Designing Monte Carlo Simulations in R

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Welcome

Monte Carlo simulations are a computational technique for investigating how well something works, or for investigating what might happen in a given circumstance. When we write a simulation, we are able to control how data are generated, which means we can know what the "right answer" is. Then, by repeatedly generating data and then applying some statistical method that data, we can assess how well a statistical method works in practice.

Monte Carlo simulations are an essential tool of inquiry for quantitative methodologists and students of statistics, useful both for small-scale or informal investigations and for formal methodological research. Despite the ubiquity of simulation work, most quantitative researchers get little formal training in the design and implementation of Monte Carlo simulations. As a result, the simulation studies presented in academic journal articles are highly variable in terms of their high-level logic, scope, programming, and presentation. Although there has long been discussion of simulation design and implementation among statisticians and methodologists, the available guidance is scattered across many different disciplines, and much of it is focused on mechanics and computing tools, rather than on principles.

In this monograph, we aim to provide an introduction to the logic and mechanics of designing simulation studies, using the R programming language. Our focus is on simulation studies for formal research purposes (i.e., as might appear in a journal article or dissertation) and for informing the design of empirical studies (e.g., power analysis). That being said, the ideas of simulation are used in many different contexts and for many different problems, and we believe the overall concepts illustrated by these "conventional" simulations readily carry over into all sorts of other types of use, even statistical inference! Our focus is on the best practices of simulation design and how to use simulation to be a more informed and effective quantitative analyst. In particular, we try to provide a guide to designing simulation studies to answer questions about statistical methodology.

Mainly, this book gives practical tools (i.e., lots of code to simply take and repurpose) along with some thoughts and guidance for writing simulations. We hope you find it to be a useful handbook to help you with your own projects, whatever they happen to be!

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About the authors

We wrote this book in full collaboration, because we thought it would be fun to have some reason to talk about how to write simulations, and we wanted more people to be writing high-quality simulations. Our author order is alphabetical, but perhaps imagine it as a circle, or something with no start or end:
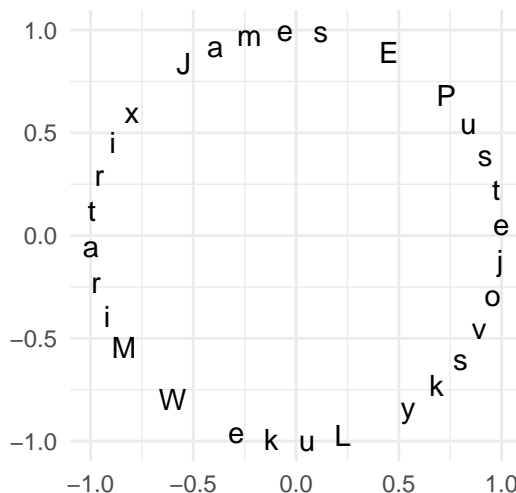
But anymore, more about us.

James E. Pustejovsky is an associate professor at the University of Wisconsin - Madison, where he teaches in the Quantitative Methods Program within the Department of Educational Psychology. He completed a Ph.D. in Statistics at Northwestern University.

Luke Miratrix: I am currently an associate professor at Harvard University's Graduate School of Education. I completed a Ph.D. in Statistics at UC Berkeley after having traveled through three different graduate programs (computer science at MIT, education at UC Berkeley, and then finally statistics at UC Berkeley). I then ended up as an assistant professor in Harvard's statistics department, and moved (back) to Education a few years later.

Over the years, simulation has become a way for me to think. This might be because I am fundamentally lazy, and the idea of sitting down and trying to do a bunch of math to figure something out seems less fun than writing up

some code "real quick" so I can see how things operate. Of course, "real quick" rarely is that quick – and before I know it I got sucked into trying to learn some esoteric aspect of how to best program something, and then a few rabbit holes later I may have discovered something interesting! I find simulation quite absorbing, and I also find them reassuring (usually with regards to whether I have correctly implemented some statistical method). This book has been a real pleasure to write, because it's given me actual license to sit down and think about why I do the various things I do, and also which way I actually prefer to approach a problem. And getting to write this book with my co-author has been a particular pleasure, for talking about the business of writing simulations is rarely done in practice. This has been a real gift, and I have learned so much.

