fit by REML. t-tests use Satterthwaite's method [
## lmerModLmerTest]
## Formula: BPSys ~ timepoint + (1 | ID)
##   Data: NHANES_sample_tidy
##
## REML criterion at convergence: 2982
##
## Scaled residuals:
##    Min       1Q   Median       3Q      Max
## -2.6985 -0.4478  0.0058  0.3996  2.7395
##
## Random effects:
##  Groups   Name                Variance Std.Dev.
```

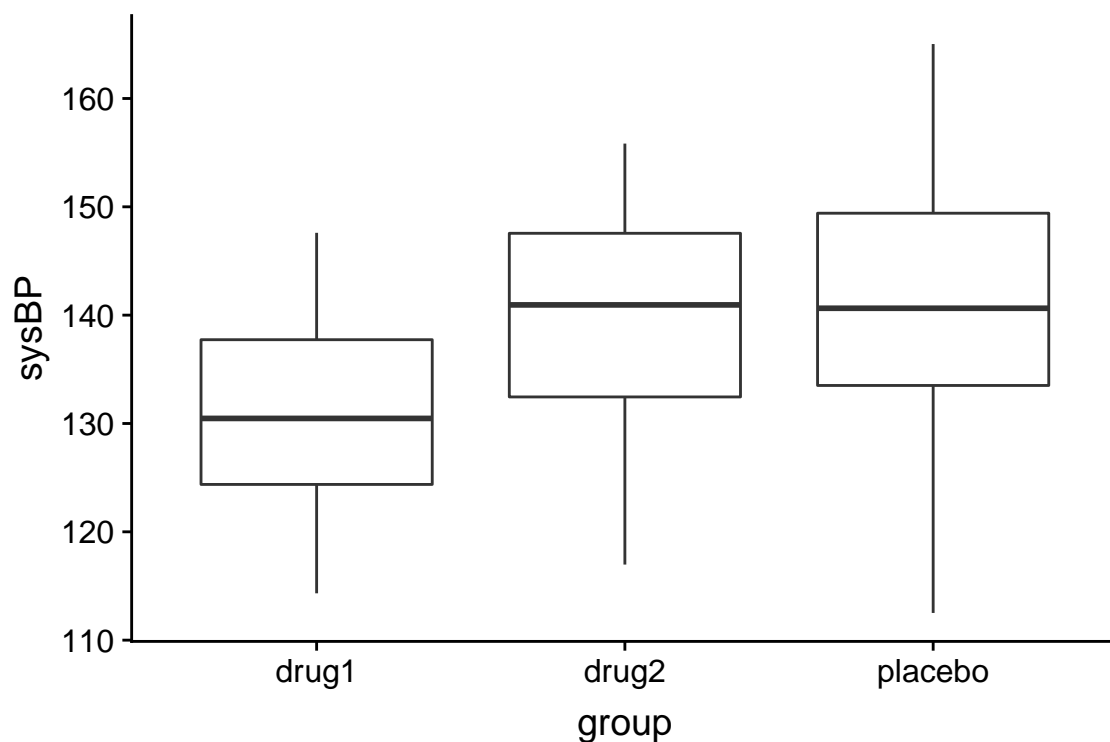


Figure 16.6: Box plots showing blood pressure for three different groups in our clinical trial.

```
## ID      (Intercept) 342      18.49
## Residual          15       3.87
## Number of obs: 400, groups: ID, 200
##
## Fixed effects:
##              Estimate Std. Error    df t value Pr(>|t|)
## (Intercept)    121.770    1.336 207.545    91.2  <2e-16 ***
## timepointBPSys2 -0.930    0.387 199.000    -2.4   0.017 *
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Correlation of Fixed Effects:
##              (Intr)
## tmpntBPSys2 -0.145
```

You can see that this shows us a p-value that is very close to the result from the paired t-test computed using the `t.test()` function.

## 16.5 Comparing more than two means

Often we want to compare more than two means to determine whether any of them differ from one another. Let's say that we are analyzing data from a clinical trial for the treatment of high blood pressure. In the study, volunteers are randomized to one of three conditions: Drug 1, Drug 2 or placebo. Let's generate some data and plot them (see Figure 16.6)

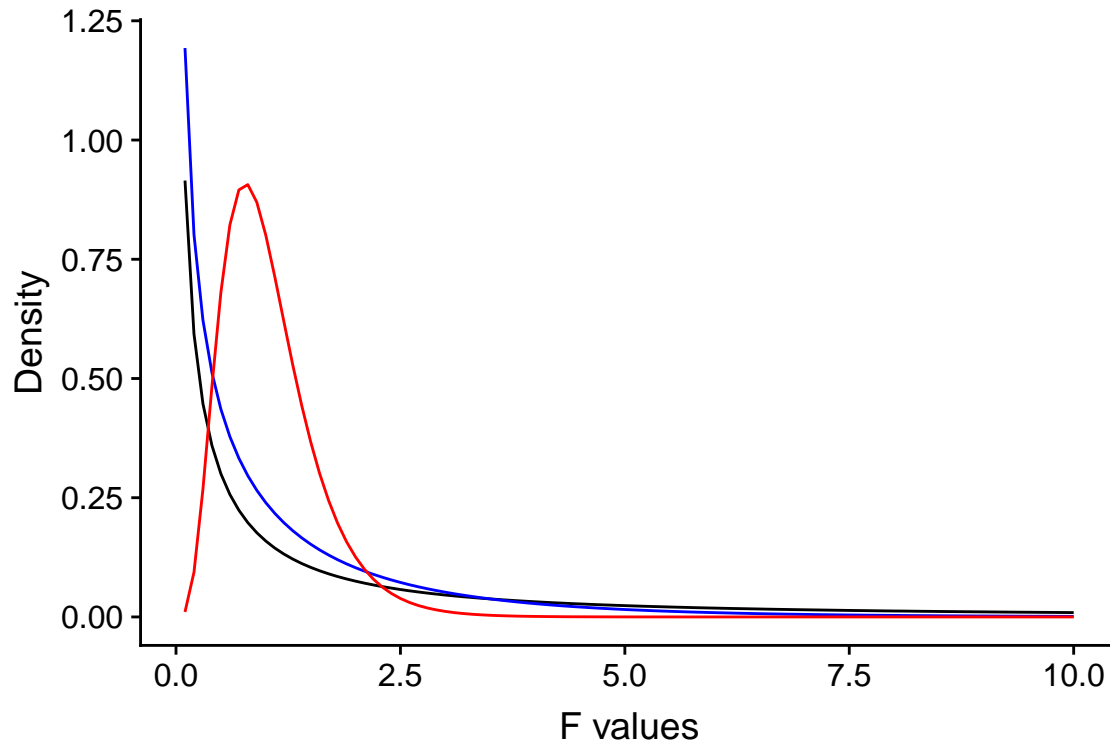


Figure 16.7: F distributions under the null hypothesis, for different values of degrees of freedom.

### 16.5.1 Analysis of variance

We would first like to test the null hypothesis that the means of all of the groups are equal – that is, neither of the treatments had any effect. We can do this using a method called *analysis of variance* (ANOVA). This is one of the most commonly used methods in psychological statistics, and we will only scratch the surface here. The basic idea behind ANOVA is one that we already discussed in the chapter on the general linear model, and in fact ANOVA is just a name for a specific implementation of such a model.

Remember from the last chapter that we can partition the total variance in the data ( $SS_{total}$ ) into the variance that is explained by the model ( $SS_{model}$ ) and the variance that is not ( $SS_{error}$ ). We can then compute a *mean square* for each of these by dividing them by their degrees of freedom; for the error this is  $N - p$  (where  $p$  is the number of means that we have computed), and for the model this is  $p - 1$ :

$$MS_{model} = \frac{SS_{model}}{df_{model}} = \frac{SS_{model}}{p - 1}$$

$$MS_{error} = \frac{SS_{error}}{df_{error}} = \frac{SS_{error}}{N - p}$$

With ANOVA, we want to test whether the variance accounted for by the model is greater than what we would expect by chance, under the null hypothesis of no differences between means. Whereas for the  $t$  distribution the expected value is zero under the null hypothesis, that's not the case here, since sums of squares are always positive numbers. Fortunately, there is another standard distribution that describes how ratios of sums of squares are distributed under the null hypothesis: The  $F$  distribution (see figure 16.7). This distribution has two degrees of freedom, which correspond to the degrees of freedom for the numerator (which in this case is the model), and the denominator (which in this case is the error).



To create an ANOVA model, we extend the idea of *dummy coding* that you encountered in the last chapter. Remember that for the t-test comparing two means, we created a single dummy variable that took the value of 1 for one of the conditions and zero for the others. Here we extend that idea by creating two dummy variables, one that codes for the Drug 1 condition and the other that codes for the Drug 2 condition. Just as in the t-test, we will have one condition (in this case, placebo) that doesn't have a dummy variable, and thus represents the baseline against which the others are compared; its mean defines the intercept of the model. Let's create the dummy coding for drugs 1 and 2.

