A User's Guide to Statistical Inference and Regression

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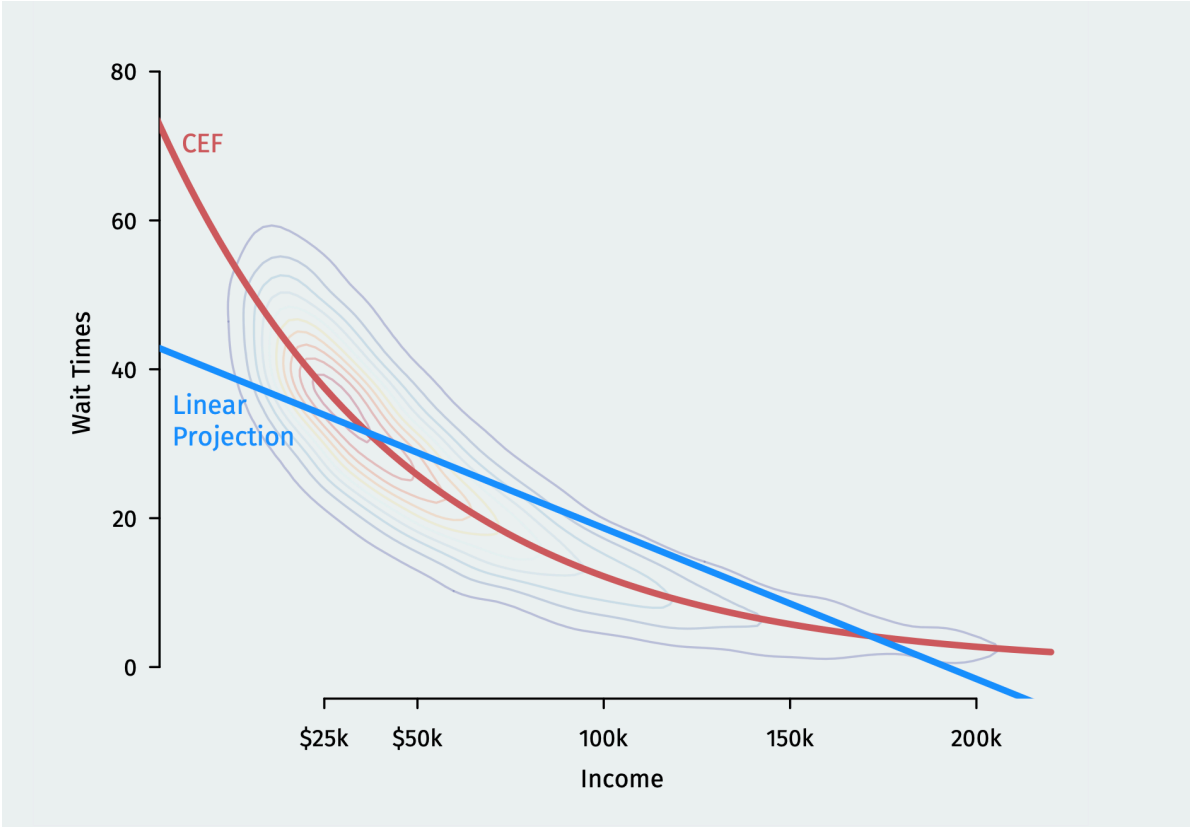
Preface



This book, like many before it, will try to teach you statistics. The field of statistics describes how we learn about the world using quantitative data. In the social sciences, an increasing share of empirical studies use statistical methods to provide evidence for or against conceptual arguments. And, while it is possible to conduct quantitative research without understanding statistics at an intuitive level, it is not a good idea. Quantitative research involves a host of *choices* about the model to use, variables to include, tuning parameters to set, assumptions to make, and so on. Without a deep understanding of statistics, you may find these choices bewildering and confusing, and you may simply (and possibly erroneously) yield to the default settings of your statistical software.

The goal of this book is to give you the foundation to make methodological choices for your specific application with knowledge and with confidence. The material is intended for first-year PhD students in political science, but it may be of interest more broadly.

We will focus on two key goals:

1. **Understand the basic ways to assess estimators** With quantitative data, we often want to make statistical inferences about some unknown feature of the world. We use estimators (which are just ways of summarizing our data) to estimate these features. This book will introduce the basics of this task at a general enough level to be applicable to almost any estimator that you are likely to encounter in empirical research in the social sciences. We will also cover major concepts such as bias, sampling variance, consistency, and asymptotic normality, which are so common to such a large swath of (frequentist) inference that understanding them at a deep level will yield an enormous return on your time investment. Once you understand these core ideas, you will have a language to analyze any fancy new estimator that pops up in the next few decades.
2. **Apply these ideas to the estimation of regression models** This book will apply these ideas to one particular social science workhorse: regression. Many methods either use regression estimators like ordinary least squares or extend them in some way. Understanding how these estimators work is vital for conducting research, for reading and reviewing contemporary scholarship, and, frankly, for being a good and valuable colleague in seminars and workshops. Regression and regression estimators also provide an entry point for discussing parametric models as approximations, rather than as rigid assumptions about the truth of a given specification.

Why write a book on statistics and regression when so many already exist? While some texts at this level exist in the fields of statistics and economics, they tend to focus on applications and models less relevant to other social sciences. This book attempts to correct this. The book also seeks to introduce a fairly high level of mathematical sophistication that will challenge and push you to develop stronger foundations in the material.

Roadmap

This book has two major parts. Part I introduces the basics of statistical inference.

We start in Chapter 1 by demonstrating basic concepts of estimation and inference from the design-based perspective in which we sample from a fixed, finite population, and all uncertainty comes from randomness over who is and is not included in the sample. This framework for inference has deep roots in the statistical literature and provides a great deal of intuition for how estimation and uncertainty work in simple settings. We will discuss how to use design-based inference to estimate features of the population from samples when the analyst knows the exact sampling design. Unfortunately, researchers often lack this knowledge about how their data came to be, limiting the usefulness of this approach.

Chapter 2 introduces a more flexible approach to estimation: model-based inference. With this approach, the researcher posits a probability model for how the data came to be. This book focuses on models that posit "independent and identically distributed" data for this model. The chapter describes how estimation and inference proceed under these models and also introduces a broad class of estimators based on the plug-in principle.

These two chapters focus on finite sample properties of different estimation techniques, but we can say more about an estimator if we consider how it behaves on larger and larger samples. Chapter 3 introduces this type of asymptotic analysis. It covers the core results of asymptotic theory, such as the law of large numbers, the central limit theorem, and the delta method, but also shows why these results are important for statistical inference. In particular, the chapter shows how these results enable the creation of asymptotically valid confidence intervals.

Chapter 4 wraps up Part I of the book by introducing statistical inference with hypothesis testing. This chapter shows how to build hypothesis tests and provides intuition for all their aspects. We also cover power analyses for planning studies and the connection between confidence intervals and hypothesis tests.

Part II of the book focuses on one particular estimator of great importance to quantitative social sciences: the least squares estimator.

Chapter 5 begins by describing exactly what quantity of interest we are targeting when we discuss "linear models." In particular, we discuss how a population best linear predictor exists even if the relationship between two variables is nonlinear. This provides a coherent basis for linear regression estimation as a linear approximation to a potentially nonlinear function. The chapter also shows how to interpret the coefficients in these linear regression models.

Chapter 6 introduces the more mechanical properties of the least squares estimator: how the estimator is constructed, its geometrical interpretation, and how influential observa-

tions may affect the estimates it returns. This chapter introduces the least squares estimator in matrix form and provides key intuition for understanding this compact notation.

Finally, Chapter 7 describes the statistical properties of the least squares estimator. The chapter shows how modeling assumptions affect the kinds of properties we can obtain. The weakest modeling assumptions allow us to derive the surprisingly strong asymptotic properties of least squares that we depend on in most settings. The chapter then shows how stronger assumptions such as linearity and normally distributed errors can provide even stronger results but that they do so at the expense of potential model misspecification.

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Colophon

You can find the source for this book at https://github.com/mattblackwell/gov2002-book. Any typos or errors can be reported at https://github.com/mattblackwell/gov2002-book/issues. Thanks for reading.

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Part I

Statistical Inference

1 Design-based Inference

1.1 Introduction

Quantitative analysis of social data has an alluring exactness to it. It allows us to estimate the average number of minutes of YouTube videos watched to the millisecond, and in doing so it gives us the aura of true scientists. But the advantage of quantitative analyses lies not in the ability to derive precise three-decimal point estimates; rather, quantitative methods shine because they allow us to communicate methodological goals, assumptions, and results in a (hopefully) common, compact, and precise mathematical language. It is this language that helps clarify *exactly* what researchers are doing with their data and why.

This dewy view of quantitative methods is unfortunately often at odds with how these methods are used in the real world. All too often we as researchers find some arbitrary data, apply a statistical tool with which we are familiar, and then shoehorn the results into a theoretical story that may or may not have a (tenuous) connection. Quantitative methods applied this way will provide us with a very specific answer to a murky question about a shapeless target.

This book is a guide to a better foundation for quantitative analysis and, in particular, for statistical inference. Inference is the task of using the data we have to learn something about the data we do not have.

The organizing motto of this book is to help us as researchers be

> Precise in stating our goals, transparent in stating our assumptions, and honest in evaluating our results.

These goals are the target of our inference – or what do we want to learn and about whom.

In pursuing these goals, this book will focus on a general workflow for statistical inference. The workflow boils down to answering a series of questions about the goals, assumptions, and methods of our analysis:

1. **Population**: who or what do we want to learn about?
2. **Design/model**: how will we collect the data, or, what assumptions are we making about how the data came to be?
3. **Quantity of Interest**: what do we want to learn about the population?

4. **Estimator**: how will we use the data to produce an estimate?
5. **Uncertainty**: how will we estimate and convey the error associated with the estimate?

These questions form the core of any quantitative research endeavor. And the answers to these will draw on a mixture of substantive interests, feasibility, and statistical theory, and this mixture will vary from question to question. For example, the population of interest can vary greatly from study to study, whereas many disparate studies may employ the same estimand and estimator.

The third core question is particularly important, since it highlights an essential division in how researchers approach statistical inference – specifically, **design-based inference** vs **model-based inference**. Design-based inference typically focuses on situations in which we have precise knowledge of how our sample was randomly selected from the population. Uncertainty here comes exclusively from the random nature of which observations are included in the sample. By contrast, in the **model-based** framework, we treat our data as random variables and propose a probabilistic model for how the data came to exist. The models then vary in the strength of their assumptions.

Design-based inference is the framework that addresses the core inferential questions most crisply, and so it is the focus of this chapter. Its main disadvantages are that it is considerably less general than the model-based approach and that the mathematics of the framework are slightly more complicated.

We will now go over each of the core questions in more detail.

1.2 Question 1: Population

Inference is the task of using the data that we have to learn facts about the world (i.e., the data we do not have). The most straightforward setting is when we have a fixed set of units that we want to learn something about. These units are what we call the **population** or **target population**. We are going to focus on random sampling from this population, but, to do so, we need to have a list of units from the population. This list of N units is called the **frame** or **sampling frame**, and we will index these units in the sampling frame by $i \in \mathcal{U} = \{1, \ldots, N\}$. Here we assume that N, the size of the population, is known, but note that this may not always be true.

The sampling frame may differ from the target population simply for feasibility reasons. For example, the target population might include all the households in a given city, but the sampling frame might be the list of all residential telephone numbers for that city. Of course, many households do not have landline telephones and rely on mobile phone exclusively. This gap between the target population and the sampling frame is called **undercoverage** or **coverage bias**.

Example 1.1. An early but prominent example of frame bias in survey sampling is the infamous *Literary Digest* poll of the 1936 U.S. presidential election. *Literary Digest*, a (now defunct) magazine, sent over 10 million ballots to addresses found in automobile registration lists and telephone books, trying to figure out who would win the important 1936 presidential race. The sample size was huge: over 2 million respondents. In the end, the results predicted that Alf Landon, the Republican candidate, would receive 55% of the vote, while the incumbent, Democratic President Franklin D. Roosevelt, would only win 41% of the vote. Unfortunately for the *Literary Digest*, Landon only received 37% of the vote.

There are many possible reasons for this massive polling error. Most obviously, the sampling frame was different from that of the target population. Why? Only those with either a car or a telephone were included in the sampling frame, and people without either overwhelmingly supported the Democrat, Roosevelt. While this is not the only source of bias – differential nonresponse seems to be a particularly big problem –the frame bias contributes a large part of the error. For more about this poll, see SQUIRE (1988).

One advantage of design-based inference is how precisely we must articulate the sampling frame. We can be extremely clear about the group of units we are trying to learn

about. We shall see that in model-based inference the concept of the population and sampling frame become more amorphous.

Example 1.2 (American National Election Survey, Population)**.** According to the materials from the American National Election Survey (ANES) in 2012, its target population is all U.S. citizens age 18 or older. The sampling frame for the face-to-face portion of the survey "consisted of the Delivery Sequence File (DSF) used by the United States Postal Service" for residential delivery of mail." Unfortunately, there are housing units that are covered by mail delivery by the postal service which would result in the potential for frame bias. The designers of the ANES used the Decennial Census to add many of these units to the final sampling frame.

1.3 Question 2: Sampling design

Now that we have a clearly defined population and sampling frame, we can consider how to select a sample from the population. We will focus on **probabilistic samples**, where units are selected into the sample by chance, and each unit in the sampling frame has a non-0 probability of being included. Let $\mathcal{S} \subset \mathcal{U}$ be a sample and let $\mathbf{Z} = (Z_1, Z_2, \ldots, Z_N)$ to be a vector of inclusion indicators such that $Z_i = 1$ if $i \in \mathcal{S}$ and $Z_i = 0$ otherwise. We denote these indicators as upper-case letters because they are random variables. We assume the sample size is $|\mathcal{S}| = n$.

Suppose our sampling frame was the hobbits who are members of the Fellowship of the Ring, an exclusive group brought into being by a wizened elf lord. This group of four hobbits is a valid – albeit small and fictional population – with $\mathcal{U} =$ {Frodo, Sam, Pip, Merry}.

Suppose we want to sample two hobbits from this group. We can list all six possible samples of size two from this population in terms of the sample members $\mathcal{S}$ or, equivalently, the inclusion indicators $\mathbf{Z}$:

- $\mathcal{S}_1 =$ {Frodo, Sam} with $\mathbf{Z}_1 = (1, 1, 0, 0)$
- $\mathcal{S}_2 =$ {Frodo, Pip} with $\mathbf{Z}_2 = (1, 0, 1, 0)$
- $\mathcal{S}_3 =$ {Frodo, Merry} with $\mathbf{Z}_3 = (1, 0, 0, 1)$
- $\mathcal{S}_4 =$ {Sam, Pip} with $\mathbf{Z}_4 = (0, 1, 1, 0)$
- $\mathcal{S}_5 =$ {Sam, Merry} with $\mathbf{Z}_5 = (0, 1, 0, 1)$
- $\mathcal{S}_6 =$ {Pip, Merry} with $\mathbf{Z}_6 = (0, 0, 1, 1)$

A **sampling design** is a complete specification of how likely to be selected each of these samples is. That is, we need to determine a selection probability π_j for each sample $\mathcal{S}_j$. The most widely used and widely studied design is one that places equal probability on each of the possible samples of size n.

Definition 1.1. A **simple random sample** (srs) is a probability sampling design where each possible sample of size n has the same probability of occurring. More specifically, let $\mathbf{z} = (z_1, \dots, z_N)$ be a particular possible sampling, then,

$$\mathbb{P}(\mathbf{Z} = \mathbf{z}) = \begin{cases} \binom{N}{n}^{-1} & \text{if } \sum_{i=1}^{N} z_i = n, \\ 0 & \text{otherwise} \end{cases}$$

If we sampled two hobbits, the srs (the simple random sample) would place $1/\binom{4}{2} = 1/6$ probability of each of the above samples $\mathcal{S}_j$. Note that the srs gives zero probability to any sample that does not have exactly n units in the sample.

Another common sampling design –the **Bernoulli sampling** design – works by choosing each unit independently with the same probability.

Definition 1.2. Bernoulli sampling is a probability sampling design where independent Bernoulli trials with probability of success q determine whether each unit in the population will be included in the sample. More specifically, let $\mathbf{z} = (z_1, \dots, z_N)$ be a particular possible sampling. Bernoulli sampling will then be

$$\mathbb{P}(\mathbf{Z} = \mathbf{z}) = \mathbb{P}(Z_1 = z_1) \cdots \mathbb{P}(Z_N = z_N) = \prod_{i=1}^{N} q_i^{Z_i} (1 - q_i)^{1 - Z_i}$$

Bernoulli sampling is very straightforward because independently selecting units simplifies many calculations. However, this "coin flipping" approach means that the sample size, $N_s = \sum_{i=1}^{N} Z_i$, will be itself a random variable because it is the result of how many of the coin flips land on "heads."

Simple random samples and Bernoulli random samples are simple to understand and implement. For large surveys, the sampling designs are often much more complicated for cost-saving reasons. We now describe the sampling design for the ANES, which contains many design features typical of similar large surveys.

Example 1.3 (American National Election Survey, Sampling Design)**.** The ANES uses a typical yet complicated design for its 2012 face-to-face survey. First, the designers divided (or stratified) U.S. states into nine Census divisions (which are based on geography). Within each division, designers then randomly sampled a number of census tracts (with higher number of sampled tracts for divisions with higher populations). The census tracts with larger populations are selected with higher probability.

The second stage randomly samples addresses from the sampling frame (described in Example 1.2). More households were sampled from tracts with higher proportion of Black and Latino residents to obtain an oversample of these groups.

Finally, the third stage of sampling was to randomly select one eligible person per household for completion of the survey.

1.4 Question 3: Quantity of Interest

The **quantity of interest** is a numerical summary of the population that we want to learn about. These quantities are also called **estimands** (Latin for "the thing to be estimated").

Let $x_1, x_2, \dots, x_N$ be a fixed set of characteristics, or items, about the population. Using the statistician's favorite home decor, we might think about our population as a set of marbles in a jar where the x_i values indicate, for example, the color of the i-th marble. In a survey, x_i might represent the age, ideology, or income of the i-th person in the population.

We can define many useful quantities of interest based on the population characteristics. These quantities generally summarize the values $x_1, \dots, x_N$. One of the most common, and certainly one of the most useful, is the **population mean**, defined as

$$\overline{x} = \frac{1}{N} \sum_{i=1}^{N} x_i.$$

The population mean is fixed because N and the population characteristics $x_1, \dots, x_N$ are fixed. Another common estimand in the survey sampling literature is the population total,

$$t = \sum_{i=1}^{N} x_i = N\overline{x}.$$

Example 1.4 (Subpopulation means)**.** We may also be interested in quantities for different subdomains. Suppose we are interested in estimating the fraction of (say) conservative-identifying respondents who support increasing legal immigration. Let $d = 1, \dots, D$ be the number of subdomains or subpopulations. In this case, we might have $d = 1$ as liberal identifiers, $d = 2$ as moderate identifiers, and $d = 3$ as conservative identifiers. We will refer to the subpopulation for each of these groups as $\mathcal{U}_d \subset \{1, \dots, N\}$ and we define the size of these groups as $N_d = |\mathcal{U}_d$. So, N_3 would be the number of conservative-identifying citizens in the population.

The mean for each group is then

$$\overline{x}_d = \frac{1}{N_d} \sum_{i \in \mathcal{U}_d} x_i.$$

Subpopulation estimation can be slightly more complicated than population estimation because we may not know who is in which subpopulation until we actually sample the population. For example, our sampling frame probably may not information about 'potential respondents' ideology. Thus, N_d will be unknown to the researcher, unlike N for the population mean, which is known.

We may be interested in many other quantities of interest, but design-based inference is largely focused on these types of population and subpopulation means and totals.

1.5 Question 4: Estimator

Now that we have a sampling design and a quantity of interest, we can consider what we can learn about this quantity of interest from our sample. An **estimator** is a function of the sample measurements intended as a best guess about our quantity of interest.

If the most common estimand is the population mean, the most popular estimator is the **sample mean**, defined as

$$\overline{X}_n = \frac{1}{n} \sum_{i=1}^{N} Z_i x_i$$

The sample mean is a **random** quantity since it varies from sample to sample, and those samples are chosen probabilistically. For example, suppose we have height measurements from our small population of hobbits in Table 1.1.

Table 1.1: A small population of hobbits

Unit (i)	Height in cm (x_i)
1 (Frodo)	124
2 (Sam)	127
3 (Pip)	123
4 (Merry)	127

If we consider a simple random sample of size $n = 2$ from this population, we can list the probability of all possible sample means associated with this sampling design as we do in Table 1.2. Table 1.3 combines the equivalent values of the sample mean to arrive at the **sampling distribution** of the sample mean of hobbit height under a srs of size 2.

Table 1.2: All possible simple random samples of size 2 from the hobbit population

Sample (j)	Probability (π_j)	Sample mean ($\overline{X}_n$)
1 (Frodo, Sam)	1/6	(124 + 127) / 2 = 125.5
2 (Frodo, Pip)	1/6	(124 + 123) / 2 = 123.5
3 (Frodo, Merry)	1/6	(124 + 127) / 2 = 125.5
4 (Sam, Pip)	1/6	(127 + 123) / 2 = 125
5 (Sam, Merry)	1/6	(127 + 127) / 2 = 127
6 (Pip, Merry)	1/6	(123 + 127) / 2 = 125

Table 1.3: Sampling distribution of the sample mean for simple random samples of size 2 from the hobbit population

Sample mean	Probability
123.5	1/6
125	1/3
125.5	1/3
127	1/6

Thus, the sampling distribution tells us what values of an estimator are more or less likely and depends on both the population distribution and the sampling design.

> **Note**
>
> Notice that the sampling distribution of an estimator will depend on the sampling design. Here, we used a simple random sample. Bernoulli sampling would have produced a different distribution. Using Bernoulli sampling, we could end up with a sample of just Frodo, in which case the sample mean would be his height (124cm), a sample mean value that is impossible with simple random sampling of size $n = 2$.

1.5.1 Properties of the sampling distribution of an estimator

Generally speaking, we want "good" estimators. But what makes an estimator "good'"? The best estimator would obviously be the one that is right all of the time ($\overline{X}_n = \overline{x}$ with probability 1), but this is only possible if we conduct a census –that is, sample everyone in the population – or the population does not vary. Neither situation is typical for most researchers.

We instead focus on properties of the sampling distribution of an estimator. The following types of questions get at these properties:

- Are the estimator's observed values (realizations) centered on the true value of the quantity of interest? (unbiasedness)
- Is there a lot or a little variation in the realizations of the estimator across different samples from the population? (sample variance)
- On average, how close to the truth is the estimator? (mean square error)

The answers to these questions will depend on (a) the estimator and (b) the sampling design.

To back up, the sampling distribution shows us all the possible values of an estimator across different samples from the population. If we want to summarize this distribution with a single number, we would focus on its expectation, which is a measure of central tendency of the distribution. Roughly speaking, we want the center of the distribution to be close to and ideally equal to the true quantity of interest. If this is not the case, that means the estimator systematically over- or under-estimates the truth. We call this difference the **bias** of an estimator, which can be written mathematically as

$$\text{bias}[\overline{X}_n] = \mathbb{E}[\overline{X}_n] - \overline{x}.$$

Any estimator that has bias equal to zero is call an **unbiased** estimator.

We can calculate the bias of our hobbit srs (where we sampled two hobbits from the Fellowship of the Ring with equal probability) by first calculating the expected value of the estimator,

$$\mathbb{E}[\overline{X}_n] = \frac{1}{6} \cdot 123.5 + \frac{1}{3} \cdot 125 + \frac{1}{3} \cdot 125.5 + \frac{1}{6} \cdot 127 = 125.25,$$

and comparing this to the population mean,

$$\overline{x} = \frac{1}{4}(124 + 127 + 123 + 127) = 125.25.$$

The two are the same, meaning the sample mean in this simple random sample is unbiased.

> **Warning**
>
> Note that the word "bias" sometimes also refers to research that is systematically incorrect in other ways. For example, we might complain that a survey question is biased if it presents a leading or misleading question or if it mismeasures the concept of interest. To see this, suppose we wanted to estimate the proportion of a population that regularly donates money to a political campaign, but x_i actually measures whether a person donated on the day of the survey. In this case, $\overline{x}$ would be quite a bit lower than the quantity of interest because it only captures one day of donation patterns, not regular donations made over time. Textbooks often refer to this gap between the measures we obtain and the measures we want as **measurement bias**. This is distinct from the bias of the sample mean. Using our donations example, taking an srs from the population of daily donors, $\overline{X}_n$ would still result in an unbiased estimate for $\overline{x}$, even if that is entirely the wrong quantity of interest.

Is the unbiasedness of our hobbit sampling unique to this example? Thankfully no. We can prove that the sample mean will be unbiased for the population mean under a simple random sample. Relying on the definition of the sample mean, we can obtain:

$$\mathbb{E}[\overline{X}_n] = \mathbb{E}\left[\frac{1}{n}\sum_{i=1}^{N} Z_i x_i\right] = \frac{1}{n}\sum_{i=1}^{N} \mathbb{E}[Z_i]x_i = \frac{1}{n}\sum_{i=1}^{N} \frac{n}{N} x_i = \frac{1}{N}\sum_{i=1}^{N} x_i = \overline{x}$$

Using $\mathbb{E}[Z_i] = n/N$ for the simple random sample in the second equality is key. Intuitively, the probability of being included in the sample is simply the fraction of the sample being selected, n/N.

The second salient feature of an estimator's sampling distribution is its spread. Generally speaking, we prefer an estimator whose estimates are very similar from sample to sample over an estimator whose estimates vary wildly from one sample to the next. We quantify this spread with the **sampling variance**, which is simply the variance of the sampling distribution of the estimator, or

$$\mathbb{V}[\overline{X}_n] = \mathbb{E}[(\overline{X}_n - \mathbb{E}[\overline{X}_n])^2].$$

An alternative measure of spread is the **standard error** of the estimator, which is the square root of the sampling variance,

$$\mathsf{se}[\overline{X}_n] = \sqrt{\mathbb{V}[\overline{X}_n]}.$$

The standard error is often more interpretable because it is on the same scale as the original variable. Using our hobbits' heights example, the sampling variance would be measured in centimeters squared but the standard error would be measured in centimeters and, thus, easier to interpret.

The final important property is the **mean squared error** or **MSE**, which (as its name implies) measures the average of the squared error:

$$\text{MSE} = \mathbb{E}[(\overline{X}_n - \overline{x})^2].$$

Keen-eyed readers might find this quantity redundant because, as we showed above, the sample mean is unbiased, so $\mathbb{E}[\overline{X}_n] = \overline{x}$. This, in turn, means that the sampling variance of the sample mean is just the mean squared error. However, circumstances will often conspire to make us use biased estimators, so these two quantities will differ. In fact, if we have an estimator $\widehat{\theta}$ for some population quantity θ,

$$\begin{aligned}
\text{MSE}[\widehat{\theta}] &= \mathbb{E}[(\widehat{\theta} - \theta)^2] \\
&= \mathbb{E}[(\widehat{\theta} - \mathbb{E}[\widehat{\theta}] + \mathbb{E}[\widehat{\theta}] - \theta)^2] \\
&= \mathbb{E}[(\widehat{\theta} - \mathbb{E}[\widehat{\theta}])^2] + \Big(\mathbb{E}[\widehat{\theta}] - \theta\Big)^2 + 2\mathbb{E}[(\widehat{\theta} - \mathbb{E}[\widehat{\theta}])]\Big(\mathbb{E}[\widehat{\theta}] - \theta\Big) \\
&= \text{bias}[\widehat{\theta}_n]^2 + \mathbb{V}[\widehat{\theta}_n]
\end{aligned}$$

Thus, the MSE is low when bias and variance are low.

Note that connecting these concepts to notions of precision and accuracy is useful. In particular, estimators with low sampling variance are **precise**, whereas estimators with low MSE are **accurate**. An estimator can be very precise, but the same estimator can be inaccurate because it is biased.

1.6 Question 5: Uncertainty

We now have a population, a quantity of interest, a sampling design, an estimator, and, with data, an actual estimate. But if we sampled, say, Sam and Merry from the hobbit population and obtained a sample mean height of 127, a reasonable worry would be that different samples – for example, Sam and Frodo or Merry and Pippin – would give us a different sample mean. So is the estimate of 127 inches that we get from our sample of Sam and Merry close to the true population mean? We cannot truly know without conducting a complete census of all four hobbits, which would render our sampling pointless. Can we instead figure out how far we might be from the truth – i.e., the true population mean? The sampling variance addresses this exact question, but the sampling variance depends on the sampling distribution, and we only have a single sample draw from this distribution, which gave the estimate of 127.

If we have a specific estimator and a sampling design, we can usually derive an analytical expression for the sampling variance (and, thus, the standard error), which in turn will identify the factors influencing the sampling variance. To aid in this endeavor, we need to define an additional feature of the population distribution, the **population variance**,

$$s^2 = \frac{1}{N-1}\sum_{i=1}^{N}(x_i - \overline{x})^2.$$

The population variance measures the spread of the x_i values in the population. As such it is a fixed quantity and not a random variable.

We now write the sampling variance of $\overline{X}_n$ under simple random sampling as

$$\mathbb{V}[\overline{X}_n] = \left(1 - \frac{n}{N}\right)\frac{s^2}{n}$$

Several features stand out from this expression. First, if the data x_i is more spread out in the population, the sample mean will also be more spread out. Second, the larger the sample size, n, the smaller the sampling variance (for a fixed population size). Third, the larger the population size, N, the smaller the sampling variance (again for a fixed sample size).

1.6.1 Deriving the sampling variance of the sample mean

How did we obtain this expression for the sampling variance under simple random sampling? It would be tempting to simply say "someone else proved it for me," but blind faith

in statistical theory limits our own understanding of this situation and the ability to navigate novel scenarios that routinely arise in research.

To derive the sampling variance of the sample mean, let's begin with a simple application of the rules of variance that would be valid for any sampling design:

$$\mathbb{V}[\overline{X}_n] = \mathbb{V}\left[\frac{1}{n}\sum_{i=1}^{N} x_i Z_i\right] = \frac{1}{n^2}\left[\sum_{i=1}^{N} x_i^2 \mathbb{V}[Z_i] + \sum_{i=1}^{N}\sum_{j\neq i} x_i x_j \text{cov}[Z_i, Z_j]\right].$$

Note in the second equality that the x_i and x_j values come out of the variance and covariance operators as if they are constants. This is because, in design-based inference, they are exactly constants. The only source of variation and uncertainty comes from the sampling, indicated by the inclusion indicators, Z_i. To make progress, we need to know the variance and covariance of these inclusion indicators. Recall that the variance of a binary indicator with probability p of being 1 is $p(1-p)$. So if $\mathbb{P}(Z_i = 1) = n/N$ for a simple random sample, then

$$\mathbb{V}[Z_i] = \frac{n}{N}\left(1 - \frac{n}{N}\right) = \frac{n(N-n)}{N^2}.$$

If you are used to the "independent and identically distributed" framework (to which we will turn in the next chapter), the covariances in the sampling variances might surprise. Aren't units usually assumed to be independent? While this assumption would (and will) make our math lives easier, it is not true for the simple random sample. The srs samples units without replacement, which implies that units' inclusion into the sample is not independent—knowing that unit i was included in the sample means that another unit j has only a $(n-1)/(N-1)$ probability of being included in the sample. To derive an expression for the covariance, note that $\text{cov}(Z_i, Z_j) = \mathbb{E}[Z_i Z_j] - \mathbb{E}[Z_i]\mathbb{E}[Z_j]$ and

$$\mathbb{E}[Z_i Z_j] = \mathbb{P}(Z_i = 1, Z_j = 1) = \mathbb{P}(Z_i = 1)\mathbb{P}(Z_j = 1 \mid Z_i = 1) = \frac{n}{N} \cdot \frac{n-1}{N-1}.$$

Plugging this into our covariance statement, we get

$$\begin{aligned}
\text{cov}(Z_i, Z_j) &= \mathbb{E}[Z_i Z_j] - \mathbb{E}[Z_i]\mathbb{E}[Z_j] \\
&= \frac{n}{N} \cdot \frac{n-1}{N-1} - \frac{n^2}{N^2}. \\
&= \frac{n}{N}\left(\frac{n-1}{N-1} - \frac{n}{N}\right) \\
&= \frac{n}{N}\left(\frac{Nn - N - Nn + n}{N(N-1)}\right) \\
&= -\frac{n(N-n)}{N^2(N-1)} \\
&= -\frac{\mathbb{V}[Z_i]}{N-1}.
\end{aligned}$$

Given that variances and population sizes must be positive, the covariance between the inclusions of two units is negative. Going back to our hobbits, there are a fixed number of spots in the sample, and so Frodo being included lowers the chance that Sam is included, so we end up with this negative covariance.

With the covariance and variance now calculated, we can derive the sampling variance of the sample mean:

$$\begin{aligned}
\mathbb{V}[\overline{X}_n] &= \frac{1}{n^2}\left[\sum_{i=1}^{N} x_i^2 \mathbb{V}[Z_i] + \sum_{i=1}^{N}\sum_{j\neq i} x_i x_j \text{cov}[Z_i, Z_j]\right] \\
&= \frac{1}{n^2}\left[\sum_{i=1}^{N} x_i^2 \mathbb{V}[Z_i] - \frac{1}{N-1}\sum_{i=1}^{N}\sum_{j\neq i} x_i x_j \mathbb{V}[Z_i]\right] \\
&= \frac{\mathbb{V}[Z_i]}{n^2}\left[\sum_{i=1}^{N} x_i^2 - \frac{1}{N-1}\sum_{i=1}^{N}\sum_{j\neq i} x_i x_j\right] \\
&= \frac{N-n}{nN^2}\left[\sum_{i=1}^{N} x_i^2 - \frac{1}{N-1}\sum_{i=1}^{N}\sum_{j\neq i} x_i x_j\right]
\end{aligned}$$

Where do we go from here? Unfortunately, we have arrived at the non-obvious and seemingly magical step of "adding and subtracting a crucial quantity." (One needs to know the step before completing the proof, so how could you complete the proof without knowing this step?) In this case, it is necessary to add and subtract the quantity $(N-1)^{-1}\sum_{i=1}^{N} x_i^2$.

To see why, rewrite the population variance in a slightly different way:

$$s^2 = \frac{1}{N-1}\sum_{i=1}^{N}(x_i - \overline{x})^2 = \frac{1}{N-1}\left(\sum_{i=1}^{N} x_i^2 - N\overline{x}^2\right)$$

Note that we can write

$$N^2\overline{x}^2 = \sum_{i=1}^{N} x_i^2 + \sum_{i=1}^{N}\sum_{j\neq i} x_i x_j,$$

which provides a hint as to the quantity that we will add and subtract

$$\begin{aligned}
\mathbb{V}[\overline{X}_n] &= \frac{N-n}{nN^2}\left[\sum_{i=1}^{N} x_i^2 \underbrace{+ \frac{1}{N-1}\sum_{i=1}^{N} x_i^2 - \frac{1}{N-1}\sum_{i=1}^{N} x_i^2}_{\text{add and subtract}} - \frac{1}{N-1}\sum_{i=1}^{N}\sum_{j\neq i} x_i x_j\right] \\
&= \frac{N-n}{nN^2}\left[\frac{N}{N-1}\sum_{i=1}^{N} x_i^2 - \frac{1}{N-1}\sum_{i=1}^{N}\sum_{j=i}^{N} x_i x_j\right] \\
&= \frac{N-n}{nN^2}\left[\frac{N}{N-1}\sum_{i=1}^{N} x_i^2 - \frac{N^2}{N-1}\overline{x}\right] \\
&= \frac{N-n}{nN(N-1)}\left[\sum_{i=1}^{N} x_i^2 - N\overline{x}\right] \\
&= \frac{N-n}{nN(N-1)}\sum_{i=1}^{N}(x_i - \overline{x})^2 \\
&= \frac{(N-n)}{N}\frac{s^2}{n} = \left(1 - \frac{n}{N}\right)\frac{s^2}{n}.
\end{aligned}$$

This proof is rather involved but does display some commonly used approaches to deriving statistical results. It also highlights how the sampling scheme leads to dependence, making the result more complicated. The next chapter will discuss how the variance of the sample mean under independent and identically distributed sampling is much simpler.

1.6.2 Estimating the sampling variance

An unfortunate aspect of the sampling variance, $\mathbb{V}[\overline{X}_n]$, is that it depends on the population variance, s^2, which we cannot know unless we have a census of the entire population

(If we had that information, we would not need to worry about uncertainty.) Thus, we need to estimate the sampling variance. Since we already know n, the sample size, and N, the population size, the most straightforward way to do this is to find an estimator for the population variance.

A good estimator for this is the **sample variance**, which is simply the variance formula applied to the sample itself,

$$S^2 = \frac{1}{n-1}\sum_{i=1}^{N} Z_i(x_i - \overline{X}_n)^2.$$

We can obtain an estimator for the sampling variance by substituting this in for the population variance,

$$\hat{\mathbb{V}}[\overline{X}_n] = \left(1 - \frac{n}{N}\right)\frac{S^2}{n}.$$

> **Mind your variances**
>
> It is easy to get confused about the difference between the population variance, the variance of the sample, and the sampling variance (just as it is to get confused about the population, the distribution of the sample, and the sampling distribution). Adding to the confusion, these are all variances but for very distinct distributions.

Why is $\hat{\mathbb{V}}[\overline{X}_n]$ a "good" estimator for $\mathbb{V}[\overline{X}_n]$? To answer this, we apply the same criteria as above in Question 4. Ideally, the estimator would be unbiased, meaning it does not systematically over- or underestimate how much variation is in the sample mean across repeated samples.

$$\begin{aligned}
\mathbb{E}[S^2] &= \frac{1}{n-1}\sum_{i=1}^{N}\mathbb{E}[Z_i(x_i - \overline{X}_n)^2] \\
&= \frac{1}{n-1}\mathbb{E}\left[\sum_{i=1}^{N} Z_i(x_i - \overline{x} - (\overline{X}_n - \overline{x}))^2\right] \\
&= \frac{1}{n-1}\mathbb{E}\left[\sum_{i=1}^{N} Z_i(x_i - \overline{x})^2 - 2Z_i(x_i - \overline{x})(\overline{X}_n - \overline{x}) + Z_i(\overline{X}_n - \overline{x})^2\right]
\end{aligned}$$

Notice that $(\overline{X}_n - \overline{x})$ does not depend on i so we can pull it out of the summations:

$$
\begin{aligned}
\mathbb{E}[S^2] &= \frac{1}{n-1}\mathbb{E}\left[\sum_{i=1}^{N} Z_i(x_i - \overline{x})^2 - 2(\overline{X}_n - \overline{x})\sum_{i=1}^{N} Z_i(x_i - \overline{x}) + (\overline{X}_n - \overline{x})^2 \sum_{i=1}^{N} Z_i\right] \\
&= \frac{1}{n-1}\mathbb{E}\left[\sum_{i=1}^{N} Z_i(x_i - \overline{x})^2 - 2n(\overline{X}_n - \overline{x})^2 + n(\overline{X}_n - \overline{x})^2\right] \\
&= \frac{1}{n-1}\left[\sum_{i=1}^{N} \mathbb{E}[Z_i](x_i - \overline{x})^2 - n\mathbb{E}[(\overline{X}_n - \overline{x})^2]\right] \\
&= \frac{n}{N}\frac{1}{n-1}\sum_{i=1}^{N}(x_i - \overline{x})^2 - \frac{n}{n-1}\mathbb{V}[\overline{X}_n] \\
&= \frac{n(N-1)}{N(n-1)}s^2 - \frac{(N-n)}{N(n-1)}s^2 \\
&= s^2
\end{aligned}
$$

This shows that the sample variance is unbiased for the population variance. To complete the derivation, we can just plug this into the estimated sampling variance,

$$
\mathbb{E}\left[\hat{\mathbb{V}}[\overline{X}_n]\right] = \left(1 - \frac{n}{N}\right)\frac{\mathbb{E}\left[S^2\right]}{n} = \left(1 - \frac{n}{N}\right)\frac{s^2}{n} = \mathbb{V}[\overline{X}_n],
$$

which establishes that the estimator is unbiased.

1.7 Stratified sampling and survey weights

True to its name, the simple random sample is perhaps the most straightforward way to take a random sample of a fixed size. With more information about the population, however, we might obtain better estimates of the population quantities by incorporating this information into the sampling scheme. We can do this by conducting a **stratified random sample**, where we divide up the population into several strata (or groups) and conduct simple random samples within each stratum. We create these strata (or "stratify the population" in the usual jargon) based on the additional information about the population.

Consider an expanded population of the entire Fellowship of the Ring, which included 9 adventurous members – the four hobbits plus two humans (Aragorn and the doomed

Boromir), an elf (Legolas of the Woodland Elves), a dwarf (Gimli), and a wizard (Gandalf the Grey)

Unit (i)	Race	Height in cm (x_i)
1 (Frodo)	Hobbit	124
2 (Sam)	Hobbit	127
3 (Pip)	Hobbit	123
4 (Merry)	Hobbit	127
5 (Gimli)	Dwarf	137
6 (Gandalf)	Wizard	168
7 (Aragorn)	Human	198
8 (Boromir)	Human	193
9 (Legolas)	Elf	183

If we were taking a sample of size 5 from this population, we could use a simple random sample, but note that the sample could be lopsided. We could, for instance, sample mostly or all non-hobbits. We could instead conduct stratified sampling here by splitting our population into two strata: hobbits and non-hobbits, making up 4/9ths $\approx$ 44% and 5/9ths $\approx$ 56% of the population, respectively. To get to a sample of 5, we could take simple random samples of size 2 for the hobbits and size 3 for the non-hobbits. This would guarantee our sample would be 40% hobbit every time while still maintaining randomness in our selection of which hobbits and non-hobbits go into the sample.

Another reason to conduct a stratified random sample is to guarantee a level of precision for a certain subgroup of the population. Social science researchers often conduct nationally representative surveys but have a specific interest in obtaining estimates for certain minority populations – for example, African Americans, Latinos, people who are LGBTQ+, and others. In modest sample sizes, the number of respondents in one of these groups might be too small to learn much about their opinions. Sampling a higher proportion of the group of interest will help ensure that we can make precise statements about that group.

In a simple random sample, we have $\pi_i = n/N$ for all i. By contrast, stratified random sampling is an example of a broad class of sampling methods that have unequal inclusion probabilities, which we denote $\pi_i = \mathbb{P}(Z_i = 1)$. In the Fellowship of the Ring example, we were sampling 2 hobbits and 3 non-hobbits, so we have the following inclusion probabilities:

Unit (i)	Race	Inclusion probability (π_i)
1 (Frodo)	Hobbit	0.5
2 (Sam)	Hobbit	0.5
3 (Pip)	Hobbit	0.5
4 (Merry)	Hobbit	0.5
5 (Gimli)	Dwarf	0.6
6 (Gandalf)	Wizard	0.6
7 (Aragorn)	Man	0.6
8 (Boromir)	Man	0.6
9 (Legolas)	Elf	0.6

There are additional ways to conduct a random sample with unequal inclusion probabilities. For example, suppose the goal is to randomly sample 5 U.S. cities for study. We might want to bias our sample toward larger cities in order to capture a larger number of citizens in the overall sample. If the number of inhabitants for city i is b_i, then our inclusion probabilities for sampling with replacement[1] is

$$\pi_i = \frac{b_i}{\sum_{i=1}^{N} b_i}.$$

Note that we use information about the population in our sampling design, though this information is continuous whereas the information in the stratified estimator is discrete.

Using a sampling design with unequal inclusion probabilities means that we have changed our sampling design (question 3), but the population and estimands (questions 1 and 2) remain the same. We are still interested in estimating the population mean, $\overline{x}$. We now turn to the estimator (question 4), since we will need to use a new estimator that matches the design.

Two estimators are commonly used to estimate the population mean when sampling with unequal inclusion probabilities. The first, the **Horvitz-Thompson (HT) estimator**, has the form

$$\widetilde{X}_{HT} = \frac{1}{N} \sum_{i=1}^{N} \frac{Z_i x_i}{\pi_i},$$

[1]This description is true for sampling with replacement. When sampling without replacement, we would need to adjust the probabilities to account for how being selected first means that a unit cannot be selected second.

This takes the weighted average of those in the sample, with the weights being the inverse of the inclusion probabilities. This is why the estimator is sometimes called the inverse probability weighting, or IPW, estimator.

We can show that the HT estimator is unbiased for the population mean by noting that $\mathbb{E}[Z_i] = \mathbb{P}(Z_i = 1) = \pi_i$, so that

$$\mathbb{E}[\widetilde{X}_{HT}] = \frac{1}{N}\sum_{i=1}^{N}\frac{\mathbb{E}[Z_i]x_i}{\pi_i} = \frac{1}{N}\sum_{i=1}^{N} x_i = \overline{x}.$$

A downside of the HT estimator is that it can be unstable if a unit with a very small inclusion probability is selected since that unit's weight $(1/\pi_i)$ will be very large. This instability is the cost of being unbiased for the stratified design. Also note that the formula for the sampling variance is rather complicated and requires notation that is less important to the task at hand.