Acknowledgements

Part I

An Introductory Look

Chapter 1

Introduction

Monte Carlo simulations are a tool for studying the behavior of random processes, such as the behavior of a statistical estimation procedure when applied to a sample of data. Within quantitatively oriented fields, researchers developing new statistical methods or evaluating the use of existing methods nearly always use Monte Carlo simulations as part of their research process. In the context of methodological development, researchers use simulations in a way analogous to how a chef would use their test kitchen to develop new recipes before putting them on the menu, how a manufacturer would use a materials testing laboratory to evaluate the safety and durability of a new consumer good before bringing it to market, or how an astronaut would prepare for a spacewalk by practicing the process in an underwater mock-up. Simulation studies provide a clean and controlled environment for testing out data analysis approaches before putting them to use with real empirical data.

More broadly, Monte Carlo studies are an essential tool in many different fields of science—climate science, engineering, and education research are three examples—and are used for a variety of different purposes. Simulations are used to model complex stochastic processes such as weather patterns (Jones et al., 2012; Robert and Casella, 2010); to generate parameter estimates from complex statistical models, as in Markov Chain Monte Carlo sampling (Gelman et al., 2013); and even to estimate uncertainty in statistical summaries, as in bootstrapping (Davison and Hinkley, 1997). In this book, we shall focus on using simulation for the development and validation of methods for data analysis, which are everyday concerns within the fields of statistics and quantitative methodology. However, we also believe that many of the general principles of simulation design and execution that we will discuss are broadly applicable to these other purposes, and we note connections as they occur.

At a very high level, Monte Carlo simulation provides a method for understanding the performance of a statistical model or data analysis method under

conditions where the truth is known and can be controlled. The basic approach for doing so is as follows:

1. Create artificial data using random number generators based on a specific statistical model, or more generally, a *Data-Generating Process* (DGP).
2. Apply one or more data-analysis procedures to the artificial data. (These procedures might be something as simple as calculating a difference in sample means or fitting a regression model, or it might be an involved, multi-step procedure involving cleansing the data of apparent outliers, imputing missing values, applying a machine-learning algorithm, and carrying out further calculations on the predictions of the algorithm.)
3. Repeat Steps 1 and 2 many times.
4. Summarize the results across these repetitions in order to understand the general trends or patterns in how the method works.

Simulation is useful because one can control the data-generating process and therefore fully know the truth—something that is almost always uncertain when analyzing real, empirical data. Having full control of the data-generating process makes it possible to assess how well a procedure works by comparing the estimates produced by the data analysis procedure against this known truth. For instance, we can see if estimates from a statistical procedure are consistently too high or too low (i.e., whether an estimator is systematically biased). We can also compare multiple data analysis procedures by assessing the degree of error in each set of results to determine which procedure is generally more accurate when applied to the same collection of artificial datasets.

This basic process of simulation can be used to investigate an array of different questions that arise in statistics and quantitative methodology. To seed the field, we now give a high-level overview of some of the major use cases. We then discuss some of the major limitations and common pitfalls of simulation studies, which are important to keep in mind as we proceed.

1.1   Some of simulation's many uses

Monte Carlo simulations allow for rapid exploration of different data analysis procedures and, even more broadly, different approaches to designing studies and collecting measurements. Simulations are especially useful because they provide a means to answer questions that are difficult or impossible to answer by other means. Many statistical models and estimation methods *can* be analyzed mathematically, but only by using asymptotic approximations that describe how the methods work as sample size increases towards infinity. In contrast, simulation methods provide answers for specific, finite sample sizes. Thus, they allow researchers to study models and estimation methods where relevant mathematical formulas are not available, not easily applied, or not sufficiently accurate.

Circumstances where simulations are helpful—or even essential—occur in a

range of different situations within quantitative research. To set the stage for our subsequent presentation, consider the following areas where one might find need of simulation.

1.1.1 Comparing statistical approaches

One of the more common uses of Monte Carlo simulation is to compare alternative statistical approaches to analyzing the same type of data. In the academic literature on statistical methodology, authors frequently report simulation studies comparing a newly proposed method against more traditional approaches, to make a case for the utility of their method. A classic example of such work is Brown and Forsythe (1974), who compared four different procedures for conducting a hypothesis test for equality of means in several populations (i.e., one-way ANOVA) when the population variances are not equal. A subsequent study by Mehrotra (1997) built on Brown and Forsythe's work, proposing a more refined method and using simulations to demonstrate that it is superior to the existing methods. We explore the Brown and Forsythe (1974) study in the case study of Chapter 5.