```
# create dummy variables for drug1 and drug2
df <-
  df %>%
  mutate(
    d1 = as.integer(group == "drug1"), # 1s for drug1, 0s for all other drugs
    d2 = as.integer(group == "drug2")  # 1s for drug2, 0s for all other drugs
  )
```

Now we can fit a model using the same approach that we used in the previous chapter:

```
# fit ANOVA model
lmResultANOVA <- lm(sysBP ~ d1 + d2, data = df)
summary(lmResultANOVA)
```

```
##
## Call:
## lm(formula = sysBP ~ d1 + d2, data = df)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -29.084  -7.745  -0.098   7.687  23.431
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)    141.60      1.66   85.50 < 2e-16 ***
## d1             -10.24      2.34   -4.37 2.9e-05 ***
## d2              -2.03      2.34   -0.87  0.39
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 9.9 on 105 degrees of freedom
## Multiple R-squared:  0.169, Adjusted R-squared:  0.154
## F-statistic: 10.7 on 2 and 105 DF, p-value: 5.83e-05
```

The output from this command provides us with two things. First, it shows us the result of a t-test for each of the dummy variables, which basically tell us whether each of the conditions separately differs from placebo; it appears that Drug 1 does whereas Drug 2 does not. However, keep in mind that if we wanted to interpret these tests, we would need to correct the p-values to account for the fact that we have done multiple hypothesis tests; we will see an example of how to do this in the next chapter.

Remember that the hypothesis that we started out wanting to test was whether there was any difference between any of the conditions; we refer to this as an *omnibus* hypothesis test, and it is the test that is provided by the F statistic. The F statistic basically tells us whether our model is better than a simple model that just includes an intercept. In this case we see that the F test is highly significant, consistent with our impression that there did seem to be differences between the groups (which in fact we know there were, because we created the data).



## Chapter 17

# The process of statistical modeling: A practical example

In this chapter we will bring together everything that we have learned to apply our knowledge to a practical example.

### 17.1 The process of statistical modeling

There is a set of steps that we generally go through when we want to use our statistical model to test a scientific hypothesis:

1. Specify your question of interest
2. Identify or collect the appropriate data
3. Prepare the data for analysis
4. Determine the appropriate model
5. Fit the model to the data
6. Criticize the model to make sure it fits properly
7. Test hypothesis and quantify effect size

Let's look at a real example. In 2007, Christopher Gardner and colleagues from Stanford published a study in the *Journal of the American Medical Association* titled “Comparison of the Atkins, Zone, Ornish, and LEARN Diets for Change in Weight and Related Risk Factors Among Overweight Premenopausal Women The A TO Z Weight Loss Study: A Randomized Trial” (Gardner et al. 2007).

#### 17.1.1 1: Specify your question of interest

According to the authors, the goal of their study was:

To compare 4 weight-loss diets representing a spectrum of low to high carbohydrate intake for effects on weight loss and related metabolic variables.

#### 17.1.2 2: Identify or collect the appropriate data

To answer their question, the investigators randomly assigned each of 311 overweight/obese women to one of four different diets (Atkins, Zone, Ornish, or LEARN), and followed their weight and other measures of health over time.

The authors recorded a large number of variables, but for the main question of interest let's focus on a single variable: Body Mass Index (BMI). Further, since our goal is to measure lasting changes in BMI, we will only look at the measurement taken at 12 months after onset of the diet.

### 17.1.3 3: Prepare the data for analysis

The actual data from the A to Z study are not publicly available, so we will use the summary data reported in their paper to generate some synthetic data that roughly match the data obtained in their study.

*# generate a dataset based on the results of Gardner et al. Table 3*

```
set.seed(123456)
dietDf <-
  data.frame(diet=c(rep('Atkins',77),
                    rep('Zone',79),
                    rep('LEARN',79),
                    rep('Ornish',76))) %>%

  mutate(
    BMICChange12Months=ifelse(diet=='Atkins',
                              rnorm(n=77,mean=-1.65,sd=2.54),
                              ifelse(diet=='Zone',
                                      rnorm(n=79,mean=-0.53,sd=2.0),
                                      ifelse(diet=='LEARN',
                                            rnorm(n=79,mean=-0.92,sd=2.0),
                                            rnorm(n=76,mean=-0.77,sd=2.14))))),
    physicalActivity=ifelse(diet=='Atkins',
                            rnorm(n=77,mean=34,sd=6),
                            ifelse(diet=='Zone',
                                    rnorm(n=79,mean=34,sd=6.0),
                                    ifelse(diet=='LEARN',
                                          rnorm(n=79,mean=34,sd=5.0),
                                          rnorm(n=76,mean=35,sd=7) )))