The second estimator for the the population mean when sampling with unequal inclusion probabilities is the **Hájek estimator**, which normalizes the weights so they sum to N and has the form

$$\widetilde{X}_{hj} = \frac{\sum_{i=1}^{N} Z_i x_i/\pi_i}{\sum_{i=1}^{N} Z_i/\pi_i}.$$

This estimator is **biased** for the population mean since there is a random quantity in the denominator. The Hajek estimator is often considered the better estimator in many situations, though, because it has lower sampling variance than the HT estimator.

1.7.1 Sampling weights

The HT and Hajek estimators are both functions of what are commonly called the **sampling weights**,

$$w_i = \frac{1}{\pi_i}$$

. We can write the HT estimator as

$$\widetilde{X}_{HT} = \frac{1}{N}\sum_{i=1}^{N} w_i Z_i x_i,$$

and we can write the Hajek estimator as

$$\widetilde{X}_{hj} = \frac{\sum_{i=1}^{N} w_i Z_i x_i}{\sum_{i=1}^{N} w_i Z_i}.$$

These weights, w_i, are usually included in final survey data sets because they contain all the information about the sampling design a researcher needs to analyze the survey responses even without knowledge of the exact design.[2]

The sampling weights have a nice interpretation in terms of a pseudo-population: each unit in the sample "represents" $w_i = 1/\pi_i$ units in the population. This makes the sample more representative of the population.

Finally, note that statistical software often is a little confusing in how it handles weights. It may not be obvious what estimator function `weighted.mean(x, w)` in R is using. In fact, the source code basically calls

```
sum(x * w) / sum(w)
```

which is equivalent to the Hajek estimator above.

1.8 Summary

This chapter covered the basic structure of design-based inference in the context of sampling from a population. We introduced the basic questions of statistical inference, including specifying a population and quantity of interest, choosing a sampling design and estimator, and assessing uncertainty of the estimator. Of course, we have only scratched the surface of the types of designs and estimators used in the practice of sampling. Professional probability surveys often use clustering, which means randomly selecting larger clusters of units and then randomly sampling within these units. However complex the sampling design, the core steps of design-based statistical inference remain the same. A researcher must identify a population, determine a sampling design, choose a quantity of interest, select an estimator, and describe the uncertainty of any estimates.

[2] If we want design-based estimators of the sampling variance, we would also need to know the joint inclusion probabilities, which are the probabilities of any two units being sampled together.

2 Model-based inference

2.1 Introduction

Suppose you have been tasked with estimating the fraction of a population that supports increasing legal immigration limits. You have a sample of data on some individual respondents' support for the policy, but you don't know exactly how this data was sampled. How should you use the information you know (the data) to make a best guess about the information you don't know (the fraction of the population)?

The design-based approach that we discussed in the previous chapter is a coherent and internally consistent framework for estimating quantities and quantifying uncertainty, but this crisp conceptual clarity comes from having exact knowledge of the sampling design. Going back to our immigration example, a reasonable approach is to use the fraction of the sample that supports the policy as the best guess about the fraction of the population. As we saw in the last chapter, a simple random sample would justify this approach.

But how does one perform estimation and inference when lacking complete information about the sampling design? How do we proceed with inference if outcomes are random due to nonresponse or measurement error? What if we would like to make inferences about a population not covered in the sampling frame? In these cases, inference requires additional information that can be incorporated via a **statistical model**. A model-based approach to statistical inference views the data $X_1, \ldots, X_n$ as a set of random variables that follow some probability distribution. The measurements in the actual sample, $x_1, \ldots, x_n$, are realizations of these random variables. The probability distribution of $X_1, \ldots, X_n$ is the model for the data and all inferences are based on it. Models can be very specific – for example, a researcher might assume the data are normally distributed – or can be very general – for example, the distribution of the data has finite mean and variance.

The focus of this chapter (and most of introductory statistics) will be on statistical models that assume units are **independent and identically distributed** or, more succinctly, **iid**.

This assumption means that each unit gives us new information about the same underlying data-generating process. Because this assumption is often motivated by a probability sample from a population, some authors also refer to this as a **random sampling** assumption. The "sample" refers to the idea that our data is a subset of some larger **population**. The "random" modifier means that the subset was chosen by an uncertain process that did not favor one type of person versus another.

Why focus on iid/random samples even though many data sets are at least partially non-random or represent the entire population rather than a subset? Consider the famous story of a drunkard's search for a two-dollar bill lost in downtown Boston:[1]

> "I lost a $2 bill down on Atlantic Avenue," said the man.
>
> "What's that?" asked the puzzled officer. "You lost a $2 bill on Atlantic Avenue? Then why are you hunting around here in Copley Square?"
>
> "Because," said the man as he turned away and continued his hunt on his hands and knees, "the light's better up here."

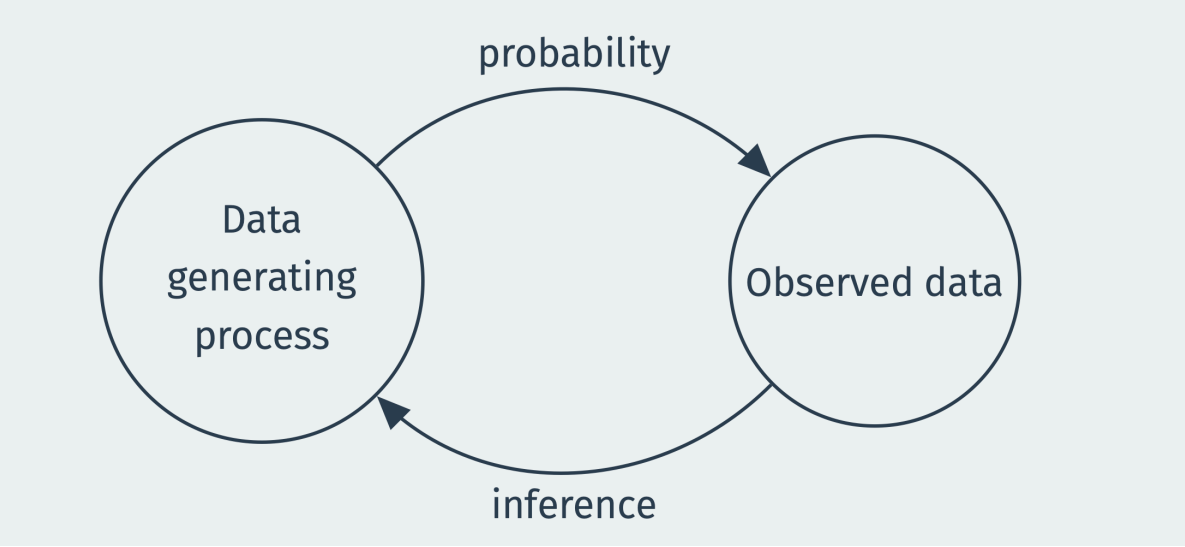
Like the poor drunkard, we focus on searching an area (random samples) that are easier to search because there is more light or, more accurately, easier math. Unlike this apocryphal tale, our search will help us better understand the darkness of non-random samples because the core ideas and intuitions from random sampling form the basis for the theoretical extensions into more exotic settings.

This chapter has two goals. First, we will introduce the entire model-based framework of estimation and estimators. We will discuss different ways to compare the properties of estimators. Most of these properties will be similar to those of the design-based framework, except the properties will be with respect to the model rather than the sampling design. (The core questions of quantitative research largely remain the same, but we replace specifying the sampling design with the specification of a probabilistic model for our data.) Second, we will establish key properties for a general class of estimators that can be written as a sample mean. These results are useful in their own right since these estimators are ubiquitous, but the derivations also provide examples of how we establish such results. Building comfort with these proofs helps us understand the arguments about novel estimators that we inevitably see over the course of our careers.

[1] 1924 May 24, Boston Herald, Whiting's Column: Tammany Has Learned That This Is No Time for Political Bosses, Quote Page 2, Column 1, Boston, Massachusetts. (GenealogyBank)

2.2 Probability vs inference: the big picture

Probability is the mathematical study of uncertain events and is the basis of the mathematical study of estimation. In probability, we assume we know the truth of the world (how many blue and red balls are in the urn) and calculate the probability of possible events (getting more than five red balls when drawing ten from the urn). Estimation works in reverse. Someone hands you five balls, 2 red and 3 blue, and your task is to guess the contents of the urn from which they came. With estimation, we use our observed data to make an **inference** about the data-generating process.



An estimator is a rule for converting our data into a best guess about some unknown quantity, such as the percent of balls in the urn, or, to use our example from the introduction, the fraction of the public supporting increasing legal immigration limits. For example, an estimator could be a rule that the proportion of red balls that you draw from the urn is a good guess for the proportion of red balls that you would find if you looked inside the urn.

We prefer to use **good** estimators rather than **bad** estimators. But what makes an estimator good or bad? In our red ball example, an estimator that always returns the value 3 is probably bad. Still, it will be helpful for us to formally define and explore properties of estimators that will allow us to compare them and choose the good over the bad. We begin with an example that highlights two estimators that at first glance may seem similar.

Example 2.1 (Randomized control trial)**.** Suppose we are conducting a randomized experiment on framing effects. All respondents receive factual information about current immigration levels. Those in the treatment group ($D_i = 1$) receive additional information about the positive benefits of immigration, while those in the control group ($D_i = 0$) receive no additional framing. The outcome is a binary outcome, whether the respondent supports increasing legal immigration limits ($Y_i = 1$) or not ($Y_i = 0$). The observed data consists of n pairs of random variables, the outcome, and the treatment assignment: $\{(Y_1, D_1), \ldots, (Y_n, D_n)\}$.

Define the two sample means/proportions in each group as

$$\overline{Y}_1 = \frac{1}{n_1} \sum_{i:D_i=1} Y_i, \qquad \overline{Y}_0 = \frac{1}{n_0} \sum_{i:D_i=0} Y_i,$$

where $n_1 = \sum_{i=1}^{n} D_i$ is the number of treated units and $n_0 = n - n_1$ is the number of control units.

A standard estimator for the treatment effect in a study such as this would be the difference in means, $\overline{Y}_1 - \overline{Y}_0$. But this is only one of many possible estimators. We could also estimate the effect by taking this difference in means separately by party identification and then averaging those party-specific effects by the size of those groups. This estimator is commonly called a **poststratification** estimator. Which of these two estimators we should prefer is at first glance unclear.

We now turn to the same key questions that we used to motivate design-based inference, but adapt these to consider model-based inference.

2.3 Question 1: Population

The main advantage and disadvantage of relying on models is that they are abstract and theoretical, which means the connection between a model and the population it helps explain is less direct than with the design-based framework. Nevertheless, we need to clearly articulate our population of study – that is, who or what we want to learn about – since it is crucial for evaluating the types of modeling assumptions that will be sustainable.

As in the design-based setting, there is often a clear and distinct population such as "all registered voters" or "all Boston residents." In other cases, the population may be more

abstract. For example, a large multi-field literature has studied how the size of minority populations affects the views of the local majority population. Researchers in this space may be interested in making claims beyond the particular geographic region or minority/majority group, instead implicitly or explicitly considering a "superpopulation" of such cases that their model might explain. While there is nothing theoretically wrong with this approach, these ideas are often neglected in practice and the "scope conditions" of a particular model go unarticulated. The best quantitative work will be clear about what units or processes it is trying to learn about so that readers can evaluate how well the modeling assumptions fit that task.

2.4 Question 2: Statistical model

Let's begin by building a bare-bones probability model for how our data came to be. As an example, suppose we have a data set with a series of numbers representing the ages, political party affiliations, and policy opinions of 1000 survey respondents. But we know that row 58 of our data could have produced a different set of numbers if another respondent had been selected as row 58 or if the original respondent gave a different opinion about immigration because they happened to see an immigration news story just before responding. To reason about this type of uncertainty precisely, we write X_i as the random variable representing the value that row i of some variable will take, before we see the data. The distribution of this random variable would tell us what types of data we should expect to see.

Why represent the data with random variables when we already know the value of the data itself? Why pretend we haven't seen the data? The study of estimation from a frequentist perspective (which is the perspective of this book) focuses on the properties of estimators across **repeated samples**. In the example of the policy survey, this is akin to drawing a 1000 person sample repeatedly, each time including possibly different respondents in the sample. The random variable X_i represents our uncertainty about what value, say, age will take for respondent i in any of these samples, and the set $\{X_1, \dots, X_n\}$ represents our uncertainty about the entire column of ages for all n respondents. At the most general, the model-based approach says that these n random variables follow some joint distribution, $F_{X_1,\dots,X_n}$,

$$\{X_1, \dots, X_n\} \sim F_{X_1,\dots,X_n}$$

The joint distribution F here represents the probability model for the data. We have made no assumptions about it so far, so it could be any joint probability distribution over n

random variables. Note that this level of generality is difficult to work with in practice because there is essentially one draw from this joint distribution (the n measurements in the data). The core question of modeling is about what restrictions a researcher puts on this joint distribution to make learning about it more tractable.

We focus on a relatively simple setting where we assume the data $\{X_1, \dots, X_n\}$ are **independent and identically distributed** (iid) draws from a distribution with cumulative distribution function (cdf) F. They are independent in that information about any subset of random variable is not informative about any other subset of random variables, or, more formally,

$$F_{X_1,\dots,X_n}(x_1, \dots, x_n) = F_{X_1}(x_1) \cdots F_{X_n}(x_n) = \prod_{i=1}^{n} F(x_i)$$

where $F_{X_1,\dots,X_n}(x_1, \dots, x_n)$ is the joint cdf of the random variable and $F_{X_j}(x_j)$ is the marginal cdf of the jth random variable. They are "identically distributed" in the sense that each of the random variables X_i have the same marginal distribution, F.

Note that we are being purposely vague about this cdf—it simply represents the unknown distribution of the data, otherwise known as the **data generating process** (DGP). Sometimes F is also referred to as the **population distribution** or even just **population**, which has its roots in viewing the data as a random sample from some larger population.[^model] As a shorthand, we often say that the collection of random variables $\{X_1, \dots, X_n\}$ is a **random sample** from population F if $\{X_1, \dots, X_n\}$ is iid with distribution F. The **sample size** n is the number of units in the sample.

> **Note**
>
> You might wonder why we reference the distribution of X_i with the cdf, F. Mathematical statistics tends to do this to avoid having to deal with discrete and continuous random variables separately. Every random variable – whether discrete or continuous – has a cdf, and the cdf contains all information about the distribution of a random variable.

Two metaphors help build intuition behind viewing the data as an iid draw from F:

1. **Random sampling**. Suppose we have a population of size N that is much larger than our sample size n, and we take a random sample of size n from this population with replacement. The distribution of the data in the random sample will be

iid draws from the population distribution of the variables we are sampling. For example, suppose the population proportion of Democratic party identifiers among U.S. citizens is 0.33. If we randomly sample $n = 100$ U.S. citizens, each data point X_i will be distributed Bernoulli with a probability of success (i.e., Democratic Party identifier) of 0.33.

Note that the last chapter explored simple random samples *without replacement*, which is a more common type of sampling – since generally people are selected into a survey once and they do not go back into the pool of potential survey takers. Sampling without replacement creates dependence across units, which would violate the iid assumption. However, if the population size N is very large relative to the sample size n, this dependence will be very small, and the iid assumption will be relatively innocuous.

2. **Groundhog Day**. Random sampling does not always make sense as a justification for iid data, especially when the units are not samples at all but rather countries, states, or subnational units. (In these cases, the population can be the same as the sample – for example, using all 50 states to draw conclusions on the efficacy of state policy.) In this case, we have to appeal to a thought experiment where F represents the fundamental uncertainty in the data-generating process. The metaphor here is that if we could re-run history many times, such as what happens to the protagonist played by Bill Murray in the 1993 American comedy movie *Groundhog Day* when he is magically forced to relive February 2 over and over again. Under this fiction, data and outcomes would change slightly due to the inherently stochastic nature of the world. In the movie, for example, Murray's character starts off the same day in exactly the same way, but he begins to change his actions and the outcomes at the end of each day change in subtle ways. The iid assumption, then, is that each of the units in our data has the same DGP producing this data or the same distribution of outcomes under the *Groundhog Day* scenario. The set of all these infinite possible draws from the DGP is sometimes referred to as the **superpopulation**.

Note that there are other situations where the iid assumption is not appropriate, which we discuss in later chapters. But much of the innovation and growth in statistics over the last 50 years has been in figuring out how to make statistical inferences when iid does not hold. The solutions are often specific to the type of iid violation (e.g., spatial, time-series, network, clustered). As a rule of thumb, however, if the iid assumption may not be valid, any uncertainty statements will likely be overconfident. For example, confidence intervals, which we will cover in later chapters, are too small.

Finally, we introduced the data as a scalar random variable, but often our data has multiple variables. In that case, we easily modify X_i to be a random vector (that is, a vector of random variables) and then F becomes the joint distribution of that random vector. Nothing substantive changes about the above discussion.

Warning

Survey sampling is one of the most popular ways of obtaining samples from a population, but modern sampling practices rarely produce a "clean" set of n iid responses. There are several reasons for this:

- Modern random sampling techniques generally do not select every unit with the same probability. We might *oversample* certain groups for which we want more precise estimates, leading those groups to have a higher likelihood of being in the sample.
- Response rates to surveys have been in steep decline and can often dip below 10%. Such non-random selection into the observed sample might lead to problems.
- Internet polling is less costly than other forms of polling, but obtaining a list of population email addresses (or other digital contact information) to randomly sample is basically impossible. Large survey firms instead recruit large groups of panelists with known demographic information from which they can randomly sample in a way that matches population demographic information. Because the initial opt-in panel is not randomly sampled from the population, this procedure does not produce a true "random sample," but, under certain assumptions, we can treat it like it is.

As discussed in the last chapter, there are ways to handle all of these issues (mostly through the use of survey weights), but it is important to realize that using a modern survey "as if" it was a simple random sample might lead to poor performance and incorrect inferences.

2.5 Question 3: Quantities of interest

In model-based inference, our goal is to learn about the data-generating process. Each data point X_i represents a draw from a distribution, captured by the cdf F, and we would like to know more about this distribution. We might be interested in estimating the cdf at a general level or only some feature of the distribution, like a mean or conditional expectation function. We call these numerical features the **quantities of interest**. (Similarly, in the design-based inference framework we discussed in the previous chapter, the quantity of interest was a numerical summary of the finite population.)

The following are examples of frequently used quantities of interest:

Example 2.2 (Population mean)**.** We may be interested in where the typical member of a population falls on some questions. Suppose we wanted to know the proportion of US citizens who support increasing legal immigration For citizen i, denote support as $Y_i = 1$. Our quantity of interest is then the mean of this random variable, $\mu = \mathbb{E}[Y_i] = \mathbb{P}(Y_i = 1)$. This is the same as the probability of randomly drawing someone from the population who supports increasing legal immigration.

Example 2.3 (Population variance)**.** We may also be interested in variation in the population. For example, feeling thermometer scores are a common way to assess how survey respondents feel about a particular person or group. These ask each respondent to say how warmly he or she feels toward a group on a scale from 0 (cool) to 100 (warm), which we will denote Y_i. We might be interested in how polarized views are toward a group in the population, and one measure of polarization could be the variance, or spread, of the distribution of Y_i around the mean. In this case, $\sigma^2 = \mathbb{V}[Y_i] = \mathbb{E}[(Y_i - \mathbb{E}[Y_i])^2]$ would be our quantity of interest.

Example 2.4 (RCT continued)**.** Example 2.1 discussed a typical estimator for an experimental study with a binary treatment. The goal of that experiment is to learn about the difference between two conditional probabilities (or expectations): 1) the average support for increasing legal immigration in the treatment group, $\mu_1 = \mathbb{E}[Y_i \mid D_i = 1]$, and 2) the same average in the control group, $\mu_0 = \mathbb{E}[Y_i \mid D_i = 0]$. This difference, $\mu_1 - \mu_0$, is a function of unknown features of these two conditional distributions.

Each of these is a function of the (possibly joint) distribution of the data, F. In each of these, we are not necessarily interested in the entire distribution, just summaries of it

(central tendency, spread). Of course, there are situations where we are also interested in the complete distribution. To speak about estimation in general, we will let θ represent some generic quantity of interest. **Point estimation** describes how we obtain a single "best guess" about θ.

> **Note**
>
> Some refer to quantities of interest as **parameters** or **estimands** (that is, the target of estimation).

2.6 Question 4: Estimator

Having a target in mind, we can estimate it with our data. To do so, we first need a rule or algorithm or function that takes as inputs the data and returns a best guess about the quantity of interest. One of the most popular and useful algorithm would be to sum all the data points and divide by the number of points:

$$\frac{X_1 + X_2 + \cdots + X_n}{n}.$$

This, the much-celebrated sample mean, provides a rule for how produce a single-number summary of the data. To go one pedantic step further and define it as a function of the data more explicitly:

$$\mathsf{mean}(X_1, X_2, \ldots, X_n) = \frac{X_1 + X_2 + \cdots + X_n}{n}.$$

We can use this model to provide a definition for an arbitrary estimator for an arbitrary quantity of interest.

Definition 2.1. An **estimator** $\widehat{\theta}_n = \theta(X_1, \ldots, X_n)$ for some parameter θ, is a function of the data intended as a guess about θ.

> **Note**
>
> It is widespread, though not universal, to use the "hat" notation to define an estimator and its estimand. For example, $\widehat{\theta}$ (or "theta hat") indicates that this estimator is

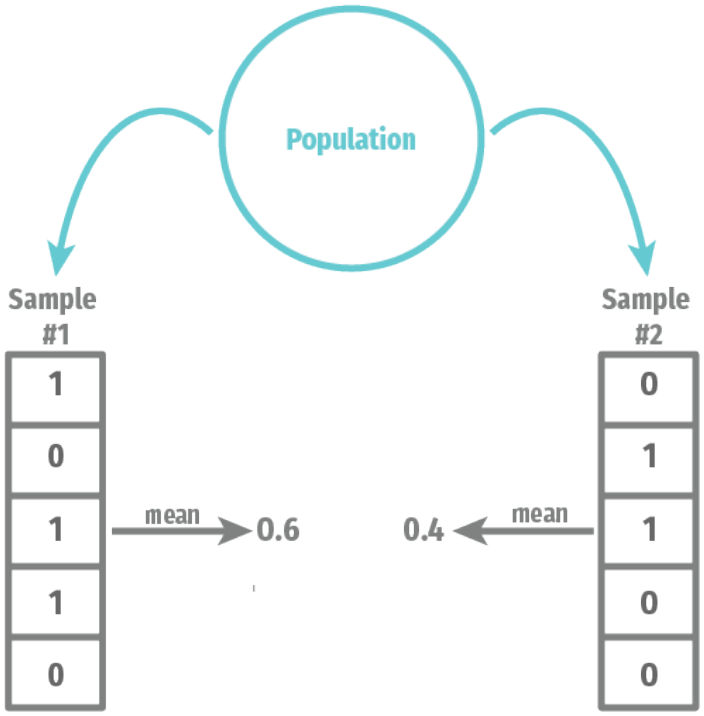
targeting the parameter θ.

Example 2.5 (Estimators for the population mean)**.** Suppose our goal is to estimate the population mean of F, which we will represent as $\mu = \mathbb{E}[X_i]$. We could choose from several estimators, all with different properties.

$$\hat{\theta}_{n,1} = \frac{1}{n}\sum_{i=1}^{n} X_i, \quad \hat{\theta}_{n,2} = X_1, \quad \hat{\theta}_{n,3} = \max(X_1, \dots, X_n), \quad \hat{\theta}_{n,4} = 3$$

The first is just the sample mean, which is an intuitive and natural estimator for the population mean. The second just uses the first observation. While this seems silly, this is a valid statistic since it is a function of the data! The third takes the maximum value in the sample, and the fourth always returns three, regardless of the data. These are also valid statistics.

When we view the data $\{X_1, \dots, X_n\}$ as a collection of random variables, then any function of them is also a random variable. Thus, we can view $\hat{\theta}_n$ as a random variable that has a distribution induced by the randomness of the sample. Drawing two different samples of respondents will lead to two different estimates. For example, here we illustrate two samples of size $n = 5$ from the population distribution of a binary variable:



We can see that the mean of the variable depends on what exact values end up in our sample. We refer to the distribution of $\hat{\theta}_n$ across repeated samples as its **sampling distribution**. The sampling distribution of an estimator will be the basis for all of the formal statistical properties of an estimator.

> ⚠ Warning
>
> One important distinction of jargon is between an estimator and an estimate. The estimator is a function of the data, whereas the **estimate** is the *realized value* of the estimator once we see the data (that is, the data are realized). The estimator is a random variable that has uncertainty over what value it will take, and we represent the estimator as a function of random variables, $\hat{\theta}_n = \theta(X_1, \dots, X_n)$. An estimate is a single number, such as 0.38, that we calculated in R with our data (our draw from F). Formally, the estimate is $\theta(x_1, \dots, x_n)$ when the data is $\{X_1, \dots, X_n\} = \{x_1, \dots, x_n\}$, whereas we represent the estimator as a function of random variables, $\hat{\theta}_n = \theta(X_1, \dots, X_n)$.

2.7 How to find estimators

Where do estimators come from? That may seem like a question reserved for statisticians or methodologists or others responsible for "developing new methods." But knowing how estimators are derived is valuable even if we never plan to do it ourselves. Knowing where an estimator comes from provides strong insights into its strengths and weaknesses. We will briefly introduce estimators based on parametric models, before turning to the main focus of this book, plug-in estimators.

2.7.1 Parametric models and maximum likelihood

The first method for generating estimators relies on **parametric models**, in which the researcher specifies the exact distribution (up to some unknown parameters) of the DGP. Let θ be the parameters of this distribution, where $\{X_1, \dots, X_n\}$ be iid draws from F_θ. We should also formally state the set of possible values the parameters can take, which we call the **parameter space**, denoted by Θ. Because we assume we know the distribution of the data, we can write the probability density function, or pdf, as $f(X_i \mid \theta)$ and define the likelihood function as the product of these pdfs over the units as a function of the parameters:

$$L(\theta) = \prod_{i=1}^{n} f(X_i \mid \theta).$$

We can then define the **maximum likelihood** estimator (MLE) for θ as the values of the parameter that, well, maximize the likelihood:

$$\hat{\theta}_{mle} = \underset{\theta \in \Theta}{\arg\max}\ L(\theta)$$

Sometimes we can use calculus to derive a closed-form expression for the MLE. At other times we use iterative techniques that search the parameter space for the maximum.

Maximum likelihood estimators have nice properties, especially in large samples. Unfortunately, they also require the correct knowledge of the parametric model, which is often difficult to justify. Do we really know if we should model a given event count variable as Poisson or Negative Binomial? The attractive properties of MLE are only as good as the ability to specify the parametric model.

> **No free lunch**
>
> Building up intuition about the **assumptions-precision tradeoff** is essential. Researchers can usually get more precise estimates if they make stronger and potentially more fragile assumptions. Conversely, they will almost always get less accurate estimates when weakening the assumptions.

2.7.2 Plug-in estimators

The second broad class of estimators is **semiparametric** in that we specify some finite-dimensional parameters of the DGP but leave the rest of the distribution unspecified. For example, we might define a population mean, $\mu = \mathbb{E}[X_i]$ and a population variance, $\sigma^2 = \mathbb{V}[X_i]$ but leave the shape of the distribution unrestricted. This ensures that our estimators will be less dependent on correctly specifying distributions about which we have little intuition or knowledge.

The primary method for constructing estimators in this setting is to use the **plug-in estimator**, or the estimator that replaces any population mean with a sample mean. Obviously, in the case of estimating the population mean, μ, we will use the **sample mean** as the estimate:

$$\overline{X}_n = \frac{1}{n}\sum_{i=1}^{n} X_i \quad \text{estimates} \quad \mathbb{E}[X_i] = \int_x x f(x) dx$$

In plain language, we are replacing the unknown population distribution $f(x)$ in the population mean with a discrete uniform distribution over our data points, with $1/n$ probability assigned to each unit. Why do this? It encodes that, if we have a random sample, our best guess about the population distribution of X_i is the sample distribution in our observed data. If this intuition fails, you can hold onto an analog principle: sample means of random variables are natural estimators of population means.

What about estimating something more complicated, like the expected value of a function of the data, $\theta = \mathbb{E}[r(X_i)]$? The key is to see that $r(X_i)$ is also a random variable. Let this random variable be $Y_i = r(X_i)$. Now we can see that θ is just the population expectation of this random variable. Using the plug-in estimator gives us:

$$\hat{\theta} = \frac{1}{n}\sum_{i=1}^{n} Y_i = \frac{1}{n}\sum_{i=1}^{n} r(X_i).$$

These facts enable us to describe a more general plug-in estimator. To estimate some quantity of interest that is a function of population means, we can generate a plug-in estimator by replacing any population mean with a sample mean. Formally, let $\alpha = g\left(\mathbb{E}[r(X_i)]\right)$ be a parameter that is defined as a function of the population mean of a (possibly vector-valued) function of the data. We can then estimate this parameter by plugging in the sample mean for the population mean to get the **plug-in estimator**,

$$\hat{\alpha} = g\left(\frac{1}{n}\sum_{i=1}^{n} r(X_i)\right) \quad \text{estimates} \quad \alpha = g\left(\mathbb{E}[r(X_i)]\right)$$

This approach to plug-in estimation with sample means is very general and will allow us to derive estimators in various settings.

Example 2.6 (Estimating population variance)**.** The population variance of a random variable is $\sigma^2 = \mathbb{E}[(X_i - \mathbb{E}[X_i])^2]$. To derive a plug-in estimator for this quantity, we replace the inner $\mathbb{E}[X_i]$ with $\overline{X}_n$ and the outer expectation with another sample mean:

$$\hat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^{n}(X_i - \overline{X}_n)^2.$$

This plug-in estimator differs from the standard sample variance, which divides by $n-1$ rather than n. This minor difference does not matter in moderate to large samples.

Example 2.7 (Estimating population covariance)**.** Suppose we have two variables, (X_i, Y_i). A natural quantity of interest here is the population covariance between these variables,

$$\sigma_{xy} = \text{Cov}[X_i, Y_i] = \mathbb{E}[(X_i - \mathbb{E}[X_i])(Y_i - \mathbb{E}[Y_i])],$$

which has the plug-in estimator,

$$\hat{\sigma}_{xy} = \frac{1}{n}\sum_{i=1}^{n}(X_i - \overline{X}_n)(Y_i - \overline{Y}_n).$$

> **Notation alert**
>
> Given the connection between the population mean and the sample mean, you may

see the $\mathbb{E}_n[\cdot]$ operator used as a shorthand for the sample average:

$$\mathbb{E}_n[r(X_i)] \equiv \frac{1}{n}\sum_{i=1}^{n} r(X_i).$$

Finally, plug-in estimation goes beyond just replacing population means with sample means. We can derive estimators of the population quantiles like the median with sample versions of those quantities. These approaches are unified in replacing the unknown population cdf, F, with the empirical cdf,

$$\widehat{F}_n(x) = \frac{\sum_{i=1}^{n} \mathbb{I}(X_i \leq x)}{n},$$

where $\mathbb{I}(A)$ is an *indicator function* that takes the value 1 if the event A occurs and 0 otherwise. For a more complete and technical treatment of these ideas, see Wasserman (2004) Chapter 7.

2.8 The three distributions: population, empirical, and sampling

Once we start to wade into estimation, there are several distributions to keep track of, and things can quickly become confusing. Three specific distributions are all related and easy to confuse, but keeping them distinct is crucial.

The **population distribution** is the distribution of the random variable, X_i, which we have labeled F and is our target of inference. The **empirical distribution** is the distribution of the actual realizations of the random variables in our samples, $X_1, \ldots, X_n$ (that is, the values that we eventually observe in our data frame). Because this is a random sample from the population distribution and can serve as an estimator of F, we sometimes call this $\widehat{F}_n$.

Separately from both is the **sampling distribution of an estimator**, which is the probability distribution of $\widehat{\theta}_n$. This represents the uncertainty around our estimate before we see the data. Remember that our estimator is itself a random variable because it is a function of random variables: the data itself. That is, we defined the estimator as $\widehat{\theta}_n = \theta(X_1, \ldots, X_n)$.

Example 2.8 (Likert responses)**.** Suppose X_i is the answer to the question "How much do you agree with the following statement: Immigrants are a net positive for the United States," where $X_i = 0$ is "strongly disagree," $X_i = 1$ is "disagree," $X_i = 2$ is "neither agree nor disagree," $X_i = 3$ is "agree," and $X_i = 4$ is "strongly agree."

The population distribution describes the probability of randomly selecting a person with each one of these values, $\mathbb{P}(X_i = x)$. The empirical distribution would be the fraction of our observed data taking each value. And the sampling distribution of the sample mean, $\overline{X}_n$, would be the distribution of the sample mean recalculated across repeated samples from the population.

Suppose the population distribution of X_i followed a binomial distribution with five trials and probability of success in each trial of $p = 0.4$. We could generate one sample with $n = 10$ and thus one empirical distribution using `rbinom()`:

```
my_samp <- rbinom(n = 10, size = 4, prob = 0.4)
my_samp
```

```
 [1] 1 2 1 3 3 0 2 3 2 1
```

```
table(my_samp)
```

```
my_samp
0 1 2 3
1 3 3 3
```

We obtain one draw from the sampling distribution of $\overline{X}_n$ by taking the mean of this sample:

```
mean(my_samp)
```

```
[1] 1.8
```

If we had a different sample,however, we would obtain a different empirical distribution and thus get a different estimate of the sample mean:

```r
my_samp2 <- rbinom(n = 10, size = 4, prob = 0.4)
mean(my_samp2)
```

```
[1] 1.6
```

The sampling distribution is the distribution of these sample means across repeated sampling.

2.9 Finite-sample properties of estimators

As discussed in our introduction to estimators, their usefulness depends on how well they help us learn about the quantity of interest. If we get an estimate $\widehat{\theta} = 1.6$, we would like to know that this is "close" to the true parameter θ. The sampling distribution is key to answering these questions. Intuitively, we would like the sampling distribution of $\widehat{\theta}_n$ to be as tightly clustered around the true θ as possible. Here, though, we run into a problem: the sampling distribution depends on the population distribution since it is about repeated samples of the data from that distribution filtered through the function $\theta()$. Since F is unknown, this implies that the sampling distribution will also usually be unknown.

Even though we cannot precisely pin down the entire sampling distribution, we can use assumptions to derive specific properties of the sampling distribution that are useful in comparing estimators. Note that the properties here will be very similar to the

2.9.1 Bias

The first property of the sampling distribution concerns its central tendency. In particular, we define the **bias** (or **estimation bias**) of estimator $\widehat{\theta}$ for parameter θ as

$$\text{bias}[\widehat{\theta}] = \mathbb{E}[\widehat{\theta}] - \theta,$$

which is the difference between the mean of the estimator (across repeated samples) and the true parameter. All else equal, we would like the estimation bias to be as small as possible. The smallest possible bias, obviously, is 0, and we define an **unbiased estimator** as one with $\text{bias}[\widehat{\theta}] = 0$ or equivalently, $\mathbb{E}[\widehat{\theta}] = \theta$.

However, all else is not always equal, and unbiasedness is not a property to which we should become overly attached. Many biased estimators have other attractive properties, and many popular modern estimators are biased.

Example 2.9 (Unbiasedness of the sample mean)**.** The sample mean is unbiased for the population mean when the data is iid and $\mathbb{E}|X| < \infty$. In particular, we apply the rules of expectations:

$$\begin{aligned}
\mathbb{E}\left[\overline{X}_n\right] &= \mathbb{E}\left[\frac{1}{n}\sum_{i=1}^{n} X_i\right] && \text{(definition of } \overline{X}_n\text{)} \\
&= \frac{1}{n}\sum_{i=1}^{n} \mathbb{E}[X_i] && \text{(linearity of } \mathbb{E}\text{)} \\
&= \frac{1}{n}\sum_{i=1}^{n} \mu && (X_i \text{ identically distributed}) \\
&= \mu.
\end{aligned}$$

Notice that we only used the "identically distributed" part of iid. Independence is not needed.

> **Warning**
>
> Properties like unbiasedness might only hold for a subset of DGPs. For example, we just showed that the sample mean is unbiased but only when the population mean is finite. There are probability distributions like the Cauchy that are not finite and where the expected value diverges. Thus, here we are dealing with a restricted class of DGPs that rules out such distributions. This is sometimes formalized by defining a class $\mathcal{F}$ of distributions; unbiasedness might hold in that class if it is unbiased for all $F \in \mathcal{F}$.

2.10 Question 5: Uncertainty

The spread of the sampling distribution is also important. We define the **sampling variance** as the variance of an estimator's sampling distribution, $\mathbb{V}[\hat{\theta}]$, which measures how spread out the estimator is around its mean. For an unbiased estimator, lower sampling

variance implies the distribution of $\hat{\theta}$ is more concentrated around the true value of the parameter.

Example 2.10 (Sampling variance of the sample mean)**.** We can prove that the sampling variance of the sample mean of iid data for all F such that $\mathbb{V}[X_i]$ is finite (more precisely, $\mathbb{E}[X_i^2] < \infty$)

$$\begin{aligned}
\mathbb{V}\left[\overline{X}_n\right] &= \mathbb{V}\left[\frac{1}{n}\sum_{i=1}^{n} X_i\right] && \text{(definition of } \overline{X}_n\text{)} \\
&= \frac{1}{n^2}\mathbb{V}\left[\sum_{i=1}^{n} X_i\right] && \text{(property of } \mathbb{V}\text{)} \\
&= \frac{1}{n^2}\sum_{i=1}^{n} \mathbb{V}[X_i] && \text{(independence)} \\
&= \frac{1}{n^2}\sum_{i=1}^{n} \sigma^2 && (X_i \text{ identically distributed}) \\
&= \frac{\sigma^2}{n}
\end{aligned}$$

As we discussed before, an alternative measure of spread for any distribution is the standard deviation, which is on the same scale as the original random variable. The standard deviation of the sampling distribution of $\hat{\theta}$ is known as the **standard error** of $\hat{\theta}$: $\mathsf{se}(\hat{\theta}) = \sqrt{\mathbb{V}[\hat{\theta}]}$.

Given the above derivation, the standard error of the sample mean under iid sampling is $\sigma/\sqrt{n}$.

2.10.1 Mean squared error

Bias and sampling variance measure two properties of "good" estimators because they capture the fact that we want the estimator to be as close as possible to the true value. One summary measure of the quality of an estimator is the **mean squared error** or **MSE**, which is

$$\text{MSE} = \mathbb{E}[(\hat{\theta}_n - \theta)^2].$$

We would ideally have this be as small as possible!

The MSE also relates to the bias and the sampling variance (provided it is finite) via the following decomposition result:

$$\text{MSE} = \text{bias}[\hat{\theta}_n]^2 + \mathbb{V}[\hat{\theta}_n] \tag{2.1}$$

This decomposition implies that, for unbiased estimators, MSE is the sampling variance. It also highlights why we might accept some bias for significant reductions in variance for lower overall MSE.

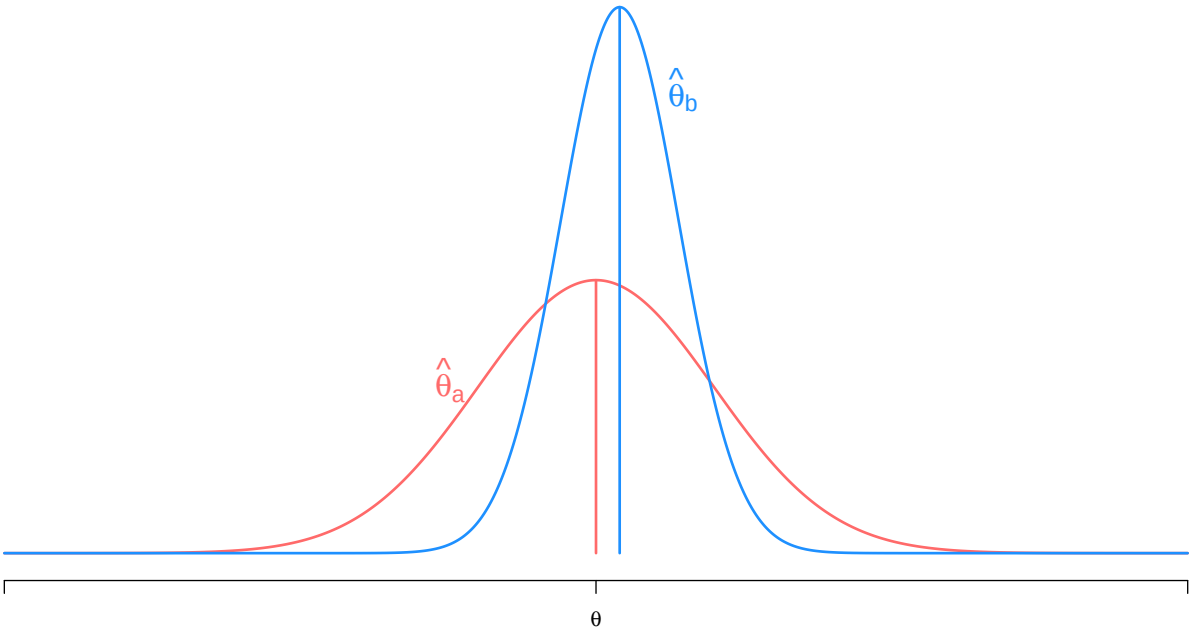


Figure 2.1: Two sampling distributions

This figure shows the sampling distributions of two estimators: (1) $\hat{\theta}_a$, which is unbiased (centered on the true value θ) but with a high sampling variance, and (2) $\hat{\theta}_b$, which is slightly biased but with much lower sampling variance. Even though $\hat{\theta}_b$ is biased, the probability of drawing a value close to the truth is higher than for $\hat{\theta}_a$. The MSE helps capture this balancing between bias and variance, and, indeed, in this case, $MSE[\hat{\theta}_b] < MSE[\hat{\theta}_a]$.

2.11 Summary

In this chapter, we introduced **model-based inference**, in which we posit a probability model for the data-generating process. These models can be **parametric** in the sense that we specify the probability distribution of the data up to some parameters. They can also be **semiparametric** where we only specify certain features of the distribution such as a finite mean and variance. This chapter mostly focused on the latter, where we assumed the observed data were **independent and identically distributed** draws from a population distribution with finite mean and variance.

An **estimator** is a function of the data meant as a guess for some quantity of interest in the population. Because it is a function of random variables (the data), estimators are also random variables and have distributions, called **sampling distributions**, across repeated draws from the population. If this distribution is centered on the true value of the quantity of interest, we call the estimator **unbiased**. The variance of the sampling distribution, called the **sampling variance**, tells us how variable we should expect the estimator to be across draws from the population. The mean-squared error is an overall measure of the accuracy of an estimator that combines notions of bias and sampling variance.

We showed in this chapter that the sample mean is unbiased for the population mean and that the sampling variance of the sample mean is the ratio of the population variance to the sample size. We also saw that **plug-in estimators** are a powerful way of constructing estimators as functions of sample means. That said, the focus of this chapter was finite-sample properties (that is, properties that are true no matter the sample size). In the next chapter, we will derive even more powerful results using large-sample approximations.

3 Asymptotics

3.1 Introduction

Suppose we are still interested in estimating the proportion of citizens who prefer increasing legal immigration. Based on the last chapter, a good strategy would be to use the sample proportion of immigration supporters in a random sample of citizens. You would have good reason to be confident with this estimator, with its finite-sample properties like unbiasedness and a sampling variance. We call these "finite-sample" properties since they hold at any sample size—they are as true for random samples of size for $n = 10$ as they are for random samples of size $n = 1,000,000$.

Finite-sample results, though, are of limited value because they only tell us about the center and spread of the sampling distribution of $\overline{X}_n$. Suppose we found that $\overline{X}_n = 0.47$ or 47% of respondents in a single survey supported increasing immigration. We might want to know how plausible it would be for the true population proportion – which is distinct from the sample proportion – to be 50% or greater. Questions like this are critical for a decision maker and, to answer this, we need to know the (approximate) distribution of $\overline{X}_n$ in addition to its mean and variance. We can often derive the exact distribution of an estimator if we are willing to make certain, sometimes strong assumptions about the underlying data (for example, if the population is normal, then the sample means will also be normal). Still, this approach is brittle: if our parametric assumption is false, we are back to square one.

In this chapter, we take a different approach by asking what happens to the sampling distribution of estimators as the sample size gets very large, which we refer to as **asymptotic theory**. While asymptotics will often simplify derivations, an essential point is that everything we do with asymptotics will be an approximation. No one ever has infinite data, but we hope that the approximations will be closer to the truth as our samples get larger.

Asymptotic results are key to modern statistical methods because many methods of quantifying uncertainty about estimates rely on asymptotic approximations. We will rely on the asymptotic results we derive in this chapter to estimate standard errors, construct confidence intervals, and perform hypothesis tests, all without assuming a fully parametric model.