Comparative simulation can also have a practical application: In many situations, more than one data analysis approach is possible for addressing a given research question (or estimating a specified target parameter). Simulations comparing multiple approaches can be quite informative and can help to guide the design of an analytic plan (such as plans included in a pre-registered study protocol). For instance, researchers designing a multi-site randomized experiment might wonder whether they should use an analytic model that allows for variation in the site-specific impact estimates (Miratrix et al., 2021) or a simpler model that treats the impact as homogeneous across sites. What are the practical benefits and costs of using the more complex model? In the ideal case, simulations can identify best practices for how to approach analysis of a certain type of data and can surface trade-offs between competing approaches that occur in practice.

1.1.2 Assessing performance of complex pipelines

In practice, statistical methods are often used as part of a multi-step workflow. For instance, in a regression model, one might first use a statistical test for heteroskedasticity (e.g., the White test or the Breusch-Pagan test) and then determine whether to use conventional or heteroskedasticity-robust standard errors depending on the result of the test. This combination of an initial diagnostic test followed by contingent use of different statistical procedures is quite difficult to analyze mathematically, but it is straight-forward to simulate (see, for example, Long and Ervin, 2000). In particular, simulations are a straightfoward way to assess whether a proposed workflow is *valid*—that is, whether the conclusions from a pipeline are correct at a given level of certainty.

Beyond just evaluating the performance characteristics of a workflow, simulating

a multi-step workflow can actually be used as a technique for *conducting* statistical inference with real data. Data analysis approaches such as randomization inference and bootstrapping involve repeatedly simulating data and putting it through an analytic pipeline, in order to assess the uncertainty of the original estimate based on real data. In bootstrapping, the variation in a point estimate across replications of the simulation is used as the standard error for the context being simulated; an argument by analogy (the bootstrap analogy) is what connects this to inference on the original data and point estimate. See the first few chapters of Davison and Hinkley (1997) or Efron (2000) for further discussion of bootstrapping, and see Good (2013) or Lehmann et al. (1975) for more on permutation inference.

1.1.3   Assessing performance under misspecification

Many statistical estimation procedures are known to perform well when the assumptions they entail are correct. However, data analysts must also be concerned with the *robustness* of estimation procedures—that is, their performance when one or more of the assumptions is violated to some degree. For example, in a multilevel model, how important is the assumption that the random effects are normally distributed? What about normality of the individual-level error terms? What about homoskedasticity of the individual-level error terms? Quantitative researchers routinely contend with such questions when analyzing empirical data, and simulation can provide some answers.

Similar concerns arise for researchers considering the trade-offs between methods that make relatively stringent assumptions versus methods that are more flexible or adaptive. When the true data-generating process meets stringent assumptions (e.g., a treatment effect that is constant across the population of participants), what are the potential gain of exploiting such structure in the estimation process? Conversely, what are the costs (in terms of computation time or precision) of using more flexible methods that do not impose strong assumptions? A researcher designing an analytic plan would want to be well-informed of such trade-offs and, ideally, would want to situate their understanding in the context of the empirical phenomena that they study. Simulation allows for such investigation and comparison.

1.1.4   Assessing the finite-sample performance of a statistical approach

Many statistical estimation procedures can be shown (through mathematical analysis) to work well *asymptotically*—that is, given an infinite amount of data—but their performance for data of a given, finite size is more difficult to quantify. Although mathematical theory can inform us about "asymptopia," empirical researchers live in a world of finite sample sizes, where it can be difficult to gauge if one's real data is large enough that the asymptotic approximations apply. For example, this is of particular concern with hierarchical data structures that

include only 20 to 40 clusters—a common circumstance in many randomized field trials in education research. Simulation is a tractable approach for assessing the small-sample performance of such estimation methods or for determining minimum required sample sizes for adequate performance.

One example of a simulation investigating questions of finite-sample behavior comes from Long and Ervin (2000), whose evaluated the performance of heteroskedasticity-robust standard errors (HRSE) in linear regression models. Asymptotic analysis indicates that HRSEs work well (in the sense of providing correct assessments of uncertainty) in sufficiently large samples (White (1980)), but what about in realistic contexts where small samples occur? Long and Ervin (2000) use extensive simulations to investigate the properties of different versions of HRSEs for linear regression across a range of sample sizes, demonstrating that the most commonly used form of these estimators often does *not* work well with sample sizes found in typical social science applications. Via simulation, they provided compelling evidence about a problem without having to wade into a technical (and potentially inaccessible) mathematical analysis of the problem.