  )

summaryDf <-
  dietDf %>%
  group_by(diet) %>%
  summarize(
    n=n(),
    meanBMICChange12Months=mean(BMICChange12Months),
    varBMICChange12Months=var(BMICChange12Months)
  ) %>%
  mutate(
    crit_val_lower = qt(.05, n - 1),
    crit_val_upper = qt(.95, n - 1),
    ci.lower=meanBMICChange12Months+(sqrt(varBMICChange12Months)*crit_val_lower)/sqrt(n),
    ci.upper=meanBMICChange12Months+(sqrt(varBMICChange12Months)*crit_val_upper)/sqrt(n)
  )

summaryDf %>%
  dplyr::select(-crit_val_lower,-crit_val_upper) %>%
  pander()
```

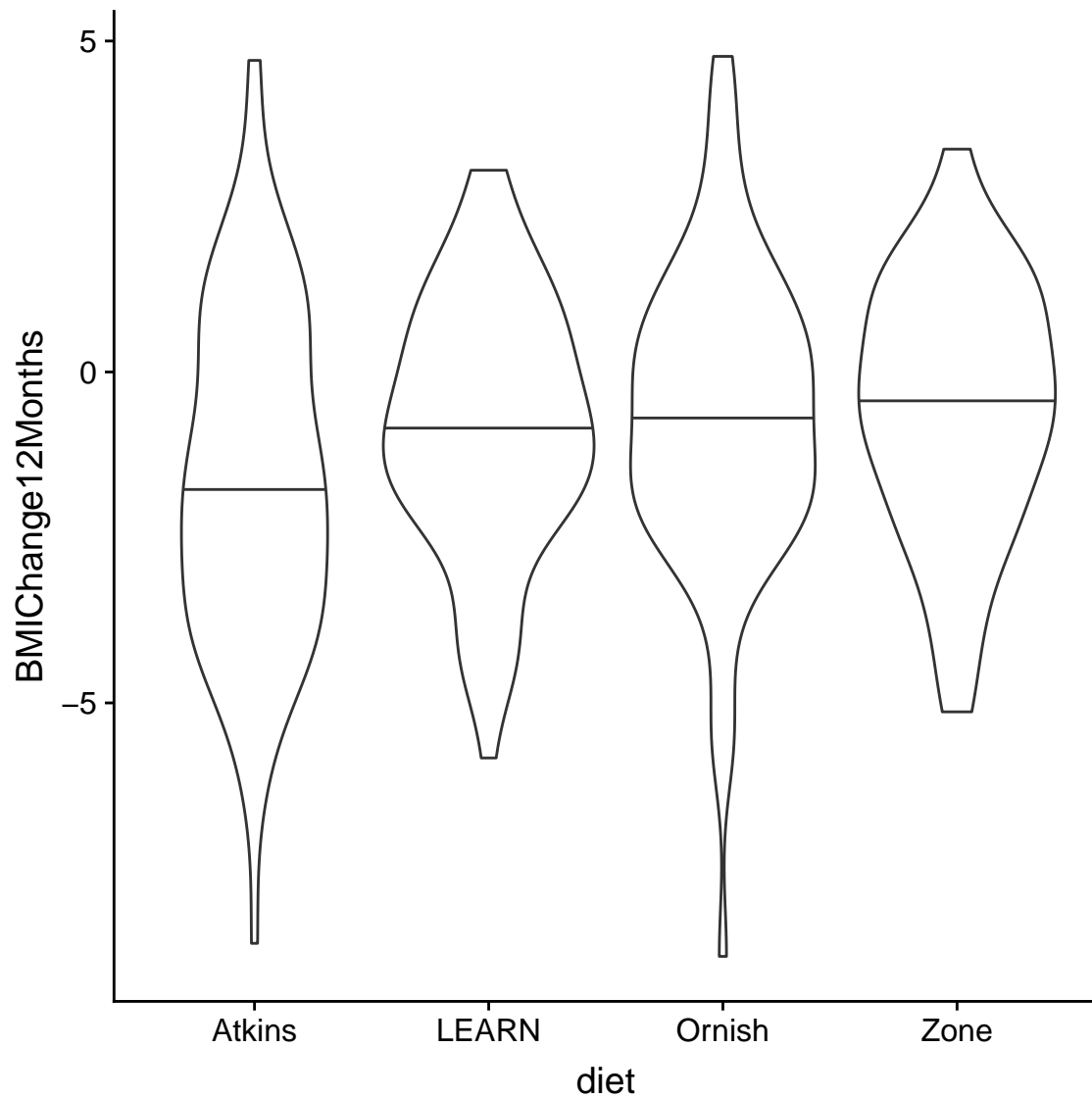


Figure 17.1: Violin plots for each condition, with the 50th percentile (i.e the median) shown as a black line for each group.

| diet   | n  | meanBMICChange12Months | varBMICChange12Months | ci.lower | ci.upper |
|--------|----|------------------------|-----------------------|----------|----------|
| Atkins | 77 | -1.62                  | 6.52                  | -2.11    | -1.14    |
| LEARN  | 79 | -0.85                  | 3.77                  | -1.21    | -0.49    |
| Ornish | 76 | -0.69                  | 5.36                  | -1.13    | -0.25    |
| Zone   | 79 | -0.57                  | 3.76                  | -0.93    | -0.21    |

Now that we have the data, let's visualize them to make sure that there are no outliers. Violin plots are useful to see the shape of the distributions, as shown in Figure 17.1. Those data look fairly reasonable - in particular, there don't seem to be any serious outliers. However, we can see that the distributions seem to vary a bit in the variance, with Atkins and Ornish showing greater variability than the others. This means that any analyses that assume the variances are equal across groups could be inappropriate.

### 17.1.4 4. Determine the appropriate model

There are several questions that we need to ask in order to determine the appropriate statistical model for our analysis.

- What kind of dependent variable?
- BMI : continuous, roughly normally distributed
- What are we comparing?
- mean BMI across four diet groups
- ANOVA is appropriate
- Are observations independent?
- random assignment and use of difference scores should ensure that IID assumption is appropriate

### 17.1.5 5. Fit the model to the data

Let's run an ANOVA on BMI change to compare it across the four diets. It turns out that we don't actually need to generate the dummy-coded variables ourselves; if we give `lm()` a categorical variable, it will automatically generate them for us.