3.2 Convergence of deterministic sequences

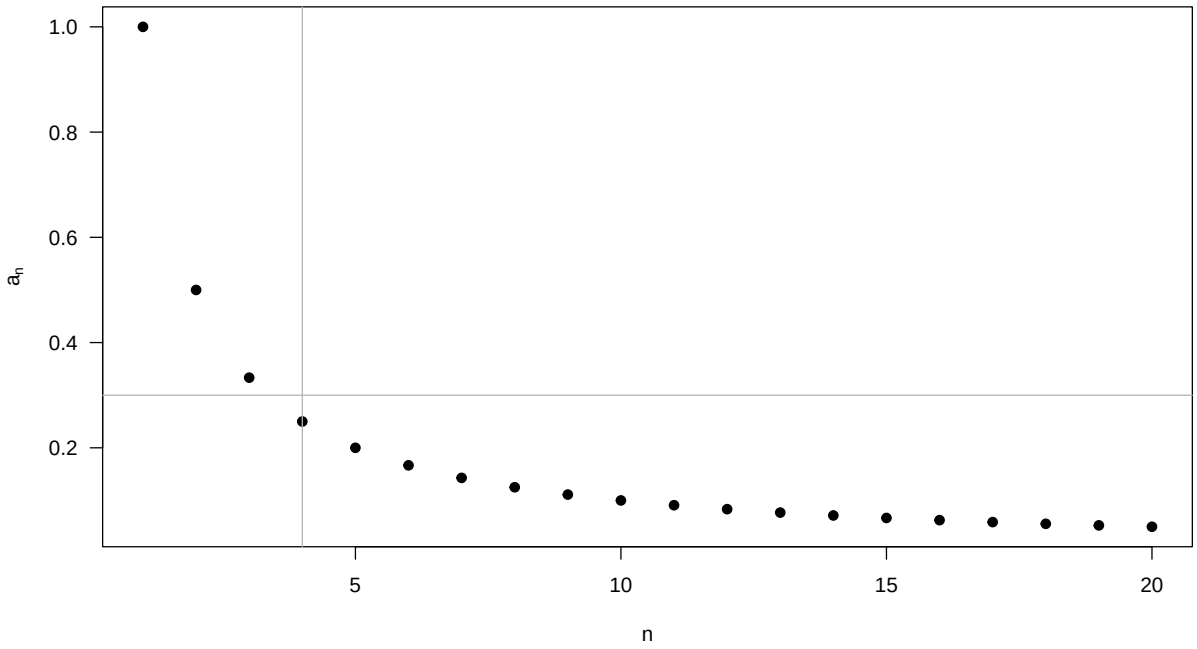
A helpful place to begin is by reviewing the basic idea of convergence in deterministic sequences from calculus:

Definition 3.1. A sequence $\{a_n : n = 1, 2, ...\}$ has the **limit** a written $a_n \to a$ as $n \to \infty$ or $\lim_{n\to\infty} a_n = a$ if for all $\epsilon > 0$ there is some $n_\epsilon < \infty$ such that for all $n \geq n_\epsilon$, $|a_n - a| \leq \epsilon$.

We say that a_n **converges** to a if $\lim_{n\to\infty} a_n = a$. Basically, a sequence converges to a number if the sequence gets closer and closer to that number as the sequence goes on.

Example 3.1. One important sequence that arises often in statistics is $1/n$ as $n \to \infty$. It may seem clear that this sequence converges to 0, but showing this using the formal definition of convergence is helpful.

Let us pick a specific value of $\epsilon = 0.3$. Now we need to find an integer n_ϵ so that $|1/n - 0| = 1/n \leq \epsilon$ for all $n \geq n_\epsilon$. Clearly, if $\epsilon = 0.3$, then $n_\epsilon = 4$ would satisfy this condition since $1/4 \leq 0.3$.



More generally, for any ϵ, $n \geq 1/\epsilon$ implies $1/n \leq \epsilon$. Thus, setting $n_\epsilon = 1/\epsilon$ ensures that the definition holds for all values of ϵ and that $\lim_{n\to\infty} 1/n = 0$.

We will mostly not use such formal definitions to establish a limit but, rather, rely on the properties of limits. For example, convergence and limits follow basic arithmetic operations. Suppose that we have two sequences with limits $\lim_{n\to\infty} a_n = a$ and $\lim_{n\to\infty} b_n = b$. Then the properties of limits imply:

- $\lim_{n\to\infty}(a_n + b_n) = a + b$
- $\lim_{n\to\infty} a_n b_n = ab$
- $\lim_{n\to\infty} ca_n = c \cdot a$
- $\lim_{n\to\infty}(a_n/b_n) = a/b$ if $b \neq 0$
- $\lim_{n\to\infty} a_n^k = a^k$

These rules plus the result in Example 3.1 allow us to prove other useful facts such as

$$\lim_{n\to\infty} \frac{2}{n} = 2 \cdot 0 = 0 \qquad \lim_{n\to\infty} \frac{1}{n^2} = 0.$$

Can we apply a similar definition of convergence to sequences of random variables (like estimators)? Possibly. Some examples clarify why this might be difficult.[1] Suppose

[1] Due to Wasserman (2004), Chapter 5.

we have a sequence of $a_n = a$ for all n (that is, a constant sequence). Then obviously $\lim_{n\to\infty} a_n = a$. Now let's say we have a sequence of random variables, $X_1, X_2, ...$, that are all independent with a standard normal distribution, $N(0,1)$. From the analogy to the deterministic case, saying that X_n converges to $X \sim N(0,1)$ would be tempting, but note that because they are all different random variables, $\mathbb{P}(X_n = X) = 0$. Thus, we must be careful about saying how one variable converges to another variable.

Another example highlights subtle problems with a sequence of random variables converging to a single value. Suppose we have a sequence of random variables $X_1, X_2, ...$ where $X_n \sim N(0, 1/n)$. Clearly, the distribution of X_n will concentrate around 0 for large values of n, so saying that X_n converges to 0 is tempting. But notice that $\mathbb{P}(X_n = 0) = 0$ because of the nature of continuous random variables.

3.3 Convergence in probability and consistency

A sequence of random variables can converge in several different ways. The first type of convergence deals with sequences converging to a single value.[2]

Definition 3.2. A sequence of random variables, $X_1, X_2, ...$, is said to **converge in probability** to a value b if for every $\varepsilon > 0$,

$$\mathbb{P}(|X_n - b| > \varepsilon) \to 0,$$

as $n \to \infty$. We write this $X_n \xrightarrow{p} b$.

What's happening in this definition? The even $|X_n - b| > \varepsilon$ says that a draw of X_n is more than ε away from b (above or below). So convergence in probability says that the probability of being some distance away from the limit value goes to zero as the n goes to ∞. With deterministic sequences, we said that a_n converges to a as it gets closer and closer to a as n gets bigger. For convergence in probability, the sequence of random variables converges to b if the probability that random variables are far away from b gets smaller and smaller as n gets big.

[2]Technically, a sequence can also converge in probability to another random variable, but the use case of converging to a single number is much more common in evaluating estimators.

Example 3.2. Let's illustrate the definition of convergence in probability by constructing a sequence of random variables,

$$X_n \sim N(0, 1/n).$$

We can see intuitively that this sequence will be centered at zero with a shrinking variance. Below, we will see that this is enough to establish convergence in probability of X_n to 0, but we can also show this in terms of its definition. To do so, we need to show that

$$\mathbb{P}(|X_n| > \varepsilon) \to 0.$$

Let $\Phi(\cdot)$ be the cdf for the standard normal. For any n, the cdf for X_n is $\mathbb{P}(X_n < x) = \Phi(\sqrt{n}x)$. Thus,

$$\begin{aligned}\mathbb{P}(|X_n| > \varepsilon) &= \mathbb{P}(X_n < -\varepsilon) + \mathbb{P}(X_n > \varepsilon) \\ &= \Phi(-\sqrt{n}\varepsilon) + (1 - \Phi(\sqrt{n}\varepsilon)) \to 0.\end{aligned}$$

The last limit is due to $\sqrt{n}\varepsilon \to \infty$ and thus, by the properties of the cdf, $\Phi(-\sqrt{n}\varepsilon) \to 0$ and $\Phi(\sqrt{n}\varepsilon) \to 1$. Clearly this holds for any ε, so $X_n \xrightarrow{p} 0$.

> **i** Notation alert
>
> Sometimes convergence in probability is written as $\text{plim}(Z_n) = b$ when $Z_n \xrightarrow{p} b$, plim stands for "probability limit."

Convergence in probability is crucial for evaluating estimators. While we said that unbiasedness was not the be-all and end-all of properties of estimators, the following property is an essential and fundamental property of good estimators.

Definition 3.3. An estimator is **consistent** if $\hat{\theta}_n \xrightarrow{p} \theta$.

Consistency of an estimator implies that the sampling distribution of the estimator "collapses" on the true value as the sample size gets large. An estimator is **inconsistent** if it converges in probability to any other value. As the sample size gets large, the probability that an inconsistent estimator will be close to the truth will approach 0. Generally speaking, consistency is a very desirable property of an estimator.

> **Note**
>
> Estimators can be inconsistent yet still converge in probability to an understandable quantity. For example, we will discuss in later chapters that regression coefficients estimated by ordinary least squares (OLS) are consistent for the conditional expectation if the conditional expectation is linear. If that function is non-linear, however, then OLS will be consistent for the best linear approximation to that function. While not ideal, it does mean that this estimator is at least consistent for an interpretable quantity.

We can also define convergence in probability for a sequence of random vectors, $\mathbf{X}_1, \mathbf{X}_2, ...$, where $\mathbf{X}_i = (X_{i1}, \dots, X_{ik})$ is a random vector of length k. This sequence converges in probability to a vector $\mathbf{b} = (b_1, \dots, b_k)$ if and only if each random variable in the vector converges to the corresponding element in $\mathbf{b}$, or that $X_{nj} \xrightarrow{p} b_j$ for all $j = 1, \dots, k$.

3.4 Useful inequalities

At first glance, establishing an estimator's consistency will be difficult. How can we know if a distribution will collapse to a specific value without knowing the shape or family of the distribution? It turns out that there are certain relationships between the mean and variance of a random variable and certain probability statements that hold for all distributions (that have finite variance, at least). These relationships are key to establishing results that do not depend on a specific distribution.

Theorem 3.1 (Markov Inequality)**.** *For any r.v. X and any $\delta > 0$,*

$$\mathbb{P}(|X| \geq \delta) \leq \frac{\mathbb{E}[|X|]}{\delta}.$$

Proof. Note that we can let $Y = |X|/\delta$ and rewrite the statement as $\mathbb{P}(Y \geq 1) \leq \mathbb{E}[Y]$ (since $\mathbb{E}[|X|]/\delta = \mathbb{E}[|X|/\delta]$ by the properties of expectation), which is what we will show. But also note that

$$\mathbb{I}(Y \geq 1) \leq Y.$$

Why does this hold? The two possible values of the indicator function show why. If Y is less than 1, then the indicator function will be 0, but recall that Y is nonnegative, so

we know that it must be at least as big as 0 so that inequality holds. If $Y \geq 1$, then the indicator function will take the value one, but we just said that $Y \geq 1$, so the inequality holds. If we take the expectation of both sides of this inequality, we obtain the result (remember, the expectation of an indicator function is the probability of the event). □

In words, Markov's inequality says that the probability of a random variable being large in magnitude cannot be high if the average is not large in magnitude. Blitzstein and Hwang (2019) provide an excellent intuition behind this result using income as an example. Let X be the income of a randomly selected individual in a population and set $\delta = 2\mathbb{E}[X]$ so that the inequality becomes $\mathbb{P}(X > 2\mathbb{E}[X]) < 1/2$ (assuming that all income is nonnegative). Here, the inequality says that the share of the population with an income twice the average must be less than 0.5 since if more than half the population were making twice the average income, then the average would have to be higher.

It's pretty astounding how general this result is since it holds for all random variables. Of course, its generality comes at the expense of not being very informative. If $\mathbb{E}[|X|] = 5$, for instance, the inequality tells us that $\mathbb{P}(|X| \geq 1) \leq 5$, which is not very helpful since we already know that probabilities are less than 1! We can get tighter bounds if we are willing to make some assumptions about X.

Theorem 3.2 (Chebyshev Inequality)**.** *Suppose that X is r.v. for which $\mathbb{V}[X] < \infty$. Then, for every real number $\delta > 0$,*

$$\mathbb{P}(|X - \mathbb{E}[X]| \geq \delta) \leq \frac{\mathbb{V}[X]}{\delta^2}.$$

Proof. To prove this, we only need to square both sides of the inequality inside the probability statement and apply Markov's inequality:

$$\mathbb{P}\left(|X - \mathbb{E}[X]| \geq \delta\right) = \mathbb{P}((X - \mathbb{E}[X])^2 \geq \delta^2) \leq \frac{\mathbb{E}[(X - \mathbb{E}[X])^2]}{\delta^2} = \frac{\mathbb{V}[X]}{\delta^2},$$

with the last equality holding by the definition of variance. □

Chebyshev's inequality is a straightforward extension of the Markov result: the probability of a random variable being far from its mean (that is, $|X - \mathbb{E}[X]|$ being large) is limited by the variance of the random variable. If we let $\delta = c\sigma$, where σ is the standard deviation of X, we can use this result to bound the normalized deviation from the mean:

$$\mathbb{P}\left(\frac{|X - \mathbb{E}[X]|}{\sigma} > c\right) \leq \frac{1}{c^2}.$$

This statement says the probability of being two standard deviations away from the mean must be less than 1/4 = 0.25. Notice that this bound can be fairly wide. If X has a normal distribution, we know that about 5% of draws will be greater than 2 SDs away from the mean, much lower than the 25% bound implied by Chebyshev's inequality.

3.5 The law of large numbers

We can now use these inequalities to show how estimators can be consistent for their target quantities of interest without making parametric assumptions. Why are these inequalities helpful? Remember that convergence in probability was about the probability of an estimator being far away from a value going to zero. Chebyshev's inequality shows that we can bound these exact probabilities.

The most famous consistency result has a special name.

Theorem 3.3 (Weak Law of Large Numbers)**.** *Let $X_1, \ldots, X_n$ be i.i.d. draws from a distribution with mean $\mu = \mathbb{E}[X_i]$ and variance $\sigma^2 = \mathbb{V}[X_i] < \infty$. Let $\overline{X}_n = \frac{1}{n}\sum_{i=1}^{n} X_i$. Then, $\overline{X}_n \xrightarrow{p} \mu$.*

Proof. Recall that the sample mean is unbiased, so $\mathbb{E}[\overline{X}_n] = \mu$ with sampling variance σ^2/n. We can then apply Chebyshev to the sample mean to get

$$\mathbb{P}(|\overline{X}_n - \mu| \geq \delta) \leq \frac{\mathbb{V}[\overline{X}_n]}{\delta} = \frac{\sigma^2}{n\delta^2}$$

An $n \to \infty$, the right-hand side goes to 0, which means that the left-hand side also must go to 0, which is the definition of $\overline{X}_n$ converging in probability to μ. □

The weak law of large numbers (WLLN) shows that, under general conditions, the sample mean gets closer to the population mean as $n \to \infty$. This result holds even when the variance of the data is infinite, though researchers will rarely face such a situation.

> **Note**
>
> The naming of the "weak" law of large numbers seems to imply the existence of a "strong" law of large numbers (SLLN), which is true. The SLLN states that the sample mean converges to the population mean with probability 1. This type of con-

vergence, called **almost sure convergence**, is stronger than convergence in probability, which only says that the probability of the sample mean being close to the population mean converges to 1. While it is nice to know that this stronger form of convergence holds for the sample mean under the same assumptions, it is rare for researchers outside of theoretical probability and statistics to rely on almost sure convergence.

Example 3.3. Seeing how the distribution of the sample mean changes as a function of the sample size allows us to appreciate the WLLN. We can see this by taking repeated iid samples of different sizes from an exponential random variable with rate parameter 0.5 so that $\mathbb{E}[X_i] = 2$. In Figure 3.1, we show the distribution of the sample mean (across repeated samples) when the sample size is 15 (black), 30 (violet), 100 (blue), and 1000 (green). The sample mean distribution "collapses" on the true population mean, 2. The probability of being far away from 2 becomes progressively smaller as the sample size increases.

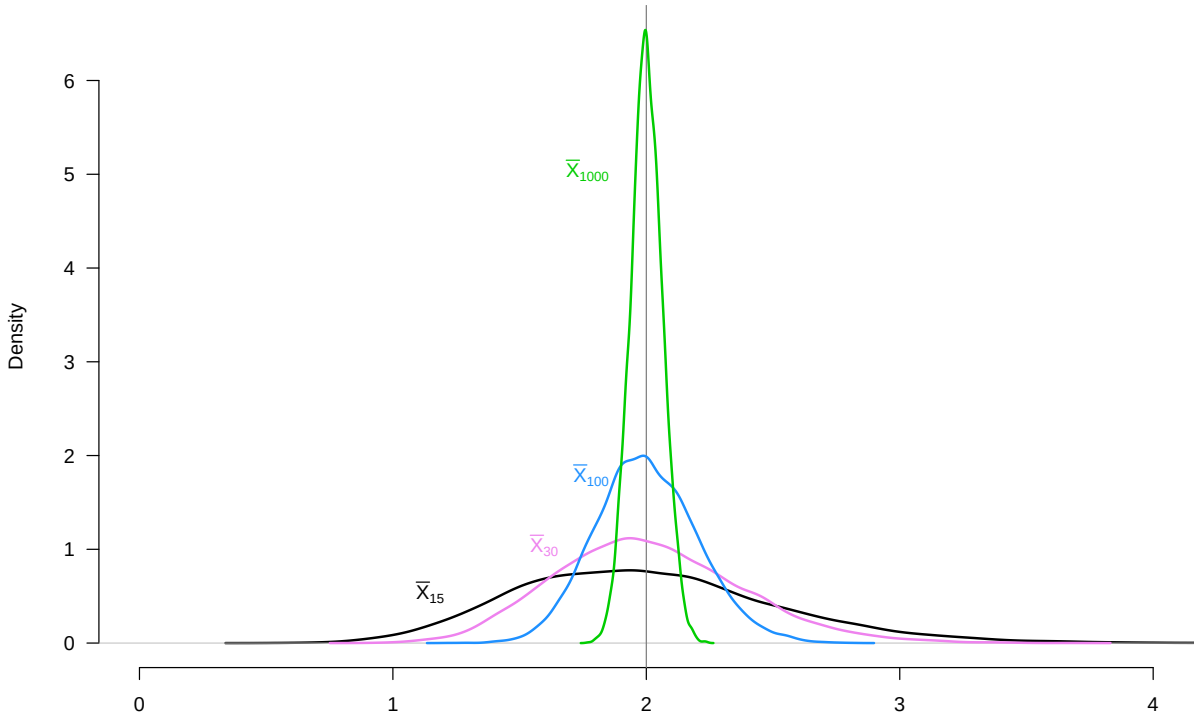


Figure 3.1: Sampling distribution of the sample mean as a function of sample size.

The WLLN also holds for random vectors in addition to random variables. Let $(\mathbf{X}_1, \dots, \mathbf{X}_n)$ be an iid sample of random vectors of length k, $\mathbf{X}_i = (X_{i1}, \dots, X_{ik})$. We can define the vector sample mean as just the vector of sample means for each of the entries:

$$\overline{\mathbf{X}}_n = \frac{1}{n}\sum_{i=1}^{n} \mathbf{X}_i = \begin{pmatrix} \overline{X}_{n,1} \\ \overline{X}_{n,2} \\ \vdots \\ \overline{X}_{n,k} \end{pmatrix}$$

Since this is just a vector of sample means, each random variable in the random vector will converge in probability to the mean of that random variable. Fortunately, this is the exact definition of convergence in probability for random vectors. We formally write this in the following theorem.

Theorem 3.4. *If $\mathbf{X}_i \in \mathbb{R}^k$ are iid draws from a distribution with $\mathbb{E}[X_{ij}] < \infty$ for all $j = 1, \dots, k$ then as $n \to \infty$*

$$\overline{\mathbf{X}}_n \xrightarrow{p} \mathbb{E}[\mathbf{X}] = \begin{pmatrix} \mathbb{E}[X_{i1}] \\ \mathbb{E}[X_{i2}] \\ \vdots \\ \mathbb{E}[X_{ik}] \end{pmatrix}.$$

i Notation alert

Note that many of the formal results presented so far have "moment conditions" that certain moments are finite. For the vector WLLN, we saw that applied to the mean of each variable in the vector. Some books use a shorthand for this: $\mathbb{E}\|\mathbf{X}_i\| < \infty$, where

$$\|\mathbf{X}_i\| = \left(X_{i1}^2 + X_{i2}^2 + \dots + X_{ik}^2\right)^{1/2}.$$

This expression has slightly more compact notation, but why does it work? One can show that this function, called the **Euclidean norm** or L_2-norm, is a **convex** function, so we can apply Jensen's inequality to show that:

$$\mathbb{E}\|\mathbf{X}_i\| \geq \|\mathbb{E}[\mathbf{X}_i]\| = (\mathbb{E}[X_{i1}]^2 + \dots + \mathbb{E}[X_{ik}]^2)^{1/2}.$$

So if $\mathbb{E}\|\mathbf{X}_i\|$ is finite, all the component means are finite. Otherwise, the right-hand side of the previous equation would be infinite.

3.6 Consistency of estimators

The WLLN shows that the sample mean of iid draws is consistent for the population mean, which is a massive result given that so many estimators are sample means of potentially complicated functions of the data. What about other estimators? The proof of the WLLN points to one way to determine that an estimator is consistent: if it is unbiased and the sampling variance shrinks as the sample size grows.

Theorem 3.5. *For any estimator $\hat{\theta}_n$, if bias$[\hat{\theta}_n] = 0$ and $\mathbb{V}[\hat{\theta}_n] \to 0$ as $n \to \infty$, then $\hat{\theta}_n$ is consistent.*

Thus, for unbiased estimators, if we can characterize its sampling variance, we should be able to tell if it is consistent. This result is handy since working with the probability statements used for the WLLN can sometimes be confusing.

What about biased estimators? Consider a situation where we calculate average household income, $\overline{X}_n$, from a random sample with mean μ, but our actual interest is in the log of average income, $\alpha = \log(\mu)$. We can obviously use the standard plug-in estimator $\hat{\alpha} = \log(\overline{X}_n)$, but, for nonlinear functions like logarithms we have $\log(\mathbb{E}[Z]) \neq \mathbb{E}[\log(Z)]$, so $\mathbb{E}[\hat{\alpha}] \neq \log(\mathbb{E}[\overline{X}_n])$ and the plug-in estimator will be biased for $\log(\mu)$. Obtaining an expression for the bias in terms of n is also difficult. Is the quest doomed? Must we give up on consistency? No, and, in fact, a few key properties of consistency make working with it much easier compared to unbiasedness.

Theorem 3.6 (Properties of convergence in probability)**.** *Let X_n and Z_n be two sequences of random variables such that $X_n \xrightarrow{p} a$ and $Z_n \xrightarrow{p} b$, and let $g(\cdot)$ be a continuous function. Then,*

1. $g(X_n) \xrightarrow{p} g(a)$ *(continuous mapping theorem)*
2. $X_n + Z_n \xrightarrow{p} a + b$
3. $X_n Z_n \xrightarrow{p} ab$
4. $X_n / Z_n \xrightarrow{p} a/b$ *if* $b > 0$.

We can now see that many of the nasty problems with expectations and nonlinear functions are made considerably easier with convergence in probability in the asymptotic setting. So while we know that $\log(\overline{X}_n)$ is biased for $\log(\mu)$, we know that it is consistent since $\log(\overline{X}_n) \xrightarrow{p} \log(\mu)$ because log is a continuous function.

Example 3.4. Suppose we implemented a survey by randomly selecting a sample from the population of size n, but not everyone responds to the survey. Let the data consist of pairs of random variables, $(Y_1, R_1), \ldots, (Y_n, R_n)$, where Y_i is the question of interest and R_i is a binary indicator for if the respondent answered the question ($R_i = 1$) or not ($R_i = 0$). Our goal is to estimate the mean of the question for responders: $\mathbb{E}[Y_i \mid R_i = 1]$. We can use the law of iterated expectation to obtain

$$\begin{aligned} \mathbb{E}[Y_i R_i] &= \mathbb{E}[Y_i \mid R_i = 1]\mathbb{P}(R_i = 1) + \mathbb{E}[0 \mid R_i = 0]\mathbb{P}(R_i = 0) \\ \implies \mathbb{E}[Y_i \mid R_i = 1] &= \frac{\mathbb{E}[Y_i R_i]}{\mathbb{P}(R_i = 1)} \end{aligned}$$

The relevant estimator for this quantity is the mean of the outcome among those who responded, which is slightly more complicated than a typical sample mean because the denominator is a random variable:

$$\hat{\theta}_n = \frac{\sum_{i=1}^n Y_i R_i}{\sum_{i=1}^n R_i}.$$

Notice that this estimator is the ratio of two random variables. The numerator has mean $n\mathbb{E}[Y_i R_i]$ and the denominator has mean $n\mathbb{P}(R_i = 1)$. It is then tempting to say that we can take the ratio of these means as the mean of $\hat{\theta}_n$, but expectations are not preserved in nonlinear functions like this.

We can establish consistency of our estimator, though, by noting that we can rewrite the estimator as a ratio of sample means

$$\hat{\theta}_n = \frac{(1/n)\sum_{i=1}^n Y_i R_i}{(1/n)\sum_{i=1}^n R_i},$$

where by the WLLN the numerator $(1/n)\sum_{i=1}^n Y_i R_i \xrightarrow{p} \mathbb{E}[Y_i R_i]$ and the denominator $(1/n)\sum_{i=1}^n R_i \xrightarrow{p} \mathbb{P}(R_i = 1)$. Thus, by Theorem 3.6, we have

$$\hat{\theta}_n = \frac{(1/n)\sum_{i=1}^n Y_i R_i}{(1/n)\sum_{i=1}^n R_i} \xrightarrow{p} \frac{\mathbb{E}[Y_i R_i]}{\mathbb{P}[R_i = 1]} = \mathbb{E}[Y_i \mid R_i = 1],$$

so long as the probability of responding is greater than zero. This establishes that our sample mean among responders, while biased for the conditional expectation among responders, is consistent for that quantity.

Keeping the difference between unbiased and consistent clear in your mind is essential. You can easily create ridiculous unbiased estimators that are inconsistent. Let's return to our iid sample, $X_1, \dots, X_n$, from a population with $E[X_i] = \mu$. There is nothing in the rule book against defining an estimator $\hat{\theta}_{first} = X_1$ that uses the first observation as the estimate. This estimator is silly, but it is unbiased since $\mathbb{E}[\hat{\theta}_{first}] = \mathbb{E}[X_1] = \mu$. It is inconsistent since the sampling variance of this estimator is just the variance of the population distribution, $\mathbb{V}[\hat{\theta}_{first}] = \mathbb{V}[X_i] = \sigma^2$, which does not change as a function of the sample size. Generally speaking, we can regard "unbiased but inconsistent" estimators as silly and not worth our time (along with biased and inconsistent estimators).

Some estimators are biased but consistent that are often much more interesting. We already saw one such estimator in Example 3.4, but there are many more. Maximum likelihood estimators, for example, are (under some regularity conditions) consistent for the parameters of a parametric model but are often biased.

To study these estimator, we can broaden Theorem 3.5 to the class of **asymptotically unbiased** estimators that have bias that vanishes as the sample size grows.

Theorem 3.7. *For any estimator $\hat{\theta}_n$, if bias$[\hat{\theta}_n] \to 0$ and $\mathbb{V}[\hat{\theta}_n] \to 0$ as $n \to \infty$, then $\hat{\theta}_n$ is consistent.*

Proof. Using Markov's inequality, we have

$$\mathbb{P}\left(|\hat{\theta}_n - \theta| \geq \delta\right) = \mathbb{P}((\hat{\theta}_n - \theta)^2 \geq \delta^2) \leq \frac{\mathbb{E}[(\hat{\theta}_n - \theta)^2]}{\delta^2} = \frac{\text{bias}[\hat{\theta}_n]^2 + \mathbb{V}[\hat{\theta}]}{\delta^2} \to 0.$$

The last inequality follows from the bias-variance decomposition of the mean squared error in Equation 2.1. □

We can use this result to show consistency for a large range of estimators.

Example 3.5 (Plug-in variance estimator)**.** In the last chapter, we introduced the plug-in estimator for the population variance,

$$\hat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^{n}(X_i - \overline{X}_n)^2,$$

which we will now show is biased but consistent. To see the bias note that we can rewrite the sum of square deviations

$$\sum_{i=1}^{n}(X_i - \overline{X}_n)^2 = \sum_{i=1}^{n} X_i^2 - n\overline{X}_n^2.$$

Then, the expectation of the plug-in estimator is

$$\begin{aligned}
\mathbb{E}[\hat{\sigma}^2] &= \mathbb{E}\left[\frac{1}{n}\sum_{i=1}^{n} X_i^2\right] - \mathbb{E}[\overline{X}_n^2] \\
&= \mathbb{E}[X_i^2] - \frac{1}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n}\mathbb{E}[X_i X_j] \\
&= \mathbb{E}[X_i^2] - \frac{1}{n^2}\sum_{i=1}^{n}\mathbb{E}[X_i^2] - \frac{1}{n^2}\sum_{i=1}^{n}\sum_{j\neq i}\underbrace{\mathbb{E}[X_i]\mathbb{E}[X_j]}_{\text{independence}}. \\
&= \mathbb{E}[X_i^2] - \frac{1}{n}\mathbb{E}[X_i^2] - \frac{1}{n^2}n(n-1)\mu^2 \\
&= \frac{n-1}{n}\left(\mathbb{E}[X_i^2] - \mu^2\right) \\
&= \frac{n-1}{n}\sigma^2 = \sigma^2 - \frac{1}{n}\sigma^2
\end{aligned}$$

Thus, we can see that the bias of the plug-in estimator is $-(1/n)\sigma^2$, so it slightly underestimates the variance. Nicely, though, the bias shrinks as a function of the sample size, so according to Theorem 3.7, it will be consistent so long as the sampling variance of $\hat{\sigma}^2$ shrinks as a function of the sample size, which it does (though omit that proof here). Of course, simply multiplying this estimator by $n/(n-1)$ will give an unbiased and consistent estimator that is also the typical sample variance estimator.

3.7 Convergence in distribution and the central limit theorem

Convergence in probability and the law of large numbers are beneficial for understanding how our estimators will (or will not) collapse to their estimand as the sample size increases. But what about the shape of the sampling distribution of our estimators? For statistical

inference, we would like to be able to make probability statements such as $\mathbb{P}(a \leq \widehat{\theta}_n \leq b)$. These statements will be the basis of hypothesis testing and confidence intervals. But to make those types of statements, we need to know the entire distribution of $\widehat{\theta}_n$, not just the mean and variance. Luckily, established results will allow us to approximate the sampling distribution of a vast swath of estimators when our sample sizes are large.

We need first to describe a weaker form of convergence to see how we will develop these approximations.

Definition 3.4. Let $X_1, X_2, ...$, be a sequence of r.v.s, and for $n = 1, 2, ...$ let $F_n(x)$ be the c.d.f. of X_n. Then it is said that $X_1, X_2, ...$ **converges in distribution** to r.v. X with c.d.f. $F(x)$ if

$$\lim_{n \to \infty} F_n(x) = F(x),$$

for all values of x for which $F(x)$ is continuous. We write this as $X_n \xrightarrow{d} X$ or sometimes $X_n \rightsquigarrow X$.

Essentially, convergence in distribution means that as n gets large, the distribution of X_n becomes more and more similar to the distribution of X, which we often call the **asymptotic distribution** of X_n (other names include the **large-sample distribution**). If we know that $X_n \xrightarrow{d} X$, then we can use the distribution of X as an approximation to the distribution of X_n, and that distribution can be reasonably accurate.

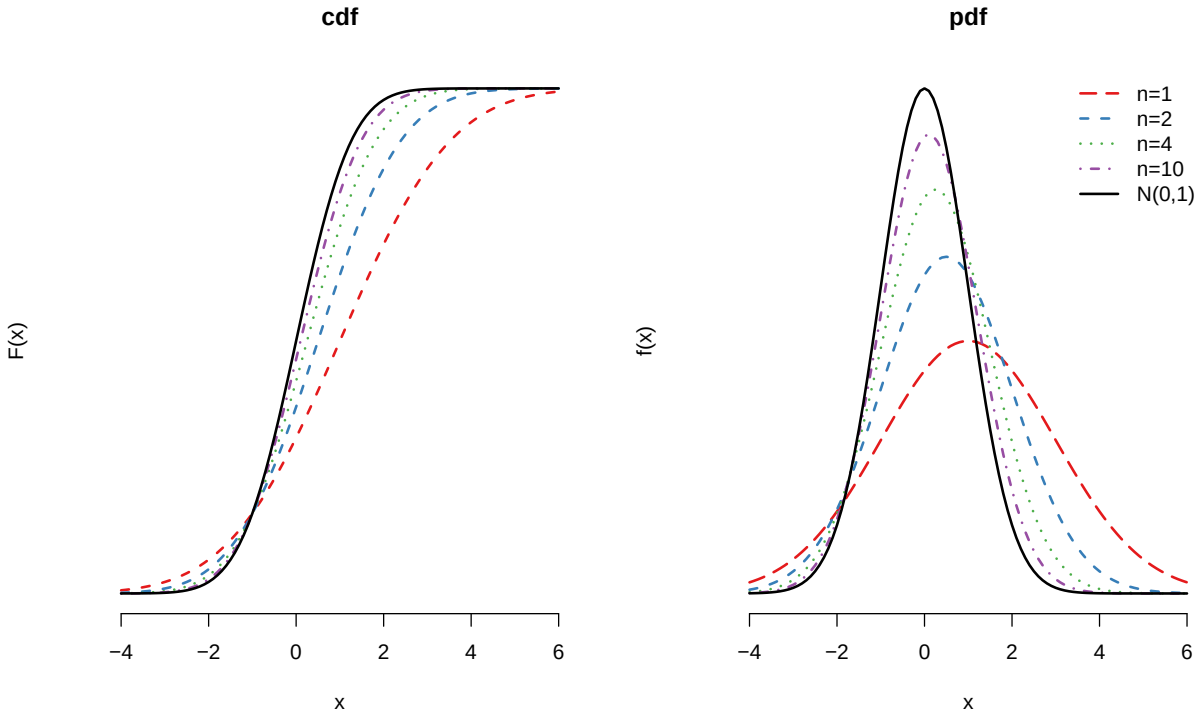
Example 3.6. A simple example of convergence in distribution would be the sequence

$$X_n \sim N\left(\frac{1}{n}, 1 + \frac{1}{n}\right),$$

which, of course, has the cdf,

$$\Phi\left(\frac{x - 1/n}{1 + 1/n}\right).$$

By inspection, this converges to $\Phi(x)$, which is the cdf for the standard normal. This implies $X_n \xrightarrow{d} N(0, 1)$.



One of the most remarkable results in probability and statistics is that a large class of estimators will converge in distribution to one particular family of distributions: the normal. This result is one reason we study the normal so much and why investing in building intuition about it will pay off across many domains of applied work. We call this broad class of results the "central limit theorem" (CLT), but it would probably be more accurate to refer to them as "central limit theorems" since much of statistics is devoted to showing the result in different settings. We now present the simplest CLT for the sample mean.

Theorem 3.8 (Central Limit Theorem)**.** *Let $X_1, \dots, X_n$ be i.i.d. r.v.s from a distribution with mean $\mu = \mathbb{E}[X_i]$ and variance $\sigma^2 = \mathbb{V}[X_i]$. Then if $\mathbb{E}[X_i^2] < \infty$, we have*

$$\frac{\overline{X}_n - \mu}{\sqrt{\mathbb{V}[\overline{X}_n]}} = \frac{\sqrt{n}\left(\overline{X}_n - \mu\right)}{\sigma} \xrightarrow{d} \mathcal{N}(0,1).$$

In words: the sample mean of a random sample from a population with finite mean and variance will be approximately normally distributed in large samples. Notice how we have not made any assumptions about the distribution of the underlying random variables, X_i. They could be binary, event count, continuous, or anything. The CLT is incredibly broadly applicable.

Notation alert

Why do we state the CLT in terms of the sample mean after centering and scaling by its standard error? Suppose we don't normalize the sample mean in this way. In that case, it isn't easy to talk about convergence in distribution because we know from the WLLN that $\overline{X}_n \xrightarrow{p} \mu$, so in the limit, the distribution of $\overline{X}_n$ is concentrated at point mass around that value. Normalizing by centering and rescaling ensures that the variance of the resulting quantity will not depend on n, so it makes sense to talk about its distribution converging. Sometimes you will see the equivalent result as

$$\sqrt{n}\left(\overline{X}_n - \mu\right) \xrightarrow{d} \mathcal{N}(0, \sigma^2).$$

We can use this result to state approximations that we can use when discussing estimators such as

$$\overline{X}_n \overset{a}{\sim} N(\mu, \sigma^2/n),$$

where we use $\overset{a}{\sim}$ to be "approximately distributed as in large samples." This approximation allows us to say things like: "in large samples, we should expect the sample mean to between within $2\sigma/\sqrt{n}$ of the true mean in 95% of repeated samples." These statements will be essential for hypothesis tests and confidence intervals! Estimators so often follow the CLT that we have an expression for this property.

Definition 3.5. An estimator $\hat{\theta}_n$ is **asymptotically normal** if for some θ

$$\sqrt{n}\left(\hat{\theta}_n - \theta\right) \xrightarrow{d} N\left(0, \mathbb{V}_\theta\right).$$

Example 3.7. To illustrate how the CLT works, we can simulate the sampling distribution of the (normalized) sample mean at different sample sizes. Let $X_1, \ldots, X_n$ be iid samples from a Bernoulli with probability of success 0.25. We then draw repeated samples of size $n = 30$ and $n = 100$ and calculate $\sqrt{n}(\overline{X}_n - 0.25)/\sigma$ for each random sample. Figure 3.2 plots the density of these two sampling distributions along with a standard normal reference. We can see that even at $n = 30$, the rough shape of the density looks normal, with spikes and valleys due to the discrete nature of the data (the sample mean can only take on 31 possible values in this case). By $n = 100$, the sampling distribution is very close to the true standard normal.

There are several properties of convergence in distribution that are helpful to us.

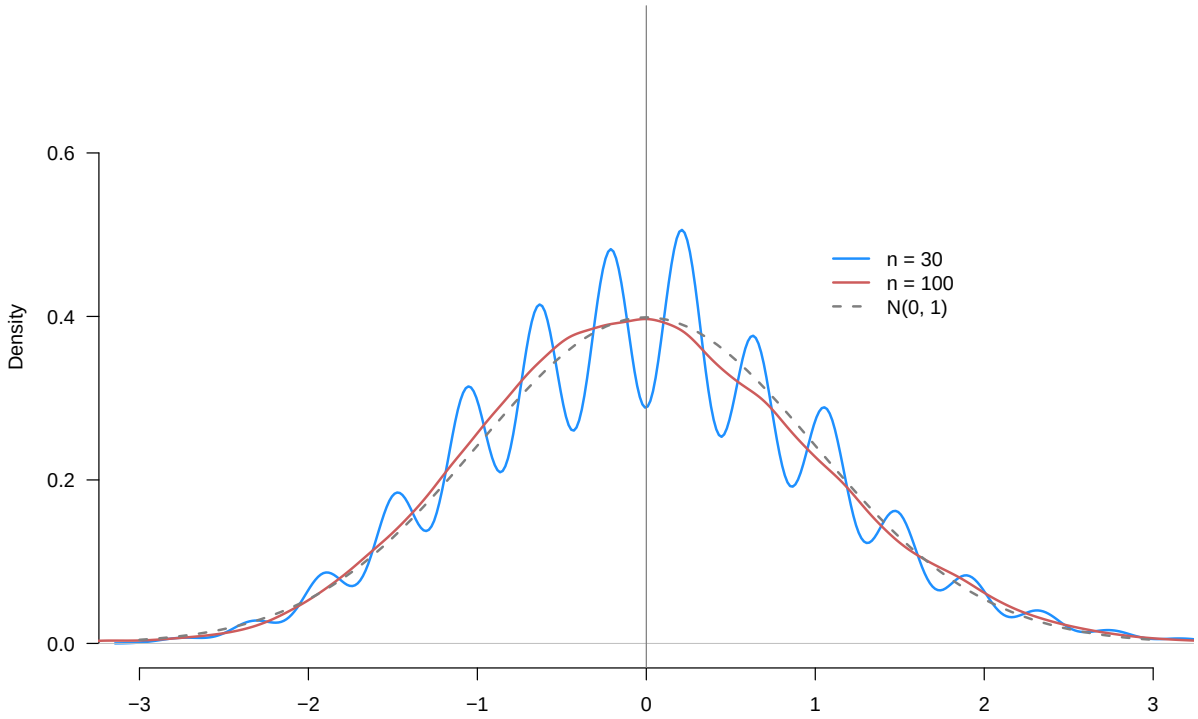


Figure 3.2: Sampling distributions of the normalized sample mean at n=30 and n=100.

Theorem 3.9 (Properties of convergence in distribution)**.** *Let X_n be a sequence of random variables $X_1, X_2, \ldots$ that converges in distribution to some rv X and let Y_n be a sequence of random variables $Y_1, Y_2, \ldots$ that converges in probability to some number, c. Then,*

1. $g(X_n) \xrightarrow{d} g(X)$ *for all continuous functions g.*
2. $X_n Y_n$ *converges in distribution to* cX
3. $X_n + Y_n$ *converges in distribution to* $X + c$
4. X_n / Y_n *converges in distribution to* X/c *if* $c \neq 0$

We refer to the last three results as **Slutsky's theorem**. These results are often crucial for determining an estimator's asymptotic distribution.

A critical application of Slutsky's theorem is when we replace the (unknown) population variance in the CLT with an estimate. Recall the definition of the **sample variance** as

$$S_n^2 = \frac{1}{n-1} \sum_{i=1}^{n} (X_i - \overline{X}_n)^2,$$

with the **sample standard deviation** defined as $S_n = \sqrt{S_n^2}$. It's easy to show that these are consistent estimators for their respective population parameters

$$S_n^2 \xrightarrow{p} \sigma^2 = \mathbb{V}[X_i], \qquad S_n \xrightarrow{p} \sigma,$$

which, by Slutsky's theorem, implies that

$$\frac{\sqrt{n}\left(\overline{X}_n - \mu\right)}{S_n} \xrightarrow{d} \mathcal{N}(0,1)$$

Comparing this result to the statement of CLT, we see that replacing the population variance with a consistent estimate of the variance (or standard deviation) does not affect the asymptotic distribution.

Like with the WLLN, the CLT holds for random vectors of sample means, where their centered and scaled versions converge to a multivariate normal distribution with a covariance matrix equal to the covariance matrix of the underlying random vectors of data, $\mathbf{X}_i$.

Theorem 3.10. *If $\mathbf{X}_i \in \mathbb{R}^k$ are i.i.d. and $\mathbb{E}\|\mathbf{X}_i\|^2 < \infty$, then as $n \to \infty$,*

$$\sqrt{n}\left(\overline{\mathbf{X}}_n - \boldsymbol{\mu}\right) \xrightarrow{d} \mathcal{N}(0, \boldsymbol{\Sigma}),$$

where $\boldsymbol{\mu} = \mathbb{E}[\mathbf{X}_i]$ and $\boldsymbol{\Sigma} = \mathbb{V}[\mathbf{X}_i] = \mathbb{E}\left[(\mathbf{X}_i - \boldsymbol{\mu})(\mathbf{X}_i - \boldsymbol{\mu})'\right]$.

Notice that $\boldsymbol{\mu}$ is the vector of population means for all the random variables in $\mathbf{X}_i$ and $\boldsymbol{\Sigma}$ is the variance-covariance matrix for that vector.

> **Note**
>
> As with the notation alert with the WLLN, we are using shorthand here, $\mathbb{E}\|\mathbf{X}_i\|^2 < \infty$, which implies that $\mathbb{E}[X_{ij}^2] < \infty$ for all $j = 1, \ldots, k$, or equivalently, that the variances of each variable in the sample means has finite variance.

3.8 Confidence intervals

We now turn to an essential application of the central limit theorem: confidence intervals.

Suppose we have run an experiment with a treatment and control group and have presented readers with our single best guess about the treatment effect using the difference in sample means. We have also presented the estimated standard error of this estimate to give readers a sense of how variable it is. But none of these approaches answer a fairly compelling question: what range of values of the treatment effect is **plausible** given the data we observe?

A point estimate of the difference in sample means typically has 0 probability of being the exact true value, but intuitively we hope that the true treatment effect is close to our estimate. **Confidence intervals** make this kind of intuition more formal by instead estimating ranges of values with a fixed percentage of these ranges containing the actual unknown parameter value.

We begin with the basic definition of a confidence interval.

Definition 3.6. A $1-\alpha$ **confidence interval** for a real-valued parameter θ is a pair of statistics $L = L(X_1, \dots, X_n)$ and $U = U(X_1, \dots, X_n)$ such that $L < U$ for all values of the sample and such that

$$\mathbb{P}(L \leq \theta \leq U \mid \theta) \geq 1 - \alpha, \quad \forall \theta \in \Theta.$$

We say that a $1-\alpha$ confidence interval covers (or contains, captures, traps, etc.) the true value at least $100(1-\alpha)\%$ of the time, and we refer to $1-\alpha$ as the **coverage probability** or simply **coverage**. Typical confidence intervals include 95% percent ($\alpha = 0.05$), 90% ($\alpha = 0.1$), and 99% ($\alpha = 0.01$). All else equal, larger coverage will imply larger intervals.