1.1.5 Conducting Power Analyses

During the process of proposing, seeking funding for, and planning an empirical research study, researchers need to justify the design of the study, including the size of the sample that they aim to collect. Part of such justifications may involve a *power analysis*, or an approximation of the probability that the study will show a statistically significant effect, given assumptions about the magnitude of true effects and other aspects of the data-generating process. Researchers may also wish to compare the power of different possible designs in order to inform decisions about how to carry out the proposed study given a set of monetary and temporal constraints.

Many guidelines and tools are available for conducting power analysis for various research designs, including software such as PowerUp! (Dong and Maynard, 2013), the Generalizer (Tipton, 2013), G*Power (Faul et al., 2009), and PUMP (Hunter et al., 2024). These tools use analytic formulas for power, which are often derived using approximations and simplifying assumptions about a planned design. Simulation provides a very general-purpose alternative for power calculations, which can avoid such approximations and simplifications. By repeatedly simulating data based on a hypothetical process and then analyzing data following a specific protocol, one can *computationally* approximate the power to detect an effect of a specified size.

Using simulation instead of analytic formulas allows for power analyses that are more nuanced and more tailored to the researcher's circumstance than what can be obtained from available software. For example, simulation can be useful for the following:

- When estimating power in multi-site, block- or cluster-randomized trials,

the formulas implemented in available software assume that sites are of equal size and that outcome distributions are unrelated to the size of each site. Small deviations from these assumptions are unlikely to change the results, but in practice, researchers may face situations where sites vary quite widely in size or where site-level outcomes are related to site size. Simulation can estimate power in this case.

- Available software such as PowerUp! allows investigators to build in assumptions about anticipated rates of attrition in cluster-randomized trials, under the assumption that attrition is completely at random and unrelated to anything. However, researchers might anticipate that, in practice, attrition will be related to baseline characteristics. Simulation can be used to assess how this might affect the power of a planned study.

- There are some closed-form expressions for power to test mediational relations (i.e., indirect and direct effects) in a variety of different experimental designs, and these formulas are now available in PowerUp!. However, the formulas involve a large number of parameters (including some where it may be difficult to develop credible assumptions) and they apply only to a specific analytic model for the mediating relationships. Researchers planning a study to investigate mediation might therefore find it useful to generate realistic data structures and conduct power analysis via simulation.

1.1.6   Simulating processess

Yet another common use for Monte Carlo simulation is as a way to emulate a complex process as a means to better understand it or to evaluate the consequences of modifying it. A famous area of process simulation are climate models, where researchers simulate the process of climate change. These physical simulations mimic very complex systems to try and understand how perturbations (e.g., more carbon release) will impact downstream trends.

Another example of process simulation arises in education research. Some large school districts such as New York City have centralized lotteries for school assignment, which entail having families rank schools by order of preference. The central office then assigns students to schools via a lottery procedure where each student gets a lottery number that breaks ties when there are too many students desiring to go to certain schools. Students' school assignments are therefore based in part on random chance, but the the process is quite complex: each student has some probability of assignment to each school on their list, but the probabilities depend on their choices and the choices of other students.

The school lottery process creates a natural experiment, based on which researchers can estimate the causal impact of being assigned to one school vs. another. A defensible analysis of the process requires knowing the probabilities of school assignment. Abdulkadiroğlu et al. (2017) conducted such an evaluation using the school lottery process in New York City. They calculated school

assignment probabilities via simulation, by running the school lottery over and over, changing only students' lottery numbers, and recording students' school assignments in each repetition of the process. Simulating the lottery process a large number of times provided precise estimates of each students' assignment probabilities, based on which Abdulkadiroğlu et al. (2017) were able to estimate causal impacts of school assignment.

For another example, one that possibly illustrates the perils of simulation as taking us away from results that pass face validity, Staiger and Rockoff (2010) simulated the process of firing teachers depending on their estimated value-added scores. Based on their simulations, which model firing different proportions of teachers, they suggest that firing substantial portions of the teacher workforce annually would substantially improve student test scores. Their work offers a clear illustration of how simulations can be used to examine the potential consequences of various policy decisions, assuming the underlying assumptions hold true. This example also brings home a core concern of simulation: we only learn about the world we are simulating, and the relevance of simulation evidence to the real world is by no means guaranteed.