```
# perform ANOVA and print result

lmResult <- lm(BMIChange12Months ~ diet, data = dietDf)
lmResult

##
## Call:
## lm(formula = BMIChange12Months ~ diet, data = dietDf)
##
## Coefficients:
## (Intercept)    dietLEARN    dietOrnish    dietZone
##      -1.622         0.772         0.932         1.050
```

Note that `lm` automatically generated dummy variables that correspond to three of the four diets, leaving the Atkins diet without a dummy variable. This means that the intercept models the Atkins diet, and the other three variables model the difference between each of the those diets and the Atkins diet.

### 17.1.6 6. Criticize the model to make sure it fits properly

The first thing we want to do is to critique the model to make sure that it is appropriate. One thing we can do is to look at the residuals from the model. In Figure 17.2, we will plot the residuals for each individual grouped by diet. We have jittered the points so that we can see all of them. There are no obvious differences in the residuals across conditions, suggesting that we can move forward and interpret the model outputs.

### 17.1.7 7. Test hypothesis and quantify effect size

First let's look at the summary of results from the ANOVA:

```
# print summary of ANOVA statistics

summary(lmResult)

##
## Call:
## lm(formula = BMIChange12Months ~ diet, data = dietDf)
```

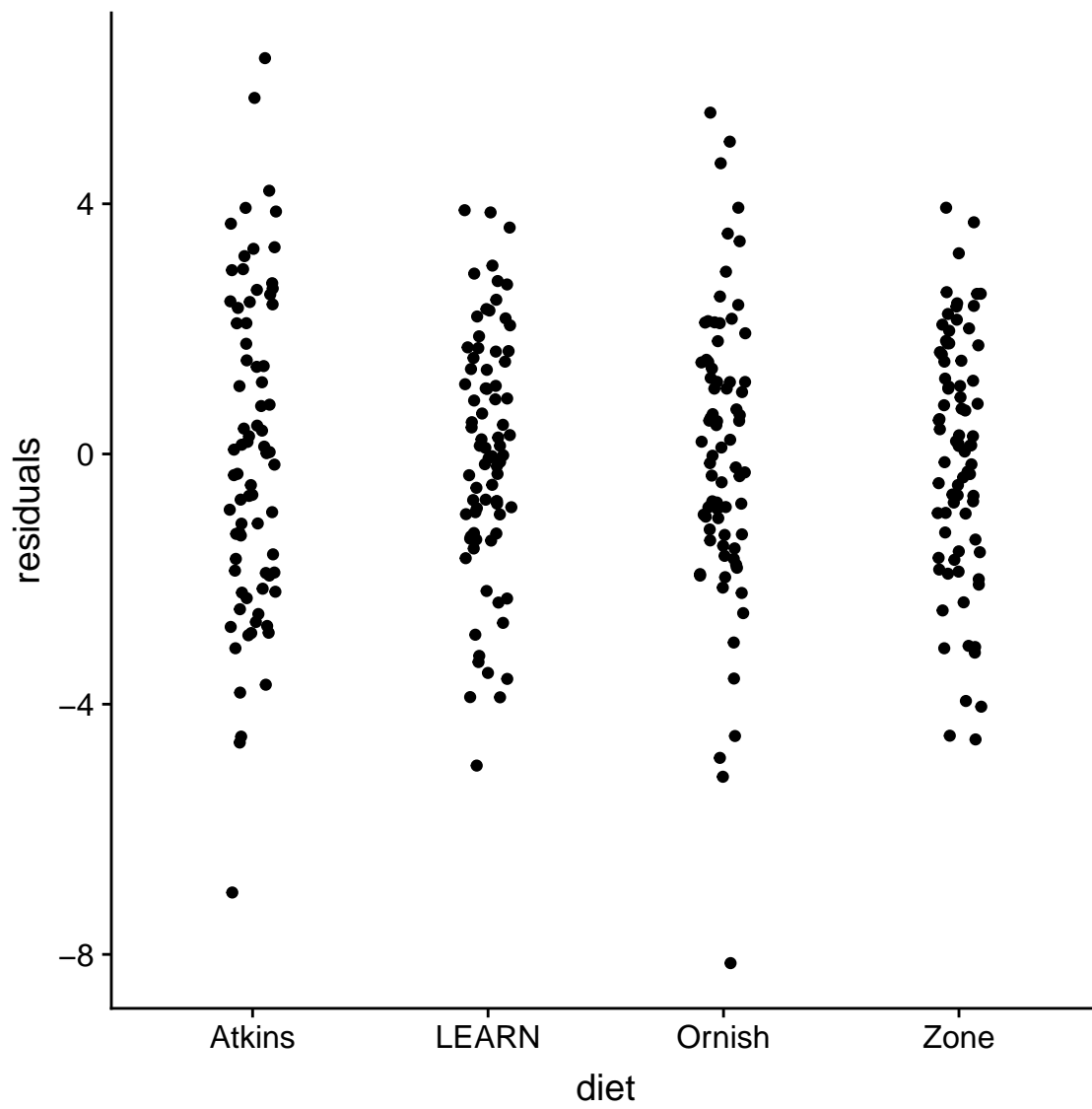


Figure 17.2: Residuals from model plotted for each group separately.

```
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -8.14  -1.37   0.07   1.50   6.33
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  -1.622     0.251   -6.47  3.8e-10 ***
## dietLEARN     0.772     0.352    2.19  0.0292 *
## dietOrnish    0.932     0.356    2.62  0.0092 **
## dietZone      1.050     0.352    2.98  0.0031 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 2.2 on 307 degrees of freedom
## Multiple R-squared:  0.0338, Adjusted R-squared:  0.0243
## F-statistic: 3.58 on 3 and 307 DF,  p-value: 0.0143
```

The significant F test shows us that there is a significant difference between diets, but we should also note that the model doesn't actually account for much variance in the data; the R-squared value is only 0.03, showing that the model is only accounting for a few percent of the variance in weight loss. Thus, we would not want to overinterpret this result.

The significant result also doesn't tell us which diets differ from which others. We can find out more by comparing means across conditions using the `emmeans()` (“estimated marginal means”) function:

```
# compute the differences between each of the means
leastsquare <- emmeans(lmResult,
                      pairwise ~ diet,
                      adjust="tukey")

# display the results by grouping using letters

CLD(leastsquare$emmeans,
    alpha=.05,
    Letters=letters)
```

```
## diet    emmean    SE df lower.CL upper.CL .group
## Atkins  -1.62 0.25 307     -2.1   -1.129    a
## LEARN   -0.85 0.25 307     -1.3   -0.363   ab
## Ornish  -0.69 0.25 307     -1.2   -0.193    b
## Zone    -0.57 0.25 307     -1.1   -0.085    b
##
## Confidence level used: 0.95
## P value adjustment: tukey method for comparing a family of 4 estimates
## significance level used: alpha = 0.05
```

The letters in the rightmost column show us which of the groups differ from one another, using to a method that adjusts for the number of comparisons being performed. This shows that Atkins and LEARN diets don't differ from one another (since they share the letter a), and the LEARN, Ornish, and Zone diets don't differ from one another (since they share the letter b), but the Atkins diet differs from the Ornish and Zone diets (since they share no letters).



### 17.1.7.1 Bayes factor

Let's say that we want to have a better way to describe the amount of evidence provided by the data. One way we can do this is to compute a Bayes factor, which we can do by fitting the full model (including diet) and the reduced model (without diet) and then comparing their fit. For the reduced model, we just include a 1, which tells the fitting program to only fit an intercept.