So a confidence interval is a random interval with a particular guarantee about how often it will contain the true value of the unknown population parameter (in our example, the true treatment effect). Remember what is random and what is fixed in this setup. The interval varies from sample to sample, but the true value of the parameter stays fixed even if it is unknown, and the coverage is how often we should expect the interval to contain that true value. The "repeating my sample over and over again" analogy can break down very quickly, so it is sometimes helpful to interpret it as giving guarantees across confidence intervals across different experiments. In particular, suppose that a journal publishes 100 quantitative articles annually, each producing a single 95% confidence interval for their quantity of interest. Then, if the confidence intervals are valid and each is constructed in the exact same way, we should expect 95 of those confidence intervals to contain the true value.

> **Warning**
>
> Suppose we have a 95% confidence interval, $[0.1, 0.4]$. It would be tempting to make a probability statement like $\mathbb{P}(0.1 \leq \theta \leq 0.4 \mid \theta) = 0.95$ or that there's a 95% chance that the parameter is in $[0.1, 0.4]$. But looking at the probability statement, everything on the left-hand side of the conditioning bar is fixed, so the probability either has to be 0 (θ is outside the interval) or 1 (θ is in the interval); the unknown parameter is a fixed value, so it is either in the interval or it is not. Another way to think about this is that the coverage probability of a confidence interval refers to its status as a pair of random variables, (L, U), not any particular realization of those variables like $(0.1, 0.4)$. As an analogy, consider if we calculated the sample mean as 0.25 and then tried to say that 0.25 is unbiased for the population mean. This statement doesn't make sense because unbiasedness refers not to a fixed value but how the sample mean varies from sample to sample.

In most cases, we will not be able to derive exact confidence intervals but rather confidence intervals that are **asymptotically valid**, which means that if we write the interval as a function of the sample size, (L_n, U_n), they would have **asymptotic coverage**

$$\lim_{n \to \infty} \mathbb{P}(L_n \leq \theta \leq U_n) \geq 1 - \alpha \quad \forall \theta \in \Theta.$$

We can show asymptotic coverage for most confidence intervals since we usually rely on large-sample approximations based on the central limit theorem.

3.8.1 Deriving confidence intervals

To derive confidence intervals, consider the standard formula for the 95% confidence interval of the sample mean,

$$\left[\overline{X}_n - 1.96\frac{s}{\sqrt{n}},\ \overline{X}_n + 1.96\frac{s}{\sqrt{n}}\right],$$

where s is the sample standard deviation and $s/\sqrt{n}$ is the estimate of the standard error of the sample mean. If this is a 95% confidence interval, then the probability that it contains the true population mean μ should be 0.95, but how can we derive this? We can justify this logic using the central limit theorem, and the argument will hold for any asymptotically normal estimator.

Suppose we have an estimator, $\hat{\theta}_n$ for the parameter θ with estimated standard error $\widehat{\mathsf{se}}[\hat{\theta}_n]$. If the estimator is asymptotically normal, then in large samples, we know that

$$\frac{\hat{\theta}_n - \theta}{\widehat{\mathsf{se}}[\hat{\theta}_n]} \sim \mathcal{N}(0, 1).$$

Then we use our knowledge of the standard normal to find

$$\mathbb{P}\left(-1.96 \leq \frac{\hat{\theta}_n - \theta}{\widehat{\mathsf{se}}[\hat{\theta}_n]} \leq 1.96\right) = 0.95.$$

Multiplying each part of the inequality by $\widehat{\mathsf{se}}[\hat{\theta}_n]$ gives us

$$\mathbb{P}\left(-1.96\,\widehat{\mathsf{se}}[\hat{\theta}_n] \leq \hat{\theta}_n - \theta \leq 1.96\,\widehat{\mathsf{se}}[\hat{\theta}_n]\right) = 0.95,$$

We then subtract all parts by the estimator to get

$$\mathbb{P}\left(-\hat{\theta}_n - 1.96\,\widehat{\mathsf{se}}[\hat{\theta}_n] \leq -\theta \leq -\hat{\theta}_n + 1.96\,\widehat{\mathsf{se}}[\hat{\theta}_n]\right) = 0.95,$$

and finally we multiply all parts by -1 (and flipping the inequalities) to arrive at

$$\mathbb{P}\left(\hat{\theta}_n - 1.96\,\widehat{\mathsf{se}}[\hat{\theta}_n] \leq \theta \leq \hat{\theta}_n + 1.96\,\widehat{\mathsf{se}}[\hat{\theta}_n]\right) = 0.95.$$

To connect back to the definition of the confidence interval, we have now shown that the random interval $[L, U]$ where

$$\begin{aligned} L &= L(X_1, \ldots, X_n) = \hat{\theta}_n - 1.96\,\widehat{\mathsf{se}}[\hat{\theta}_n] \\ U &= U(X_1, \ldots, X_n) = \hat{\theta}_n + 1.96\,\widehat{\mathsf{se}}[\hat{\theta}_n], \end{aligned}$$

is an asymptotically valid estimator.[3] Replacing $\overline{X}_n$ for $\hat{\theta}_n$ and $s/\sqrt{n}$ for $\widehat{\mathsf{se}}[\hat{\theta}_n]$ establishes how the standard 95% confidence interval for the sample mean above is asymptotically valid.

How can we generalize this to $1 - \alpha$ confidence intervals? For a random variable that is distributed following a standard normal, Z, we know that

$$\mathbb{P}(-z_{\alpha/2} \leq Z \leq z_{\alpha/2}) = 1 - \alpha$$

[3]The analysis here largely comes from Senn (2012).

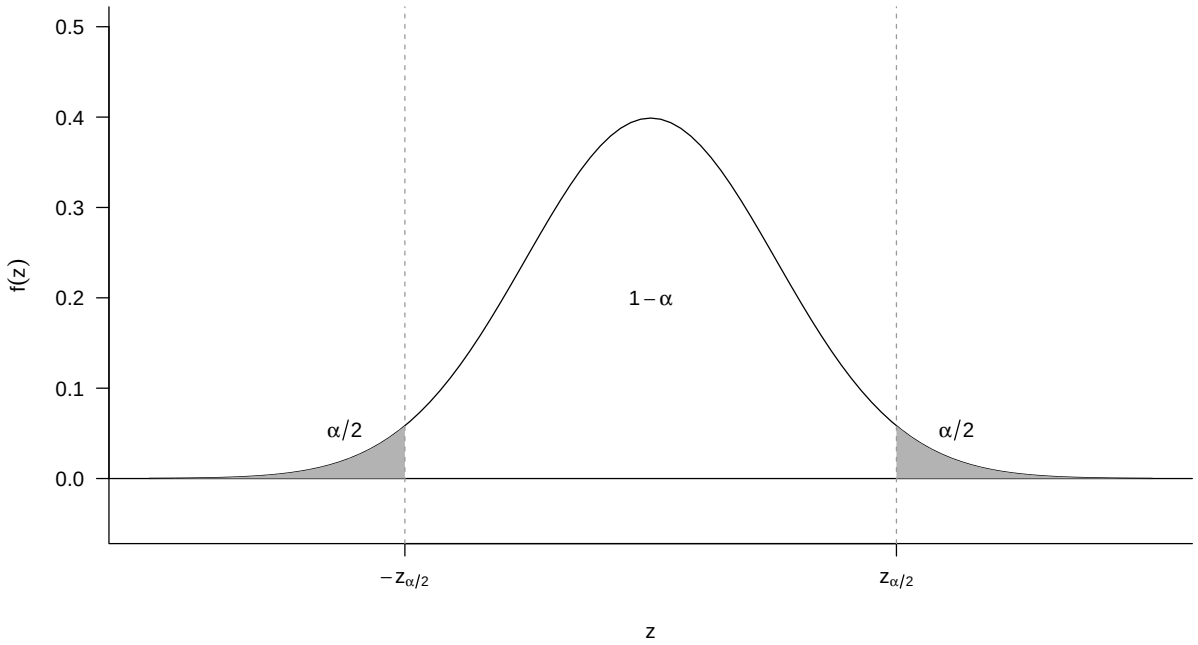


Figure 3.3: Critical values for the standard normal.

which implies that we can obtain a $1 - \alpha$ asymptotic confidence intervals by using the interval $[L, U]$, where

$$L = \hat{\theta}_n - z_{\alpha/2}\widehat{\mathsf{se}}[\hat{\theta}_n], \quad U = \hat{\theta}_n + z_{\alpha/2}\widehat{\mathsf{se}}[\hat{\theta}_n].$$

This is sometimes shortened to $\hat{\theta}_n \pm z_{\alpha/2}\widehat{\mathsf{se}}[\hat{\theta}_n]$. Remember that we can obtain the values of $z_{\alpha/2}$ easily from R:

```
## alpha = 0.1 for 90% CI
qnorm(0.1 / 2, lower.tail = FALSE)
```

```
[1] 1.644854
```

As a concrete example, then, we could derive a 90% asymptotic confidence interval for the sample mean as

$$\left[\overline{X}_n - 1.64\frac{\hat{\sigma}}{\sqrt{n}}, \overline{X}_n + 1.64\frac{\hat{\sigma}}{\sqrt{n}}\right]$$

3.8.2 Interpreting confidence intervals

A very important point is that the interpretation of confidence is how the random interval performs over repeated samples. A valid 95% confidence interval is a random interval that contains the true population value in 95% of samples. Simulating repeated samples helps clarify this.

Example 3.8. Suppose we are taking samples of size $n = 500$ of random variables where $X_i \sim \mathcal{N}(1, 10)$, and we want to estimate the population mean $\mathbb{E}[X] = 1$. To do so, we repeat the following steps:

1. Draw a sample of $n = 500$ from $\mathcal{N}(1, 10)$.
2. Calculate the 95% confidence interval sample mean $\overline{X}_n \pm 1.96\hat{\sigma}/\sqrt{n}$.
3. Plot the intervals along the x-axis and color them blue if they contain the truth (1) and red if not.

Figure 3.4 shows 100 iterations of these steps. We see that, as expected, most calculated CIs do contain the true value. Five random samples produce intervals that fail to include 1, an exact coverage rate of 95%. Of course, this is just one simulation, and a different set of 100 random samples might have produced a slightly different coverage rate. The guarantee of the 95% confidence intervals is that if we were to continue to take these repeated samples, the long-run frequency of intervals covering the truth would approach 0.95.

3.9 Delta method

Suppose that we know that an estimator follows the CLT, and so we have

$$\sqrt{n}\left(\hat{\theta}_n - \theta\right) \xrightarrow{d} \mathcal{N}(0, V),$$

but we actually want to estimate $h(\theta)$ so we use the plug-in estimator, $h(\hat{\theta}_n)$. It seems like we should be able to apply part 1 of Theorem 3.9 to obtain the asymptotic distribution of $h(\hat{\theta}_n)$. Still, the CLT established the large-sample distribution of the centered and scaled random sequence, $\sqrt{n}(\hat{\theta}_n - \theta)$, not to the original estimator itself, and we would need the latter to investigate the asymptotic distribution of $h(\hat{\theta}_n)$. We can use a little bit of calculus to get an approximation of the distribution we need.

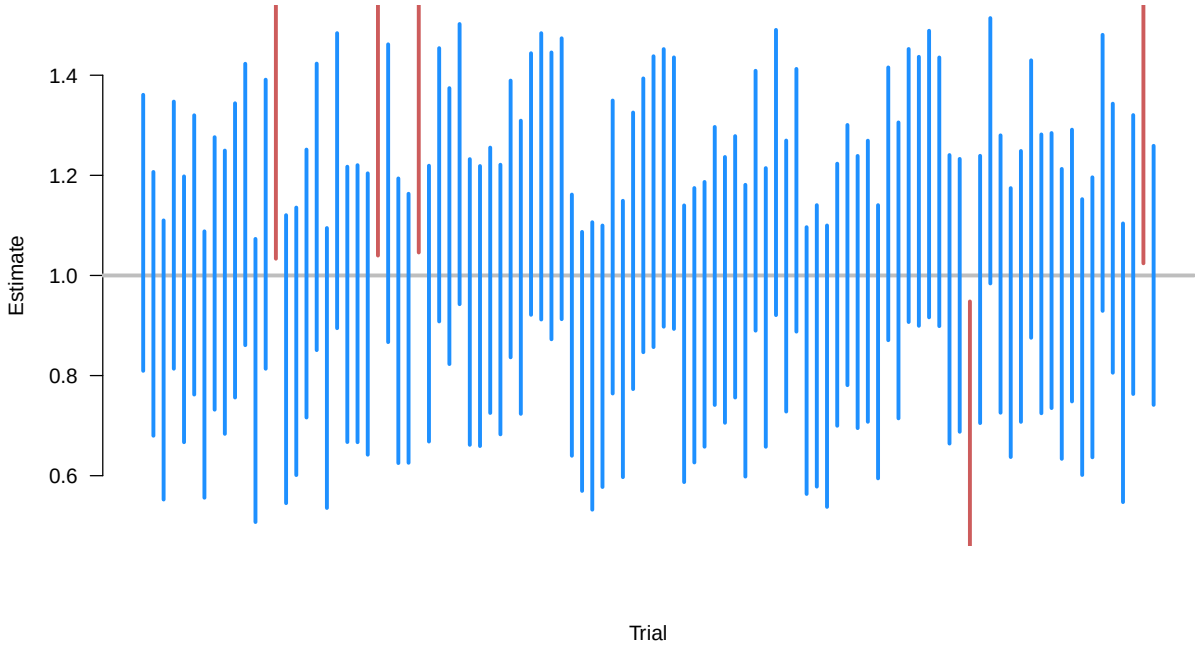


Figure 3.4: 95% confidence intervals from 100 random samples. Intervals are blue if they contain the truth and red if they do not.

Theorem 3.11. *If* $\sqrt{n}\left(\hat{\theta}_n - \theta\right) \xrightarrow{d} \mathcal{N}(0, V)$ *and* $h(u)$ *is continuously differentiable in a neighborhood around* θ*, then as* $n \to \infty$*,*

$$\sqrt{n}\left(h(\hat{\theta}_n) - h(\theta)\right) \xrightarrow{d} \mathcal{N}(0, (h'(\theta))^2 V).$$

Understanding what is happening here provides intuition as to when this might go wrong. Why do we focus on continuously differentiable functions, $h()$? These functions can be well-approximated with a line in a neighborhood around a given point like θ. In Figure 3.5, we show this at the point where the tangent line at θ_0, which has slope $h'(\theta_0)$, is very similar to $h(\theta)$ for values close to θ_0. Because of this, we can approximate the difference between $h(\hat{\theta}_n)$ and $h(\theta_0)$ with the what this tangent line would give us:

$$\underbrace{\left(h(\widehat{\theta_n}) - h(\theta_0)\right)}_{\text{change in } y} \approx \underbrace{h'(\theta_0)}_{\text{slope}} \underbrace{\left(\hat{\theta}_n - \theta_0\right)}_{\text{change in } x},$$

and then multiplying both sides by the $\sqrt{n}$ gives

$$\sqrt{n}\left(h(\widehat{\theta_n}) - h(\theta_0)\right) \approx h'(\theta_0)\sqrt{n}\left(\hat{\theta}_n - \theta_0\right).$$

The right-hand side of this approximation converges to $h'(\theta_0)Z$, where Z is a random variable with $\mathcal{N}(0, V)$. The variance of this quantity will be

$$\mathbb{V}[h'(\theta_0)Z] = (h'(\theta_0))^2\mathbb{V}[Z] = (h'(\theta_0))^2V,$$

by the properties of variances.

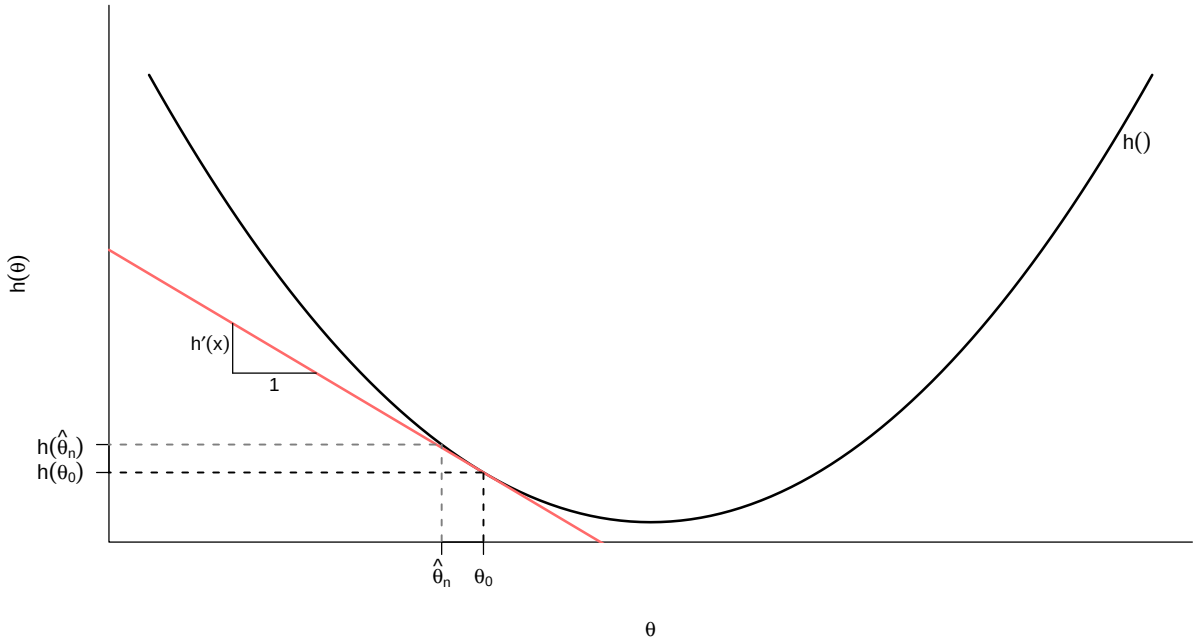


Figure 3.5: Linear approximation to nonlinear functions.

Example 3.9. Let's return to the iid sample $X_1, \ldots, X_n$ with mean $\mu = \mathbb{E}[X_i]$ and variance $\sigma^2 = \mathbb{V}[X_i]$. From the CLT, we know that $\sqrt{n}(\overline{X}_n - \mu) \xrightarrow{d} \mathcal{N}(0, \sigma^2)$. Suppose that we want to estimate $\log(\mu)$, so we use the plug-in estimator $\log(\overline{X}_n)$ (assuming that $X_i > 0$ for all i so that we can take the log). What is the asymptotic distribution of this estimator? This is a situation where $\widehat{\theta}_n = \overline{X}_n$ and $h(\mu) = \log(\mu)$. From basic calculus, we know that

$$h'(\mu) = \frac{\partial \log(\mu)}{\partial \mu} = \frac{1}{\mu},$$

so applying the delta method, we can determine that

$$\sqrt{n}\left(\log(\overline{X}_n) - \log(\mu)\right) \xrightarrow{d} \mathcal{N}\left(0, \frac{\sigma^2}{\mu^2}\right).$$

Example 3.10. What about estimating the $\exp(\mu)$ with $\exp(\overline{X}_n)$? Recall that

$$h'(\mu) = \frac{\partial \exp(\mu)}{\partial \mu} = \exp(\mu)$$

so applying the delta method, we have

$$\sqrt{n}\left(\exp(\overline{X}_n) - \exp(\mu)\right) \xrightarrow{d} \mathcal{N}(0, \exp(2\mu)\sigma^2),$$

since $\exp(\mu)^2 = \exp(2\mu)$.

Like all of the results in this chapter, there is a multivariate version of the delta method that is incredibly useful in practical applications. For example, suppose we want to combine two different estimators (or two different estimated parameters) to estimate another quantity. We now let $\mathbf{h}(\boldsymbol{\theta}) = (h_1(\boldsymbol{\theta}), \ldots, h_m(\boldsymbol{\theta}))$ map from $\mathbb{R}^k \to \mathbb{R}^m$ and be continuously differentiable (we make the function bold since it returns an m-dimensional vector). It will help us to use more compact matrix notation if we introduce a $m \times k$ Jacobian matrix of all partial derivatives

$$\mathbf{H}(\boldsymbol{\theta}) = \boldsymbol{\nabla}_{\boldsymbol{\theta}} \mathbf{h}(\boldsymbol{\theta}) = \begin{pmatrix} \frac{\partial h_1(\boldsymbol{\theta})}{\partial \theta_1} & \frac{\partial h_1(\boldsymbol{\theta})}{\partial \theta_2} & \cdots & \frac{\partial h_1(\boldsymbol{\theta})}{\partial \theta_k} \\ \frac{\partial h_2(\boldsymbol{\theta})}{\partial \theta_1} & \frac{\partial h_2(\boldsymbol{\theta})}{\partial \theta_2} & \cdots & \frac{\partial h_2(\boldsymbol{\theta})}{\partial \theta_k} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial h_m(\boldsymbol{\theta})}{\partial \theta_1} & \frac{\partial h_m(\boldsymbol{\theta})}{\partial \theta_2} & \cdots & \frac{\partial h_m(\boldsymbol{\theta})}{\partial \theta_k} \end{pmatrix},$$

which we can use to generate the equivalent multivariate linear approximation

$$\left(\mathbf{h}(\hat{\boldsymbol{\theta}}_n) - \mathbf{h}(\boldsymbol{\theta}_0)\right) \approx \mathbf{H}(\boldsymbol{\theta}_0)' \left(\hat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_0\right).$$

We can use this fact to derive the multivariate delta method.

Theorem 3.12. *Suppose that* $\sqrt{n}\left(\hat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_0\right) \xrightarrow{d} \mathcal{N}(0, \boldsymbol{\Sigma})$*, then for any function* $\mathbf{h}$ *that is continuously differentiable in a neighborhood of* $\boldsymbol{\theta}_0$*, we have*

$$\sqrt{n}\left(\mathbf{h}(\hat{\boldsymbol{\theta}}_n) - \mathbf{h}(\boldsymbol{\theta}_0)\right) \xrightarrow{d} \mathcal{N}(0, \mathbf{H}\boldsymbol{\Sigma}\mathbf{H}'),$$

where $\mathbf{H} = \mathbf{H}(\boldsymbol{\theta}_0)$.

This result follows from the approximation above plus rules about variances of random vectors. Recall that for any compatible matrix of constants, $\mathbf{A}$, we have $\mathbb{V}[\mathbf{A}'\mathbf{Z}] = \mathbf{A}\mathbb{V}[\mathbf{Z}]\mathbf{A}'$. The matrix of constants appears twice here, like the matrix version of the "squaring the constant" rule for variance.

The delta method is handy for generating closed-form approximations for asymptotic standard errors, but the math is often quite complex for even simple estimators. It is usually more straightforward for applied researchers to use computational tools such as the bootstrap to approximate the needed standard errors. The bootstrap has the trade-off of taking more computational time to implement compared to the delta method, but it is more easily adaptable across different estimators and domains.

3.10 Summary

In this chapter, we covered asymptotic analysis, which considers how estimators behave as we feed them larger and larger samples. While we never actually have infinite data, asymptotic results provide approximations that work quite well in practice. A **consistent** estimator converges in probability to a desired quantity of interest. We saw several ways of establishing consistency, including the **Law of Large Numbers** for the sample mean, which converges in probability to the population mean. The **Central Limit Theorem** tells us that the sample mean will be approximately normally distributed when we have large, iid samples. We also saw how the **continuous mapping theorem** and **Slutsky's theorem** allow us to determine asymptotic results for a broad class of estimators. Knowing the asymptotic normality of an estimator allows us to derive **confidence intervals** that are valid in large samples. Finally, the **delta method** is a general tool for finding the asymptotic distribution of an estimator that is a function of another estimator with a known asymptotic distribution.

In the next chapter, we will leverage these asymptotic results to introduce another important tool for statistical inference: the hypothesis test.

4 Hypothesis tests

We have up to now discussed the properties of estimators that allow us to characterize their distributions in finite and large samples. These properties allow us to say, for example, that our estimated difference in means is equal to a true average treatment effect on average across repeated samples or that it will converge to the true value in large samples. These properties, however, are properties of repeated samples. Most researchers, on the other hand, will only have access to a single sample. **Statistical inference** is the process of using a single sample to learn about population parameters. As we will see, many common techniques of statistical inference are intuitively closely connected. One of the most ubiquitous in the social sciences is the hypothesis test, a kind of statistical thought experiment.

4.1 The Lady Tasting Tea

The story of the Lady Tasting Tea exemplifies the core ideas behind hypothesis testing.[1] The story goes like this. R.A. Fisher, the early 20th-century British polymath and statistical pioneer, had prepared tea for his colleague, the algologist Muriel Bristol. Knowing that she preferred milk in her tea, he poured milk into a tea cup and then poured the hot tea into the milk and swirled it around. But Bristol rejected the cup, stating that she preferred pouring the tea first, then the milk. Fisher was skeptical of the idea that anyone could tell the difference between a cup poured milk-first versus tea-first, and so he and another colleague, William Roach, devised a test to see if Bristol could tell the difference between the two preparation methods.

Fisher and Roach prepared 8 cups of tea, four with the milk poured first and four with the tea poured first. Then they presented the cups to Bristol in a random order (though she knew there were four of each type), and she proceeded to identify all of the cups correctly. At first glance, this seems like good evidence that she could tell the difference between the

[1] The analysis here largely comes from Senn (2012).

two types of tea, but Fisher, being a natural skeptic, raised the question, "Could she have just been randomly guessing and got lucky?" This led Fisher to a **statistical thought experiment**: what would the probability of identifying the correct cups be *if* she was guessing randomly?

To calculate the probability of Bristol identifying the four milk-first cups correctly, note that "randomly guessing" would mean that she was selecting a group of 4 cups to be labeled milk-first from the 8 cups available. Using basic combinatorics, there are 70 ways to choose 4 cups among 8, but only 1 of those arrangements would be correct. Thus, if randomly guessing means choosing among those 70 options with equal chance, then the probability of guessing the right set of cups is $1/70$ or ≈ 0.014. The low probability implies that the hypothesis of random guessing may be implausible.

The story of the Lady Tasting Tea encapsulates many of the core elements of hypothesis testing. Hypothesis testing is about taking our observed estimate (Bristol identifying all four cups correctly) and seeing how likely that observed estimate would be under some assumption, or hypothesis, about the data-generating process (Bristol was randomly guessing). When the observed estimate is unlikely under the maintained hypothesis, we might view this as evidence against that hypothesis. Thus, hypothesis tests help us assess evidence for particular guesses about the DGP.

> **i** Notation alert
>
> For the rest of this chapter, we will introduce the concepts following the notation in the past chapters. We will assume a random (iid) sample of random variables $X_1, \dots, X_n$ from a distribution, F. We'll focus on estimating some parameter, θ, of this distribution (like the mean, median, variance, etc.), and we will refer to Θ as the set of possible values of θ or the **parameter space**.

4.2 Hypotheses

In the context of hypothesis testing, hypotheses are simply statements about the population distribution. In particular, we will make statements that $\theta = \theta_0$ where $\theta_0 \in \Theta$ is the hypothesized value of θ, a population parameter. Hypotheses are ubiquitous in empirical work. Examples include:

- The population proportion of US citizens who identify as Democrats is 0.33.

- The population difference in average voter turnout between households who received get-out-the-vote mailers vs. those who did not is 0.
- The difference in the average incidence of human rights abuse in countries that signed a human rights treaty vs. those countries that did not sign is 0.

Each of these is a statement about the true DGP. The latter two are examples where the hypothesis is phrased as a possible non-difference, which is very common. When θ represents the difference in means between two groups, then $\theta = 0$ is the hypothesis of no actual difference in population means or no treatment effect (if the causal effect is identified).

The goal of hypothesis testing is to adjudicate between two complementary hypotheses.

Definition 4.1. The two hypotheses in a hypothesis test are called the **null hypothesis** and the **alternative hypothesis**, denoted as H_0 and H_1, respectively.

These hypotheses are complementary, so if the null hypothesis is $H_0 : \theta \in \Theta_0$, then the alternative hypothesis is $H_1 : \theta \in \Theta_0^c$. The "null" in null hypothesis may seem odd until you realize that most null hypotheses are that there is no effect of some treatment or no difference in means. For example, suppose that θ is the difference in mean support for increasing legal immigration between a treatment group that received a pro-immigrant message with some facts about immigration and a control group that just received the immigration facts. The usual null hypothesis would be no difference in means or $H_0 : \theta = 0$, and the alternative would be $H_1 : \theta \neq 0$. Substantively, the null hypothesis would posit no average difference in the outcome – in this case support for increasing legal immigration – between the two groups.

There are two common types of tests that differ in terms of the form of their null and alternative hypotheses. A **two-sided test** is of the form

$$H_0 : \theta = \theta_0 \quad \text{versus} \quad H_1 : \theta \neq \theta_0,$$

where the "two-sided" part refers to how the alternative contains values of θ above and below the null value θ_0.

A **one-sided test** is of the form

$$H_0 : \theta \leq \theta_0 \quad \text{versus} \quad H_1 : \theta > \theta_0,$$

or

$$H_0 : \theta \geq \theta_0 \quad \text{versus} \quad H_1 : \theta < \theta_0.$$

Where the "one-sided" part refers to how the alternative contains values of θ only above or below the null value. Two-sided tests are much more common in the social sciences, mostly because we usually want to know if there is any evidence, positive or negative, against the presumption of no treatment effect or no relationship between two variables. One-sided tests are best suited for situations with clear, directional hypotheses that are ideally preregistered before collection of the data. Preregistration of the direction of a one-sided test is important because researchers changing the direction of the hypothesis after seeing the data can inflate the strength of evidence against the null. For this reason, one-sided tests outside of preregistered settings should be used with extreme caution. That said, unfortunately, the math of two-sided tests is also more complicated.

4.3 The procedure of hypothesis testing

At the most basic level, a **hypothesis test** is a rule that specifies values of the sample data for which we will decide to **reject** the null hypothesis. Let $\mathcal{X}_n$ be the range of the sample—that is, all possible vectors $(x_1, \dots, x_n)$ that have a positive probability of occurring. A hypothesis test then describes a region of this space, $R \subset \mathcal{X}_n$, called the **rejection region** where when $(X_1, \dots, X_n) \in R$ we will **reject** H_0 and when the data is outside this region, $(X_1, \dots, X_n) \notin R$ we **retain**, **accept**, or **fail to reject** the null hypothesis.[2]

How do we decide what the rejection region should be? Even though we define the rejection region in terms of the **sample space**, $\mathcal{X}_n$, working with the entire vector of data can be unwieldy. We instead usually formulate the rejection region in terms of a **test statistic**, $T = T(X_1, \dots, X_n)$, where the rejection region becomes

$$R = \{(x_1, \dots, x_n) : T(x_1, \dots, x_n) > c\},$$

where c is called the **critical value**. This expression says that the rejection region is the collection of possible data sets that make the test statistic sufficiently large. Thus, the test statistic is a function of the data that should get larger as the observed data becomes incompatible with the null hypothesis. The critical value (and thus the rejection region) demarcates when the divergence between the observed data and the null hypothesis is large enough to allow us to reject the null hypothesis. Note that the test statistic is a

[2]Different people and different textbooks describe what to do when we do not reject the null hypothesis differently. The terminology is not so important so long as you understand that rejecting the null does not mean the null is logically false and that "accepting" (or failing to reject) the null does not mean the null is logically true.

random variable and has a distribution. We will exploit this later to better understand the different properties of a hypothesis test.

Consider a simple one-sided test where you feel a bit ill and try to determine if you have a normal body temperature of 98.7 degrees Fahrenheit or if you have a fever. In this case, the thermometer reading is the test statistic since a larger reading are less consistent with a normal body temperature. Thermometers, however, are imperfect and noisy tools, so the reading might differ from 98.7 even if one's temperature is normal. Thus, we can use a rejection region such as readings over 100.5 degrees to determine when to reject the null hypothesis of a normal body temperature.

Example 4.1. Suppose that $(X_1, \dots, X_n)$ represents a sample of US citizens where $X_i = 1$ indicates support for the current US president and $X_i = 0$ means opposition (no support). A good and reasonable null hypothesis is that the president does not have the support of a majority of American citizens. Let $\mu = \mathbb{E}[X_i] = \mathbb{P}(X_i = 1)$. Then, a one-sided test would compare the two hypotheses:

$$H_0 : \mu \leq 0.5 \quad \text{versus} \quad H_1 : \mu > 0.5.$$

In this case, we might use the sample mean as the test statistic, so that $T(X_1, \dots, X_n) = \overline{X}_n$, and we have to find some threshold above 0.5 such that we would reject the null,

$$R = \left\{(x_1, \dots, x_n) : \overline{X}_n > c\right\}.$$

In words, we are asking how much support should we see for the current president before we reject the notion that he or she lacks majority support? Below we will select the critical value, c, to have beneficial statistical properties.

The structure of a reject region will depend on whether a test is one- or two-sided. This is an important point of difference between the two test types that we will raise again below. One-sided tests will take the form $T > c$, whereas two-sided tests will take the form $|T| > c$ since we want to count deviations from either side of the null hypothesis as evidence against that null.

4.4 Testing errors

Hypothesis tests end with a decision to reject the null hypothesis or not, but this might be an incorrect decision. In particular, there are two ways to make errors and two ways to

be correct in this setting, as shown in Table 4.1. The labels are confusing, but remember that **Type I errors** (said "type one") are labeled so because they are the worst of the two types of errors. Type I errors occur when we reject a null when the null is in fact true. For example, if we have a null hypothesis of no treatment effect between a treatment and control condition, and we reject that null hypothesis (and conclude substantively that there is some sort of a treatment effect), then we would be committing a Type I error if in fact the null was true – that is, there is no real treatment effect but we concluded there was one. Type I errors are what we see in the replication crisis: lots of "significant" effects that turn out later to be null.

Type II errors (said "type two") are generally considered less problematic. For such errors, There is a true relationship, but we cannot detect it with our test. That is, we do not reject a null that is false. For example, if we have a null hypothesis of no treatment effect between a treatment and control condition, we would be committing a Type II error if in fact there was a difference in the treatment and control but we concluded there wasn't (we failed to reject the null hypothesis of no difference).

Table 4.1: Typology of testing errors

	H_0 True	H_0 False
Retain H_0	Awesome	Type II error
Reject H_0	Type I error	Great

Ideally, we would minimize the chances of making either a Type I or Type II error. Unfortunately, because the test statistic is a random variable, we cannot remove the probability of an error altogether. Instead, we will derive tests with some guaranteed performance to minimize the probability of Type I error, usually the more objectionable type of error. To derive this, we can define the **power function** of a test,

$$\pi(\theta) = \mathbb{P}\left(\text{Reject } H_0 \mid \theta\right) = \mathbb{P}\left(T \in R \mid \theta\right),$$

which is the probability of rejection as a function of the parameter of interest, θ. The power function tells us, for example, how likely we are to reject the null hypothesis of no treatment effect (no difference) as we vary the actual size of the treatment effect (which in this case is θ).

We can define the probability of Type I error from the power function.

Definition 4.2. The **size** of a hypothesis test with the null hypothesis $H_0 : \theta = \theta_0$ is

$$\pi(\theta_0) = \mathbb{P}\left(\text{Reject } H_0 \mid \theta_0\right).$$

You can think of the size of a test as the rate of false positives (or false discoveries) produced by the test. Figure 4.1 shows an example of rejection regions, size, and power for a one-sided test. In the left panel, we have the distribution of the test statistic under the null, with $H_0 : \theta = \theta_0$, and the rejection region is defined by values $T > c$. We refer to the distribution of the test statistic under the null hypothesis as the **null distribution** or the **reference distribution**. The shaded gray region is the probability of rejection under this null hypothesis, or the size of the test. Sometimes, we will get extreme samples by random chance, even under the null, leading to false discoveries.[3]

In the right panel, we overlay the distribution of the test statistic under one particular alternative, $\theta = \theta_1 > \theta_0$. The red-shaded region is the probability of rejecting the null when this alternative is true for the power—it is the probability of correctly rejecting the null when it is false. Intuitively, we can see that alternatives that produce test statistics closer to the rejection region will have higher power. This makes sense: detecting big deviations from the null should be easier than detecting minor ones.

Figure 4.1 also hints at a tradeoff between size and power. Notice that we could make the size smaller (lower the false positive rate) by increasing the critical value to $c' > c$. This would make the probability of being in the rejection region smaller, $\mathbb{P}(T > c' \mid \theta_0) < \mathbb{P}(T > c \mid \theta_0)$, leading to a lower-sized test. Unfortunately, it would also reduce power in the right panel since the probability of being in the rejection region will be lower under any alternative, $\mathbb{P}(T > c' \mid \theta_1) < \mathbb{P}(T > c \mid \theta_1)$. This means we usually cannot simultaneously reduce both types of errors.

4.5 Determining the rejection region

If we cannot simultaneously optimize a test's size and power, how should we determine where the rejection region is? That is, how should we decide what empirical evidence will

[3] Eagle-eyed readers will notice that the null tested here is a point, while we previously defined the null in a one-sided test as a region $H_0 : \theta \leq \theta_0$. Technically, the size of the test will vary based on which of these nulls we choose. In this example, notice that any null to the left of θ_0 will result in a lower size. And so, the null at the boundary, θ_0, will maximize the size of the test, making it the most "conservative" null to investigate. Technically, we should define the size of a test as $\alpha = \sup_{\theta \in \Theta_0} \pi(\theta)$.

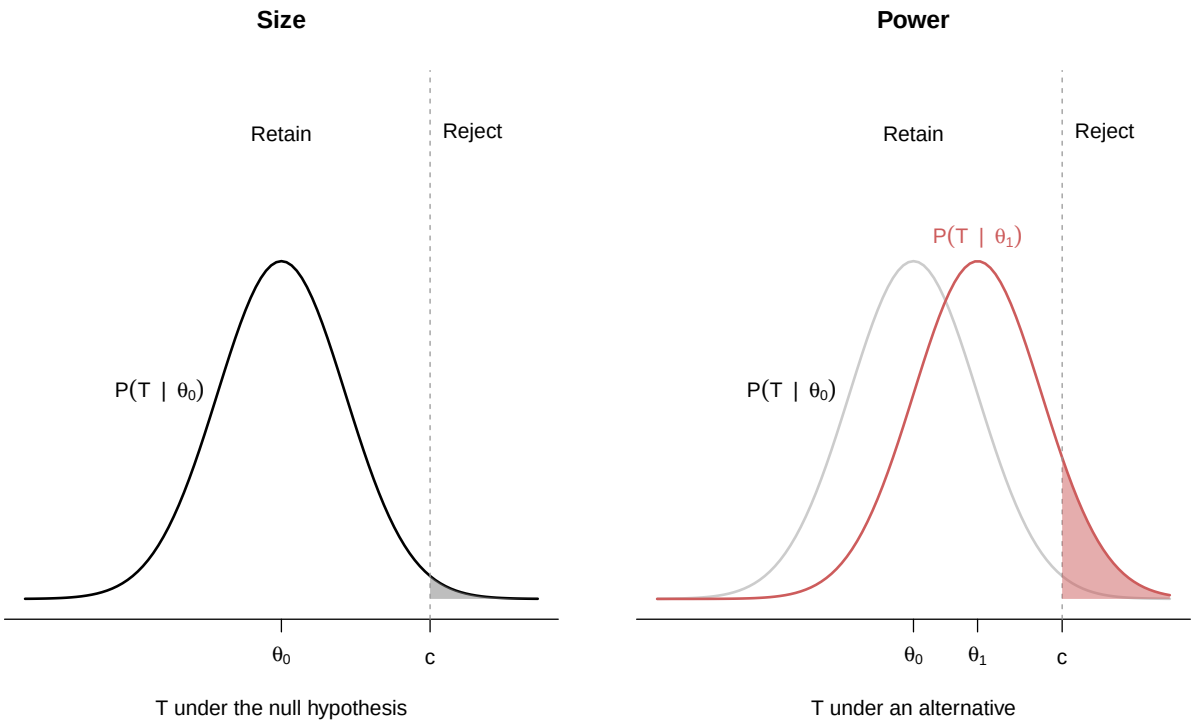


Figure 4.1: Size of a test and power against an alternative.

be strong enough for us to reject the null? The standard approach is to control the size of a test (that is, control the rate of false positives) and try to maximize the power of the test subject to that constraint. So we say, "I'm willing to accept at most X%" of findings will be false positives and do whatever we can to maximize power subject to that constraint.

Definition 4.3. A test has **significance level** α if its size is less than or equal to α, or $\pi(\theta_0) \leq \alpha$.

A test with a significance level of $\alpha = 0.05$ will have a false positive/Type I error rate no larger than 0.05. This level is widespread in the social sciences, though you also will see $\alpha = 0.01$ or $\alpha = 0.1$. Frequentists justify this by saying this means that with $\alpha = 0.05$, there will only be at most 5% of studies that will produce false discoveries.

Our task is to construct the rejection region so that the **null distribution** of the test statistic $G_0(t) = \mathbb{P}(T \leq t \mid \theta_0)$ has less than α probability in that region. One-sided tests like in Figure 4.1 are the easiest to show, even though we warned you not to use them. We want to choose c that puts no more than α probability in the tail, or

$$\mathbb{P}(T > c \mid \theta_0) = 1 - G_0(c) \leq \alpha.$$

Remember that the smaller the value of c we can use will maximize power, which implies that the critical value for the maximum power while maintaining the significance level is when $1 - G_0(c) = \alpha$. We can use the **quantile function** of the null distribution to find the exact value of c we need,

$$c = G_0^{-1}(1 - \alpha),$$

which substantively translates to say, "the value at which $1 - \alpha$ of the null distribution is below."

The determination of the rejection region follows the same principles for two-sided tests, but it is more complicated because we reject when the magnitude of the test statistic is large, $|T| > c$. Figure 4.2 shows that basic setup. Notice that because there are two (disjoint) regions, one on the left and one on the right, we can write the size (false positive rate) as

$$\pi(\theta_0) = G_0(-c) + 1 - G_0(c).$$

In most cases, the null distribution for such a test will be symmetric around 0 (usually asymptotically standard normal, actually), which means that $G_0(-c) = 1 - G_0(c)$. This in turn implies that the size is

$$\pi(\theta_0) = 2(1 - G_0(c)).$$

Solving for the critical value that would make this α gives

$$c = G_0^{-1}(1 - \alpha/2).$$

Again, this formula can seem dense, but remember what you are doing: finding the value that puts $\alpha/2$ of the probability of the null distribution in each tail.

4.6 Hypothesis tests of the sample mean

Consider the following extended example about hypothesis testing of a sample mean, sometimes called a **one-sample test** since we are usually using just one sample statistic (the sample mean in this case) and comparing that to some sort of natural conceptual benchmark. Let's say X_i represents feeling thermometer scores about "liberals" as a group on a scale of 0 to 100, with values closer to 0 indicating cooler feelings about liberals and values closer to 100 indicating warmer feelings about liberals. (This is similar to many survey items on nationally representative surveys, such as the ANES in the U.S.) We want to know if the population average differs from a value of 50, which is a good

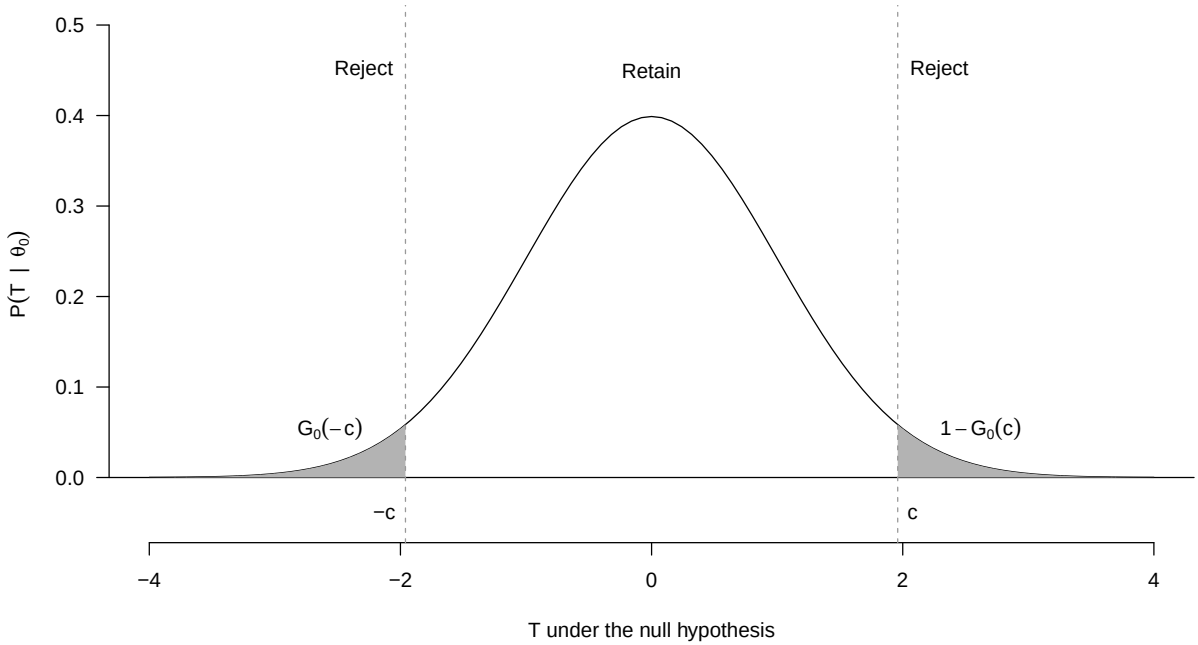


Figure 4.2: Rejection regions for a two-sided test.

benchmark that would indicate roughly neutral feelings toward liberals. We can write this two-sided test as

$$H_0 : \mu = 50 \quad \text{versus} \quad H_1 : \mu \neq 50,$$

where $\mu = \mathbb{E}[X_i]$. The standard test statistic for this type of test is the so-called **t-statistic**,

$$T = \frac{(\overline{X}_n - \mu_0)}{\sqrt{s^2/n}} = \frac{(\overline{X}_n - 50)}{\sqrt{s^2/n}},$$

where μ_0 is the null value of interest and s^2 is the sample variance. If the null hypothesis is true, then by the CLT, we know that the t-statistic is asymptotically normal, $T \xrightarrow{d} \mathcal{N}(0, 1)$. Thus, we can approximate the null distribution with the standard normal.