1.2 The perils of simulation as evidence

Simulation has the potential to be a powerful tool for investigating quantitative methods. However, evidence from simulation studies is also fundamentally limited in certain ways, and thus very susceptible to critique. The core advantage of simulation studies is that they allow for evaluation of data analysis methods under *specific and exact conditions*, avoiding the need for approximation. The core limitation of simulations stems from this same property: they provide information about the performance of data analysis methods under specified conditions, but provide no guarantee that patterns of performance hold in general. One can partially address questions of generalization by examining a wide range of conditions, looking to see whether a pattern holds consistently or changes depending on features of the data-generating process. Even this strategy has limitations, though. Except for very simple processes, we can seldom consider every possible set of conditions.

As we will see in later chapters, the design of a simulation study typically entails making choices over very large spaces of possibility. This flexibility leaves lots of room for discretion and judgement, and even for personal or professional biases (Boulesteix et al., 2020). Due to this flexibility, simulation findings are held in great skepticism by many. The following motto summarizes the skeptic's concern:

> Simulations are doomed to succeed.

As this motto captures, simulations are alluring: once a simulation framework is set up, it is easy to tweak and adjust. It is natural for us all to continue to do this until the simulation works "as it should." If our goal is to show something that

we already believe is correct (e.g., that our fancy new estimation procedure is better than existing methods), we could probably find a way to align our simulation with our intuition.[1]

Critiques of simulation studies often revolve around the *realism*, *relevance*, or *generality* of the data generating process. Are the simulated data realistic, in the sense that they follow similar patterns to what one would see in real empirical data? Are the explored aspects of the simulation relevant to what we would expect to find in practice? Was the simulation systematic in exploring a wide variety of scenarios, so that general conclusions are warranted?

We see at least three principles for addressing such questions in one's own work. Perhaps most fundamental is to be transparent in one's methods and reasoning: explicitly state what was done, and provide code so that others can reproduce one's results or tweak them to test variations of the data-generating process or alternative analysis strategies. Another important component of a robust argument is to systematically vary the conditions under examination. This is facilitated by writing code in a way to make it easy to simulate across a range of different data-generating scenarios. Once that is in place, one can systematically explore myriad scenarios and report all of the results. An aspiration of the simulation architect should be to explore the boundary conditions that separate where preferred methods work and where they break or fail. Finally, one can draw on relevant statistical theory to support the design of a simulation and interpretation of its results. Mathematical analysis might indicate that some features of a data-generating process will have a strong influence on the performance of a method, while other features will not matter at all when sample sizes are sufficiently large. Well designed simulations will examine conditions that are motivated by or complement what is known based on existing statistical theory.

In addition to these principles, methodologists have proposed broader changes in practice to counter the potential for bias in methodological simulation studies. Morris et al. (2019) introduced a formal framework, called ADEMP, to guide the reporting of methodological simulations. Boulesteix et al. (2013) argued for greater use of neutral comparison studies, in which the performance of alternative statistical methods are compared under a range of relevant conditions by methodological researchers who do not have vested interests in any specific method (see also Boulesteix et al., 2017). Further, Siepe et al. (2024) argue for more routine pre-registration of methodological simulations to bring greater transparency and reduce the possibility of bias arising from flexibility in their design.

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[1]A comment from James: I recall attending seminars in the statistics department during graduate school, where guest speakers usually presented both some theory and some simulation results. A few years into my graduate studies, I realized that the simulation part of the presentation could nearly always be replaced with a single slide that said "we did some simulations and showed that our new method works better than old methods under conditions that we have cleverly selected to be favorable for our approach." I hope that my own work is not as boring or predictable as my memory of these seminars.

1.3 Simulating to learn

Most of the examples of Monte Carlo simulation that we have mentioned thus far are drawn from formal methodological research, published in methodologically focused research journals. If you do not identify as a methodologist, you may be wondering whether there is any benefit to learning how to do simulations—what's the point, if you are never going to conduct methodological research studies or use simulation to aid in planning an empirical study? However, we believe that simulation is an incredibly useful tool—and well worth learning, even outside the context of formal methodological research—for at least two reasons.

First, in order to do any sort of quantitative data analysis, you will need to make decisions about what methods to use. Across fields, existing guidance about data analysis practice is almost certainly informed by simulation research of some form, whether well-designed and thorough or haphazard and poorly reasoned. Consequently, having a high-level understanding of the logic and limitations of simulation will help you to be a critical consumer of methods research, even if you do not intend to conduct methods research of your own.