```
brmFullModel <- brm(BMICChange12Months ~ diet, data = dietDf,
  save_all_pars = TRUE)

brmReducedModel <- brm(BMICChange12Months ~ 1, data = dietDf,
  save_all_pars = TRUE)

bayes_factor(brmFullModel, brmReducedModel)
```

```
## Iteration: 1
## Iteration: 2
## Iteration: 3
## Iteration: 4
## Iteration: 1
## Iteration: 2
## Iteration: 3
## Iteration: 4
## Iteration: 5

## Estimated Bayes factor in favor of bridge1 over bridge2: 99.86593
```

This shows us that there is very strong evidence (Bayes factor of nearly 100) for differences between the diets.

### 17.1.8 What about possible confounds?

If we look more closely at the Garder paper, we will see that they also report statistics on how many individuals in each group had been diagnosed with *metabolic syndrome*, which is a syndrome characterized by high blood pressure, high blood glucose, excess body fat around the waist, and abnormal cholesterol levels and is associated with increased risk for cardiovascular problems. Let's first add those data into the summary data frame:

```
summaryDf <-
  summaryDf %>%
  mutate(
    nMetSym=c(22,20,29,27),
    nNoMetSym=n-nMetSym,
    pMetSym=nMetSym/(nMetSym+nNoMetSym)
  )

summaryDf %>%
  dplyr::select(diet,n,pMetSym) %>%
  pandier()
```

| diet   | n  | pMetSym |
|--------|----|---------|
| Atkins | 77 | 0.29    |
| LEARN  | 79 | 0.25    |
| Ornish | 76 | 0.38    |
| Zone   | 79 | 0.34    |

Looking at the data it seems that the rates are slightly different across groups, with more metabolic syndrome cases in the Ornish and Zone diets – which were exactly the diets with poorer outcomes. Let's say that we are interested in testing whether the rate of metabolic syndrome was significantly different between the groups, since this might make us concerned that these differences could have affected the results of the diet outcomes.

### 17.1.8.1 Determine the appropriate model

- What kind of dependent variable?
- proportions
- What are we comparing?
- proportion with metabolic syndrome across four diet groups
- chi-squared test for goodness of fit is appropriate against null hypothesis of no difference

Let's compute that statistic using the `chisq.test()` function:

```
chisq.test(summaryDf$nMetSym,summaryDf$nNoMetSym)
```

```
##
## Pearson's Chi-squared test
##
## data: summaryDf$nMetSym and summaryDf$nNoMetSym
## X-squared = 10, df = 9, p-value = 0.2
```

This test shows that there is not a significant difference between means. However, it doesn't tell us how certain we are that there is no difference; remember that under NHST, we are always working under the assumption that the null is true unless the data show us enough evidence to cause us to reject this null hypothesis.

What if we want to quantify the evidence for or against the null? We can do this using the Bayes factor.

```
bf <- contingencyTableBF(as.matrix(summaryDf[,9:10]),
                        sampleType = "indepMulti",
                        fixedMargin = "cols")
bf
```