> **Warning**
>
> The names of the various tests can be quite confusing because they are so similar. Earlier, we discussed one-sided versus two-sided tests, which differed in what alternative hypotheses were being considered. One-sample and two-sample tests, on the other hand, describe how many group means we are comparing. In a one-sample

test, we compare one population mean to a fixed number. For two-sample tests (described in more detail below), we are usually making null hypotheses about the different between two population means.

Let's create a two-sided test with level $\alpha = 0.05$, our tolerance for Type I error. Then we need to find the rejection region that puts 0.05 probability in the tails of the null distribution, which we just saw was $\mathcal{N}(0, 1)$. Let $\Phi()$ be the CDF for the standard normal and let $\Phi^{-1}()$ be the quantile function for the standard normal. Drawing on what we developed above, you can find the value c so that $\mathbb{P}(|T| > c \mid \mu_0)$ is 0.05 with

$$c = \Phi^{-1}(1 - 0.05/2) \approx 1.96,$$

This means that a test where we reject when $|T| > 1.96$ would have a level of 0.05 asymptotically.

4.7 The Wald test

We can generalize the hypothesis test for the sample mean to estimators more broadly. Let $\hat{\theta}_n$ be an estimator for some parameter θ and let $\widehat{\mathsf{se}}[\hat{\theta}_n]$ be a consistent estimate of the standard error of the estimator, $\mathsf{se}[\hat{\theta}_n] = \sqrt{\mathbb{V}[\hat{\theta}_n]}$. We consider the two-sided test

$$H_0 : \theta = \theta_0 \quad \text{versus} \quad H_1 : \theta \neq \theta_0.$$

In many cases, our estimators will be asymptotically normal by a version of the CLT so that under the null hypothesis, we have

$$T = \frac{\hat{\theta}_n - \theta_0}{\widehat{\mathsf{se}}[\hat{\theta}_n]} \xrightarrow{d} \mathcal{N}(0, 1).$$

The **Wald test** rejects H_0 when $|T| > z_{\alpha/2}$, with $z_{\alpha/2}$ that puts $\alpha/2$ in the upper tail of the standard normal. That is, if $Z \sim \mathcal{N}(0, 1)$, then $z_{\alpha/2}$ satisfies $\mathbb{P}(Z \geq z_{\alpha/2}) = \alpha/2$.

> **Note**
>
> In R, you can find the $z_{\alpha/2}$ values easily with the `qnorm()` function:

```r
qnorm(0.05 / 2, lower.tail = FALSE)
```

```
[1] 1.959964
```

Theorem 4.1. *Asymptotically, the Wald test has size α such that*

$$\mathbb{P}(|T| > z_{\alpha/2} \mid \theta_0) \to \alpha.$$

This result is very general, and it means that many, many hypothesis tests based on estimators will have the same form. The main difference across estimators will be how we calculate the estimated standard error.

Example 4.2 (Difference in proportions)**.** Get-out-the-vote (GOTV) experiments are common in political science. A typical GOTV design might randomly assign a group of citizens to receive mailers encouraging them to vote, whereas a control group receives no message. We will define the turnout variables in the treatment group, $Y_1, Y_2, \ldots, Y_{n_t}$, as iid draws from a Bernoulli distribution with success p_t, which represents the population turnout rate in the treated group treated. The outcomes in the control group, $X_1, X_2, \ldots, X_{n_c}$, are iid draws from another Bernoulli distribution with success p_c, which represents the population turnout rate among citizens not receiving a mailer.

Our goal is to learn about the effect of this treatment on whether a citizen votes, $\tau = p_t - p_c$, and we will use the sample difference in means/proportions as our estimator, $\hat{\tau} = \overline{Y} - \overline{X}$. To perform a Wald test, we need to either know or estimate the standard error of this estimator. Notice that because these are independent samples, the variance is

$$\mathbb{V}[\hat{\tau}_n] = \mathbb{V}[\overline{Y} - \overline{X}] = \mathbb{V}[\overline{Y}] + \mathbb{V}[\overline{X}] = \frac{p_t(1-p_t)}{n_t} + \frac{p_c(1-p_c)}{n_c},$$

where the third equality comes from the fact that the underlying outcome variables Y_i and X_j are binary. Obviously, we do not know the true population proportions p_t and p_c (that's why we're doing the test!), but we can estimate the standard error by replacing them with their estimates

$$\widehat{\mathsf{se}}[\hat{\tau}] = \sqrt{\frac{\overline{Y}(1-\overline{Y})}{n_t} + \frac{\overline{X}(1-\overline{X})}{n_c}}.$$

The typical null hypothesis test in this **two-sample test** is "no treatment effect" vs. "some treatment effect":

$$H_0 : \tau = p_t - p_c = 0 \quad \text{versus} \quad H_1 : \tau \neq 0,$$

which gives the following test statistic for the Wald test

$$T = \frac{\overline{Y} - \overline{X}}{\sqrt{\frac{\overline{Y}(1-\overline{Y})}{n_t} + \frac{\overline{X}(1-\overline{X})}{n_c}}}.$$

If we wanted a test with level $\alpha = 0.01$, we would reject the null when $|T| > 2.58$ since

```
qnorm(0.01/2, lower.tail = FALSE)
```

```
[1] 2.575829
```

Example 4.3 (Difference in means)**.** Consider a similar example with randomly assigned treatment and control groups, but instead the treatment is now an appeal for financial donations to a political campaign and the outcomes are continuous measures of how much money a person has donated. The treatment data $Y_1, \ldots, Y_{n_t}$ are iid draws from a population with mean $\mu_t = \mathbb{E}[Y_i]$ and population variance $\sigma_t^2 = \mathbb{V}[Y_i]$. The control data $X_1, \ldots, X_{n_c}$ are iid draws (independent of the Y_i) from a population with mean $\mu_c = \mathbb{E}[X_i]$ and population variance $\sigma_c^2 = \mathbb{V}[X_i]$. The parameter of interest is similar to before: the population difference in means, $\tau = \mu_t - \mu_c$. We will form the usual hypothesis test of

$$H_0 : \tau = \mu_t - \mu_c = 0 \quad \text{versus} \quad H_1 : \tau \neq 0.$$

The only difference between this setting and the difference-in-proportions setting is that the standard error here is different because we cannot rely on binary outcomes. Instead, we'll use our knowledge of the sampling variance of the sample means and independence between the samples to derive

$$\mathbb{V}[\hat{\tau}] = \mathbb{V}[\overline{Y}] + \mathbb{V}[\overline{X}] = \frac{\sigma_t^2}{n_t} + \frac{\sigma_c^2}{n_c},$$

where we can come up with an estimate of the unknown population variance with sample variances

$$\widehat{\mathsf{se}}[\hat{\tau}] = \sqrt{\frac{s_t^2}{n_t} + \frac{s_c^2}{n_c}}.$$

We can use this estimator to derive the Wald test statistic of

$$T = \frac{\hat{\tau} - 0}{\widehat{\mathsf{se}}[\hat{\tau}]} = \frac{\overline{Y} - \overline{X}}{\sqrt{\frac{s_t^2}{n_t} + \frac{s_c^2}{n_c}}},$$

and if we want an asymptotic level of 0.05, we can reject when $|T| > 1.96$.

4.8 p-values

The hypothesis testing framework focuses on making a decision – to reject the null hypothesis or not – in the face of uncertainty. You choose a level of wrongness you are comfortable with (rate of false positives, or α) and then decide null vs. alternative based firmly on the rejection region.

That said, note that we are discarding, somewhat artificially, information on how far the observed data is from the null hypothesis. We would "accept" the null if $T = 1.95$ in the last example but would reject it if $T = 1.97$, even though these are very similar. Simply reporting the reject/retain decision also fails to give us a sense of possible other levels at which we might have rejected the null. Again, this makes sense if we need to make a single decision: other tests don't matter because we carefully considered our α level test. But in the lower-stakes world of the academic social sciences, we can afford to be more informative.

One alternative to reporting the reject/retain decision is to report a **p-value**.

Definition 4.4. The **p-value** of a test is the probability of observing a test statistic at least as extreme as the observed test statistic in the direction of the alternative hypothesis.

The line "in the direction of the alternative hypothesis" deals with the unfortunate headache of one-sided versus two-sided tests. For a one-sided test where larger values of T correspond to more evidence for H_1, the p-value is

$$\mathbb{P}(T(X_1, \ldots, X_n) > T \mid \theta_0) = 1 - G_0(T),$$

whereas for a (symmetric) two-sided test, we have

$$\mathbb{P}(|T(X_1, \dots, X_n)| > |T| \mid \theta_0) = 2(1 - G_0(|T|)).$$

In either case, the interpretation of the p-value is the same. It is the smallest size α at which a test would reject the null hypothesis. Presenting a p-value allows the reader to determine their own α level and determine quickly if the evidence would warrant rejecting H_0 in that case. Thus, the p-value is a more **continuous** measure of divergence between the observed data and the null hypothesis. Lower values indicate more divergence because the observed result is less likely under the null.

Much of the controversy surrounding p-values focuses on arbitrary p-value cutoffs for determining statistical significance and sometimes publication decisions. These problems are not the fault of p-values but, rather, the hyperfixation on the reject/retain decision for arbitrary test levels like $\alpha = 0.05$. It might be best to view p-values as a transformation of the test statistic onto a common scale between 0 and 1.

> ⚠ Warning
>
> People use many statistical shibboleths to purportedly identify people who don't understand statistics, and these criticisms sometimes hinge on seemingly subtle differences in interpretation that are easy to miss. If you have intuitively mastered the core concepts, however, avoiding these common pitfalls will be much easier.
> The shibboleth with p-values is that sometimes people interpret them as "the probability that the null hypothesis is true." But this doesn't make sense from our definition because the p-value *conditions* on the null hypothesis—it cannot tell us anything about the probability of the null hypothesis being true. A more useful metaphor is that hypothesis tests are statistical thought experiments and that p-values answer the question: how likely would my data be if the null were true?

4.9 Power analysis

Imagine you have spent a large amount of your research budget on a big experiment that tests a new and exciting theory, but the results come back, and… you fail to reject the null of no treatment effect. This can happen under two possible states of the world: (1) the null is true, and you correctly failed to reject it, or (2) the null is false but the test had insufficient power to detect the true effect (that is, to allow you to reject the null). Because this

is unwanted uncertainty after the fact, it is common for researchers to conduct **power analyses** before collecting data. These analyses forecast the necessary sample size to ensure you can reject the null under a hypothesized effect size. These hypothesized effect sizes are vital to this exercise and often come from prior studies or substantive knowledge about the domain.

Generally power analyses involve calculating the power function $\pi(\theta) = \mathbb{P}(T(X_1, \dots, X_n) \in R \mid \theta)$ for different values of θ. It might also involve sample size calculations for a particular alternative, θ_1, the hypothesized treatment effect. In that case, we try to find the sample size n to make the power $\pi(\theta_1)$ as close to a particular value (often 0.8) as possible. For simpler one-sided tests, solving for the sample size is straightforward. For more general situations or two-sided tests, however, we typically need numerical or simulation-based approaches to find the optimal sample size.

With Wald tests, we can characterize the power function quite easily, even if the test does not allow us to back out sample size calculations easily.

Theorem 4.2. *For a Wald test with an asymptotically normal estimator, the power function for a particular alternative $\theta_1 \neq \theta_0$ is*

$$\pi(\theta_1) = 1 - \Phi\left(\frac{\theta_0 - \theta_1}{\widehat{se}[\hat{\theta}_n]} + z_{\alpha/2}\right) + \Phi\left(\frac{\theta_0 - \theta_1}{\widehat{se}[\hat{\theta}_n]} - z_{\alpha/2}\right).$$

4.10 Exact tests under normal data

The Wald test above relies on large-sample approximations but these may not be valid in finate samples. Can we get **exact** inferences at any sample size? Yes, if we make stronger assumptions about the data. In particular, assume a **parametric model** for the data where $X_1, \dots, X_n$ are iid samples from $N(\mu, \sigma^2)$. Under a null hypothesis of $H_0 : \mu = \mu_0$, we can show that

$$T_n = \frac{\overline{X}_n - \mu_0}{s_n/\sqrt{n}} \sim t_{n-1},$$

where t_{n-1} is the **Student's t-distribution** with $n-1$ degrees of freedom. This result implies the null distribution is t, so we use quantiles of t for critical values. For a one-sided test, $c = G_0^{-1}(1-\alpha)$, but now G_0 is t with $n-1$ df and so we use `qt()` instead of `qnorm()` to calculate these critical values.

The critical values for the t distribution are always larger than the normal because the t distribution has fatter tails, as shown in Figure 4.3. As $n \to \infty$, however, the t converges to the standard normal, and so it is asymptotically equivalent to the Wald test but slightly more conservative in finite samples. Most software packages calculate p-values and rejection regions based on the t to exploit this conservativeness.

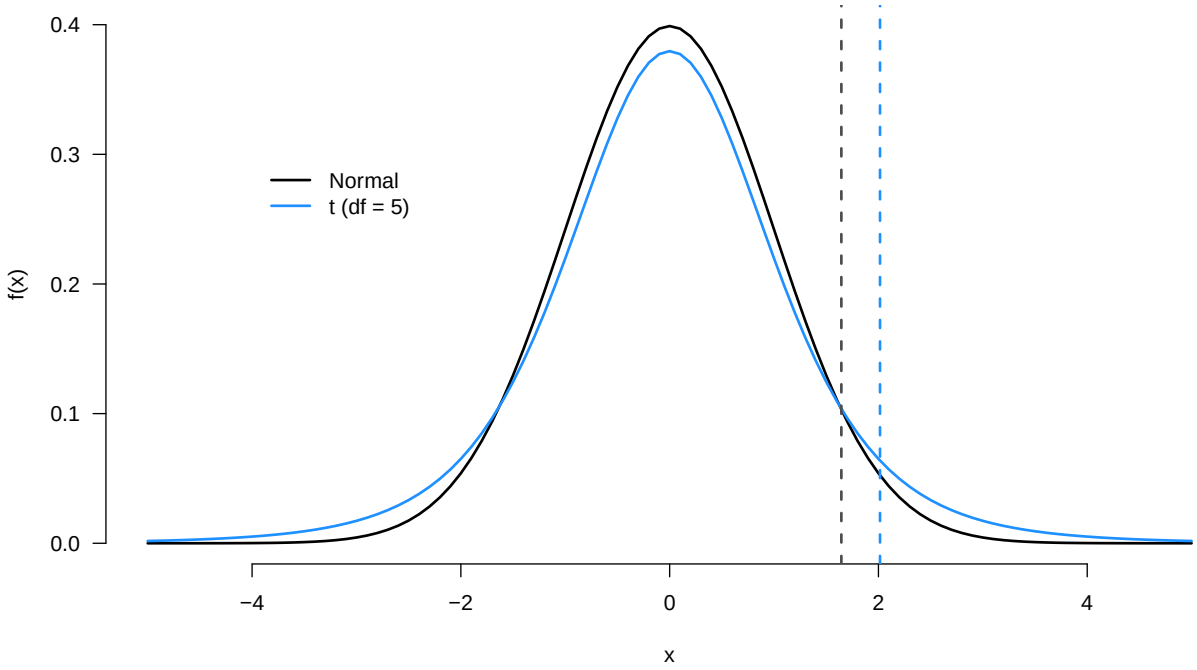


Figure 4.3: Normal versus t distribution.

4.11 Confidence intervals and hypothesis tests

At first glance, we may seem sloppy in using α in deriving a $1-\alpha$ confidence interval in the last chapter and an α-level test in this chapter. In reality, we were foreshadowing the deep connection between confidence intervals and hypothesis tests: every $1-\alpha$ confidence interval contains all null hypotheses that we **would not reject** with an α-level test.

This connection is easiest to see with an asymptotically normal estimator, $\widehat{\theta}_n$. Consider

the hypothesis test of

$$H_0 : \theta = \theta_0 \quad \text{vs.} \quad H_1 : \theta \neq \theta_0,$$

using the test statistic,

$$T = \frac{\hat{\theta}_n - \theta_0}{\widehat{\mathsf{se}}[\hat{\theta}_n]}.$$

As we discussed earlier, an $\alpha = 0.05$ test would reject this null when $|T| > 1.96$, or when

$$|\hat{\theta}_n - \theta_0| > 1.96\widehat{\mathsf{se}}[\hat{\theta}_n].$$

Notice that will be true when

$$\theta_0 < \hat{\theta}_n - 1.96\widehat{\mathsf{se}}[\hat{\theta}_n] \quad \text{or} \quad \hat{\theta}_n + 1.96\widehat{\mathsf{se}}[\hat{\theta}_n] < \theta_0$$

or, equivalently, that null hypothesis is outside of the 95% confidence interval,

$$\theta_0 \notin \left[\hat{\theta}_n - 1.96\widehat{\mathsf{se}}[\hat{\theta}_n], \hat{\theta}_n + 1.96\widehat{\mathsf{se}}[\hat{\theta}_n]\right].$$

Our choice of the null hypothesis was arbitrary, which means that any null hypothesis outside the 95% confidence interval would be rejected by a $\alpha = 0.05$ level test. And any null hypothesis inside the confidence interval is a null hypothesis that we would not reject.

This relationship holds more broadly. Any $1-\alpha$ confidence interval contains all possible parameter values that would not be rejected as the null hypothesis of an α-level hypothesis test. This connection can be handy for two reasons:

1. We can quickly determine if we would reject a null hypothesis at some level by inspecting if it falls in a confidence interval. For example, quickly looking to see whether 0 is included in the confidence interval is a fast and easy check on whether a null hypothesis of no treatment effect is or is not rejected – if it is included, the null cannot be rejected.
2. In some situations, determining a confidence interval might be difficult, but performing a hypothesis test is straightforward. Then, we can find the rejection region for the test and determine which null hypotheses would not be rejected at level α to formulate the $1-\alpha$ confidence interval. We call this process **inverting a test**. A critical application of this method is for formulating confidence intervals for treatment effects based on randomization inference in the finite population analysis of experiments.

4.12 Summary

In this chapter, we covered the basics of hypothesis tests, which are a type of statistical thought experiment. We assume that we know the true state of the world and determine how unlikely our observed data would be in that world. We described different types of tests (one-sided versus two-sided), introduced the properties of tests (size and power), and showed how to determine the rejection region of a test. We also described the Wald test, a general test that can be used in a wide variety of settings. P-values are a continuous measure of divergence between the observed data and the null hypothesis. Power analyses allow researchers to forecast how large of a sample they will need to detect different effect sizes with sufficient statistical power. Finally, confidence intervals and hypothesis tests are deeply connected since confidence intervals will contain all null hypotheses that cannot be rejected at a certain α.

We have now covered the basic tools of statistical inference at a high level and have shown how to apply them to simple estimators like the sample mean or the sample difference in means. In Part II of this book, we turn to applying many of these ideas to the predominant estimator in the quantitative social sciences—ordinary least squares.

Part II

Regression

5 Linear regression

Regression is simply a set of tools for evaluating the relationship between an **outcome variable**, Y_i, and a set of **covariates**, $\mathbf{X}_i$. In particular, these tools show how the conditional mean of Y_i varies as a function of $\mathbf{X}_i$. For example, we may want to know how wait times at voting precincts vary as a function of various socioeconomic features of the precinct, like income and racial composition. We can accomplish this by estimating the **regression function** or **conditional expectation function** (CEF) of the outcome given the covariates,

$$\mu(\mathbf{x}) = \mathbb{E}[Y_i \mid \mathbf{X}_i = \mathbf{x}].$$

Why are estimation and inference for this regression function special? Why can't we just use the approaches we have seen for the mean, variance, covariance, and so on? The fundamental problem with the CEF is that there may be many values $\mathbf{x}$ that can occur and many different conditional expectations that we will need to estimate. If any variable in $\mathbf{X}_i$ is continuous, we must estimate an infinite number of possible values of $\mu(\mathbf{x})$, and this worsens as we add covariates to $\mathbf{X}_i$. Because of that, we refer to this problem as the **curse of dimensionality**. How can we resolve this with our measly finite data?

In this chapter, we will explore two ways of "solving" the curse of dimensionality: (1) assuming it away, and (2) changing the quantity of interest to something easier to estimate.

Regression is so ubiquitous across many scientific fields that it has generated a lot of acquired notational baggage. In particular, the labels of the Y_i and $\mathbf{X}_i$ vary greatly:

- The outcome can also be called: the response variable, the dependent variable, the labels (in machine learning), the left-hand side variable, or the regressand
- The covariates are also called: the explanatory variables, the independent variables, the predictors, the right-hand side variables, the regressors, inputs, or features

5.1 Why do we need models?

At first glance, the connection between the CEF and parametric models might be hazy. For example, imagine we are interested in estimating the average wait times at a voting precinct (Y_i) for Black voters ($X_i = 1$) versus non-Black voters ($X_i = 0$). In that case, there are two parameters to estimate,

$$\mu(1) = \mathbb{E}[Y_i \mid X_i = 1] \quad \text{and} \quad \mu(0) = \mathbb{E}[Y_i \mid X_i = 0],$$

which we could estimate by using the plug-in estimators that replace the population averages with their sample counterparts,

$$\widehat{\mu}(1) = \frac{\sum_{i=1}^{n} Y_i \mathbb{1}(X_i = 1)}{\sum_{i=1}^{n} \mathbb{1}(X_i = 1)} \qquad \widehat{\mu}(0) = \frac{\sum_{i=1}^{n} Y_i \mathbb{1}(X_i = 0)}{\sum_{i=1}^{n} \mathbb{1}(X_i = 0)}.$$

These are just the sample averages of the wait times for Black and non-Black voters, respectively. And because the race variable here is discrete, we are simply estimating sample means within subpopulations defined by race. The same logic would apply if we had k racial categories: we would have k conditional expectations to estimate and k (conditional) sample means.

Now imagine that we want to know how the average wait time varies as a function of income so that X_i is (essentially) continuous. (Perhaps the theory here is that wait times may be lower in precincts with more affluent voters.) Now we have a different conditional expectation for every possible dollar amount from 0 to however much the wealthiest earner makes. Suppose we choose one particular income, $42,238, and that we are interested in the conditional expectation $\mu(42,238) = \mathbb{E}[Y_i \mid X_i = 42,238]$. We could use the same plug-in estimator as in the discrete case,

$$\widehat{\mu}(42,238) = \frac{\sum_{i=1}^{n} Y_i \mathbb{1}(X_i = 42,238)}{\sum_{i=1}^{n} \mathbb{1}(X_i = 42,238)}.$$

This is straightforward, but there is one glaring problem with this estimator: in all likelihood, no units in the particular dataset have that exact income, meaning this estimator is undefined because we would be dividing by zero.

One solution to this problem is to use **subclassification** to turn the continuous variable into a discrete one and then proceed with the discrete approach above. For example, we could group incomes into $25,000 bins and then calculate the average wait times

of anyone between, say, \$25,000 and \$50,000 income. When we make this estimator switch for practical purposes, we need to connect it back to the DGP of interest. We could **assume** that the CEF of interest only depends on these binned means, giving us:

$$\mu(x) = \begin{cases} \mathbb{E}[Y_i \mid 0 \leq X_i < 25,000] & \text{if } 0 \leq x < 25,000 \\ \mathbb{E}[Y_i \mid 25,000 \leq X_i < 50,000] & \text{if } 25,000 \leq x < 50,000 \\ \mathbb{E}[Y_i \mid 50,000 \leq X_i < 100,000] & \text{if } 50,000 \leq x < 100,000 \\ \vdots & \\ \mathbb{E}[Y_i \mid 200,000 \leq X_i] & \text{if } 200,000 \leq x \end{cases}$$

This approach assumes, perhaps incorrectly, that the average wait time does not vary within the bins. Figure 5.1 shows a hypothetical joint distribution between income and wait times with the true CEF, $\mu(x)$, shown in red. The figure also shows the bins created by subclassification and the implied CEF if we assume bin-constant means in blue. Note that the blue function approximates the true CEF but deviates from it close to the bin edges. The trade-off is that once we make the assumption that wait times do not vary within the bins, we only have to estimate one mean for every bin rather than an infinite number of means for each possible income.

Similarly, we could **assume** that the CEF follows a simple functional form such as a line:

$$\mu(x) = \mathbb{E}[Y_i \mid X_i = x] = \beta_0 + \beta_1 x.$$

This assumption reduces our infinite number of unknowns (the conditional mean at every possible income) to just two unknowns: (1) the slope and (2) the intercept. As we will see, we can use the standard ordinary least squares to estimate these parameters. Note that if the true CEF is nonlinear, this assumption is incorrect, and any estimate based on this assumption might be biased or even inconsistent.

We call the binning and linear assumptions on $\mu(x)$ **functional form** assumptions because they restrict the class of functions that $\mu(x)$ can take. While powerful, these types of assumptions can muddy the roles of defining the quantity of interest and estimation. If our estimator $\widehat{\mu}(x)$ performs poorly, it will be difficult to tell if this is because the estimator is flawed or our functional form assumptions are incorrect.

To clarify these issues, we will pursue a different approach: understanding what linear regression can estimate under minimal assumptions and then investigating how well this estimand approximates the true CEF.

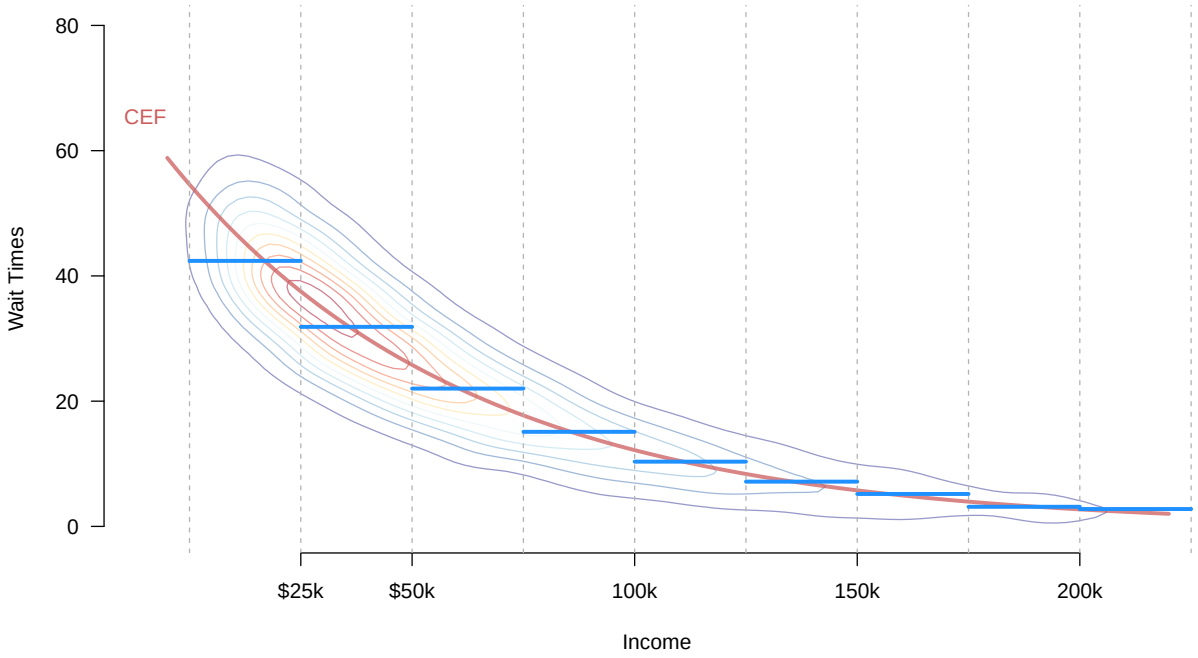


Figure 5.1: Hypothetical joint distribution of income and poll wait times (contour plot), conditional expectation function (red), and the conditional expectation of the binned income (blue).

5.2 Population linear regression

5.2.1 Bivariate linear regression

Let's set aside the idea of the conditional expectation function and instead focus on finding the **linear** function of a single covariate X_i that best predicts the outcome. Recall from your earlier mathematical training that linear functions have the form $a + bX_i$. The **best linear predictor** (BLP) or **population linear regression** of Y_i on X_i is defined as

$$m(x) = \beta_0 + \beta_1 x \quad \text{where,} \quad (\beta_0, \beta_1) = \underset{(b_0, b_1) \in \mathbb{R}^2}{\arg\min} \; \mathbb{E}[(Y_i - b_0 - b_1 X_i)^2].$$

The expression being minimized is the expected prediction error, or the (squared) distance between the observed outcome and the outcome as predicted with a particular slope and intercept. The best linear predictor is the line (that is, slope and intercept values) that results in the lowest expected prediction error. Note that this function is a feature of the

joint distribution of the data—the DGP—and so we cannot observe it directly. It must be estimated. The BLP is an alternative to the CEF for summarizing the relationship between the outcome and the covariate, though as we discuss later they will sometimes be equal. We call (β_0, β_1) the **population linear regression coefficients**. Note that $m(x)$ could differ greatly from the CEF $\mu(x)$ if the latter is nonlinear.

We can solve for the best linear predictor using standard calculus (taking the derivative with respect to each coefficient, setting those equations equal to 0, and solving the system of equations). The first-order conditions, in this case, are

$$\frac{\partial \mathbb{E}[(Y_i - b_0 - b_1 X_i)^2]}{\partial b_0} = \mathbb{E}[-2(Y_i - \beta_0 - \beta_1 X_i)] = 0$$
$$\frac{\partial \mathbb{E}[(Y_i - b_0 - b_1 X_i)^2]}{\partial b_1} = \mathbb{E}[-2(Y_i - \beta_0 - \beta_1 X_i)X_i] = 0$$

Given the linearity of expectations, it is easy to solve for β_0 in terms of β_1,

$$\beta_0 = \mathbb{E}[Y_i] - \beta_1 \mathbb{E}[X_i].$$

We can plug this into the first-order condition for β_1 to get

$$\begin{aligned} 0 &= \mathbb{E}[Y_i X_i] - (\mathbb{E}[Y_i] - \beta_1 \mathbb{E}[X_i])\mathbb{E}[X_i] - \beta_1 \mathbb{E}[X_i^2] \\ &= \mathbb{E}[Y_i X_i] - \mathbb{E}[Y_i]\mathbb{E}[X_i] - \beta_1(\mathbb{E}[X_i^2] - \mathbb{E}[X_i]^2) \\ &= \text{cov}(X_i, Y_i) - \beta_1 \mathbb{V}[X_i] \\ \beta_1 &= \frac{\text{cov}(X_i, Y_i)}{\mathbb{V}[X_i]} \end{aligned}$$

Thus, the slope on the population linear regression of Y_i on X_i is equal to the ratio of the covariance of the two variables divided by the variance of X_i. It follows from this that the covariance will determine the sign of the slope: positive covariances will lead to positive β_1 and negative covariances will lead to negative β_1. In addition, if Y_i and X_i are independent, $\beta_1 = 0$. The slope scales this covariance by the variance of the covariate, so slopes will be lower for more spread-out covariates and higher for less spread-out covariates. If we define the correlation between these variables as ρ_{YX}, then we can relate the coefficient to this quantity as

$$\beta_1 = \rho_{YX} \sqrt{\frac{\mathbb{V}[Y_i]}{\mathbb{V}[X_i]}}.$$

Collecting these various results together, we can write the population linear regression as

$$m(x) = \beta_0 + \beta_1 x = \mathbb{E}[Y_i] + \beta_1(x - \mathbb{E}[X_i]),$$

which shows how we adjust our best guess about Y_i from the mean of the outcome using the covariate.

Be sure to remember that the BLP, $m(x)$, and the CEF, $\mu(x)$, are distinct entities. If the CEF is nonlinear, as in Figure 5.2, there will be a difference between these functions, meaning that the BLP might produce subpar predictions. We will derive a formal connection between the BLP and the CEF below.

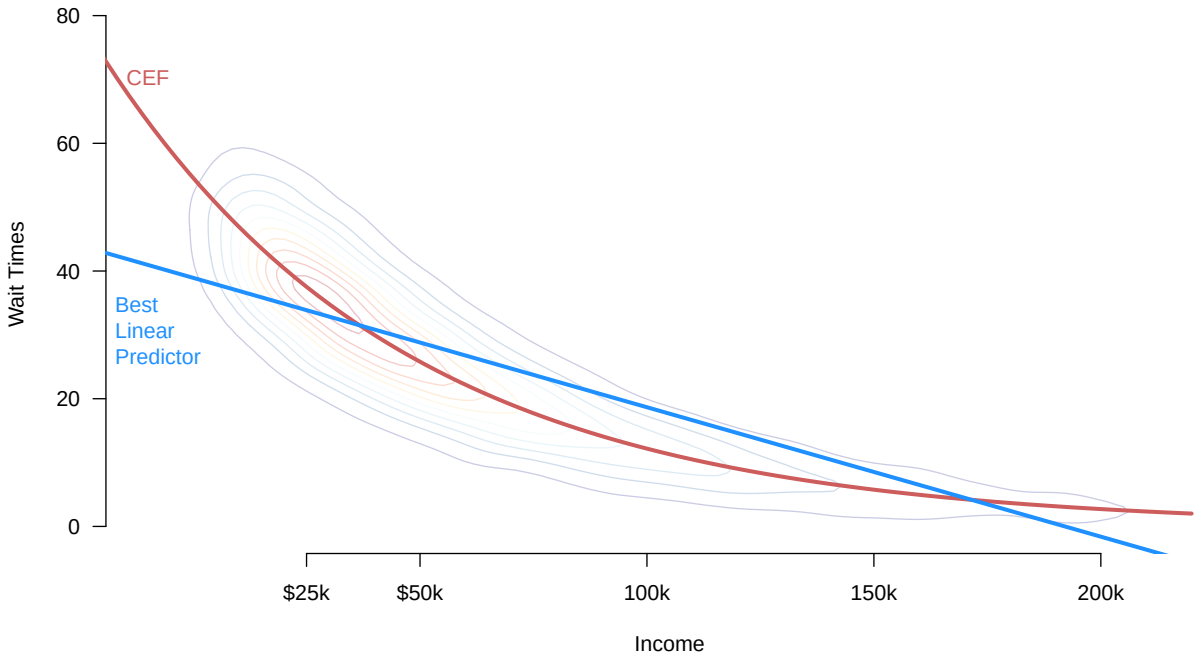


Figure 5.2: Comparison of the CEF and the best linear predictor.

5.2.2 Beyond linear approximations

The linear part of the "best linear predictor" is less restrictive than it appears at first glance. We can easily modify the minimum MSE problem to find the best quadratic, cubic, or

general polynomial function of X_i that predicts Y_i. For example, the quadratic function of X_i that best predicts Y_i would be

$$m(X_i, X_i^2) = \beta_0 + \beta_1 X_i + \beta_2 X_i^2 \quad \text{where} \quad \underset{(b_0,b_1,b_2)\in\mathbb{R}^3}{\arg\min} \; \mathbb{E}[(Y_i - b_0 - b_1 X_i - b_2 X_i^2)^2].$$

While the equation is now a quadratic function of the covariates, it is still a linear function of the unknown parameters $(\beta_0, \beta_1, \beta_2)$, so we still call this a best linear predictor.

We could include higher-order terms of X_i in the same manner, and, including more polynomial terms, X_i^p, will allow the BLP to be a more flexible function of X_i. When we estimate the BLP, however, we usually pay for this flexibility with overfitting and high variance in our estimates.

5.2.3 Linear prediction with multiple covariates

We now generalize the idea of a best linear predictor to a setting with an arbitrary number of covariates, which more flexibly captures real-life empirical research scenarios. In this setting, recall that the linear function will be

$$\mathbf{x}'\boldsymbol{\beta} = x_1\beta_1 + x_2\beta_2 + \cdots + x_k\beta_k.$$

We will define the **best linear predictor** (BLP) to be

$$m(\mathbf{x}) = \mathbf{x}'\boldsymbol{\beta}, \quad \text{where} \quad \boldsymbol{\beta} = \underset{\mathbf{b}\in\mathbb{R}^k}{\arg\min} \; \mathbb{E}\left[\left(Y_i - \mathbf{X}_i'\mathbf{b}\right)^2\right]$$

This BLP solves the same fundamental optimization problem as in the bivariate case: it chooses the set of coefficients that minimizes the expected mean-squared error, where the expectation is over the joint distribution of the data.

i Best linear projection assumptions

Without some assumptions on the joint distribution of the data, the following "regularity conditions" will ensure the existence of the BLP:

1. $\mathbb{E}[Y^2] < \infty$ (outcome has finite mean/variance)
2. $\mathbb{E}\|\mathbf{X}\|^2 < \infty$ ($\mathbf{X}$ has finite means/variances/covariances)
3. $\mathbf{Q}_{\mathbf{XX}} = \mathbb{E}[\mathbf{X}\mathbf{X}']$ is positive definite (columns of $\mathbf{X}$ are linearly independent)

Under these assumptions, it is possible to derive a closed-form expression for the **population coefficients** $\boldsymbol{\beta}$ using matrix calculus. To set up the optimization problem, we find the first-order condition by taking the derivative of the expectation of the squared errors. First, take the derivative of the squared prediction errors using the chain rule:

$$\begin{aligned}
\frac{\partial}{\partial \mathbf{b}} \left(Y_i - \mathbf{X}_i'\mathbf{b}\right)^2 &= 2\left(Y_i - \mathbf{X}_i'\mathbf{b}\right) \frac{\partial}{\partial \mathbf{b}}(Y_i - \mathbf{X}_i'\mathbf{b}) \\
&= -2\left(Y_i - \mathbf{X}_i'\mathbf{b}\right)\mathbf{X}_i \\
&= -2\mathbf{X}_i\left(Y_i - \mathbf{X}_i'\mathbf{b}\right) \\
&= -2\left(\mathbf{X}_i Y_i - \mathbf{X}_i\mathbf{X}_i'\mathbf{b}\right),
\end{aligned}$$

where the third equality comes from the fact that $(Y_i - \mathbf{X}_i'\boldsymbol{\beta})$ is a scalar. We can plug this into the expectation to get the first-order condition and solve for $\boldsymbol{\beta}$,

$$\begin{aligned}
0 &= -2\mathbb{E}[\mathbf{X}_i Y_i - \mathbf{X}_i\mathbf{X}_i'\boldsymbol{\beta}] \\
\mathbb{E}[\mathbf{X}_i\mathbf{X}_i']\boldsymbol{\beta} &= \mathbb{E}[\mathbf{X}_i Y_i],
\end{aligned}$$

which implies the population coefficients are

$$\boldsymbol{\beta} = \left(\mathbb{E}[\mathbf{X}_i\mathbf{X}_i']\right)^{-1}\mathbb{E}[\mathbf{X}_i Y_i] = \mathbf{Q}_{\mathbf{XX}}^{-1}\mathbf{Q}_{\mathbf{X}Y}$$

This gives us an expression for the coefficients for the population best linear predictor in terms of the joint distribution $(Y_i, \mathbf{X}_i)$.

A couple of facts might be useful for interpreting this expression substantively. Recall that $\mathbf{Q}_{\mathbf{XX}} = \mathbb{E}[\mathbf{X}_i\mathbf{X}_i']$ is a $k \times k$ matrix and $\mathbf{Q}_{\mathbf{X}Y} = \mathbb{E}[\mathbf{X}_i Y_i]$ is a $k \times 1$ column vector, which implies that $\boldsymbol{\beta}$ is also a $k \times 1$ column vector.

> **Note**
>
> What does the expression for the population regression coefficients mean? It is helpful to separate the intercept or constant term so that we have
>
> $$Y_i = \beta_0 + \mathbf{X}'\boldsymbol{\beta} + e_i,$$
>
> so $\boldsymbol{\beta}$ refers to just the vector of coefficients for the covariates. In this case, we can write the coefficients in a more interpretable way:
>
> $$\boldsymbol{\beta} = \mathbb{V}[\mathbf{X}]^{-1}\text{Cov}(\mathbf{X}, Y), \qquad \beta_0 = \mu_Y - \boldsymbol{\mu}_{\mathbf{X}}'\boldsymbol{\beta}$$

Thus, the population coefficients take the covariance between the outcome and the covariates and "divide" it by information about variances and covariances of the covariates. The intercept recenters the regression so that projection errors are mean zero. This means that these coefficients generalize the bivariate formula to this multiple covariate context.

With an expression for the population linear regression coefficients, we can write the linear projection as

$$m(\mathbf{X}_i) = \mathbf{X}_i' \left(\mathbb{E}[\mathbf{X}_i\mathbf{X}_i']\right)^{-1} \mathbb{E}[\mathbf{X}_i Y_i] = \mathbf{X}_i'\mathbf{Q}_{\mathbf{XX}}^{-1}\mathbf{Q}_{\mathbf{X}Y}$$

5.2.4 Projection error

The **projection error** or is the difference between the actual value of Y_i and the projection,

$$e_i = Y_i - m(\mathbf{X}_i) = Y_i - \mathbf{X}_i'\boldsymbol{\beta},$$

where we have made no assumptions about this error yet. The projection error is simply the prediction error of the best linear prediction for a particular unit in the data. Rewriting this definition, we can see that we can always write the outcome as the linear projection plus the projection error,

$$Y_i = \mathbf{X}_i'\boldsymbol{\beta} + e_i.$$

Notice that this looks suspiciously similar to a linearity assumption on the CEF, but we haven't made any assumptions here. Instead, we just used the definition of the projection error to write a tautological statement:

$$Y_i = \mathbf{X}_i'\boldsymbol{\beta} + e_i = \mathbf{X}_i'\boldsymbol{\beta} + Y_i - \mathbf{X}_i'\boldsymbol{\beta} = Y_i.$$

The critical difference between this representation and the usual linear model assumption is what properties e_i possesses.

A key property of the projection errors is that when the covariate vector includes an "intercept" or constant term, the projection errors are uncorrelated with the covariates. To see this, first note that $\mathbb{E}[\mathbf{X}_i e_i] = 0$ since

$$\begin{aligned}
\mathbb{E}[\mathbf{X}_i e_i] &= \mathbb{E}[\mathbf{X}_i(Y_i - \mathbf{X}_i'\boldsymbol{\beta})] \\
&= \mathbb{E}[\mathbf{X}_i Y_i] - \mathbb{E}[\mathbf{X}_i\mathbf{X}_i']\boldsymbol{\beta} \\
&= \mathbb{E}[\mathbf{X}_i Y_i] - \mathbb{E}[\mathbf{X}_i\mathbf{X}_i'] \left(\mathbb{E}[\mathbf{X}_i\mathbf{X}_i']\right)^{-1} \mathbb{E}[\mathbf{X}_i Y_i] \\
&= \mathbb{E}[\mathbf{X}_i Y_i] - \mathbb{E}[\mathbf{X}_i Y_i] = 0
\end{aligned}$$

Thus, for every X_{ij} in $\mathbf{X}_i$, we have $\mathbb{E}[X_{ij}e_i] = 0$. If one of the entries in $\mathbf{X}_i$ is a constant 1, then this also implies that $\mathbb{E}[e_i] = 0$. Together, these facts imply that the projection error is uncorrelated with each X_{ij}, since

$$\text{cov}(X_{ij}, e_i) = \mathbb{E}[X_{ij}e_i] - \mathbb{E}[X_{ij}]\mathbb{E}[e_i] = 0 - 0 = 0$$

Note that we still have made no assumptions about these projection errors except for some mild regularity conditions on the joint distribution of the outcome and covariates. Thus, in very general settings, we can write the linear projection model $Y_i = \mathbf{X}_i'\boldsymbol{\beta} + e_i$ where $\boldsymbol{\beta} = \left(\mathbb{E}[\mathbf{X}_i\mathbf{X}_i']\right)^{-1}\mathbb{E}[\mathbf{X}_iY_i]$ and conclude that $\mathbb{E}[\mathbf{X}_ie_i] = 0$ by definition, not by assumption.