Second, we believe conducting simulations deepens one's understanding of the logic of statistical modeling and statistical inference. Learning a new statistical model (such as generalized linear mixed models) or analytic technique (such as multiple imputation by chained equations) requires taking in *a lot* of detailed information, from the assumptions of the model to the interpretation of parameter estimates to the best practices for estimation and what to do if some part of the process goes off. To thoroughly digest all these details, we have found it invaluable to *simulate* data based on the model under consideration. This usually requires translating mathematical notation into computer code, an exercise which makes the components of the model more tangible than just a jumble of Greek letters. The simulated data is then available for inspection, summarizing, graphing, and further calculation, all of which can aid comprehension and interpretation. Moreover, the process of simulating yields a dataset which can then be used to practice implementing the analysis procedure and interpreting the results. We have found that building a habit of simulating is a highly effective way to learn new models and methods, worthwhile even if one has no intention of carrying out methodological research. We might even go so far as to argue that *whatever you might think, you don't really understand a statistical model until you've done a simulation of it.*

1.4 Why R?

This book aims not only to introduce the conceptual principles of Monte Carlo simulation, but also to provide a practical guide to actually *conducting* simulation studies (whether for personal learning purposes or for formal methodological research). And conducting simulations requires writing computer code (some-

times, lots of code!). The computational principles and practices that we will describe are very general, not specific to any particular programming language, but for purposes of demonstrating, presenting examples, and practicing the process of developing a simulation, it helps to be specific. To that end, we will be using R, a popular programming language that is widely used among statisticians, quantitative methodologists, and data scientists. Our presentation will assume that readers are comfortable with writing R scripts to carry out tasks such as cleaning variables, summarizing data, creating data-based graphics, and running regression models (or more generally, estimating statistical models).

We have chosen to focus on R (rather than some other programming language) because both of us are intimately familiar with R and use it extensively in our day-to-day work. Simply put, it is much easier to write in your native language than in one in which you are less fluent. But beyond our own habits and preferences, there are several more principled reasons for using R.

R is free and open source software, which can be run under many different operating systems (Windows, Mac, Linux, etc.). This is advantageous not only because of the cost, but also because it means that anyone with a computer—anywhere in the world—can access the software and could, if they wanted, re-run our provided code for themselves. This makes R a good choice for practicing transparent and open science processes.

There is a very large, active, and diverse community of people who use, teach, and develop R. It is used widely for applied data analysis and statistical work in such fields as education, psychology, economics, epidemiology, public health, and political science, and is widely taught in quantitative methods and applied statistics courses. Integral to the appeal of R is that it includes tens of thousands of contributed packages, which extend the core functionality of the language in myriad ways. New statistical techniques are often quickly available in R, or can be accessed through R interfaces. Increasingly, R can also be used to interface with other languages and platforms, such as running Python code via the `reticulate` package, running Stan programs for Bayesian modeling via `RStan`, or calling the h2o machine learning library using the `h2o` package (Fryda et al., 2014). The huge variety of statistical tools available in R makes it a fascinating place to learn and practice.

R does have a persistent reputation as being a challenging and difficult language to use. This reputation might be partly attributable to its early roots, having been developed by highly technical statisticians who did not necessarily prioritize accessibility, legibility of code, or ease of use. However, as the R community has grown, the availability of introductory documentation and learning materials has improved drastically, so that it is now much easier to access pedagogical materials and find help.

R's reputation also probably partly stems from being a decentralized, open source project with many, many contributors. Contributed R packages vary hugely in quality and depth of development; there are some amazingly powerful

tools available but also much that is half-baked, poorly executed, or flat out wrong. Because there is no central oversight or quality control, the onus is on the user to critically evaluate the packages that they use. For newer users especially, we recommend focusing on more established and widely used packages, seeking input and feedback from more knowledgeable users, and taking time to validate functionality against other packages or software when possible.

A final contributor to R's intimidating reputation might be its extreme flexibility. As both a statistical analysis package and a fully functional programming language, R can do many things that other software packages cannot, but this also means that there are often many different ways to accomplish the same task. In light of this situation, it is good to keep in mind that knowing a single way to do something is usually adequate—there is no need to learn six different words for hello, when one is enough to start a conversation.