```
## Bayes factor analysis
## -----
## [1] Non-indep. (a=1) : 0.058 ±0%
##
## Against denominator:
##   Null, independence, a = 1
## ---
## Bayes factor type: BFcontingencyTable, independent multinomial
```

This shows us that the alternative hypothesis is 0.058 times more likely than the null hypothesis, which means that the null hypothesis is  $1/0.058 \sim 17$  times more likely than the alternative hypothesis given these data. This is fairly strong, if not completely overwhelming, evidence.

### 17.1.8.2 Addressing confounds in the model

We generally use random assignment to treatments (as Gardner et al. did) because we think that, on average, it will prevent the effects of other variables (which we call *confounds*) on the outcome. However, as we see in this case, in any particular study there could be a confound that occurs randomly. It is important to make sure that the differences between conditions are not due to differences between groups in the presence of metabolic syndrome, and to do this we can include the metabolic syndrome variable in our statistical model.

By doing this, any variance that is associated with metabolic syndrome will be removed from the effect of the diet, so that we are left with a cleaner measurement of the effect of the diet.

In this case we don't have the original data



## Chapter 18

# Doing reproducible research

Most people think that science is a reliable way to answer questions about the world. When our physician prescribes a treatment we trust that it has been shown to be effective through research, and we have similar faith that the airplanes that we fly in aren't going to fall from the sky. However, since 2005 there has been an increasing concern that science may not always work as well as we have long thought that it does. In this chapter we will discuss these concerns about reproducibility of scientific research, and outline the steps that one can take to make sure that our statistical results are as reproducible as possible.

### 18.1 How we think science should work

Let's say that we are interested in a research project on how children choose what to eat. This is a question that was asked in a study by the well-known eating researcher Brian Wansink and his colleagues in 2012. The standard (and, as we will see, somewhat naive) view goes something like this:

- You start with a hypothesis
- Branding with popular characters should cause children to choose “healthy” food more often
- You collect some data
- Offer children the choice between a cookie and an apple with either an Elmo-branded sticker or a control sticker, and record what they choose
- You do statistics to test the null hypothesis
- “The preplanned comparison shows Elmo-branded apples were associated with an increase in a child's selection of an apple over a cookie, from 20.7% to 33.8% ( $\chi^2=5.158$ ;  $P=.02$ )” (Wansink, Just, and Payne 2012)
- You make a conclusion based on the data \*“this study suggests that the use of branding or appealing branded characters may benefit healthier foods more than they benefit indulgent, more highly processed foods. Just as attractive names have been shown to increase the selection of healthier foods in school lunchrooms, brands and cartoon characters could do the same with young children.”(Wansink, Just, and Payne 2012)

### 18.2 How science (sometimes) actually works

Brian Wansink is well known for his books on “Mindless Eating”, and his fee for corporate speaking engagements is in the tens of thousands of dollars. In 2017, a set of researchers began to scrutinize some of his published research, starting with a set of papers about how much pizza people ate at a buffet. The researchers asked Wansink to share the data from the studies but he refused, so they dug into his published papers and found a large number of inconsistencies and statistical problems in the papers. The publicity

around this analysis led a number of others to dig into Wansink’s past, including obtaining emails between Wansink and his collaborators. As reported by Stephanie Lee at Buzzfeed, these emails showed just how far Wansink’s actual research practices were from the naive model:

... back in September 2008, when Payne was looking over the data soon after it had been collected, he found no strong apples-and-Elmo link — at least not yet. ... “I have attached some initial results of the kid study to this message for your report,” Payne wrote to his collaborators. “Do not despair. It looks like stickers on fruit may work (with a bit more wizardry).” ... Wansink also acknowledged the paper was weak as he was preparing to submit it to journals. The p-value was 0.06, just shy of the gold standard cutoff of 0.05. It was a “sticking point,” as he put it in a Jan. 7, 2012, email. ... “It seems to me it should be lower,” he wrote, attaching a draft. “Do you want to take a look at it and see what you think. If you can get the data, and it needs some tweeking, it would be good to get that one value below .05.” ... Later in 2012, the study appeared in the prestigious JAMA Pediatrics, the 0.06 p-value intact. But in September 2017, it was retracted and replaced with a version that listed a p-value of 0.02. And a month later, it was retracted yet again for an entirely different reason: Wansink admitted that the experiment had not been done on 8- to 11-year-olds, as he’d originally claimed, but on preschoolers.

This kind of behavior finally caught up with Wansink; fifteen of his research studies have been retracted and in 2018 he resigned from his faculty position at Cornell University.

## 18.3 The reproducibility crisis in science

One might hope that Brian Wansink was a rare outlier, but it has become increasingly clear that problems with reproducibility are much more widespread in science than previously thought. This became clear in 2015, when a large group of researchers published a study in the journal *Science* titled “Estimating the reproducibility of psychological science” (Open Science Collaboration 2015). In this study, the researchers took 100 published studies in psychology and attempted to reproduce the results originally reported in the papers. Their findings were shocking: Whereas 97% of the original papers had reported statistically significant findings, only 37% of these effects were statistically significant in the replication study. Although these problems in psychology have received a great deal of attention, they seem to be present in nearly every area of science, from cancer biology (Errington et al. 2014) and chemistry (Baker 2017) to economics (Christensen and Miguel 2016) and the social sciences (Camerer et al. 2018).

The reproducibility crisis that emerged after 2010 was actually predicted by John Ioannidis, a physician from Stanford who wrote a paper in 2005 titled “Why most published research findings are false” (Ioannidis 2005). In this article, Ioannidis argued that the use of null hypothesis statistical testing in the context of modern science will necessarily lead to high levels of false results.

### 18.3.1 Positive predictive value and statistical significance

Ioannidis’ analysis focused on a concept known as the *positive predictive value*, which is defined as the proportion of positive results (which generally translates to “statistically significant findings”) that are true:

$$PPV = \frac{p(\text{true positive result})}{p(\text{true positive result}) + p(\text{false positive result})}$$

Assuming that we know the probability that our hypothesis is true ( $p(hIsTrue)$ ), then the probability of a true positive result is simply  $p(hIsTrue)$  multiplied by the statistical power of the study:

$$p(\text{true positive result}) = p(hIsTrue) * (1 - \beta)$$