The projection error is uncorrelated with the covariates, so does this mean that the CEF is linear? Unfortunately, no. Recall that while independence implies this lack of correlation, the reverse does not hold. So when we look at the CEF, we have

$$\mathbb{E}[Y_i \mid \mathbf{X}_i] = \mathbf{X}_i'\boldsymbol{\beta} + \mathbb{E}[e_i \mid \mathbf{X}_i],$$

and the last term $\mathbb{E}[e_i \mid \mathbf{X}_i]$ would only be 0 if the errors were independent of the covariates, so $\mathbb{E}[e_i \mid \mathbf{X}_i] = \mathbb{E}[e_i] = 0$. But nowhere in the linear projection model did we assume this. So while we can (almost) always write the outcome as $Y_i = \mathbf{X}_i'\boldsymbol{\beta} + e_i$ and have those projection errors be uncorrelated with the covariates, it will require additional assumptions to ensure that the true CEF is, in fact, linear $\mathbb{E}[Y_i \mid \mathbf{X}_i] = \mathbf{X}_i'\boldsymbol{\beta}$.

To step back for a moment, what have we shown here? In a nutshell, we showed that a population linear regression exists under very general conditions and that we can write the coefficients of that population linear regression as a function of expectations of the joint distribution of the data. We did not, however, assume that the CEF was linear nor that the projection errors were normally distributed.

Why is this important? The ordinary least squares estimator, the workhorse regression estimator of the social sciences, targets this quantity of interest in large samples, regardless of whether the true CEF is linear or not. Thus, even when a linear CEF assumption is incorrect and the projection errors are not normally distributed, OLS still targets a perfectly valid quantity of interest: the coefficients from this population linear projection.

5.3 Linear CEFs without assumptions

What is the relationship between the best linear predictor (which we just saw generally exists) and the CEF? To draw the connection, remember that the conditional expectation is

importantly the function of $\mathbf{X}_i$ that best predicts Y_i. The population regression was the best **linear** predictor, but the CEF is the best predictor among all nicely behaved functions of $\mathbf{X}_i$, linear or nonlinear. In particular, if we label L_2 to be the set of all functions of the covariates $g()$ that have finite squared expectation, $\mathbb{E}[g(\mathbf{X}_i)^2] < \infty$, then we can show that the CEF has the lowest squared prediction error in this class of functions:

$$\mu(\mathbf{X}) = \mathbb{E}[Y_i \mid \mathbf{X}_i] = \underset{g(\mathbf{X}_i) \in L_2}{\arg\min} \; \mathbb{E}\left[(Y_i - g(\mathbf{X}_i))^2\right],$$

So we have established that the CEF is the best predictor and the population linear regression $m(\mathbf{X}_i)$ is the best linear predictor. These two facts allow us to connect the CEF to the population regression.

Theorem 5.1. *If $\mu(\mathbf{X}_i)$ is a linear function of $\mathbf{X}_i$, then $\mu(\mathbf{X}_i) = m(\mathbf{X}_i) = \mathbf{X}_i'\boldsymbol{\beta}$.*

This theorem says that if the true CEF is linear, it must equal the population linear regression. The proof of this is straightforward: the CEF is the best predictor, so if it is linear, it must also be the best linear predictor.

In general, we are in the business of learning about the CEF, so we are unlikely to know if it genuinely is linear or not. In some situations, however, we can show that the CEF is linear without any additional assumptions. These are situations where the covariates take on a finite number of possible values. Going back to the example from the chapter introduction, suppose we are interested in the CEF of wait times at voting precincts for Black ($X_i = 1$) vs. non-Black ($X_i = 0$) voters. In this case, there are two possible values of the CEF, $\mu(1) = \mathbb{E}[Y_i \mid X_i = 1]$, the average wait time for Black voters, and $\mu(0) = \mathbb{E}[Y_i \mid X_i = 0]$, the average wait time for non-Black voters. Notice that we can write the CEF as

$$\mu(x) = x\mu(1) + (1 - x)\mu(0) = \mu(0) + x\left(\mu(1) - \mu(0)\right) = \beta_0 + x\beta_1,$$

which is clearly a linear function of x. Based on this derivation, we obtain coefficients of this linear CEF that have clear substantive interpretations:

- $\beta_0 = \mu(0)$: the expected wait time for a Black voter.
- $\beta_1 = \mu(1) - \mu(0)$: the difference in average wait times between Black and non-Black voters. How X_i is defined here is important since the intercept will always be the average outcome when $X_i = 0$, and the slope will always be the difference in means between the $X_i = 1$ group and the $X_i = 0$ group.

What about a categorical covariate with more than two levels? For example, we may be interested in wait times by party identification, where $X_i = 1$ indicates Democratic voters, $X_i = 2$ indicates Republican voters, and $X_i = 3$ indicates Independent voters. We could write the CEF of wait times as a linear function of this variable, but that would assume that the difference between Democrats and Republicans is exactly the same as for Independents and Republicans – which is probably false. With more than two levels, we can represent a categorical variable as a vector of binary variables, $\mathbf{X}_i = (X_{i1}, X_{i2})$, where

$$X_{i1} = \begin{cases} 1 & \text{if Republican} \\ 0 & \text{if not Republican} \end{cases}$$

$$X_{i2} = \begin{cases} 1 & \text{if independent} \\ 0 & \text{if not independent} \end{cases}$$

These two indicator variables encode the same information as the original single three-level variable, X_i, so if we know the values of X_{i1} and X_{i2}, then we know exactly to which party i belongs. Thus, the CEFs for X_i and the pair of indicator variables, $\mathbf{X}_i$, are precisely the same, but the latter allows for a lovely linear representation,

$$\mathbb{E}[Y_i \mid X_{i1}, X_{i2}] = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2},$$

where

- $\beta_0 = \mathbb{E}[Y_i \mid X_{i1} = 0, X_{i2} = 0]$ is the average wait time for the group who does not get an indicator variable (Democrats in this case). This group is sometimes called the baseline group or the omitted group.
- $\beta_1 = \mathbb{E}[Y_i \mid X_{i1} = 1, X_{i2} = 0] - \mathbb{E}[Y_i \mid X_{i1} = 0, X_{i2} = 0]$ is the difference in means between Republican voters and Democratic voters, or the difference between the first indicator group and the baseline group.
- $\beta_2 = \mathbb{E}[Y_i \mid X_{i1} = 0, X_{i2} = 1] - \mathbb{E}[Y_i \mid X_{i1} = 0, X_{i2} = 0]$ is the difference in means between independent voters and Democratic voters, or the difference between the second indicator group and the baseline group.

This approach easily generalizes to categorical variables with an arbitrary number of levels.

What have we shown? The CEF is linear without additional assumptions when there is a categorical covariate. We can show that this continues to hold even when we have multiple categorical variables. We now have two binary covariates: $X_{i1} = 1$ indicating

a Black voter, and $X_{i2} = 1$ indicating a retired voter versus a working-age voter. These two binary variables give us four possible values of the CEF:

$$\mu(x_1, x_2) = \begin{cases} \mu_{00} & \text{if } x_1 = 0 \text{ and } x_2 = 0 \text{ (non-Black, working age)} \\ \mu_{10} & \text{if } x_1 = 1 \text{ and } x_2 = 0 \text{ (Black, working age)} \\ \mu_{01} & \text{if } x_1 = 0 \text{ and } x_2 = 1 \text{ (non-Black, retired)} \\ \mu_{11} & \text{if } x_1 = 1 \text{ and } x_2 = 1 \text{ (Black, retired)} \end{cases}$$

We can write this as

$$\mu(x_1, x_2) = (1 - x_1)(1 - x_2)\mu_{00} + x_1(1 - x_2)\mu_{10} + (1 - x_1)x_2\mu_{01} + x_1x_2\mu_{11},$$

which we can rewrite as

$$\mu(x_1, x_2) = \beta_0 + x_1\beta_1 + x_2\beta_2 + x_1x_2\beta_3,$$

where the substantive interpretations are

- $\beta_0 = \mu_{00}$: average wait times for working-age non-Black voters.
- $\beta_1 = \mu_{10} - \mu_{00}$: difference in means for working-age Black vs. working-age non-Black voters.
- $\beta_2 = \mu_{01} - \mu_{00}$: difference in means for retired non-Black vs. working-age non-Black voters.
- $\beta_3 = (\mu_{11} - \mu_{01}) - (\mu_{10} - \mu_{00})$: difference in retired racial difference vs working-age racial difference.

Thus, we can write the CEF with two binary covariates as linear when the linear specification includes a multiplicative interaction between them (x_1x_2). This result holds for all pairs of binary covariates, and we can generalize the interpretation of the coefficients in the CEF as

- $\beta_0 = \mu_{00}$: average outcome when both variables are 0.
- $\beta_1 = \mu_{10} - \mu_{00}$: difference in average outcomes for the first covariate when the second covariate is 0.
- $\beta_2 = \mu_{01} - \mu_{00}$: difference in average outcomes for the second covariate when the first covariate is 0.
- $\beta_3 = (\mu_{11} - \mu_{01}) - (\mu_{10} - \mu_{00})$: change in the "effect" of the first (second) covariate when the second (first) covariate goes from 0 to 1.

This result also generalizes to an arbitrary number of binary covariates. If we have p binary covariates, then the CEF will be linear with all two-way interactions, x_1x_2, all three-way interactions, $x_1x_2x_3$, up to the p-way interaction $x_1 \times \cdots \times x_p$. Furthermore, we can generalize to arbitrary numbers of categorical variables by expanding each into a series of binary variables and then including all interactions between the resulting binary variables.

We have established that when we have a set of categorical covariates, the true CEF will be linear, and we have seen the various ways to represent that CEF. Note that when we use, for example, ordinary least squares, we are free to choose how to include our variables. We could run a regression of Y_i on X_{i1} and X_{i2} without an interaction term, but this model will only be correct if β_3 is equal to 0, and so the interaction term is irrelevant. We call a model **saturated** if there are as many coefficients as the CEF's unique values. A saturated model can, by its nature, always be written as a linear function without assumptions. The above examples show how to construct saturated models in various situations.

5.4 Interpretation of the regression coefficients

We have seen how to interpret population regression coefficients when the CEF is linear without assumptions. How do we interpret the population coefficients $\boldsymbol{\beta}$ in other settings?

Consider the simplest case, one in which every entry in $\mathbf{X}_i$ represents a different covariate and no covariate is any function of another (we will see why this caveat is necessary below). In this simple case, the kth coefficient, β_k, represents the change in the predicted outcome for a one-unit change in the kth covariate X_{ik}, holding all other covariates fixed. We can see this from

$$\begin{aligned} m(x_1 + 1, x_2) &= \beta_0 + \beta_1(x_1 + 1) + \beta_2 x_2 \\ m(x_1, x_2) &= \beta_0 + \beta_1 x_1 + \beta_2 x_2, \end{aligned}$$

so that the change in the predicted outcome for increasing X_{i1} by one unit is

$$m(x_1 + 1, x_2) - m(x_1, x_2) = \beta_1$$

Notice that nothing changes in this interpretation when adding more covariates to the vector,

$$m(x_1 + 1, \mathbf{x}_2) - m(x_1, \mathbf{x}_2) = \beta_1,$$

The coefficient on a particular variable is the change in the predicted outcome corresponding to a one-unit change in the covariate holding all other covariates constant. Each coefficient summarizes the "all else equal" difference in the predicted outcome for each covariate.

5.4.1 Polynomial functions of the covariates

The interpretation of the population regression coefficients becomes more complicated when including nonlinear functions of the covariates. In that case, multiple coefficients control how a change in a covariate will change the predicted value of Y_i. For example, suppose we have a quadratic function of X_{i1},

$$m(x_1, x_1^2, x_2) = \beta_0 + \beta_1 x_1 + \beta_2 x_1^2 + \beta_3 x_2,$$

and try to look at a one-unit change in x_1,

$$\begin{aligned} m(x_1 + 1, (x_1 + 1)^2, x_2) &= \beta_0 + \beta_1 (x_1 + 1) + \beta_2 (x_1 + 1)^2 + \beta_3 x_2 \\ m(x_1, x_1^2, x_2) &= \beta_0 + \beta_1 x_1 + \beta_2 x_1^2 + \beta_3 x_2, \end{aligned}$$

resulting in $\beta_1 + \beta_2(2x_1 + 1)$. This formula might be an interesting quantity, but we more commonly use the derivative of $m(\mathbf{x})$ with respect to x_1 as a measure of the marginal effect of X_{i1} on the predicted value of Y_i (holding all other variables constant), where "marginal" here means the change in prediction for a very small change in X_{i1}.[1] In the case of the quadratic covariate, we have

$$\frac{\partial m(x_1, x_1^2, x_2)}{\partial x_1} = \beta_1 + 2\beta_2 x_1,$$

so the marginal effect on prediction varies as a function of x_1. From this, we see that the individual interpretations of the coefficients are less interesting: β_1 is the marginal effect when $X_{i1} = 0$ and $\beta_2/2$ describes how a one-unit change in X_{i1} changes the marginal effect. As is hopefully clear, it will often be more straightforward to visualize the nonlinear predictor function (perhaps using the orthogonalization techniques in Section 5.5).

[1] Note the choice of language here. The marginal effect is on the predicted value of Y_i, not on Y_i itself. So these marginal effects are associational, not necessarily causal quantities.

5.4.2 Interactions

Another common nonlinear function occurs when including **interaction terms** or covariates that are products of two other covariates,

$$m(x_1, x_2, x_1 x_2) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2.$$

In these situations, we can use the derivative of the BLP to measure the marginal effect of one variable or the other on the predicted value of Y_i. In particular, we have

$$\frac{\partial m(x_1, x_2, x_1 x_2)}{\partial x_1} = \beta_1 + \beta_3 x_2,$$
$$\frac{\partial m(x_1, x_2, x_1 x_2)}{\partial x_2} = \beta_2 + \beta_3 x_1.$$

Here, the coefficients are slightly more interpretable:

- β_1: the marginal effect of X_{i1} on predicted Y_i when $X_{i2} = 0$.
- β_2: the marginal effect of X_{i2} on predicted Y_i when $X_{i1} = 0$.
- β_3: the change in the marginal effect of X_{i1} due to a one-unit change in X_{i2} **OR** the change in the marginal effect of X_{i2} due to a one-unit change in X_{i1}.

If we add more covariates to this BLP, these interpretations change to "holding all other covariates constant."

Interactions are a standard part of social science research because they allow us to assess how the relationship between the outcome and an independent variable varies by the values of another variable. In the context of our study of wait times at a voting precinct, if X_{i1} is income and X_{i2} is the Black/non-Black voter indicator, then β_3 represents the change in the slope of the wait time-income relationship between Black and non-Black voters.

> **i** Centering variables to improve interpretability
>
> In many cases, the so-called marginal coefficients on the lower-order terms (β_1 for X_{i1} and β_2 for X_{i2}) are uninteresting because they represent the marginal effect of one variable when the other is 0. If X_{i1} is age and X_{i2} is the Black/non-Black indicator, then β_2 is the estimated difference in average voter wait times for voters who are zero years old, an obviously nonsensical parameter. We can improve the interpretability of the coefficient by recentering the age variable. Suppose we include a

mean-centered version of age,

$$\widetilde{X}_{i1} = X_{i1} - \overline{X}_1$$

in place of X_{i1}. That is, we regress Y_i on $\widetilde{X}_{i1}$, X_{i2}, and $\widetilde{X}_{i1}X_{i2}$. In this case, β_2 (the coefficient on the race indicator X_{i2}) is the marginal effect of X_{i2} when $\widetilde{X}_{i1} = 0$ or when $X_{i1} = \overline{X}_1$. Thus, this coefficient is now the estimated difference in average voter wait times for the average-aged voter, which is far more interpretable. This recentering has no effect on either β_1 or β_3, which is rather remarkable.

5.5 Multiple regression from bivariate regression

With a regression of an outcome on two covariates, understanding how the coefficients of one variable relate to the other is helpful. Consider the following best linear projection:

$$(\alpha, \beta, \gamma) = \underset{(a,b,c)\in\mathbb{R}^3}{\arg\min}\ \mathbb{E}[(Y_i - (a + bX_i + cZ_i))^2] \tag{5.1}$$

Can we understand the β coefficient here in terms of a bivariate regression? As it turns out, yes. From the above results, we know that the intercept has a simple form:

$$\alpha = \mathbb{E}[Y_i] - \beta\mathbb{E}[X_i] - \gamma\mathbb{E}[Z_i].$$

Let's investigate the first order condition for β:

$$\begin{aligned}
0 &= \mathbb{E}[Y_iX_i] - \alpha\mathbb{E}[X_i] - \beta\mathbb{E}[X_i^2] - \gamma\mathbb{E}[X_iZ_i] \\
&= \mathbb{E}[Y_iX_i] - \mathbb{E}[Y_i]\mathbb{E}[X_i] + \beta\mathbb{E}[X_i]^2 + \gamma\mathbb{E}[X_i]\mathbb{E}[Z_i] - \beta\mathbb{E}[X_i^2] - \gamma\mathbb{E}[X_iZ_i] \\
&= \text{cov}(Y, X) - \beta\mathbb{V}[X_i] - \gamma\text{cov}(X_i, Z_i)
\end{aligned}$$

We can see from this that if $\text{cov}(X_i, Z_i) = 0$, then the coefficient on X_i will be the same as in the simple regression case, $\text{cov}(Y_i, X_i)/\mathbb{V}[X_i]$. When X_i and Z_i are uncorrelated, we sometimes call them **orthogonal**.

To write a simple formula for β when the covariates are not orthogonal, we **orthogonalize** X_i by obtaining the prediction errors from a population linear regression of X_i on Z_i:

$$\widetilde{X}_i = X_i - (\delta_0 + \delta_1 Z_i) \quad \text{where} \quad (\delta_0, \delta_1) = \underset{(d_0,d_1)\in\mathbb{R}^2}{\arg\min}\ \mathbb{E}[(X_i - (d_0 + d_1 Z_i))^2]$$

Given the properties of projection errors, we know that this orthogonalized version of X_i will be uncorrelated with Z_i since $\mathbb{E}[\widetilde{X}_i Z_i] = 0$. Remarkably, the coefficient on X_i from the "long" BLP in Equation 5.1 is the same as the regression of Y_i on this orthogonalized $\widetilde{X}_i$,

$$\beta = \frac{\text{cov}(Y_i, \widetilde{X}_i)}{\mathbb{V}[\widetilde{X}_i]}$$

We can expand this idea to when there are several other covariates. Suppose now that we are interested in a regression of Y_i on $\mathbf{X}_i$ and we are interested in the coefficient on the kth covariate. Let $\mathbf{X}_{i,-k}$ be the vector of covariates omitting the kth entry and let $m_k(\mathbf{X}_{i,-k})$ represent the BLP of X_{ik} on these other covariates. We can define $\widetilde{X}_{ik} = X_{ik} - m_k(\mathbf{X}_{i,-k})$ as the kth variable orthogonalized with respect to the rest of the variables and we can write the coefficient on X_{ik} as

$$\beta_k = \frac{\text{cov}(Y_i, \widetilde{X}_{ik})}{\mathbb{V}[\widetilde{X}_{ik}]}.$$

Thus, the population regression coefficient in the BLP is the same as from a bivariate regression of the outcome on the projection error for X_{ik} projected on all other covariates. One interpretation of coefficients in a population multiple regression is that they represent the relationship between the outcome and the covariate after removing the linear relationships of all other variables.

5.6 Omitted variable bias

In many situations, we may need to choose whether to include a variable in a regression, so it can be helpful to understand how this choice might affect the population coefficients on the other variables in the regression. Suppose we have a variable Z_i that we may add to our regression, which currently has $\mathbf{X}_i$ as the covariates. We can write this new projection as

$$m(\mathbf{X}_i, Z_i) = \mathbf{X}_i'\boldsymbol{\beta} + Z_i\gamma, \qquad m(\mathbf{X}_i) = \mathbf{X}_i'\boldsymbol{\delta},$$

where we often refer to $m(\mathbf{X}_i, Z_i)$ as the long regression and $m(\mathbf{X}_i)$ as the short regression.

From the definition of the BLP, we can write the short coefficients as

$$\boldsymbol{\delta} = \left(\mathbb{E}[\mathbf{X}_i\mathbf{X}_i']\right)^{-1}\mathbb{E}[\mathbf{X}_i Y_i].$$

Letting $e_i = Y_i - m(\mathbf{X}_i, Z_i)$ be the projection errors from the long regression, we can write this as

$$\begin{aligned}\boldsymbol{\delta} &= \left(\mathbb{E}[\mathbf{X}_i\mathbf{X}_i']\right)^{-1}\mathbb{E}[\mathbf{X}_i(\mathbf{X}_i'\boldsymbol{\beta} + Z_i\gamma + e_i)] \\ &= \left(\mathbb{E}[\mathbf{X}_i\mathbf{X}_i']\right)^{-1}\left(\mathbb{E}[\mathbf{X}_i\mathbf{X}_i']\boldsymbol{\beta} + \mathbb{E}[\mathbf{X}_i Z_i]\gamma + \mathbb{E}[\mathbf{X}_i e_i]\right) \\ &= \boldsymbol{\beta} + \left(\mathbb{E}[\mathbf{X}_i\mathbf{X}_i']\right)^{-1}\mathbb{E}[\mathbf{X}_i Z_i]\gamma\end{aligned}$$

Note that the vector in the second term is the vector of linear projection coefficients of a population linear regression of Z_i on the $\mathbf{X}_i$. If we call these coefficients $\boldsymbol{\pi}$, then the short coefficients are

$$\boldsymbol{\delta} = \boldsymbol{\beta} + \boldsymbol{\pi}\gamma.$$

We can rewrite this to show that the difference between the coefficients in these two projections is $\boldsymbol{\delta} - \boldsymbol{\beta} = \boldsymbol{\pi}\gamma$ or the product of the coefficient on the "excluded" Z_i and the coefficient of the included $\mathbf{X}_i$ on the excluded. Most textbooks refer to this difference as the **omitted variable bias** of omitting Z_i under the idea that $\boldsymbol{\beta}$ is the true target of inference. But the result is much broader than this since it tells us how to relate the coefficients of two nested projections.

The last two results (multiple regressions from bivariate and omitted variable bias) are sometimes presented as results for the ordinary least squares estimator that we will show in the next chapter. We introduce them here as features of a particular population quantity, the linear projection or population linear regression.

5.7 Drawbacks of the BLP

The best linear predictor is, of course, a *linear* approximation to the CEF, and this approximation could be quite poor if the true CEF is highly nonlinear. A more subtle issue with the BLP is that it is sensitive to the marginal distribution of the covariates when the CEF is nonlinear. Let's return to our example of wait times at voting precincts and income. In Figure 5.3, we show the true CEF and the BLP when we restrict income below \$50,000 or above \$100,000. The BLP can vary quite dramatically here. This figure is an extreme example, but the essential point still holds as the marginal distribution of X_i changes.

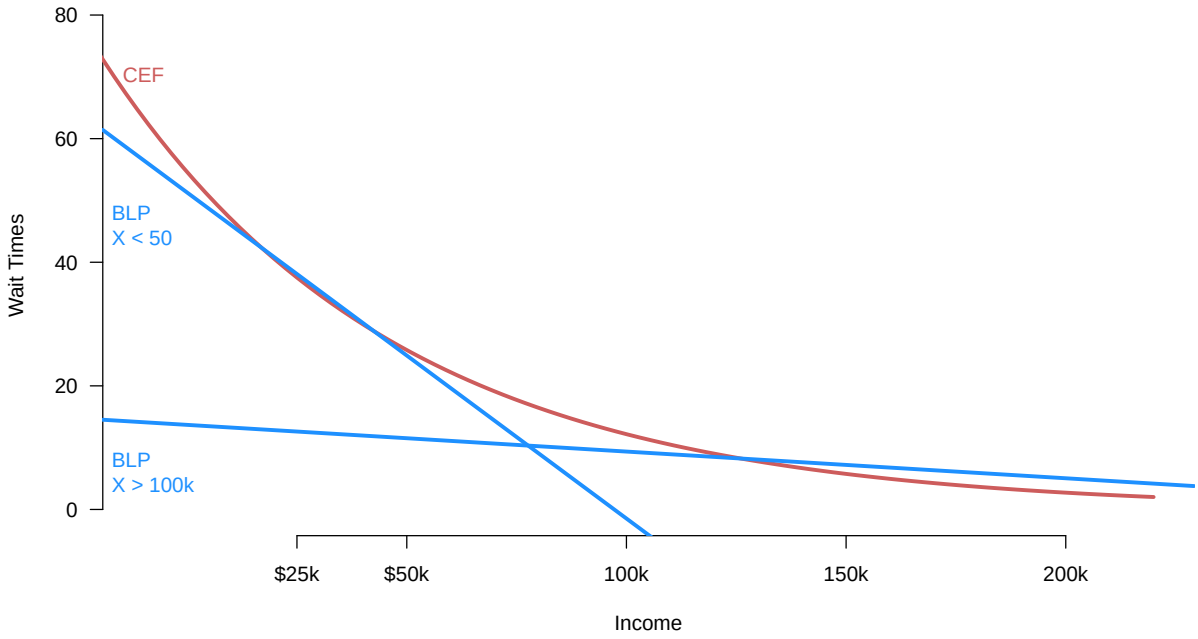


Figure 5.3: Linear projections for when truncating income distribution below $50k and above $100k.

5.8 Summary

As we discussed in this chapter, with even a moderate number of covariates, conditional expectation functions (also known as regressions) become very difficult to estimate because of the high dimensionality involved. To avoid this problem, we can focus on a different quantity, the **best linear predictor** which is the linear function of the covariates that best predicts the outcome in mean-squared error. The BLP exists under very mild conditions and has very interpretable parameters. Another strategy is to impose a linearity assumption on the **conditional expectation function** to make it more estimable, in which case, the BLP and the CEF are the same function. With a small number of discrete covariates it is possible to **saturate** a model so that linearity holds mechanically. Coefficients on population linear regressions with multiple independent variables can always be written in terms of a regression of the outcome on one variable orthogonalized relative to the rest of the independent variables. The **omitted variable bias** formula shows how leaving a variable out of the best linear affects the coefficients on other independent variables. In the next chapter, we will turn to using data to estimate the coefficients for these population linear regressions.

6 The mechanics of least squares

This chapter explores the most widely used estimator for population linear regressions: **ordinary least squares** (OLS). OLS is a plug-in estimator for the best linear projection (or population linear regression) described in the last chapter. Its popularity is partly due to its ease of interpretation, computational simplicity, and statistical efficiency. Because most people in the quantitative social sciences rely extensively on OLS for their own research, the time you spend developing deep familiarity with this approach will serve you well.

In this chapter, we focus on motivating the estimator and the mechanical or algebraic properties of the OLS estimator. In the next chapter, we will investigate its statistical assumptions. Textbooks often introduce OLS under the assumption of a linear model for the conditional expectation, but this is unnecessary if we view the inference target as the best linear predictor. We discuss this point more fully in the next chapter.

6.1 Deriving the OLS estimator

The last chapter on the linear model and the best linear projection operated purely in the population, not samples. We derived the population regression coefficients $\boldsymbol{\beta}$, representing the coefficients on the line of best fit in the population. We now take these as our quantity of interest. We now focus on how to use a sample from the population to make inferences about the line of best fit in the population and the population coefficients. To do this, we will focus on the OLS estimator for these population quantities.

> **i** Assumption
>
> The variables $\{(Y_1, \mathbf{X}_1), \dots, (Y_i, \mathbf{X}_i), \dots, (Y_n, \mathbf{X}_n)\}$ are i.i.d. draws from a common distribution F.

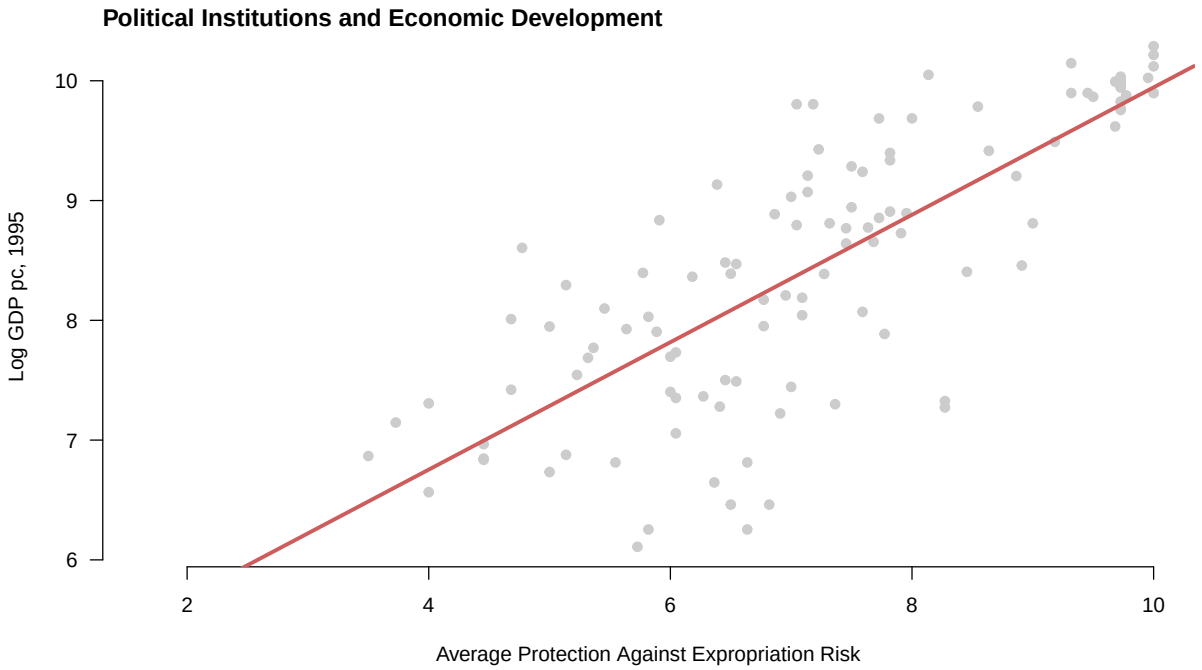


Figure 6.1: Relationship between political institutions and economic development from Acemoglu, Johnson, and Robinson (2001).

Recall the population linear coefficients (or best linear predictor coefficients) that we derived in the last chapter,

$$\boldsymbol{\beta} = \underset{\mathbf{b}\in\mathbb{R}^k}{\arg\min}\ \mathbb{E}\left[\left(Y_i - \mathbf{X}_i'\mathbf{b}\right)^2\right] = \left(\mathbb{E}[\mathbf{X}_i\mathbf{X}_i']\right)^{-1}\mathbb{E}[\mathbf{X}_i Y_i]$$

We will consider two different ways to derive the OLS estimator for these coefficients, both of which are versions of the plug-in principle. The first approach is to use the closed-form representation of the coefficients and then to replace any expectations with sample means,

$$\widehat{\boldsymbol{\beta}} = \left(\frac{1}{n}\sum_{i=1}^{n}\mathbf{X}_i\mathbf{X}_i'\right)^{-1}\left(\frac{1}{n}\sum_{i=1}^{n}\mathbf{X}_i Y_i\right),$$

which exists if $\sum_{i=1}^{n}\mathbf{X}_i\mathbf{X}_i'$ is **positive definite** and thus invertible. We will return to this assumption below.

In a simple bivariate linear projection model $m(X_i) = \beta_0 + \beta_1 X_i$, we saw that the population slope was $\beta_1 = \text{cov}(Y_i, X_i)/\mathbb{V}[X_i]$. This approach means that the estimator

for the slope should be the ratio of the sample covariance of Y_i and X_i to the sample variance of X_i, or

$$\hat{\beta}_1 = \frac{\hat{\sigma}_{Y,X}}{\hat{\sigma}_X^2} = \frac{\frac{1}{n-1}\sum_{i=1}^n (Y_i - \overline{Y})(X_i - \overline{X})}{\frac{1}{n-1}\sum_{i=1}^n (X_i - \overline{X})^2}.$$

This plug-in approach is widely applicable and tends to have excellent properties in large samples under iid data. But the simplicity of the plug-in approach also hides some features of the estimator that become more apparent when deriving the estimator more explicitly using calculus. The second approach applies the plug-in principle not to the closed-form expression for the coefficients but to the optimization problem itself. We call this the **least squares** estimator because it minimizes the empirical (or sample) squared prediction error,

$$\widehat{\boldsymbol{\beta}} = \underset{\mathbf{b}\in\mathbb{R}^k}{\arg\min}\ \frac{1}{n}\sum_{i=1}^n \left(Y_i - \mathbf{X}_i'\mathbf{b}\right)^2 = \underset{\mathbf{b}\in\mathbb{R}^k}{\arg\min}\ SSR(\mathbf{b}),$$

where,

$$SSR(\mathbf{b}) = \sum_{i=1}^n \left(Y_i - \mathbf{X}_i'\mathbf{b}\right)^2$$

is the sum of the squared residuals. To distinguish it from other, more complicated least squares estimators, we call this the **ordinary least squares** estimator, or OLS.

Let's solve this minimization problem. We write down the first-order conditions as

$$0 = \frac{\partial SSR(\widehat{\boldsymbol{\beta}})}{\partial \boldsymbol{\beta}} = 2\left(\sum_{i=1}^n \mathbf{X}_i Y_i\right) - 2\left(\sum_{i=1}^n \mathbf{X}_i\mathbf{X}_i'\right)\widehat{\boldsymbol{\beta}}.$$

We can rearrange this system of equations to

$$\left(\sum_{i=1}^n \mathbf{X}_i\mathbf{X}_i'\right)\widehat{\boldsymbol{\beta}} = \left(\sum_{i=1}^n \mathbf{X}_i Y_i\right).$$

To obtain the solution for $\widehat{\boldsymbol{\beta}}$, notice that $\sum_{i=1}^n \mathbf{X}_i\mathbf{X}_i'$ is a $(k+1)\times(k+1)$ matrix and $\widehat{\boldsymbol{\beta}}$ and $\sum_{i=1}^n \mathbf{X}_i Y_i$ are both $k+1$ length column vectors. If $\sum_{i=1}^n \mathbf{X}_i\mathbf{X}_i'$ is invertible, then we can multiply both sides of this equation by that inverse to arrive at

$$\widehat{\boldsymbol{\beta}} = \left(\sum_{i=1}^n \mathbf{X}_i\mathbf{X}_i'\right)^{-1}\left(\sum_{i=1}^n \mathbf{X}_i Y_i\right),$$

which is the same expression as the plug-in estimator (after canceling the $1/n$ terms). To confirm that we have found a minimum, we also need to check the second-order condition,

$$\frac{\partial^2 SSR(\widehat{\boldsymbol{\beta}})}{\partial \boldsymbol{\beta} \boldsymbol{\beta}'} = 2\left(\sum_{i=1}^{n} \mathbf{X}_i \mathbf{X}_i'\right) > 0.$$

What does the matrix being "positive" mean? In matrix algebra, this condition means that the matrix $\sum_{i=1}^{n} \mathbf{X}_i \mathbf{X}_i'$ is **positive definite**, a condition that we discuss in Section 6.4.

Both the plug-in or least squares approaches yield the same estimator for the best linear predictor/population linear regression coefficients.

Theorem 6.1. *If the $\sum_{i=1}^{n} \mathbf{X}_i \mathbf{X}_i'$ is positive definite, then the ordinary least squares estimator is*

$$\widehat{\boldsymbol{\beta}} = \left(\sum_{i=1}^{n} \mathbf{X}_i \mathbf{X}_i'\right)^{-1} \left(\sum_{i=1}^{n} \mathbf{X}_i Y_i\right).$$

i Formula for the OLS slopes

Almost all regression will contain an intercept term, usually represented as a constant 1 in the covariate vector. It is also possible to obtain expressions for the OLS estimates of the intercept and variable coefficients separately. We can rewrite the best linear predictor decomposition as

$$Y_i = \alpha + \mathbf{X}_i' \boldsymbol{\beta} + \boldsymbol{\epsilon}_i.$$

Defined this way, we can write the OLS estimator for the "slopes" on $\mathbf{X}_i$ as the OLS estimator with all variables demeaned:

$$\widehat{\boldsymbol{\beta}} = \left(\frac{1}{n}\sum_{i=1}^{n} (\mathbf{X}_i - \overline{\mathbf{X}})(\mathbf{X}_i - \overline{\mathbf{X}})'\right) \left(\frac{1}{n}\sum_{i=1}^{n} (\mathbf{X}_i - \overline{\mathbf{X}})(Y_i - \overline{Y})\right)$$

which is the inverse of the sample covariance matrix of $\mathbf{X}_i$ times the sample covariance of $\mathbf{X}_i$ and Y_i. The intercept is

$$\hat{\alpha} = \overline{Y} - \overline{\mathbf{X}}' \widehat{\boldsymbol{\beta}}.$$

When dealing with actual data and not the population, we refer to the prediction errors $\hat{e}_i = Y_i - \mathbf{X}_i'\widehat{\boldsymbol{\beta}}$ as the **residuals**. The predicted value itself, $\widehat{Y}_i = \mathbf{X}_i'\widehat{\boldsymbol{\beta}}$, is also called the **fitted value**. With the population linear regression, we saw that the projection errors, $e_i = Y_i - \mathbf{X}_i'\boldsymbol{\beta}$, were mean zero and uncorrelated with the covariates $\mathbb{E}[\mathbf{X}_i e_i] = 0$. The residuals have a similar property with respect to the covariates in the sample:

$$\sum_{i=1}^{n} \mathbf{X}_i \hat{e}_i = 0.$$

The residuals are *exactly* uncorrelated with the covariates (when the covariates include a constant/intercept term), which is a mechanical artifact of the OLS estimator.

Figure 6.2 shows how OLS works in the bivariate case. It displays three possible regression lines as well as the sum of the squared residuals for each line. OLS aims to find the line that minimizes the function on the right.

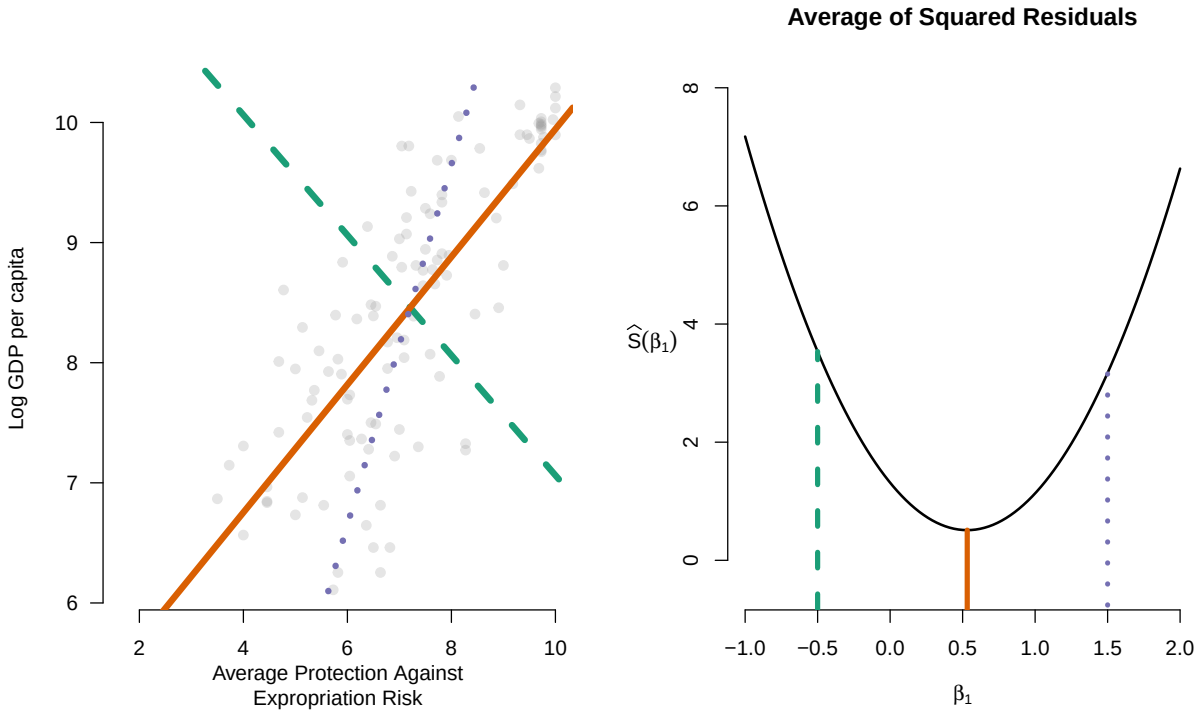


Figure 6.2: Different possible lines and their corresponding sum of squared residuals.

6.2 Model fit

We have learned how to use OLS to obtain an estimate of the best linear predictor, but an open question is whether that prediction is any good. Does using $\mathbf{X}_i$ help us predict Y_i? To investigate this, we consider two different prediction errors: (1) those using covariates and (2) those that do not.

We have already seen the prediction error when using the covariates; it is just the **sum of the squared residuals**,

$$SSR = \sum_{i=1}^{n} (Y_i - \mathbf{X}_i' \widehat{\boldsymbol{\beta}})^2.$$

Recall that the best predictor for Y_i without any covariates is simply its sample mean $\overline{Y}$. The prediction error without covariates is what we call the **total sum of squares**,

$$TSS = \sum_{i=1}^{n} (Y_i - \overline{Y})^2.$$

Figure 6.3 shows the difference between these two types of prediction errors.

We can use the **proportion reduction in prediction error** from adding those covariates to measure how much those covariates improve the regression's predictive ability. This value, called the **coefficient of determination** or R^2, is simply

$$R^2 = \frac{TSS - SSR}{TSS} = 1 - \frac{SSR}{TSS}.$$

The numerator, $TSS - SSR$, is the reduction in prediction error moving from $\overline{Y}$ to $\mathbf{X}_i' \widehat{\boldsymbol{\beta}}$ as the predictor. The denominator is the prediction error using $\overline{Y}$. Thus, the R^2 value is the fraction of the total prediction error eliminated by using $\mathbf{X}_i$ to predict Y_i. Another way to think about this value is that it measures how much less noisy the residuals are relative to the overall variation in Y. One thing to note is that OLS with covariates will *always* improve in-sample fit so that $TSS \geq SSR$ even if $\mathbf{X}_i$ is unrelated to Y_i. This phantom improvement occurs because the point of OLS is to minimize the SSR, and it will do that even if it is just chasing noise.

Since regression always improves in-sample fit, R^2 will fall between 0 and 1. A value 0 zero would indicate exactly 0 estimated coefficients on all covariates (except the intercept) so that Y_i and $\mathbf{X}_i$ are perfectly orthogonal in the data. (This is very unlikely to occur because there will likely be some minimal but nonzero relationship by random chance.) A value of 1 indicates a perfect linear fit, which occurs when all data points are perfectly predicted by the model with zero residuals.

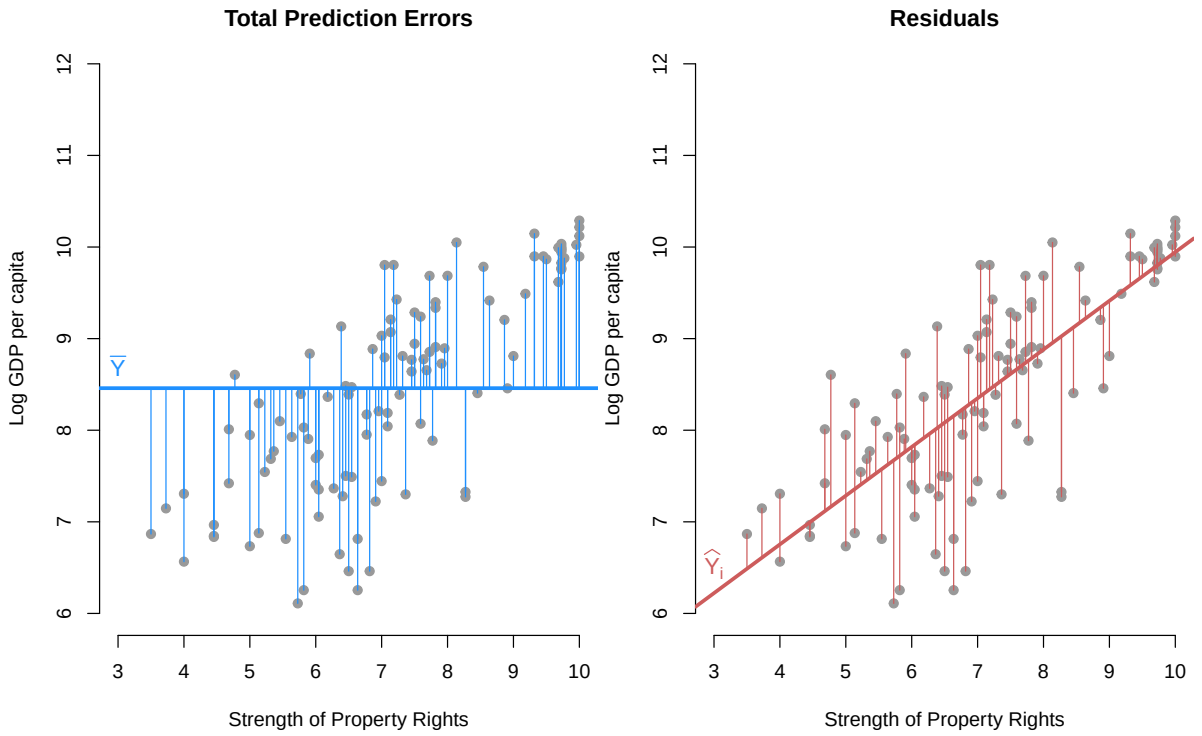


Figure 6.3: Total sum of squares vs. the sum of squared residuals.