On balance, we think that the many strengths of R make it worthwhile to learn and continue exploring. For simulation, in particular, R's facility to easily write functions (bundles of commands that you can easily call in different manners), to work with multiple datasets in play at the same time, and to leverage the vast array of other people's work all make it a very attractive language.

1.5   Organization of the text

We think of simulation studies as falling on a spectrum of formality. On the least formal end, we may use simulations to learn a statistical model, investigating questions purely to satisfy our own curiosity. On the most formal end, we may conduct carefully designed, pre-registered simulations that compare the performance of competing statistical methods across an array of data-generating conditions designed to inform practice in a particular research area.

Our central goal is to help you learn to work anywhere along this spectrum, from the most casual to the most principled. To support that goal, the book is designed with a spiral structure, where we first present simpler and less formal examples that illustrate high-level principles, then revisit the component pieces, dissecting and exploring them in greater depth. We defer discussion of concepts that are relevant only to more formal use-cases (such as the ADEMP framework of Morris et al. (2019)) until later chapters. We have also included many case studies throughout the book; these are designed to make the topics under discussion tangible, and are also designed to provide chunks of code that you emulate or even directly copy and use for your own purposes.

We divided the book into several parts. In Part I (which you are reading now), we lay out our case for learning simulation, introduces some guidance on programming, and presents an initial, very simple simulation to set the stage for later discussion of design principles. Part II lays out the core components (generating artificial data, applying analytic procedures, executing the simulations, and analyzing the simulation results) for simulating a single scenario. It then

presents some more involved case studies that illustrate the principles of modular, tidy simulation design. Part III moves to multifactor simulations, meaning simulations that look at more than one scenario or context. Multifactor simulation is central to the design of more formal simulation studies because it is only by evaluating or comparing estimation procedures across multiple scenarios that we can begin to understand their general properties.

The book closes with two final parts. Part IV covers some technical challenges that are commonly encountered when programming simulations, including reproducibility, parallel computing, and error handling. Part V covers three extensions to specialized forms of simulation: simulating to calculate power, simulating within a potential outcomes framework for causal inference, and the parametric bootstrap. The specialized applications underscore how simulation can be used to answer a wide variety of questions across a range of contexts, thus connecting back to the broader purposes discussed above. The book also includes appendices with some further guidance on writing R code and pointers to further resources.

Chapter 2

Programming Preliminaries

In this chapter, we introduce some essential programming concepts that may be less familiar to readers, but which are central to how we approach writing code for simulation studies. We also explain some of the rationale and reasoning behind how we present example code throughout the book.

2.1   Welcome to the tidyverse

Layered on top of R are a collection of contributed packages that make data wrangling and management much, much easier. This collection is called `tidyverse` and it includes popular packages such as `dplyr`, `tidyr`, and `ggplot2`. We use methods from the "tidyverse" throughout the book because it facilitates writing clean, concise code. In particular, we make heavy use of the `dplyr` package for group-wise data manipulation, the `purrr` package for functional programming, and the `ggplot2` package for statistical graphics. The 1st edition or 2nd edition of the free online textbook *R for Data Science* provide an excellent, thorough introduction to these packages, along with much more background on the tidyverse. We will cite portions of this text throughout the book.

Loading the tidyverse packages is straightforward:

```r
library( tidyverse )
options(list(dplyr.summarise.inform = FALSE))
```

(The second line is to turn off some of the persistent warnings generated by the `dplyr` function `summarize()`.) These lines of code appear in the header of nearly every script we use.

2.2   Functions

If you are comfortable using R for data analysis tasks, you will be familiar with many of R's functions. R has function to do things like calculate a summary statistic from a list of numbers (e.g., `mean()`, `median()`, or `sd()`), calculate linear regression coefficient estimates from a dataset (`lm()`), or count the number of rows in a dataset (`nrow()`). In the abstract, a function is a little machine for transforming ingredients into outputs, like a microwave (put a bag of kernels in and it will return hot, crunchy popcorn), a cheese shredder (put a block of mozzarella in and it transforms it into topping for your pizza), or a washing machine (put in dirty clothes and detergent and it will return clean but damp clothes). A function takes in pieces of information specified by the user (the inputs), follows a set of instructions for transforming or summarizing those inputs, and then returns the result of the calculations (the outputs).