where  $\beta$  is the false negative rate. The probability of a false positive result is determined by  $p(hIsTrue)$  and the false positive rate  $\alpha$ :

$$p(\text{false positive result}) = (1 - p(hIsTrue)) * \alpha$$

PPV is then defined as:

$$PPV = \frac{p(hIsTrue) * (1 - \beta)}{p(hIsTrue) * (1 - \beta) + (1 - p(hIsTrue)) * \alpha}$$

Let's first take an example where the probability of our hypothesis being true is high, say 0.8 - though note that in general we cannot actually know this probability. Let's say that we perform a study with the standard values of  $\alpha = 0.05$  and  $\beta = 0.2$ . We can compute the PPV as:

$$PPV = \frac{0.8 * (1 - 0.2)}{0.8 * (1 - 0.2) + (1 - 0.8) * 0.05} = 0.98$$

This means that if we find a positive result in a study where the hypothesis is likely to be true and power is high, then its likelihood of being true is high. Note, however, that a research field where the hypotheses have such a high likelihood of being true is probably not a very interesting field of research; research is most important when it tells us something new!

Let's do the same analysis for a field where  $p(hIsTrue) = 0.1$  - that is, most of the hypotheses being tested are false. In this case, PPV is:

$$PPV = \frac{0.1 * (1 - 0.2)}{0.1 * (1 - 0.2) + (1 - 0.1) * 0.05} = 0.307$$

This means that in a field where most of the hypotheses are likely to be wrong (that is, an interesting scientific field where researchers are testing risky hypotheses), even when we find a positive result it is more likely to be false than true! In fact, this is just another example of the base rate effect that we discussed in the context of hypothesis testing - when an outcome is unlikely, then it's almost certain that most positive outcomes will be false positives.

We can simulate this to show how PPV relates to statistical power, as a function of the prior probability of the hypothesis being true (see Figure 18.1)

Unfortunately, statistical power remains low in many areas of science (Smaldino and McElreath 2016), suggesting that many published research findings are false.

### 18.3.2 The winner's curse

Another kind of error can also occur when statistical power is low: Our estimates of the effect size will be inflated. This phenomenon often goes by the term "winner's curse", which comes from economics, where it refers to the fact that for certain types of auctions (where the value is the same for everyone, like a jar of quarters, and the bids are private), the winner almost always pays more than the good is worth. In science, the winner's curse refers to the fact that the effect size estimated from a significant result (i.e. a winner) is almost always an overestimate of the true effect size.

We can simulate this in order to see how the estimated effect size for significant results is related to the actual underlying effect size. Let's generate data for which there is a true effect size of 0.2, and estimate the effect size for those results where there is a significant effect detected. Figure 18.2 shows that when power is low, the estimated effect size for significant results can be highly inflated compared to the actual effect size.

We can look at a single simulation to see why this is the case. In Figure 18.3, you can see a histogram of the estimated effect sizes for 1000 samples, separated by whether the test was statistically significant. It should be clear from the figure that if we estimate the effect size only based on significant results, then our estimate

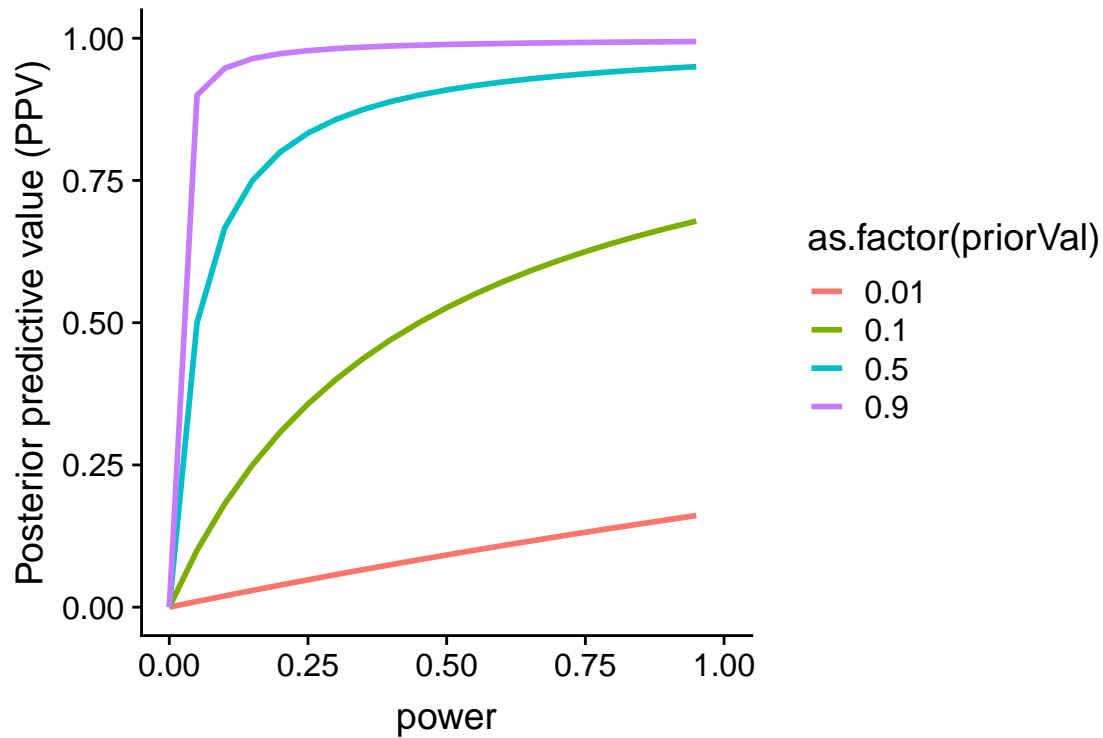


Figure 18.1: A simulation of posterior predictive value as a function of statistical power (plotted on the x axis) and prior probability of the hypothesis being true (plotted as separate lines).

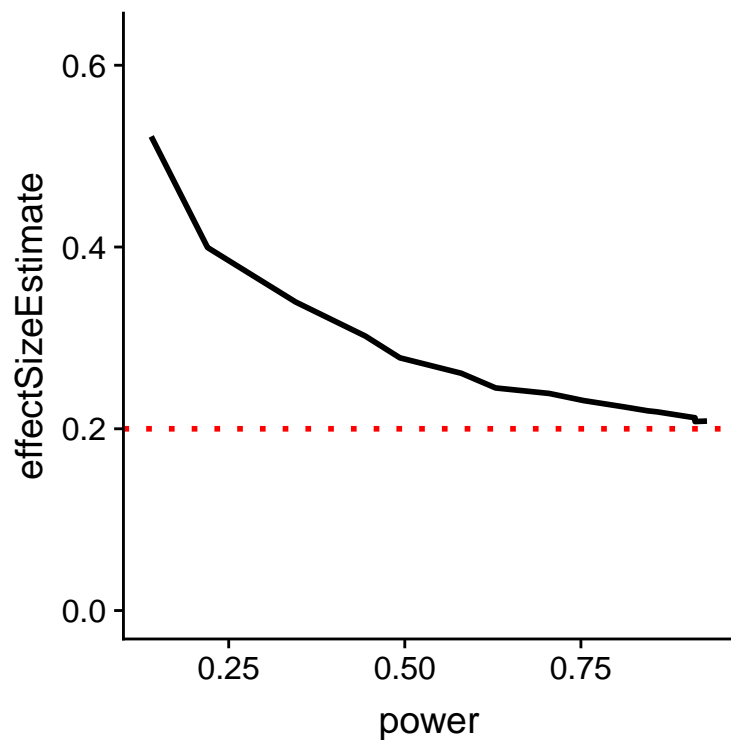


Figure 18.2: A simulation of the winner's curse as a function of statistical power (x axis). The black line shows the estimated effect size, and the red dashed line shows the actual effect size.



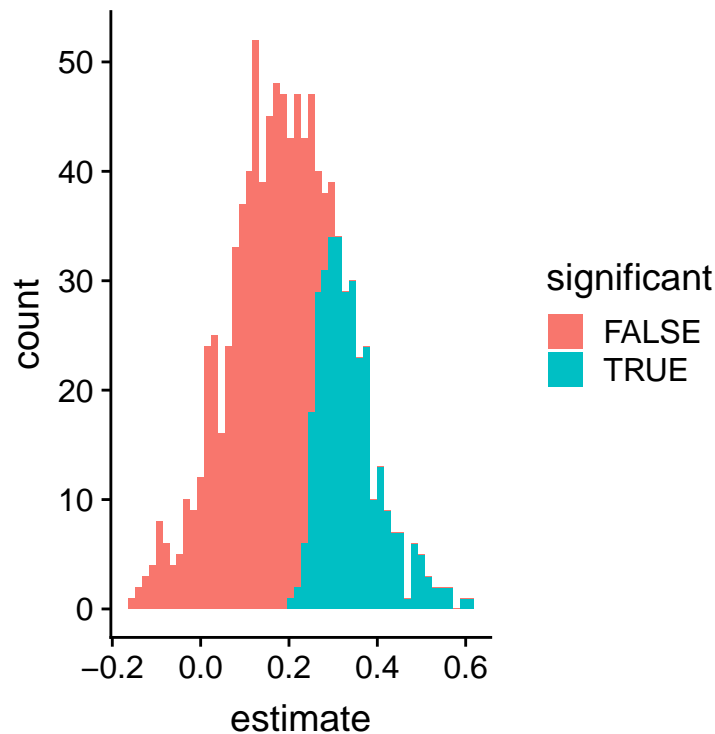


Figure 18.3: A histogram showing sample sizes for a number of samples from a dataset, with significant results shown in blue and non-significant results in red.

will be inflated; only when most results are significant (i.e. power is high and the effect is relatively large) will our estimate come near the actual effect size.

## 18.4 Questionable research practices

A popular book entitled “The Compleat Academic: A Career Guide”, published by the American Psychological Association (Darley, Zanna, and Roediger 2004), aims to provide aspiring researchers with guidance on how to build a career. In a chapter by well-known social psychologist Daryl Bem titled “Writing the Empirical Journal Article”, Bem provides some suggestions about how to write a research paper. Unfortunately, the practices that he suggests are deeply problematic, and have come to be known as *questionable research practices* (QRPs).

**Which article should you write?** There are two possible articles you can write: (1) the article you planned to write when you designed your study or (2) the article that makes the most sense now that you have seen the results. They are rarely the same, and the correct answer is (2).

What Bem suggests here is known as *HARKing* (Hypothesizing After the Results are Known) (Kerr 1998). This might seem innocuous, but is problematic because it allows the research to re-frame a post-hoc conclusion (which we should take with a grain of salt) as an a priori prediction (in which we would have stronger faith). In essence, it allows the researcher to rewrite their theory based on the facts, rather than using the theory to make predictions and then test them – akin to moving the goalpost so that it ends up wherever the ball goes. It thus becomes very difficult to disconfirm incorrect ideas, since the goalpost can always be moved to match the data.

**Analyzing data** Examine them from every angle. Analyze the sexes separately. Make up new composite indices. If a datum suggests a new hypothesis, try to find further evidence for it

elsewhere in the data. If you see dim traces of interesting patterns, try to reorganize the data to bring them into bolder relief. If there are participants you don't like, or trials, observers, or interviewers who gave you anomalous results, drop them (temporarily). Go on a fishing expedition for something — anything — interesting. No, this is not immoral.

What Bem suggests here is known as *p-hacking*, which refers to trying many different analyses until one finds a significant result. Bem is correct that if one were to report every analysis done on the data then this approach would not be “immoral”. However, it is rare to see a paper discuss all of the analyses that were performed on a dataset; rather, papers often only present the analyses that *worked* - which usually means that they found a statistically significant result. There are many different ways that one might p-hack:

- Analyze data after every subject, and stop collecting data once  $p < .05$
- Analyze many different variables, but only report those with  $p < .05$
- Collect many different experimental conditions, but only report those with  $p < .05$
- Exclude participants to get  $p < .05$
- Transform the data to get  $p < .05$

A well-known paper by Simmons, Nelson, and Simonsohn (2011) showed that the use of these kinds of p-hacking strategies could greatly increase the actual false positive rate, resulting in a high number of false positive results.

### 18.4.1 ESP or QRP?

In 2011, Daryl Bem published an article (Bem 2011) that claimed to have found scientific evidence for extrasensory perception. The article states:

This article reports 9 experiments, involving more than 1,000 participants, that test for retroactive influence by “time-reversing” well-established psychological effects so that the individual's responses are obtained before the putatively causal stimulus events occur. . . . The mean effect size (d) in psi performance across all 9 experiments was 0.22, and all but one of the experiments yielded statistically significant results.

As researchers began to examine Bem's article, it became clear that he had engaged in all of the QRPs that he had recommended in the chapter discussed above. As Tal Yarkoni pointed out in a blog post that examined the article:

- Sample sizes varied across studies
- Different studies appear to have been lumped together or split apart
- The studies allow many different hypotheses, and it's not clear which were planned in advance
- Bem used one-tailed tests even when it's not clear that there was a directional prediction (so alpha is really 0.1)
- Most of the p-values are very close to 0.05
- It's not clear how many other studies were run but not reported

## 18.5 Doing reproducible research

In the years since the reproducibility crisis arose, there has been a robust movement to develop tools to help protect the reproducibility of scientific research.

### 18.5.1 Pre-registration

One of the ideas that has gained the greatest traction is *pre-registration*, in which one submits a detailed description of a study (including all data analyses) to a trusted repository (such as the Open Science

Framework or AsPredicted.org. By specifying one's plans in detail prior to analyzing the data, pre-registration provides greater faith that the analyses do not suffer from p-hacking or other questionable research practices.

The effects of pre-registration have been seen in clinical trials in medicine. In 2000, the National Heart, Lung, and Blood Institute (NHLBI) began requiring all clinical trials to be pre-registered using the system at ClinicalTrials.gov. This provides a natural experiment to observe the effects of study pre-registration. When Kaplan and Irvin (2015) examined clinical trial outcomes over time, they found that the number of positive outcomes in clinical trials was reduced after 2000 compared to before. While there are many possible causes, it seems likely that prior to study registration researchers were able to change their methods in order to find a positive result, which became more difficult after registration was required.

### 18.5.2 Reproducible practices

The paper by Simmons, Nelson, and Simonsohn (2011) laid out a set of suggested practices for making research more reproducible, all of which should become standard for researchers:

- Authors must decide the rule for terminating data collection before data collection begins and report this rule in the article.
- Authors must collect at least 20 observations per cell or else provide a compelling cost-of-data-collection justification.
- Authors must list all variables collected in a study.
- Authors must report all experimental conditions, including failed manipulations.
- If observations are eliminated, authors must also report what (the statistical results are if those observations are included).
- If an analysis includes a covariate, authors must report the statistical results of the analysis without the covariate.

### 18.5.3 Replication

One of the hallmarks of science is the idea of *replication* – that is, other researchers should be able to perform the same study and obtain the same result. Unfortunately, as we saw in the outcome of the Replication Project discussed earlier, many findings are not replicable. The best way to ensure replicability of one's research is to first replicate it on your own; for some studies this just won't be possible, but whenever it is possible one should make sure that one's finding holds up in a new sample. That new sample should be sufficiently powered to find the effect size of interest; in many cases, this will actually require a larger sample than the original.

It's important to keep a couple of things in mind with regard to replication. First, the fact that a replication attempt fails does not necessarily mean that the original finding was false; remember that with the standard level of 80% power, there is still a one in five chance that the result will be nonsignificant, even if there is a true effect. For this reason, we generally want to see multiple replications of any important finding before we come to believe it. Unfortunately, many fields including psychology have failed to follow this advice in the past, leading to "textbook" findings that turn out to be likely false. With regard to Daryl Bem's studies of ESP, a large replication attempt involving 7 studies failed to replicate his findings (Galak et al. 2012).

Second, remember that the p-value doesn't provide us with a measure of the likelihood of a finding to replicate. As we discussed previously, the p-value is a statement about the likelihood of one's data under a specific null hypothesis; it doesn't tell us anything about the probability that the finding is actually true (as we learned in the chapter on Bayesian analysis). In order to know the likelihood of replication we need to know the probability that the finding is true, which we generally don't know.

## 18.6 Doing reproducible data analysis

So far we have focused on the ability to replicate other researchers' findings in new experiments, but another important aspect of reproducibility is to be able to reproduce someone's analyses on their own data, which we refer to a *computational reproducibility*. This requires that researchers share both their data and their analysis code, so that other researchers can both try to reproduce the result as well as potentially test different analysis methods on the same data. There is an increasing move in psychology towards open sharing of code and data; for example, the journal *Psychological Science* now provides "badges" to papers that share research materials, data, and code, as well as for pre-registration.

The ability to reproduce analyses is one reason that we strongly advocate for the use of scripted analyses (such as those using R) rather than using a "point-and-click" software package. It's also a reason that we advocate the use of free and open-source software (like R) as opposed to commercial software packages, which will require others to buy the software in order to reproduce any analyses.

There are many ways to share both code and data. A common way to share code is via web sites that support *version control* for software, such as Github. Small datasets can also be shared via these same sites; larger datasets can be shared through data sharing portals such as Zenodo, or through specialized portals for specific types of data (such as OpenNeuro for neuroimaging data).

## 18.7 Conclusion: Doing better science

It is every scientist's responsibility to improve their research practices in order to increase the reproducibility of their research. It is essential to remember that the goal of research is not to find a significant result; rather, it is to ask and answer questions about nature in the most truthful way possible. Most of our hypotheses will be wrong, and we should be comfortable with that, so that when we find one that's right, we will be even more confident in its truth.

## 18.8 Suggested Readings

- Rigor Mortis: How Sloppy Science Creates Worthless Cures, Crushes Hope, and Wastes Billions, by Richard Harris
- Improving your statistical inferences - an online course on how to do better statistical analysis, including many of the points raised in this chapter.

# Chapter 19

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