6.3 Matrix form of OLS

We derived the OLS estimator above using simple algebra and calculus, but a more common representation of the estimator relies on vectors and matrices. We usually write the linear model for a generic unit, $Y_i = \mathbf{X}_i'\boldsymbol{\beta} + e_i$, but obviously, there are n of these equations,

$$\begin{aligned} Y_1 &= \mathbf{X}_1'\boldsymbol{\beta} + e_1 \\ Y_2 &= \mathbf{X}_2'\boldsymbol{\beta} + e_2 \\ &\vdots \\ Y_n &= \mathbf{X}_n'\boldsymbol{\beta} + e_n \end{aligned}$$

We can write this system of equations more compactly using matrix algebra. Combining the variables here into random vectors/matrices gives us:

$$\mathbf{Y} = \begin{pmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{pmatrix}, \quad \mathbb{X} = \begin{pmatrix} \mathbf{X}_1' \\ \mathbf{X}_2' \\ \vdots \\ \mathbf{X}_n' \end{pmatrix} = \begin{pmatrix} 1 & X_{11} & X_{12} & \cdots & X_{1k} \\ 1 & X_{21} & X_{22} & \cdots & X_{2k} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & X_{n1} & X_{n2} & \cdots & X_{nk} \end{pmatrix}, \quad \mathbf{e} = \begin{pmatrix} e_1 \\ e_2 \\ \vdots \\ e_n \end{pmatrix}$$

We can write the above system of equations as

$$\mathbf{Y} = \mathbb{X}\boldsymbol{\beta} + \mathbf{e},$$

Note that $\mathbb{X}$ is an $n \times (k+1)$ matrix and $\boldsymbol{\beta}$ is a $k+1$ length column vector.

Representing sums in matrix form is the critical link between the definition of OLS and matrix notation. In particular, we have

$$\sum_{i=1}^{n} \mathbf{X}_i \mathbf{X}_i' = \mathbb{X}'\mathbb{X}$$
$$\sum_{i=1}^{n} \mathbf{X}_i Y_i = \mathbb{X}'\mathbf{Y},$$

which means we can write the OLS estimator in the more recognizable form as

$$\widehat{\boldsymbol{\beta}} = \left(\mathbb{X}'\mathbb{X}\right)^{-1} \mathbb{X}'\mathbf{Y}.$$

We can of course also define the vector of residuals,

$$\hat{\mathbf{e}} = \mathbf{Y} - \mathbb{X}\widehat{\boldsymbol{\beta}} = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix} - \begin{bmatrix} 1\hat{\beta}_0 + X_{11}\hat{\beta}_1 + X_{12}\hat{\beta}_2 + \cdots + X_{1k}\hat{\beta}_k \\ 1\hat{\beta}_0 + X_{21}\hat{\beta}_1 + X_{22}\hat{\beta}_2 + \cdots + X_{2k}\hat{\beta}_k \\ \vdots \\ 1\hat{\beta}_0 + X_{n1}\hat{\beta}_1 + X_{n2}\hat{\beta}_2 + \cdots + X_{nk}\hat{\beta}_k \end{bmatrix},$$

and so the sum of the squared residuals in this case becomes

$$SSR(\boldsymbol{\beta}) = \|\mathbf{Y} - \mathbb{X}\boldsymbol{\beta}\|^2 = (\mathbf{Y} - \mathbb{X}\boldsymbol{\beta})'(\mathbf{Y} - \mathbb{X}\boldsymbol{\beta}),$$

where the double vertical lines are the Euclidean norm of the argument, $\|\mathbf{z}\| = \sqrt{\sum_{i=1}^{n} z_i^2}$. The OLS minimization problem, then, is

$$\widehat{\boldsymbol{\beta}} = \underset{\mathbf{b} \in \mathbb{R}^{(k+1)}}{\arg\min} \ \|\mathbf{Y} - \mathbb{X}\mathbf{b}\|^2$$

Finally, we can write the lack of correlation of the covariates and the residuals as

$$\mathbb{X}'\hat{\mathbf{e}} = \sum_{i=1}^{n} \mathbf{X}_i \hat{e}_i = 0,$$

which also implies these vectors are **orthogonal**.

6.4 Rank, linear independence, and multicollinearity

We noted that the OLS estimator exists when $\sum_{i=1}^{n} \mathbf{X}_i \mathbf{X}_i'$ is positive definite or that there is "no multicollinearity." This assumption is equivalent to saying that the matrix $\mathbb{X}$ is full column rank, meaning that rank$(\mathbb{X}) = (k+1)$, where $k+1$ is the number of columns of $\mathbb{X}$. Recall from matrix algebra that the column rank is the number of linearly independent columns in the matrix, and **linear independence** means that $\mathbb{X}\mathbf{b} = 0$ if and only if $\mathbf{b}$ is a column vector of 0s. In other words, we have

$$b_1\mathbb{X}_1 + b_2\mathbb{X}_2 + \cdots + b_{k+1}\mathbb{X}_{k+1} = 0 \quad \iff \quad b_1 = b_2 = \cdots = b_{k+1} = 0,$$

where $\mathbb{X}_j$ is the jth column of $\mathbb{X}$. Thus, full column rank says that all the columns are linearly independent or that there is no "multicollinearity."

Could this be violated? Suppose we accidentally included a linear function of one variable so that $\mathbb{X}_2 = 2\mathbb{X}_1$. We then have

$$\begin{aligned}\mathbb{X}\mathbf{b} &= b_1\mathbb{X}_1 + b_2 2\mathbb{X}_1 + b_3\mathbb{X}_3 + \cdots + b_{k+1}\mathbb{X}_{k+1} \\ &= (b_1 + 2b_2)\mathbb{X}_1 + b_3\mathbb{X}_3 + \cdots + b_{k+1}\mathbb{X}_{k+1}\end{aligned}$$

In this case, this expression equals 0 when $b_3 = b_4 = \cdots = b_{k+1} = 0$ and $b_1 = -2b_2$. Thus, the collection of columns is linearly dependent, so we know that the rank of $\mathbb{X}$ must be less than full column rank (that is, less than $k+1$). Hopefully it is also clear that if we removed the problematic column $\mathbb{X}_2$, the resulting matrix would have k linearly independent columns, implying that $\mathbb{X}$ is rank k.

Why does this rank condition matter for the OLS estimator? In short, linear independence of the columns of $\mathbb{X}$ ensures that the inverse $(\mathbb{X}'\mathbb{X})^{-1}$ exists and so does $\widehat{\boldsymbol{\beta}}$. This is because $\mathbb{X}$ is of full column rank if and only if $\mathbb{X}'\mathbb{X}$ is non-singular and a matrix is invertible if and only if it is non-singular. This full rank condition further implies that $\mathbb{X}'\mathbb{X} = \sum_{i=1}^{n} \mathbf{X}_i \mathbf{X}_i'$ is positive definite, implying that the estimator is truly finding the minimal sum of squared residuals.

What are common situations that lead to violations of no multicollinearity? We have seen one above, with one variable being a linear function of another. But this problem can come out in more subtle ways. Suppose we have a set of dummy variables corresponding to a single categorical variable, like the region of the world. This might mean we have $X_{i1} = 1$ for units in Asia (0 otherwise), $X_{i2} = 1$ for units in Europe (0 otherwise), $X_{i3} =$

1 for units in Africa (0 otherwise), and $X_{i4} = 1$ for units in the Americas (0 otherwise), and $X_{i5} = 1$ for countries in Oceania (0 otherwise). Each unit has to be in exactly one of these five regions, so there is a linear dependence between these variables,

$$X_{i5} = 1 - X_{i1} - X_{i2} - X_{i3} - X_{i4}.$$

That is, if a unit is not in Asia, Europe, Africa, or the Americas, we know it is in Oceania. We would get a linear dependence by including all of these variables in our regression with an intercept. (Note the 1 in the relationship between X_{i5} and the other variables, the reason why there will be linear dependence when including a constant.) Thus, we usually omit one dummy variable from each categorical variable. In that case, the coefficients on the remaining dummies are differences in means between that category and the omitted one (perhaps conditional on other variables included, if included). So if we omitted X_{i5} (Oceania), then the coefficient on X_{i1} would be the difference in mean outcomes between units in Asia and Oceania.

Collinearity can also occur when including both an intercept term and a variable that does not vary. This issue can often happen if we mistakenly subset our data, for example in this case if we subsetted the data to only the Asian units but still included the Asian dummy variable in the regression.

Finally, note that most statistical software packages will "solve" the multicollinearity by arbitrarily removing as many linearly dependent covariates as is necessary to achieve full rank. R will show the estimated coefficients as `NA` in those cases.

6.5 OLS coefficients for binary and categorical regressors

Suppose that the covariates include just the intercept and a single binary variable, $\mathbf{X}_i = (1 \;\; X_i)'$, where $X_i \in \{0, 1\}$. In other words, the right-hand side contains only one covariate, an indicator variable. In this case, the OLS coefficient on X_i, $\widehat{\beta_1}$, is exactly equal to the difference in sample means of Y_i in the $X_i = 1$ group and the $X_i = 0$ group:

$$\hat{\beta}_1 = \frac{\sum_{i=1}^n X_i Y_i}{\sum_{i=1}^n X_i} - \frac{\sum_{i=1}^n (1 - X_i) Y_i}{\sum_{i=1}^n 1 - X_i} = \overline{Y}_{X=1} - \overline{Y}_{X=0}$$

This very useful result is not an approximation: it holds exactly for any sample size.

We can generalize this idea to discrete variables more broadly. Suppose we have our region variables from the last section and include in our covariates a constant and the dummies for Asia, Europe, Africa, and the Americas (with Oceania again being the omitted variable/category). Then the coefficient on the West dummy will be

$$\hat{\beta}_{\text{Asia}} = \overline{Y}_{\text{Asia}} - \overline{Y}_{\text{Oceania}},$$

which is exactly the difference in sample means of Y_i between Asian units and units in Oceania.

Note that these interpretations only hold when the regression consists solely of the binary variable or the set of categorical dummy variables. These exact relationships fail when other covariates are added to the model.

6.6 Projection and geometry of least squares

OLS has a very nice geometric interpretation that adds a lot of intuition for various aspects of the method. In this geometric approach, we view $\mathbf{Y}$ as an n-dimensional vector in $\mathbb{R}^n$. As we saw above, OLS in matrix form is about finding a linear combination of the covariate matrix $\mathbb{X}$ closest to this vector in terms of the Euclidean distance, which is just the sum of squares.

Let $\mathcal{C}(\mathbb{X}) = \{\mathbb{X}\mathbf{b} : \mathbf{b} \in \mathbb{R}^(k+1)\}$ be the **column space** of the matrix $\mathbb{X}$. This set is all linear combinations of the columns of $\mathbb{X}$ or the set of all possible linear predictions we could obtain from $\mathbb{X}$. Note that the OLS fitted values, $\mathbb{X}\widehat{\boldsymbol{\beta}}$, are in this column space. If, as we assume, $\mathbb{X}$ has full column rank of $k+1$, then the column space $\mathcal{C}(\mathbb{X})$ will be a $k+1$-dimensional surface inside of the larger n-dimensional space. If $\mathbb{X}$ has two columns, the column space will be a plane.

Another interpretation of the OLS estimator is that it finds the linear predictor as the closest point in the column space of $\mathbb{X}$ to the outcome vector $\mathbf{Y}$. This is called the **projection** of $\mathbf{Y}$ onto $\mathcal{C}(\mathbb{X})$. Figure 6.4 shows this projection for a case with $n = 3$ and 2 columns in $\mathbb{X}$. The shaded blue region represents the plane of the column space of $\mathbb{X}$, and $\mathbb{X}\widehat{\boldsymbol{\beta}}$ is the closest point to $\mathbf{Y}$ in that space. This illustrates the whole idea of the OLS estimator: find the linear combination of the columns of $\mathbb{X}$ (a point in the column space) that minimizes the Euclidean distance between that point and the outcome vector (the sum of squared residuals).

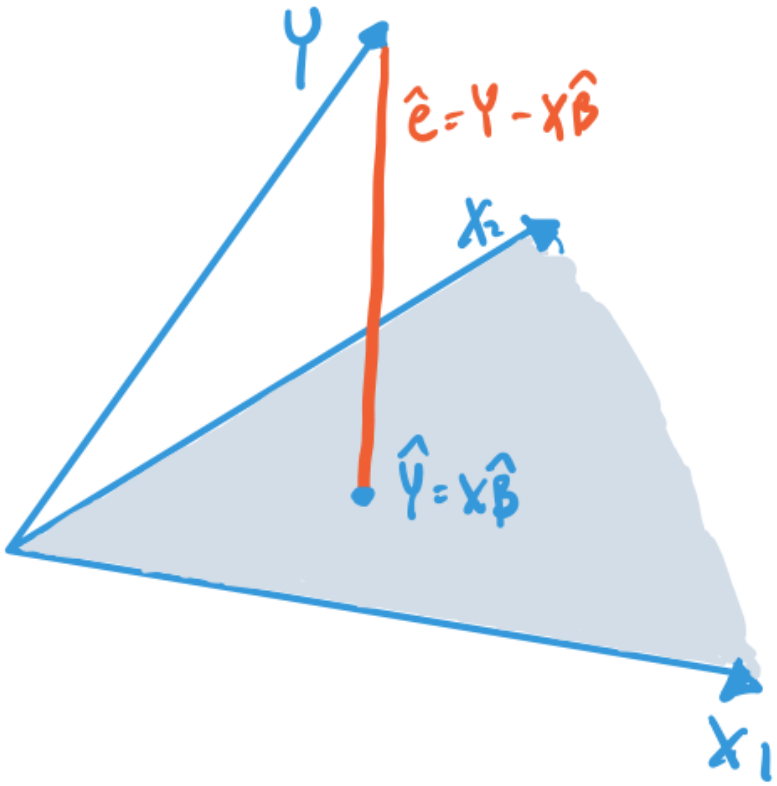


Figure 6.4: Projection of Y on the column space of the covariates.

This figure shows that the residual vector, which is the difference between the $\mathbf{Y}$ vector and the projection $\mathbb{X}\widehat{\boldsymbol{\beta}}$, is perpendicular or orthogonal to the column space of $\mathbb{X}$. This orthogonality is a consequence of the residuals being orthogonal to all the columns of $\mathbb{X}$,

$$\mathbb{X}'\mathbf{e} = 0,$$

as we established above. Being orthogonal to all the columns means it will also be orthogonal to all linear combinations of the columns.

6.7 Projection and annihilator matrices

With the idea of projection to the column space of $\mathbb{X}$ established, we can define a way to project any vector into that space. The $n \times n$ **projection matrix,**

$$\mathbf{P}_{\mathbb{X}} = \mathbb{X}(\mathbb{X}'\mathbb{X})^{-1}\mathbb{X}',$$

projects a vector into $\mathcal{C}(\mathbb{X})$. In particular, we can see that this gives us the fitted values for $\mathbf{Y}$:

$$\mathbf{P}_{\mathbb{X}}\mathbf{Y} = \mathbb{X}(\mathbb{X}'\mathbb{X})^{-1}\mathbb{X}'\mathbf{Y} = \mathbb{X}\widehat{\boldsymbol{\beta}}.$$

Because we sometimes write the linear predictor as $\widehat{\mathbf{Y}} = \mathbb{X}\widehat{\boldsymbol{\beta}}$, the projection matrix is also called the **hat matrix**. With either name, multiplying a vector by $\mathbf{P}_{\mathbb{X}}$ gives the best linear predictor of that vector as a function of $\mathbb{X}$. Intuitively, any vector that is already a linear combination of the columns of $\mathbb{X}$ (so is in $\mathcal{C}(\mathbb{X})$) should be unaffected by this projection: the closest point in $\mathcal{C}(\mathbb{X})$ to a point already in $\mathcal{C}(\mathbb{X})$ is itself. We can also see this algebraically for any linear combination $\mathbb{X}\mathbf{c}$,

$$\mathbf{P}_{\mathbb{X}}\mathbb{X}\mathbf{c} = \mathbb{X}(\mathbb{X}'\mathbb{X})^{-1}\mathbb{X}'\mathbb{X}\mathbf{c} = \mathbb{X}\mathbf{c},$$

because $(\mathbb{X}'\mathbb{X})^{-1}\mathbb{X}'\mathbb{X}$ simplifies to the identity matrix. In particular, the projection of $\mathbb{X}$ onto itself is just itself: $\mathbf{P}_{\mathbb{X}}\mathbb{X} = \mathbb{X}$.

The second matrix related to projection is the **annihilator matrix**,

$$\mathbf{M}_{\mathbb{X}} = \mathbf{I}_n - \mathbf{P}_{\mathbb{X}},$$

which projects any vector into the orthogonal complement to the column space of $\mathbb{X}$,

$$\mathcal{C}^{\perp}(\mathbb{X}) = \{\mathbf{c} \in \mathbb{R}^n \ : \ \mathbb{X}\mathbf{c} = 0\}.$$

This matrix is called the annihilator matrix because applying it to any linear combination of $\mathbb{X}$, gives us 0:

$$\mathbf{M}_{\mathbb{X}}\mathbb{X}\mathbf{c} = \mathbb{X}\mathbf{c} - \mathbf{P}_{\mathbb{X}}\mathbb{X}\mathbf{c} = \mathbb{X}\mathbf{c} - \mathbb{X}\mathbf{c} = 0.$$

Note that $\mathbf{M}_{\mathbb{X}}\mathbb{X} = 0$. Why should we care about this matrix? Perhaps a more evocative name might be the **residual maker** since it makes residuals when applied to $\mathbf{Y}$,

$$\mathbf{M}_{\mathbb{X}}\mathbf{Y} = (\mathbf{I}_n - \mathbf{P}_{\mathbb{X}})\mathbf{Y} = \mathbf{Y} - \mathbf{P}_{\mathbb{X}}\mathbf{Y} = \mathbf{Y} - \mathbb{X}\widehat{\boldsymbol{\beta}} = \hat{\mathbf{e}}.$$

The projection matrix has several useful properties:

- $\mathbf{P}_{\mathbb{X}}$ and $\mathbf{M}_{\mathbb{X}}$ are **idempotent**, which means that when applied to itself, it simply returns itself: $\mathbf{P}_{\mathbb{X}}\mathbf{P}_{\mathbb{X}} = \mathbf{P}_{\mathbb{X}}$ and $\mathbf{M}_{\mathbb{X}}\mathbf{M}_{\mathbb{X}} = \mathbf{M}_{\mathbb{X}}$.
- $\mathbf{P}_{\mathbb{X}}$ and $\mathbf{M}_{\mathbb{X}}$ are symmetric $n \times n$ matrices so that $\mathbf{P}'_{\mathbb{X}} = \mathbf{P}_{\mathbb{X}}$ and $\mathbf{M}'_{\mathbb{X}} = \mathbf{M}_{\mathbb{X}}$.
- The rank of $\mathbf{P}_{\mathbb{X}}$ is $k+1$ (the number of columns of $\mathbb{X}$) and the rank of $\mathbf{M}_{\mathbb{X}}$ is $n-k-1$.

We can use the projection and annihilator matrices to arrive at an orthogonal decomposition of the outcome vector:

$$\mathbf{Y} = \mathbb{X}\widehat{\boldsymbol{\beta}} + \hat{\mathbf{e}} = \mathbf{P}_{\mathbb{X}}\mathbf{Y} + \mathbf{M}_{\mathbb{X}}\mathbf{Y}.$$

6.8 Residual regression

There are many situations where we can partition the covariates into two groups, and we might wonder if it is possible to express or calculate the OLS coefficients for just one set of covariates. In particular, let the columns of $\mathbb{X}$ be partitioned into $[\mathbb{X}_1 \mathbb{X}_2]$, so that the linear prediction we are estimating is

$$\mathbf{Y} = \mathbb{X}_1\boldsymbol{\beta}_1 + \mathbb{X}_2\boldsymbol{\beta}_2 + \mathbf{e},$$

with estimated coefficients and residuals

$$\mathbf{Y} = \mathbb{X}_1\widehat{\boldsymbol{\beta}}_1 + \mathbb{X}_2\widehat{\boldsymbol{\beta}}_2 + \hat{\mathbf{e}}.$$

We now document another way to obtain the estimator $\widehat{\boldsymbol{\beta}}_1$ from this regression using a technique called **residual regression**, **partitioned regression**, or the **Frisch-Waugh-Lovell theorem**.

Residual regression approach

The residual regression approach is:

1. Use OLS to regress $\mathbf{Y}$ on $\mathbb{X}_2$ and obtain residuals $\tilde{\mathbf{e}}_2$.
2. Use OLS to regress each column of $\mathbb{X}_1$ on $\mathbb{X}_2$ and obtain residuals $\widetilde{\mathbb{X}}_1$.
3. Use OLS to regress $\tilde{\mathbf{e}}_2$ on $\widetilde{\mathbb{X}}_1$.

Theorem 6.2 (Frisch-Waugh-Lovell)**.** *The OLS coefficients from a regression of* $\tilde{\mathbf{e}}_2$ *on* $\widetilde{\mathbb{X}}_1$ *are equivalent to the coefficients on* $\mathbb{X}_1$ *from the regression of* $\mathbf{Y}$ *on both* $\mathbb{X}_1$ *and* $\mathbb{X}_2$*.*

An implication of this theorem is that the regression coefficient for a given variable captures the relationship between the residual variation in the outcome and that variable after accounting for the other covariates. In particular, this coefficient focuses on the variation orthogonal to those other covariates.

While perhaps unexpected, this result may not appear particularly useful. We can just run the long regression, right? But this trick can be very handy when $\mathbb{X}_2$ consists of dummy variables (or "fixed effects") for a categorical variable with many categories. For example, suppose $\mathbb{X}_2$ consists of indicators for the county of residence for a respondent. In that case, that will have over 3,000 columns, meaning that direct calculation of the $\widehat{\boldsymbol{\beta}} = (\widehat{\boldsymbol{\beta}}_1, \widehat{\boldsymbol{\beta}}_2)$ will require inverting a matrix that is bigger than $3,000 \times 3,000$. Computationally, this process will be very slow. But above, we saw that predictions of an outcome on a categorical variable are just the sample mean within each level of the variable. Thus, in this case, the residuals $\tilde{\mathbf{e}}_2$ and $\mathbb{X}_1$ can be computed by demeaning the outcome and $\mathbb{X}_1$ within levels of the dummies in $\mathbb{X}_2$, which can be considerably faster computationally.

Finally, using residual regression allows researchers to visualize the conditional relationships between the outcome and a single independent variable after adjusting for other covariates. In particular, one can check the relationship using this approach with a scatterplot of $\tilde{\mathbf{e}}_2$ on $\mathbb{X}_1$ (when it is a single column). This residualized scatterplot allows researchers to check if this conditional relationship appears linear or should be modeled in another way.

6.9 Outliers, leverage points, and influential observations

Given that OLS finds the coefficients that minimize the sum of the squared residuals, asking how much impact each residual has on that solution is very helpful. Let $\widehat{\boldsymbol{\beta}}_{(-i)}$ be the OLS estimates if we omit unit i. Intuitively, **influential observations** should significantly impact the estimated coefficients so that $\widehat{\boldsymbol{\beta}}_{(-i)} - \widehat{\boldsymbol{\beta}}$ is large in absolute value.

Under what conditions do we have influential observations? OLS tries to minimize the sum of **squared** residuals, so it will move more in order to shrink larger residuals versus

smaller ones. Where are large residuals likely to occur? Well, notice that any OLS regression line with a constant will exactly pass through the means of the outcome and the covariates: $\overline{Y} = \overline{\mathbf{X}}\widehat{\boldsymbol{\beta}}$. Thus, by definition, this means that, when an observation is close to the average of the covariates, $\overline{\mathbf{X}}$, it cannot have that much influence because OLS forces the regression line to go through $\overline{Y}$. Thus, influential points will have two properties:

1. Have high **leverage**, where leverage roughly measures how far $\mathbf{X}_i$ is from $\overline{\mathbf{X}}$, and
2. Be an **outlier** in the sense of having a large residual (if left out of the regression).

We'll take each of these in turn.

6.9.1 Leverage points

We can define the **leverage** of an observation by

$$h_{ii} = \mathbf{X}_i' \left(\mathbb{X}'\mathbb{X}\right)^{-1} \mathbf{X}_i,$$

which is the ith diagonal entry of the projection matrix, $\mathbf{P}_{\mathbb{X}}$. Notice that

$$\widehat{\mathbf{Y}} = \mathbf{P}_{\mathbb{X}}\mathbf{Y} \qquad \Longrightarrow \qquad \widehat{Y}_i = \sum_{j=1}^{n} h_{ij} Y_j,$$

so that h_{ij} is the importance of observation j for the fitted value for observation i. The leverage, then, is the importance of the observation for its own fitted value. We can also interpret these values in terms of the distribution of $\mathbf{X}_i$. Roughly speaking, these values are the weighted distance between $\mathbf{X}_i$ and $\overline{\mathbf{X}}$, where the weights normalize to the empirical variance/covariance structure of the covariates (so that the scale of each covariate is roughly the same). We can see this most clearly when we fit a simple linear regression (with one covariate and an intercept) with OLS when the leverage is

$$h_{ii} = \frac{1}{n} + \frac{(X_i - \overline{X})^2}{\sum_{j=1}^{n}(X_j - \overline{X})^2}$$

Leverage values have three key properties:

1. $0 \leq h_{ii} \leq 1$
2. $h_{ii} \geq 1/n$ if the model contains an intercept
3. $\sum_{i=1}^{n} h_{ii} = k + 1$

6.9.2 Outliers and leave-one-out regression

In the context of OLS, an **outlier** is an observation with a large prediction error for a particular OLS specification. Figure 6.5 shows an example of an outlier.

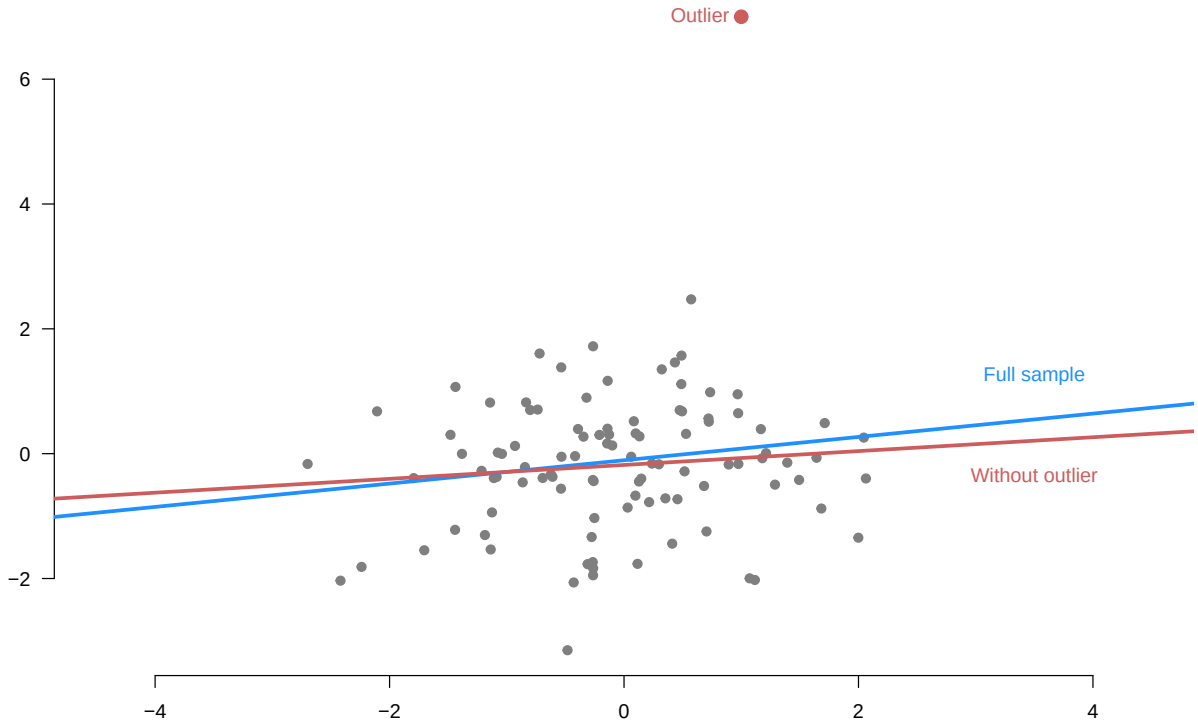


Figure 6.5: An example of an outlier.

Intuitively, it seems as though we could use the residual $\widehat{e}_i$ to assess the prediction error for a given unit. But the residuals are not valid predictions because the OLS estimator is designed to make those as small as possible (in machine learning parlance, these were in the training set). In particular, if an outlier is influential, we already noted that it might "pull" the regression line toward it, and the resulting residual might be pretty small.

To assess prediction errors more cleanly, we can use **leave-one-out regression** (LOO), which regresses $\mathbf{Y}_{(-i)}$ on $\mathbb{X}_{(-i)}$, where these omit unit i:

$$\widehat{\boldsymbol{\beta}}_{(-i)} = \left(\mathbb{X}'_{(-i)}\mathbb{X}_{(-i)}\right)^{-1}\mathbb{X}_{(-i)}\mathbf{Y}_{(-i)}.$$

We can then calculate LOO prediction errors as

$$\tilde{e}_i = Y_i - \mathbf{X}_i' \widehat{\boldsymbol{\beta}}_{(-i)}.$$

Calculating these LOO prediction errors for each unit appears to be computationally costly because it seems as though we have to fit OLS n times. Fortunately, there is a closed-form expression for the LOO coefficients and prediction errors in terms of the original regression,

$$\widehat{\boldsymbol{\beta}}_{(-i)} = \widehat{\boldsymbol{\beta}} - \left(\mathbb{X}'\mathbb{X}\right)^{-1} \mathbf{X}_i \tilde{e}_i \qquad \tilde{e}_i = \frac{\hat{e}_i}{1 - h_{ii}}. \tag{6.1}$$

This shows that the LOO prediction errors will differ from the residuals when the leverage of a unit is high. This makes sense! We said earlier that observations with low leverage would be close to $\overline{\mathbf{X}}$, where the outcome values have relatively little impact on the OLS fit (because the regression line must go through $\overline{Y}$).

6.9.3 Influential observations

An influential observation (also sometimes called an influential point) is a unit that has the power to change the coefficients and fitted values for a particular OLS specification. Figure 6.6 shows an example of such an influence point.

One measure of influence, called DFBETA$_i$, measures how much i changes the estimated coefficient vector

$$\widehat{\boldsymbol{\beta}} - \widehat{\boldsymbol{\beta}}_{(-i)} = \left(\mathbb{X}'\mathbb{X}\right)^{-1} \mathbf{X}_i \tilde{e}_i,$$

so there is one value for each observation-covariate pair. When divided by the standard error of the estimated coefficients, this is called DFBETA**S** (where the "S" is for standardized). These are helpful if we focus on a particular coefficient.

When we want to summarize how much an observation matters for the fit, we can use a compact measure of the influence of an observation by comparing the fitted value from the entire sample to the fitted value from the leave-one-out regression. Using the DFBETA above, we have

$$\widehat{Y}_i - \mathbf{X}_i \widehat{\boldsymbol{\beta}}_{(-1)} = \mathbf{X}_i'(\widehat{\boldsymbol{\beta}} - \widehat{\boldsymbol{\beta}}_{(-1)}) = \mathbf{X}_i' \left(\mathbb{X}'\mathbb{X}\right)^{-1} \mathbf{X}_i \tilde{e}_i = h_{ii} \tilde{e}_i,$$

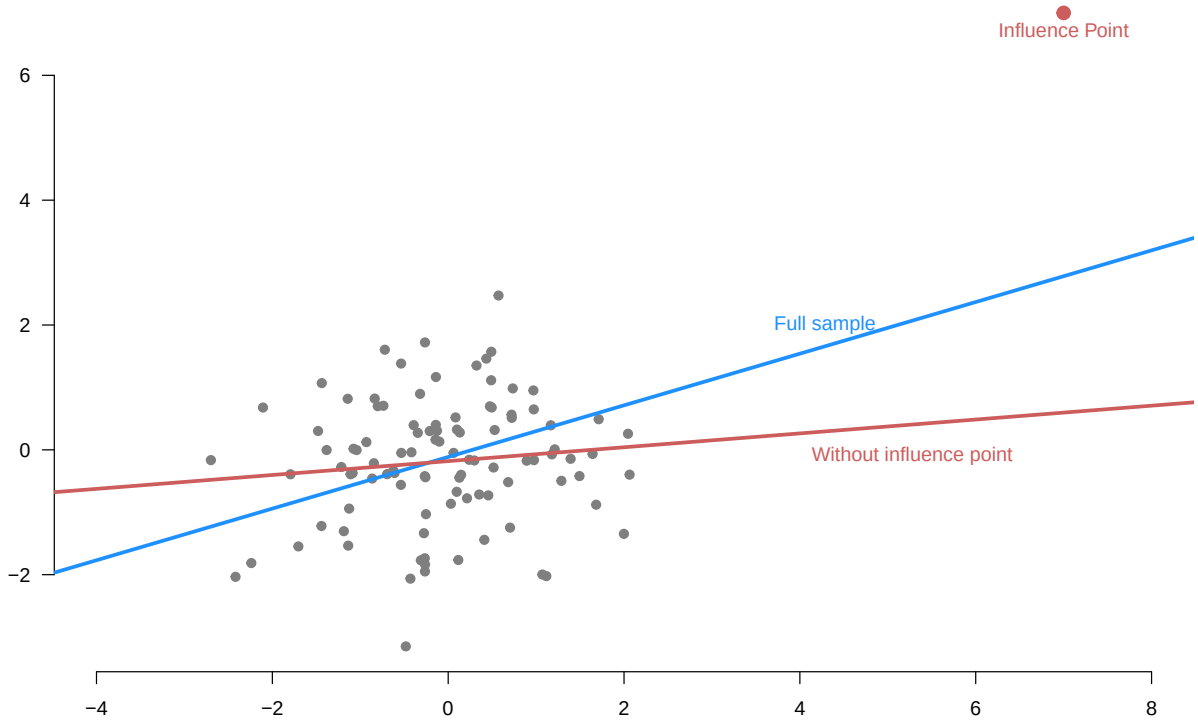


Figure 6.6: An example of an influence point.

so the influence of an observation is its leverage multiplied by how much of an outlier it is. This value is sometimes called DFFIT (difference in fit). One transformation of this quantity, **Cook's distance**, standardizes this by the sum of the squared residuals:

$$D_i = \frac{n-k-1}{k+1} \frac{h_{ii}\tilde{e}_i^2}{\hat{\mathbf{e}}'\hat{\mathbf{e}}}.$$

Different cutoffs exist for identifying "influential" observations, but they tend to be ad hoc. In any case, the more important question is "how much does this observation matter for my substantive interpretation" rather than the narrow question of a particular threshold.

It's all well and good to find influential observations, but what should be done about them? The first thing to check is that the data is not corrupted somehow. Influence points sometimes occur because of a coding or data entry error. We may consider removing the observation if the error appears in the data acquired from another source but exercise transparency if this appears to be the case. Another approach is to consider a transformation of the dependent or independent variables, like taking the natural logarithm, that might

dampen the effects of outliers. Finally, consider using methods that are robust to outliers such as least absolute deviations or least trimmed squares.

6.10 Summary

In this chapter, we introduced the **ordinary least squares** estimator, which finds the linear function of the $\mathbf{X}_i$ that minimizes the sum of the squared residuals and is the sample version of the best linear predictor in the last chapter. The R^2 statistic assesses the in-sample **model fit** of OLS by comparing how much better it predicts the outcome compared to a simple baseline predictor of the sample mean of the outcome. OLS can also be written in a very compact manner using matrix algebra, which allows us to understand the geometry of OLS as a **projection** of the outcome into space of linear functions of the independent variables. The **Frisch-Waugh-Lovell theorem** describes a residual regression approach to obtaining OLS estimates for subsets of coefficients, which can be helpful for computational efficiency or data visualization. Lastly, influential observations are those that alter the estimated coefficients when they are omitted from the OLS estimation, and there are several metrics that help to assess this. In the next chapter, we move from the mechanical properties to the statistical properties of OLS: unbiasedness, consistency, and asymptotic normality.

7 The statistics of least squares

The last chapter showcased the least squares estimator and investigated many of its more mechanical properties, which are essential for the practical application of OLS. But we still need to understand its statistical properties, as we discussed in Part I of this book: unbiasedness, sampling variance, consistency, and asymptotic normality. As we saw then, these properties fall into finite-sample (unbiasedness, sampling variance) and asymptotic (consistency, asymptotic normality).

In this chapter, we will focus on the asymptotic properties of OLS because those properties hold under the relatively mild conditions of the linear projection model introduced in Section 5.2. We will see that OLS consistently estimates a coherent quantity of interest (the best linear predictor) regardless of whether the conditional expectation is linear. That is, for the asymptotic properties of the estimator, we will not need the commonly invoked linearity assumption. Later, when we investigate the finite-sample properties, we will show how linearity will help us establish unbiasedness and also how the normality of the errors can allow us to conduct exact, finite-sample inference. But these assumptions are very strong, so understanding what we can say about OLS without them is vital.

7.1 Large-sample properties of OLS

As we saw in Chapter 3, we need two key ingredients to conduct statistical inference with the OLS estimator: (1) a consistent estimate of the variance of $\widehat{\boldsymbol{\beta}}$ and (2) the approximate distribution of $\widehat{\boldsymbol{\beta}}$ in large samples. Remember that, since $\widehat{\boldsymbol{\beta}}$ is a vector, the variance of that estimator will actually be a variance-covariance matrix. To obtain the two key ingredients, we first establish the consistency of OLS and then use the central limit theorem to derive its asymptotic distribution, which includes its variance.

We begin by setting out the assumptions needed for establishing the large-sample properties of OLS, which are the same as the assumptions needed to ensure that the best linear predictor, $\widehat{\boldsymbol{\beta}} = \mathbb{E}[\mathbf{X}_i\mathbf{X}_i']^{-1}\mathbb{E}[\mathbf{X}_i Y_i]$, is well-defined and unique.

Linear projection assumptions

The linear projection model makes the following assumptions:

1. $\{(Y_i, \mathbf{X}_i)\}_{i=1}^n$ are iid random vectors
2. $\mathbb{E}[Y_i^2] < \infty$ (finite outcome variance)
3. $\mathbb{E}[\|\mathbf{X}_i\|^2] < \infty$ (finite variances and covariances of covariates)
4. $\mathbb{E}[\mathbf{X}_i\mathbf{X}_i']$ is positive definite (no linear dependence in the covariates)

Recall that these are mild conditions on the joint distribution of $(Y_i, \mathbf{X}_i)$ and in particular, we are **not** assuming linearity of the CEF, $\mathbb{E}[Y_i \mid \mathbf{X}_i]$, nor are we assuming any specific distribution for the data.

We can helpfully decompose the OLS estimator into the actual BLP coefficient plus estimation error as

$$\widehat{\boldsymbol{\beta}} = \left(\frac{1}{n}\sum_{i=1}^n \mathbf{X}_i\mathbf{X}_i'\right)^{-1}\left(\frac{1}{n}\sum_{i=1}^n \mathbf{X}_i Y_i\right) = \boldsymbol{\beta} + \underbrace{\left(\frac{1}{n}\sum_{i=1}^n \mathbf{X}_i\mathbf{X}_i'\right)^{-1}\left(\frac{1}{n}\sum_{i=1}^n \mathbf{X}_i e_i\right)}_{\text{estimation error}}.$$

This decomposition will help us quickly establish the consistency of $\widehat{\boldsymbol{\beta}}$. By the law of large numbers, we know that sample means will converge in probability to population expectations, so we have

$$\frac{1}{n}\sum_{i=1}^n \mathbf{X}_i\mathbf{X}_i' \xrightarrow{p} \mathbb{E}[\mathbf{X}_i\mathbf{X}_i'] \equiv \mathbf{Q}_{\mathbf{XX}} \qquad \frac{1}{n}\sum_{i=1}^n \mathbf{X}_i e_i \xrightarrow{p} \mathbb{E}[\mathbf{X}_i e_i] = \mathbf{0},$$

which implies by the continuous mapping theorem (the inverse is a continuous function) that

$$\widehat{\boldsymbol{\beta}} \xrightarrow{p} \boldsymbol{\beta} + \mathbf{Q}_{\mathbf{XX}}^{-1}\mathbb{E}[\mathbf{X}_i e_i] = \boldsymbol{\beta},$$

The linear projection assumptions ensure that the LLN applies to these sample means and that $\mathbb{E}[\mathbf{X}_i\mathbf{X}_i']$ is invertible.

Theorem 7.1. *Under the above linear projection assumptions, the OLS estimator is consistent for the best linear projection coefficients, $\widehat{\boldsymbol{\beta}} \xrightarrow{p} \boldsymbol{\beta}$.*

Thus, OLS should be close to the population linear regression in large samples under relatively mild conditions. Remember that this may not equal the conditional expectation if the CEF is nonlinear. What we can say is that OLS converges to the best *linear* approximation to the CEF. Of course, this also means that, if the CEF is linear, then OLS will consistently estimate the coefficients of the CEF.

To emphasize, the only assumptions made about the dependent variable are that it (1) has finite variance and (2) is iid. Under this assumption, the outcome could be continuous, categorical, binary, or event count.

Next, we would like to establish an asymptotic normality result for the OLS coefficients. We first review some key ideas about the Central Limit Theorem.

CLT reminder

Suppose that we have a function of the data iid random vectors $\mathbf{X}_1, \ldots, \mathbf{X}_n$, $g(\mathbf{X}_i)$ where $\mathbb{E}[g(\mathbf{X}_i)] = 0$ and so $\mathbb{V}[g(\mathbf{X}_i)] = \mathbb{E}[g(\mathbf{X}_i)g(\mathbf{X}_i)']$. Then if $\mathbb{E}[\|g(\mathbf{X}_i)\|^2] < \infty$, the CLT implies that

$$\sqrt{n}\left(\frac{1}{n}\sum_{i=1}^{n} g(\mathbf{X}_i) - \mathbb{E}[g(\mathbf{X}_i)]\right) = \frac{1}{\sqrt{n}}\sum_{i=1}^{n} g(\mathbf{X}_i) \xrightarrow{d} \mathcal{N}(0, \mathbb{E}[g(\mathbf{X}_i)g(\mathbf{X}_i')]) \tag{7.1}$$

We now manipulate our decomposition to arrive at the *stabilized* version of the estimator,

$$\sqrt{n}\left(\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta}\right) = \left(\frac{1}{n}\sum_{i=1}^{n} \mathbf{X}_i\mathbf{X}_i'\right)^{-1}\left(\frac{1}{\sqrt{n}}\sum_{i=1}^{n} \mathbf{X}_i e_i\right).$$

Recall that we stabilize an estimator to ensure it has a fixed variance as the sample size grows, allowing it to have a non-degenerate asymptotic distribution. The stabilization works by asymptotically centering it (that is, subtracting the value to which it converges) and multiplying by the square root of the sample size. We have already established that the first term on the right-hand side will converge in probability to $\mathbf{Q}_{\mathbf{XX}}^{-1}$. Notice that $\mathbb{E}[\mathbf{X}_i e_i] = 0$, so we can apply Equation 7.1 to the second term. The covariance matrix of $\mathbf{X}_i e_i$ is

$$\boldsymbol{\Omega} = \mathbb{V}[\mathbf{X}_i e_i] = \mathbb{E}[\mathbf{X}_i e_i (\mathbf{X}_i e_i)'] = \mathbb{E}[e_i^2 \mathbf{X}_i \mathbf{X}_i'].$$

The CLT will imply that

$$\frac{1}{\sqrt{n}}\sum_{i=1}^{n} \mathbf{X}_i e_i \xrightarrow{d} \mathcal{N}(0, \boldsymbol{\Omega}).$$

Combining these facts with Slutsky's Theorem implies the following theorem.

Theorem 7.2. *Suppose that the linear projection assumptions hold and, in addition, we have* $\mathbb{E}[Y_i^4] < \infty$ *and* $\mathbb{E}[\|\mathbf{X}_i\|^4] < \infty$*. Then the OLS estimator is asymptotically normal with*

$$\sqrt{n}\left(\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta}\right) \xrightarrow{d} \mathcal{N}(0, \mathbf{V}_{\boldsymbol{\beta}}),$$

where

$$\mathbf{V}_{\boldsymbol{\beta}} = \mathbf{Q}_{\mathbf{XX}}^{-1}\boldsymbol{\Omega}\mathbf{Q}_{\mathbf{XX}}^{-1} = \left(\mathbb{E}[\mathbf{X}_i\mathbf{X}_i']\right)^{-1}\mathbb{E}[e_i^2\mathbf{X}_i\mathbf{X}_i']\left(\mathbb{E}[\mathbf{X}_i\mathbf{X}_i']\right)^{-1}.$$

Thus, with a large enough sample size we can approximate the distribution of $\widehat{\boldsymbol{\beta}}$ with a multivariate normal distribution with mean $\boldsymbol{\beta}$ and covariance matrix $\mathbf{V}_{\boldsymbol{\beta}}/n$. In particular, the square root of the jth diagonals of this matrix will be standard errors for $\hat{\beta}_j$. Knowing the shape of the OLS estimator's multivariate distribution will allow us to conduct hypothesis tests and generate confidence intervals for both individual coefficients and groups of coefficients. But, first, we need an estimate of the covariance matrix.

7.2 Variance estimation for OLS

The asymptotic normality of OLS from the last section is of limited value without some way to estimate the covariance matrix,

$$\mathbf{V}_{\boldsymbol{\beta}} = \mathbf{Q}_{\mathbf{XX}}^{-1}\boldsymbol{\Omega}\mathbf{Q}_{\mathbf{XX}}^{-1}.$$

Since each term here is a population mean, this is an ideal place in which to drop a plug-in estimator. For now, we will use the following estimators:

$$\mathbf{Q}_{\mathbf{XX}} = \mathbb{E}[\mathbf{X}_i\mathbf{X}_i'] \qquad \widehat{\mathbf{Q}}_{\mathbf{XX}} = \frac{1}{n}\sum_{i=1}^{n}\mathbf{X}_i\mathbf{X}_i' = \frac{1}{n}\mathbb{X}'\mathbb{X}$$

$$\boldsymbol{\Omega} = \mathbb{E}[e_i^2\mathbf{X}_i\mathbf{X}_i'] \qquad \widehat{\boldsymbol{\Omega}} = \frac{1}{n}\sum_{i=1}^{n}\hat{e}_i^2\mathbf{X}_i\mathbf{X}_i'.$$

Under the assumptions of Theorem 7.2, the LLN will imply that these are consistent for the quantities we need, $\widehat{\mathbf{Q}}_{\mathbf{XX}} \xrightarrow{p} \mathbf{Q}_{\mathbf{XX}}$ and $\widehat{\boldsymbol{\Omega}} \xrightarrow{p} \boldsymbol{\Omega}$. We can plug these into the variance

formula to arrive at

$$\begin{aligned}\widehat{\mathbf{V}}_{\boldsymbol{\beta}} &= \widehat{\mathbf{Q}}_{\mathbf{XX}}^{-1}\widehat{\boldsymbol{\Omega}}\widehat{\mathbf{Q}}_{\mathbf{XX}}^{-1} \\ &= \left(\frac{1}{n}\mathbb{X}'\mathbb{X}\right)^{-1}\left(\frac{1}{n}\sum_{i=1}^{n}\hat{e}_i^2\mathbf{X}_i\mathbf{X}_i'\right)\left(\frac{1}{n}\mathbb{X}'\mathbb{X}\right)^{-1},\end{aligned}$$

which by the continuous mapping theorem is consistent, $\widehat{\mathbf{V}}_{\boldsymbol{\beta}} \xrightarrow{p} \mathbf{V}_{\boldsymbol{\beta}}$.

This estimator is sometimes called the **robust variance estimator** or, more accurately, the **heteroskedasticity-consistent (HC) variance estimator**. Why is it robust? Consider the standard **homoskedasticity** assumption that most statistical software packages make when estimating OLS variances: the variance of the errors does not depend on the covariates, or $\mathbb{V}[e_i^2 \mid \mathbf{X}_i] = \mathbb{V}[e_i^2]$. This assumption is stronger than needed, and we can rely on a weaker assumption that the squared errors are uncorrelated with a specific function of the covariates:

$$\mathbb{E}[e_i^2\mathbf{X}_i\mathbf{X}_i'] = \mathbb{E}[e_i^2]\mathbb{E}[\mathbf{X}_i\mathbf{X}_i'] = \sigma^2\mathbf{Q}_{\mathbf{XX}},$$

where σ^2 is the variance of the residuals (since $\mathbb{E}[e_i] = 0$). Homoskedasticity simplifies the asymptotic variance of the stabilized estimator, $\sqrt{n}(\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta})$, to

$$\mathbf{V}_{\boldsymbol{\beta}}^{\texttt{lm}} = \mathbf{Q}_{\mathbf{XX}}^{-1}\sigma^2\mathbf{Q}_{\mathbf{XX}}\mathbf{Q}_{\mathbf{XX}}^{-1} = \sigma^2\mathbf{Q}_{\mathbf{XX}}^{-1}.$$

We already have an estimator for $\mathbf{Q}_{\mathbf{XX}}$, but we need one for σ^2. We can easily use the SSR,

$$\hat{\sigma}^2 = \frac{1}{n-k-1}\sum_{i=1}^{n}\hat{e}_i^2,$$

where we use $n-k-1$ in the denominator instead of n to correct for the residuals being slightly less variable than the actual errors (because OLS mechanically attempts to make the residuals small). For consistent variance estimation, $n-k-1$ or n can be used, since either way $\hat{\sigma}^2 \xrightarrow{p} \sigma^2$. Thus, under homoskedasticity, we have

$$\widehat{\mathbf{V}}_{\boldsymbol{\beta}}^{\texttt{lm}} = \hat{\sigma}^2\left(\mathbb{X}'\mathbb{X}\right)^{-1},$$

This is the standard variance estimator used by `lm()` in R and `reg` in Stata.

How do these two estimators, $\widehat{\mathbf{V}}_{\boldsymbol{\beta}}$ and $\widehat{\mathbf{V}}_{\boldsymbol{\beta}}^{\texttt{lm}}$, compare? Notice that the HC variance estimator and the homoskedasticity variance estimator will both be consistent when homoskedasticity holds. But as the "heteroskedasticity-consistent" label implies, only the

HC variance estimator will be consistent when homoskedasticity fails to hold. So $\widehat{\mathbf{V}}_{\boldsymbol{\beta}}$ has the advantage of being consistent regardless of the homoskedasticity assumption. This advantage comes at a cost, however. When homoskedasticity is correct, $\widehat{\mathbf{V}}_{\boldsymbol{\beta}}^{\texttt{lm}}$ incorporates that assumption into the estimator whereas the HC variance estimator has to estimate it. The HC estimator will therefore have higher variance (the variance estimator will be more variable!) when homoskedasticity actually does hold.

Now that we have established the asymptotic normality of the OLS estimator and developed a consistent estimator of its variance, we can proceed with all of the statistical inference tools we discussed in Part I, including hypothesis tests and confidence intervals.

We begin by defining the estimated **heteroskedasticity-consistent standard errors** as

$$\widehat{\mathsf{se}}(\hat{\beta}_j) = \sqrt{\frac{[\widehat{\mathbf{V}}_{\boldsymbol{\beta}}]_{jj}}{n}},$$

where $[\widehat{\mathbf{V}}_{\boldsymbol{\beta}}]_{jj}$ is the jth diagonal entry of the HC variance estimator. Note that we divide by $\sqrt{n}$ here because $\widehat{\mathbf{V}}_{\boldsymbol{\beta}}$ is a consistent estimator of the stabilized estimator $\sqrt{n}(\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta})$ not the estimator itself.

Hypothesis tests and confidence intervals for individual coefficients are almost precisely the same as with the most general case presented in Part I. For a two-sided test of $H_0 : \beta_j = b$ versus $H_1 : \beta_j \neq b$, we can build the t-statistic and conclude that, under the null,

$$\frac{\hat{\beta}_j - b}{\widehat{\mathsf{se}}(\hat{\beta}_j)} \xrightarrow{d} \mathcal{N}(0, 1).$$

Statistical software will typically and helpfully provide the t-statistic for the null hypothesis of no (partial) linear relationship between X_{ij} and Y_i,

$$t = \frac{\hat{\beta}_j}{\widehat{\mathsf{se}}(\hat{\beta}_j)},$$

which measures how large the estimated coefficient is in standard errors. With $\alpha = 0.05$, asymptotic normality would imply that we reject this null when $t > 1.96$. We can form asymptotically-valid confidence intervals with

$$\left[\hat{\beta}_j - z_{\alpha/2}\, \widehat{\mathsf{se}}(\hat{\beta}_j),\ \hat{\beta}_j + z_{\alpha/2}\, \widehat{\mathsf{se}}(\hat{\beta}_j)\right].$$

For reasons we will discuss below, standard software typically relies on the t distribution instead of the normal for hypothesis testing and confidence intervals. Still, this difference is of little consequence in large samples.

7.3 Inference for multiple parameters

With multiple coefficients, we might have hypotheses that involve more than one coefficient. As an example, consider a regression with an interaction between two covariates,

$$Y_i = \beta_0 + X_i\beta_1 + Z_i\beta_2 + X_iZ_i\beta_3 + e_i.$$

Suppose we wanted to test the hypothesis that X_i does not affect the best linear predictor for Y_i. That would be

$$H_0 : \beta_1 = 0 \text{ and } \beta_3 = 0 \quad \text{vs} \quad H_1 : \beta_1 \neq 0 \text{ or } \beta_3 \neq 0,$$

where we usually write the null more compactly as $H_0 : \beta_1 = \beta_3 = 0$.

To test this null hypothesis, we need a test statistic that discriminates between the two hypotheses: it should be large when the alternative is true and small enough when the null is true. With a single coefficient, we usually test the null hypothesis of $H_0 : \beta_j = b_0$ with the t-statistic,

$$t = \frac{\hat{\beta}_j - b_0}{\widehat{\mathsf{se}}(\hat{\beta}_j)},$$

and we usually take the absolute value, $|t|$, as our measure of how extreme our estimate is given the null distribution. But notice that we could also use the square of the t statistic, which is

$$t^2 = \frac{\left(\hat{\beta}_j - b_0\right)^2}{\mathbb{V}[\hat{\beta}_j]} = \frac{n\left(\hat{\beta}_j - b_0\right)^2}{[\mathbf{V}_{\boldsymbol{\beta}}]_{[jj]}}. \tag{7.2}$$

While $|t|$ is the usual test statistic we use for two-sided tests, we could equivalently use t^2 and arrive at the exact same conclusions (as long as we knew the distribution of t^2 under the null hypothesis). It turns out that the t^2 version of the test statistic will generalize more easily to comparing multiple coefficients. This version of the test statistic suggests another general way to differentiate the null from the alternative: by taking the squared distance between them and dividing by the variance of the estimate.

Can we generalize this idea to hypotheses about multiple parameters? Adding the sum of squared distances for each component of the null hypothesis is straightforward. For our interaction example, that would be

$$\hat{\beta}_1^2 + \hat{\beta}_3^2,$$

Remember, however, that some of the estimated coefficients are noisier than others, so we should account for the uncertainty just like we did for the t-statistic.

With multiple parameters and multiple coefficients, the variances will now require matrix algebra. We can write any hypothesis about linear functions of the coefficients as $H_0 : \mathbf{L}\boldsymbol{\beta} = \mathbf{c}$. For example, in the interaction case, we have

$$\mathbf{L} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \qquad \mathbf{c} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

Thus, $\mathbf{L}\boldsymbol{\beta} = \mathbf{0}$ is equivalent to $\beta_1 = 0$ and $\beta_3 = 0$. Notice that with other $\mathbf{L}$ matrices, we could represent more complicated hypotheses like $2\beta_1 - \beta_2 = 34$, though we mostly stick to simpler functions. Let $\hat{\boldsymbol{\theta}} = \mathbf{L}\widehat{\boldsymbol{\beta}}$ be the OLS estimate of the function of the coefficients. By the delta method (discussed in Section 3.9), we have

$$\sqrt{n}\left(\mathbf{L}\widehat{\boldsymbol{\beta}} - \mathbf{L}\boldsymbol{\beta}\right) \xrightarrow{d} \mathcal{N}(0, \mathbf{L}'\mathbf{V}_{\boldsymbol{\beta}}\mathbf{L}).$$

We can now generalize the squared t statistic in Equation 7.2 by taking the distances $\mathbf{L}\widehat{\boldsymbol{\beta}} - \mathbf{c}$ weighted by the variance-covariance matrix $\mathbf{L}'\mathbf{V}_{\boldsymbol{\beta}}\mathbf{L}$,

$$W = n(\mathbf{L}\widehat{\boldsymbol{\beta}} - \mathbf{c})'(\mathbf{L}'\mathbf{V}_{\boldsymbol{\beta}}\mathbf{L})^{-1}(\mathbf{L}\widehat{\boldsymbol{\beta}} - \mathbf{c}),$$

which is called the **Wald test statistic**. This statistic generalizes the ideas of the t-statistic to multiple parameters. With the t-statistic, we recenter to have mean 0 and divide by the standard error to get a variance of 1. If we ignore the middle variance weighting, we have $(\mathbf{L}\widehat{\boldsymbol{\beta}} - \mathbf{c})'(\mathbf{L}\widehat{\boldsymbol{\beta}} - \mathbf{c})$ which is just the sum of the squared deviations of the estimates from the null. Including the $(\mathbf{L}'\mathbf{V}_{\boldsymbol{\beta}}\mathbf{L})^{-1}$ weight has the effect of rescaling the distribution of $\mathbf{L}\widehat{\boldsymbol{\beta}} - \mathbf{c}$ to make it rotationally symmetric around 0 (so the resulting dimensions are uncorrelated) with each dimension having an equal variance of 1. In this way, the Wald statistic transforms the random vectors to be mean-centered and have variance 1 (just the t-statistic), but also to have the resulting random variables in the vector be uncorrelated.[1]

[1]The form of the Wald statistic is that of a weighted inner product, $\mathbf{x}'\mathbf{A}\mathbf{y}$, where $\mathbf{A}$ is a symmetric positive-definite weighting matrix.

Why transform the data in this way? Figure 7.1 shows the contour plot of a hypothetical joint distribution of two coefficients from an OLS regression. We might want to know the distance between different points in the distribution and the mean, which in this case is $(1, 2)$. Without considering the joint distribution, the circle is obviously closer to the mean than the triangle. However, looking at the two points on the distribution, the circle is at a lower contour than the triangle, meaning it is more extreme than the triangle for this particular distribution. The Wald statistic, then, takes into consideration how much of a "climb" it is for $\mathbf{L}\widehat{\boldsymbol{\beta}}$ to get to $\mathbf{c}$ given the distribution of $\mathbf{L}\widehat{\boldsymbol{\beta}}$.

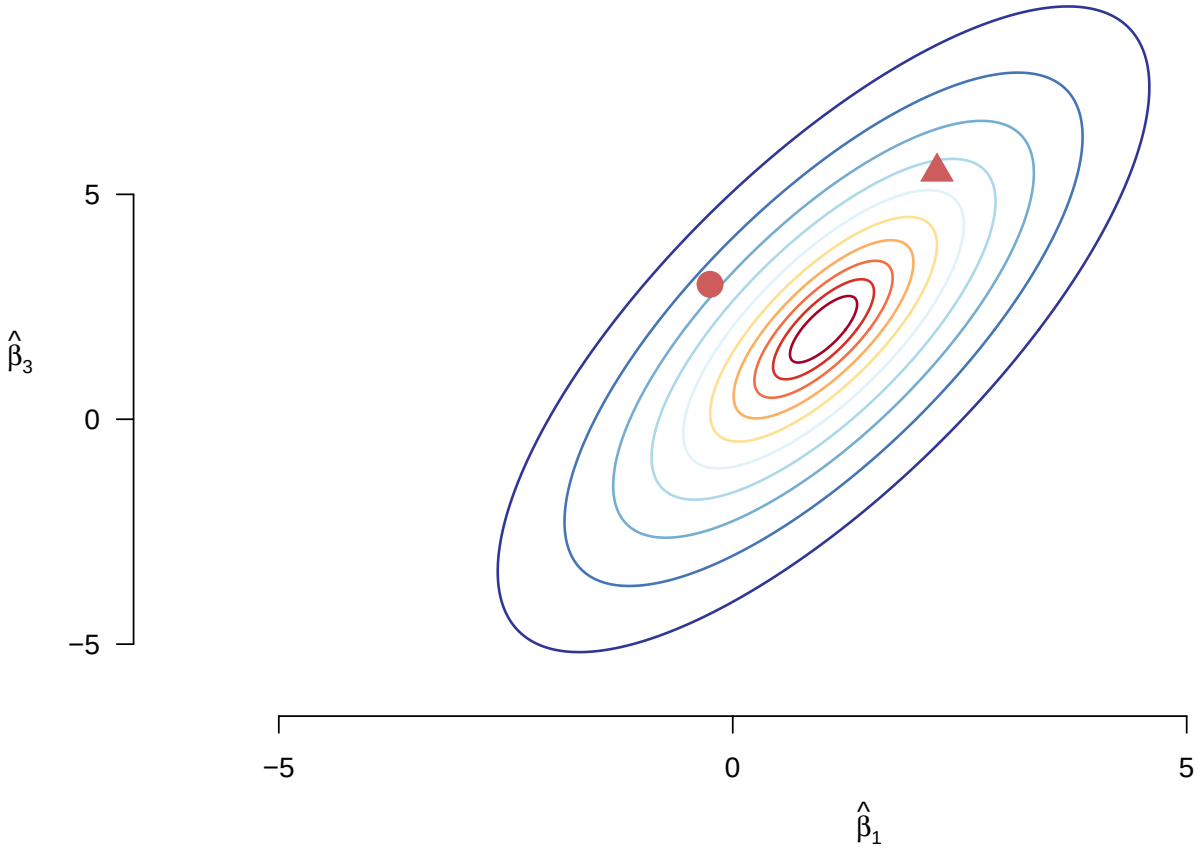


Figure 7.1: Hypothetical joint distribution of two slope coefficients. The circle is closer to the center of the distribution by the standard Euclidean distance, but the triangle is closer once you consider the joint distribution.

If $\mathbf{L}$ only has one row, our Wald statistic is the same as the squared t statistic, $W = t^2$.

This fact will help us think about the asymptotic distribution of W. Note that as $n \to \infty$, we know that by the asymptotic normality of $\widehat{\boldsymbol{\beta}}$,

$$t = \frac{\hat{\beta}_j - \beta_j}{\widehat{\mathsf{se}}[\hat{\beta}_j]} \xrightarrow{d} \mathcal{N}(0, 1)$$

so t^2 will converge in distribution to a χ^2_1 (since a χ^2_1 distribution is just one standard normal distribution squared). After recentering and rescaling by the covariance matrix, W converges to the sum of q squared independent normals, where q is the number of rows of $\mathbf{L}$, or equivalently, the number of restrictions implied by the null hypothesis. Thus, under the null hypothesis of $\mathbf{L}\widehat{\boldsymbol{\beta}} = \mathbf{c}$, we have $W \xrightarrow{d} \chi^2_q$.

We need to define the rejection region to use the Wald statistic in a hypothesis test. Because we are squaring each distance in $W \geq 0$, larger values of W indicate more disagreement with the null in either direction. Thus, for an α-level test of the joint null, we only need a one-sided rejection region of the form $\mathbb{P}(W > w_\alpha) = \alpha$. Obtaining these values is straightforward (see the above callout tip). For $q = 2$ and a $\alpha = 0.05$, the critical value is roughly 6.

i Chi-squared critical values

We can obtain critical values for the χ^2_q distribution using the `qchisq()` function in R. For example, if we wanted to obtain the critical value w such that $\mathbb{P}(W > w_\alpha) = \alpha$ for our two-parameter interaction example, we could use:

```
qchisq(p = 0.95, df = 2)
```

```
[1] 5.991465
```

The Wald statistic is not a common test provided by standard statistical software functions like `lm()` in R, though it is fairly straightforward to implement "by hand." Alternatively, packages like {aod} or {clubSandwich} have implementations of the test. What is reported by most software implementations of OLS (like `lm()` in R) is the F-statistic, which is

$$F = \frac{W}{q}.$$

This also typically uses the homoskedastic variance estimator $\mathbf{V}_{\boldsymbol{\beta}}^{\texttt{lm}}$ in W. The p-values reported for such tests use the $F_{q,n-k-1}$ distribution because this is the exact distribution of

the F statistic when the errors are (a) homoskedastic and (b) normally distributed. When these assumptions do not hold, the F distribution has no justification in statistical theory, but it is slightly more conservative than the χ^2_q distribution, and the inferences from the F statistic will converge to those from the χ^2_q distribution as $n \to \infty$. So it might be justified as an *ad hoc* small-sample adjustment to the Wald test. For example, if we used the $F_{q,n-k-1}$ with the interaction example where $q = 2$ and we have, say, a sample size of $n = 100$, then in that case, the critical value for the F test with $\alpha = 0.05$ is

```
qf(0.95, df1 = 2, df2 = 100 - 4)
```

```
[1] 3.091191
```

This result implies a critical value of 6.182 on the scale of the Wald statistic (multiplying it by $q = 2$). Compared to the earlier critical value of 5.991 based on the χ^2_2 distribution, we can see that the inferences will be very similar even in moderately-sized datasets.

Finally, note that the F-statistic reported by `lm()` in R is the test of all the coefficients being equal to 0 jointly except for the intercept. In modern quantitative social sciences, this test is seldom substantively interesting.

7.4 Finite-sample properties with a linear CEF

All the above results have been large-sample properties, and we have not addressed finite-sample properties like the sampling variance or unbiasedness. Under the linear projection assumption above, OLS is generally biased without stronger assumptions. This section introduces the stronger assumption that will allow us to establish stronger properties for OLS. As usual, however, remember that these stronger assumptions can be wrong.

Assumption: Linear Regression Model

1. The variables $(Y_i, \mathbf{X}_i)$ satisfy the linear CEF assumption.

$$\begin{aligned} Y_i &= \mathbf{X}_i'\boldsymbol{\beta} + e_i \\ \mathbb{E}[e_i \mid \mathbf{X}_i] &= 0. \end{aligned}$$

2. The design matrix is invertible $\mathbb{E}[\mathbf{X}_i\mathbf{X}_i'] > 0$ (positive definite).

We discussed the concept of a linear CEF extensively in Chapter 5. However, recall that the CEF might be linear mechanically if the model is **saturated** or when there are as many coefficients in the model as there are unique values of $\mathbf{X}_i$. When a model is not saturated, the linear CEF assumption is just that: an assumption. What can this assumption do? It can aid in establishing some nice statistical properties in finite samples.

Before proceeding, note that, when focusing on the finite sample inference for OLS, we focused on its properties **conditional on the observed covariates**, such as $\mathbb{E}[\widehat{\boldsymbol{\beta}} \mid \mathbb{X}]$ or $\mathbb{V}[\widehat{\boldsymbol{\beta}} \mid \mathbb{X}]$. The historical reason for this is that the researcher often chose these independent variables and so they were not random. Thus, sometimes $\mathbb{X}$ is treated as "fixed" in some older texts, which might even omit explicit conditioning statements.

Theorem 7.3. *Under the linear regression model assumption, OLS is unbiased for the population regression coefficients,*

$$\mathbb{E}[\widehat{\boldsymbol{\beta}} \mid \mathbb{X}] = \boldsymbol{\beta},$$

and its conditional sampling variance is

$$\mathbb{V}_{\widehat{\boldsymbol{\beta}}} = \mathbb{V}[\widehat{\boldsymbol{\beta}} \mid \mathbb{X}] = (\mathbb{X}'\mathbb{X})^{-1} \left(\sum_{i=1}^{n} \sigma_i^2 \mathbf{X}_i \mathbf{X}_i' \right) (\mathbb{X}'\mathbb{X})^{-1},$$

where $\sigma_i^2 = \mathbb{E}[e_i^2 \mid \mathbb{X}]$.

Proof. To prove the conditional unbiasedness, recall that we can write the OLS estimator as

$$\widehat{\boldsymbol{\beta}} = \boldsymbol{\beta} + (\mathbb{X}'\mathbb{X})^{-1}\mathbb{X}'\mathbf{e},$$

and so taking (conditional) expectations, we have

$$\mathbb{E}[\widehat{\boldsymbol{\beta}} \mid \mathbb{X}] = \boldsymbol{\beta} + \mathbb{E}[(\mathbb{X}'\mathbb{X})^{-1}\mathbb{X}'\mathbf{e} \mid \mathbb{X}] = \boldsymbol{\beta} + (\mathbb{X}'\mathbb{X})^{-1}\mathbb{X}'\mathbb{E}[\mathbf{e} \mid \mathbb{X}] = \boldsymbol{\beta},$$

because under the linear CEF assumption $\mathbb{E}[\mathbf{e} \mid \mathbb{X}] = 0$.

For the conditional sampling variance, we can use the same decomposition we have,

$$\mathbb{V}[\widehat{\boldsymbol{\beta}} \mid \mathbb{X}] = \mathbb{V}[\boldsymbol{\beta} + (\mathbb{X}'\mathbb{X})^{-1}\mathbb{X}'\mathbf{e} \mid \mathbb{X}] = (\mathbb{X}'\mathbb{X})^{-1}\mathbb{X}'\mathbb{V}[\mathbf{e} \mid \mathbb{X}]\mathbb{X}(\mathbb{X}'\mathbb{X})^{-1}.$$

Since $\mathbb{E}[\mathbf{e} \mid \mathbb{X}] = 0$, we know that $\mathbb{V}[\mathbf{e} \mid \mathbb{X}] = \mathbb{E}[\mathbf{e}\mathbf{e}' \mid \mathbb{X}]$, which is a matrix with diagonal entries $\mathbb{E}[e_i^2 \mid \mathbb{X}] = \sigma_i^2$ and off-diagonal entries $\mathbb{E}[e_i e_j \mathbb{X}] = \mathbb{E}[e_i \mid \mathbb{X}]\mathbb{E}[e_j \mid \mathbb{X}] = 0$,

where the first equality follows from the independence of the errors across units. Thus, $\mathbb{V}[\mathbf{e} \mid \mathbb{X}]$ is a diagonal matrix with σ_i^2 along the diagonal, which means

$$\mathbb{X}'\mathbb{V}[\mathbf{e} \mid \mathbb{X}]\mathbb{X} = \sum_{i=1}^{n} \sigma_i^2 \mathbf{X}_i \mathbf{X}_i',$$

establishing the conditional sampling variance. □

This means that, for any realization of the covariates, $\mathbb{X}$, OLS is unbiased for the true regression coefficients $\boldsymbol{\beta}$. By the law of iterated expectation, we also know that it is unconditionally unbiased[2] as well since

$$\mathbb{E}[\widehat{\boldsymbol{\beta}}] = \mathbb{E}[\mathbb{E}[\widehat{\boldsymbol{\beta}} \mid \mathbb{X}]] = \boldsymbol{\beta}.$$

The difference between these two statements usually isn't incredibly meaningful.

There are a lot of variances flying around, so reviewing them is helpful. Above, we derived the asymptotic variance of $\mathbf{Z}_n = \sqrt{n}(\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta})$,

$$\mathbf{V}_{\boldsymbol{\beta}} = \left(\mathbb{E}[\mathbf{X}_i \mathbf{X}_i']\right)^{-1} \mathbb{E}[e_i^2 \mathbf{X}_i \mathbf{X}_i'] \left(\mathbb{E}[\mathbf{X}_i \mathbf{X}_i']\right)^{-1},$$

which implies that the approximate variance of $\widehat{\boldsymbol{\beta}}$ will be $\mathbf{V}_{\boldsymbol{\beta}}/n$ because

$$\widehat{\boldsymbol{\beta}} = \frac{Z_n}{\sqrt{n}} + \boldsymbol{\beta} \quad \Longrightarrow \quad \widehat{\boldsymbol{\beta}} \overset{a}{\sim} \mathcal{N}(\boldsymbol{\beta}, n^{-1}\mathbf{V}_{\boldsymbol{\beta}}),$$

where $\overset{a}{\sim}$ means asymptotically distributed as. Under the linear CEF, the conditional sampling variance of $\widehat{\boldsymbol{\beta}}$ has a similar form and will be similar to the

$$\mathbf{V}_{\widehat{\boldsymbol{\beta}}} = \left(\mathbb{X}'\mathbb{X}\right)^{-1} \left(\sum_{i=1}^{n} \sigma_i^2 \mathbf{X}_i \mathbf{X}_i' \right) \left(\mathbb{X}'\mathbb{X}\right)^{-1} \approx \mathbf{V}_{\boldsymbol{\beta}}/n.$$

In practice, these two derivations lead to basically the same variance estimator. Recall that the heteroskedastic-consistent variance estimator

$$\widehat{\mathbf{V}}_{\boldsymbol{\beta}} = \left(\frac{1}{n}\mathbb{X}'\mathbb{X}\right)^{-1} \left(\frac{1}{n} \sum_{i=1}^{n} \hat{e}_i^2 \mathbf{X}_i \mathbf{X}_i' \right) \left(\frac{1}{n}\mathbb{X}'\mathbb{X}\right)^{-1},$$

[2] We are basically ignoring some edge cases when it comes to discrete covariates here. In particular, we assume that $\mathbb{X}'\mathbb{X}$ is nonsingular with probability one. However, this assumption can fail if we have a binary covariate since there is some chance (however slight) that the entire column will be all ones or all zeros, which would lead to a singular matrix $\mathbb{X}'\mathbb{X}$. Practically this is not a big deal, but it does mean that we have to ignore this issue theoretically or focus on conditional unbiasedness.

is a valid plug-in estimator for the asymptotic variance and

$$\widehat{\mathbf{V}}_{\widehat{\boldsymbol{\beta}}} = n^{-1}\widehat{\mathbf{V}}_{\boldsymbol{\beta}}.$$

Thus, in practice, the asymptotic and finite-sample results under a linear CEF justify the same variance estimator.

7.4.1 Linear CEF model under homoskedasticity

If we are willing to assume that the standard errors are homoskedastic, we can derive even stronger results for OLS. Stronger assumptions typically lead to stronger conclusions, but, obviously, those conclusions may not be robust to assumption violations. But homoskedasticity of errors is such a historically important assumption that statistical software implementations of OLS like `lm()` in R assume it by default.

> **i** Assumption: Homoskedasticity with a linear CEF
>
> In addition to the linear CEF assumption, we further assume that
>
> $$\mathbb{E}[e_i^2 \mid \mathbf{X}_i] = \mathbb{E}[e_i^2] = \sigma^2,$$
>
> or that variance of the errors does not depend on the covariates.

Theorem 7.4. *Under a linear CEF model with homoskedastic errors, the conditional sampling variance is*

$$\mathbf{V}_{\widehat{\boldsymbol{\beta}}}^{lm} = \mathbb{V}[\widehat{\boldsymbol{\beta}} \mid \mathbb{X}] = \sigma^2 \left(\mathbb{X}'\mathbb{X}\right)^{-1},$$

and the variance estimator

$$\widehat{\mathbf{V}}_{\widehat{\boldsymbol{\beta}}}^{lm} = \hat{\sigma}^2 \left(\mathbb{X}'\mathbb{X}\right)^{-1} \quad \textit{where,} \quad \hat{\sigma}^2 = \frac{1}{n-k-1}\sum_{i=1}^{n} \hat{e}_i^2$$

is unbiased, $\mathbb{E}[\widehat{\mathbf{V}}_{\widehat{\boldsymbol{\beta}}}^{lm} \mid \mathbb{X}] = \mathbf{V}_{\widehat{\boldsymbol{\beta}}}^{lm}$.

Proof. Under homoskedasticity $\sigma_i^2 = \sigma^2$ for all i. Recall that $\sum_{i=1}^{n} \mathbf{X}_i\mathbf{X}_i' = \mathbb{X}'\mathbb{X}$. Thus,

the conditional sampling variance from Theorem 7.3,

$$\begin{aligned}
\mathbb{V}[\widehat{\boldsymbol{\beta}} \mid \mathbb{X}] &= (\mathbb{X}'\mathbb{X})^{-1} \left(\sum_{i=1}^{n} \sigma^2 \mathbf{X}_i \mathbf{X}_i' \right) (\mathbb{X}'\mathbb{X})^{-1} \\
&= \sigma^2 (\mathbb{X}'\mathbb{X})^{-1} \left(\sum_{i=1}^{n} \mathbf{X}_i \mathbf{X}_i' \right) (\mathbb{X}'\mathbb{X})^{-1} \\
&= \sigma^2 (\mathbb{X}'\mathbb{X})^{-1} (\mathbb{X}'\mathbb{X}) (\mathbb{X}'\mathbb{X})^{-1} \\
&= \sigma^2 (\mathbb{X}'\mathbb{X})^{-1} = \mathbf{V}_{\widehat{\boldsymbol{\beta}}}^{\texttt{lm}}.
\end{aligned}$$

For unbiasedness, we just need to show that $\mathbb{E}[\hat{\sigma}^2 \mid \mathbb{X}] = \sigma^2$. Recall that we defined $\mathbf{M}_{\mathbb{X}}$ as the residual-maker because $\mathbf{M}_{\mathbb{X}}\mathbf{Y} = \hat{\mathbf{e}}$. We can use this to connect the residuals to the standard errors,

$$\mathbf{M}_{\mathbb{X}}\mathbf{e} = \mathbf{M}_{\mathbb{X}}\mathbf{Y} - \mathbf{M}_{\mathbb{X}}\mathbb{X}\boldsymbol{\beta} = \mathbf{M}_{\mathbb{X}}\mathbf{Y} = \hat{\mathbf{e}},$$

so

$$\mathbb{V}[\hat{\mathbf{e}} \mid \mathbb{X}] = \mathbf{M}_{\mathbb{X}}\mathbb{V}[\mathbf{e} \mid \mathbb{X}] = \mathbf{M}_{\mathbb{X}}\sigma^2,$$

where the first equality holds because $\mathbf{M}_{\mathbb{X}} = \mathbf{I}_n - \mathbb{X}(\mathbb{X}'\mathbb{X})^{-1}\mathbb{X}'$ is constant conditional on $\mathbb{X}$. Notice that the diagonal entries of this matrix are the variances of particular residuals $\hat{e}_i$ and that the diagonal entries of the annihilator matrix are $1 - h_{ii}$ (since the h_{ii} are the diagonal entries of $\mathbf{P}_{\mathbb{X}}$). Thus, we have

$$\mathbb{V}[\hat{e}_i \mid \mathbb{X}] = \mathbb{E}[\hat{e}_i^2 \mid \mathbb{X}] = (1 - h_{ii})\sigma^2.$$

In the last chapter in Section 6.9.1, we established that one property of these leverage values is $\sum_{i=1}^{n} h_{ii} = k + 1$, so $\sum_{i=1}^{n} 1 - h_{ii} = n - k - 1$ and we have

$$\begin{aligned}
\mathbb{E}[\hat{\sigma}^2 \mid \mathbb{X}] &= \frac{1}{n-k-1} \sum_{i=1}^{n} \mathbb{E}[\hat{e}_i^2 \mid \mathbb{X}] \\
&= \frac{\sigma^2}{n-k-1} \sum_{i=1}^{n} 1 - h_{ii} \\
&= \sigma^2.
\end{aligned}$$

This establishes $\mathbb{E}[\widehat{\mathbf{V}}_{\widehat{\boldsymbol{\beta}}}^{\texttt{lm}} \mid \mathbb{X}] = \mathbf{V}_{\widehat{\boldsymbol{\beta}}}^{\texttt{lm}}$. □

Thus, under the linear CEF model and homoskedasticity of the errors, we have an unbiased variance estimator that is a simple function of the sum of squared residuals and the design matrix. Most statistical software packages estimate standard errors using $\widehat{\mathbf{V}}_{\widehat{\boldsymbol{\beta}}}^{\texttt{lm}}$.

The final result we can derive for the linear CEF under the homoskedasticity assumption is an optimality result. That is, we might ask if there is another estimator for $\boldsymbol{\beta}$ that would outperform OLS in the sense of having a lower sampling variance. Perhaps surprisingly, no linear estimator for $\boldsymbol{\beta}$ has a lower conditional variance, meaning that OLS is the **best linear unbiased estimator**, often jovially shortened to BLUE. This result is famously known as the Gauss-Markov Theorem.

Theorem 7.5. *Let $\widetilde{\boldsymbol{\beta}} = \mathbf{AY}$ be a linear and unbiased estimator for $\boldsymbol{\beta}$. Under the linear CEF model with homoskedastic errors,*

$$\mathbb{V}[\widetilde{\boldsymbol{\beta}} \mid \mathbb{X}] \geq \mathbb{V}[\widehat{\boldsymbol{\beta}} \mid \mathbb{X}].$$

Proof. Note that if $\widetilde{\boldsymbol{\beta}}$ is unbiased then $\mathbb{E}[\widetilde{\boldsymbol{\beta}} \mid \mathbb{X}] = \boldsymbol{\beta}$ and so

$$\boldsymbol{\beta} = \mathbb{E}[\mathbf{AY} \mid \mathbb{X}] = \mathbf{A}\mathbb{E}[\mathbf{Y} \mid \mathbb{X}] = \mathbf{A}\mathbb{X}\boldsymbol{\beta},$$

which implies that $\mathbf{A}\mathbb{X} = \mathbf{I}_n$. Rewrite the competitor as $\widetilde{\boldsymbol{\beta}} = \widehat{\boldsymbol{\beta}} + \mathbf{BY}$ where,

$$\mathbf{B} = \mathbf{A} - \left(\mathbb{X}'\mathbb{X}\right)^{-1}\mathbb{X}'.$$

and note that $\mathbf{A}\mathbb{X} = \mathbf{I}_n$ implies that $\mathbf{B}\mathbb{X} = 0$. We now have

$$\begin{aligned}
\widetilde{\boldsymbol{\beta}} &= \left(\left(\mathbb{X}'\mathbb{X}\right)^{-1}\mathbb{X}' + \mathbf{B}\right)\mathbf{Y} \\
&= \left(\left(\mathbb{X}'\mathbb{X}\right)^{-1}\mathbb{X}' + \mathbf{B}\right)\mathbb{X}\boldsymbol{\beta} + \left(\left(\mathbb{X}'\mathbb{X}\right)^{-1}\mathbb{X}' + \mathbf{B}\right)\mathbf{e} \\
&= \boldsymbol{\beta} + \mathbf{B}\mathbb{X}\boldsymbol{\beta} + \left(\left(\mathbb{X}'\mathbb{X}\right)^{-1}\mathbb{X}' + \mathbf{B}\right)\mathbf{e} \\
&= \boldsymbol{\beta} + \left(\left(\mathbb{X}'\mathbb{X}\right)^{-1}\mathbb{X}' + \mathbf{B}\right)\mathbf{e}
\end{aligned}$$

The variance of the competitor is, thus,

$$\begin{aligned}
\mathbb{V}[\widetilde{\boldsymbol{\beta}} \mid \mathbb{X}] &= \left(\left(\mathbb{X}'\mathbb{X}\right)^{-1}\mathbb{X}' + \mathbf{B}\right)\mathbb{V}[\mathbf{e} \mid \mathbb{X}]\left(\left(\mathbb{X}'\mathbb{X}\right)^{-1}\mathbb{X}' + \mathbf{B}\right)' \\
&= \sigma^2\left(\left(\mathbb{X}'\mathbb{X}\right)^{-1}\mathbb{X}' + \mathbf{B}\right)\left(\mathbb{X}\left(\mathbb{X}'\mathbb{X}\right)^{-1} + \mathbf{B}'\right) \\
&= \sigma^2\left(\left(\mathbb{X}'\mathbb{X}\right)^{-1}\mathbb{X}'\mathbb{X}\left(\mathbb{X}'\mathbb{X}\right)^{-1} + \left(\mathbb{X}'\mathbb{X}\right)^{-1}\mathbb{X}'\mathbf{B}' + \mathbf{B}\mathbb{X}\left(\mathbb{X}'\mathbb{X}\right)^{-1} + \mathbf{B}\mathbf{B}'\right) \\
&= \sigma^2\left(\left(\mathbb{X}'\mathbb{X}\right)^{-1} + \mathbf{B}\mathbf{B}'\right) \\
&\geq \sigma^2\left(\mathbb{X}'\mathbb{X}\right)^{-1} \\
&= \mathbb{V}[\widehat{\boldsymbol{\beta}} \mid \mathbb{X}]
\end{aligned}$$

The first equality comes from the properties of covariance matrices, the second is due to the homoskedasticity assumption, and the fourth is due to $\mathbf{B}\mathbb{X} = 0$, which implies that $\mathbb{X}'\mathbf{B}' = 0$ as well. The fifth inequality holds because matrix products of the form $\mathbf{B}\mathbf{B}'$ are positive definite if $\mathbf{B}$ is of full rank (which we have assumed it is). □

In this proof, we saw that the variance of the competing estimator had variance $\sigma^2\left((\mathbb{X}'\mathbb{X})^{-1} + \mathbf{B}\mathbf{B}'\right)$ which we argued was "greater than 0" in the matrix sense, which is also called positive definite. What does this mean practically? Remember that any positive definite matrix must have strictly positive diagonal entries and that the diagonal entries of $\mathbb{V}[\widehat{\boldsymbol{\beta}} \mid \mathbb{X}]$ and $V[\widetilde{\boldsymbol{\beta}} \mid \mathbb{X}]$ are the variances of the individual parameters, $\mathbb{V}[\hat{\beta}_j \mid \mathbb{X}]$ and $\mathbb{V}[\tilde{\beta}_j \mid \mathbb{X}]$. Thus, the variances of the individual parameters will be larger for $\widetilde{\boldsymbol{\beta}}$ than for $\widehat{\boldsymbol{\beta}}$.

Many textbooks cite the Gauss-Markov theorem as a critical advantage of OLS over other methods, but recognizing its limitations is essential. It requires linearity and homoskedastic error assumptions, and these can be false in many applications.

Finally, note that while we have shown this result for linear estimators, Hansen (2022) proves a more general version of this result that applies to any unbiased estimator.

7.5 The normal linear model

Finally, we add the strongest and thus least loved of the classical linear regression assumption: (conditional) normality of the errors. Historically the reason to use this assumption was that finite-sample inference hits a roadblock without some knowledge of the sampling distribution of $\widehat{\boldsymbol{\beta}}$. Under the linear CEF model, we saw that $\widehat{\boldsymbol{\beta}}$ is unbiased, and under homoskedasticity, we could produce an unbiased estimator of the conditional variance. But for hypothesis testing or for generating confidence intervals, we need to make probability statements about the estimator, and, for that, we need to know its exact distribution. When the sample size is large, we can rely on the CLT and know $\widehat{\boldsymbol{\beta}}$ is approximately normal. But how do we proceed in small samples? Historically we would have assumed (conditional) normality of the errors, basically proceeding with some knowledge that we were wrong but hopefully not too wrong.

The normal linear regression model

In addition to the linear CEF assumption, we assume that

$$e_i \mid \mathbb{X} \sim \mathcal{N}(0, \sigma^2).$$

There are a couple of important points:

- The assumption here is not that $(Y_i, \mathbf{X}_i)$ are jointly normal (though this would be sufficient for the assumption to hold), but rather that Y_i is normally distributed conditional on $\mathbf{X}_i$.
- Notice that the normal regression model has the homoskedasticity assumption baked in.

Theorem 7.6. *Under the normal linear regression model, we have*

$$\widehat{\boldsymbol{\beta}} \mid \mathbb{X} \sim \mathcal{N}\left(\boldsymbol{\beta}, \sigma^2 \left(\mathbb{X}'\mathbb{X}\right)^{-1}\right)$$

$$\frac{\hat{\beta}_j - \beta_j}{[\widehat{\mathbf{V}}^{lm}_{\widehat{\boldsymbol{\beta}}}]_{jj}/\sqrt{n}} \sim t_{n-k-1}$$

$$W/q \sim F_{q,n-k-1}.$$

This theorem says that in the normal linear regression model, the coefficients follow a normal distribution, the t-statistics follow a t-distribution, and a transformation of the Wald statistic follows an F distribution. These are **exact** results and do not rely on large-sample approximations. Under the assumption of conditional normality of the errors, the results are as valid for $n = 5$ as for $n = 500,000$.

Few people believe errors follow a normal distribution, so why even present these results? Unfortunately, most statistical software implementations of OLS implicitly assume this when calculating p-values for tests or constructing confidence intervals. In R, for example, the p-value associated with the t-statistic reported by `lm()` relies on the t_{n-k-1} distribution, and the critical values used to construct confidence intervals with `confint()` use that distribution as well. When normality does not hold, there is no principled reason to use the t or the F distributions in this way. But we might hold our nose and use this *ad hoc* procedure under two rationalizations:

- $\widehat{\beta}$ is asymptotically normal. This approximation might, however, be poor in smaller finite samples. The t distribution will make inference more conservative in these cases (wider confidence intervals, smaller test rejection regions), which might help offset its poor approximation of the normal distribution in small samples.
- As $n \to \infty$, the t_{n-k-1} will converge to a standard normal distribution, so the *ad hoc* adjustment will not matter much for medium to large samples.

These arguments are not very convincing since whether the t approximation will be any better than the normal in finite samples is unclear. But it may be the best we can do while we go and find more data.

7.6 Summary

In this chapter, we discussed the large-sample properties of OLS, which are quite strong. Under mild conditions, OLS is consistent for the population linear regression coefficients and is asymptotically normal. The variance of the OLS estimator, and thus the variance estimator, depends on whether the projection errors are assumed to be unrelated to the covariates (**homoskedastic**) or possibly related (**heteroskedastic**). Confidence intervals and hypothesis tests for individual OLS coefficients are largely the same as discussed in Part I of this book, and we can obtain finite-sample properties of OLS such as conditional unbiasedness if we assume the conditional expectation function is linear. If we further assume the errors are normally distributed, we can derive confidence intervals and hypothesis tests that are valid for all sample sizes.

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