A function can do nearly anything as long as the calculation can be expressed in code—it can even produce output that is random. For example, the `rnorm()` function takes as input a number `n` and returns that many random numbers, drawn from a standard normal distribution:

```
rnorm(3)
```

```
## [1] -1.7372203  1.9057092 -0.7121786
```

Each time the function is called, it returns a different set of numbers:

```
rnorm(3)
```

```
## [1] -0.05632604  1.03322514 -1.10335909
```

The `rnorm()` function also has further input arguments that let the user specify the mean and standard deviation of the distribution from which numbers are drawn:

```
rnorm(3, mean = 10, sd = 0.5)
```

```
## [1] 10.734061  9.756171 10.136555
```

In writing code for simulations, we will make extensive use of this particular function and other functions that produce sequences of random numbers. We will have more to say about random number generation later.

2.2.1   Rolling your own

In R, you can create your own function by specifying the pieces of input information, the steps to follow in transforming the inputs, and the result to return as output. Learning to write your own functions to carry out calculations is an immensely useful skill that will greatly enhance your ability to accomplish a range of tasks. Writing custom functions is also central to our approach to coding Monte Carlo simulations, and so we highlight some of the key considera-

tions here. Chapter 19 of R for Data Science (1st edition) provides an in-depth discussion of how to write your own functions.

Here is an example of a custom function called `one_run()`:

```r
one_run <- function( N, mn, sd ) {
  vals <- rnorm( N, mean = mn, sd = sd )
  tt <- t.test( vals )
  pvalue <- tt$p.value
  return(pvalue)
}
```

The first line specifies that we are creating a function that takes inputs `N`, `mn`, and `sd`. These are called the *parameters*, *inputs*, or *arguments* of the function. The remaining lines inside the curly brackets are called the *body* of the function. These lines specify the instructions to follow in transforming the inputs into an output:

1. Generate a random sample of `N` observations from a normal distribution with mean `mn` and store the result in `vals`.
2. Use the built-in function `t.test()` to compute a one-sample t-test for the null hypothesis that the population mean is zero, then store the result in `tt`.
3. Extract the p-value from the t-test store the result in `pvalue`.
4. Return `pvalue` as output.

Having created the function, we can then use it with any inputs that we like:

```r
one_run( 100, 5, 1 )
```

```
## [1] 1.380295e-76
```

```r
one_run( 10, 0.3, 1 )
```

```
## [1] 0.5815231
```

```r
one_run( 10, 0.3, 0.2 )
```

```
## [1] 0.0001038725
```

In each case, the output of the function is a p-value from a simulated sample of data. The function produces a different answer each time because its instructions involve generating random numbers each time it is called. In essence, our custom function is just a short-cut for carrying out its instructions. Writing it saves us from having to repeatedly write or copy-paste the lines of code inside its body.

2.2.2   A dangerous function

Writing custom functions will prove to be crucial for effectively implementing Monte Carlo simulations. However, designing custom functions does take prac-

tice to master. It also requires a degree of care above and beyond what is needed just to use R's built-in functions.

One of the common mistakes encountered in writing custom functions is to let the function depend on information that is not part of the input arguments. For example, consider the following script, which includes a nonsensical custom function called `funky()`:

```r
secret <- 3

funky <- function(input1, input2, input3) {

  # do funky stuff
  ratio <- input1 / (input2 + 4)
  funky_output <- input3 * ratio + secret

  return(funky_output)
}

funky(3, 2, 5)
```

```
## [1] 5.5
```

`funky` takes inputs `input1`, `input2`, and `input3`, but its instructions also depend on the quantity `secret`. What happens if we change the value of `secret`?

```r
secret <- 100
funky(3, 2, 5)
```

```
## [1] 102.5
```

Even though we give it the same arguments as previously, the output of the function is different. This sort of behavior is confusing. Unless the function involves generating random numbers, we would generally expect it to return the exact same output if we give it the same inputs. Even worse, we get a rather cryptic error if the value of `secret` is not compatible with what the function expects:

```r
secret <- "A"
funky(3, 2, 5)
```

```
## Error in input3 * ratio + secret: non-numeric argument to binary operator
```

If we are not careful, we will end up with very confusing code that can very easily lead to unintended results and errors.

To avoid this issue, it is important for functions to only use information that is explicitly provided to it through its arguments. This is the principle of *isolating the inputs*. If the result of a function is supposed to depend on a quantity, then we should include that quantity among the input arguments. We can fix our

example function by including `secret` as an argument:

```r
secret <- 3

funkier <- function(input1, input2, input3, secret) {

  # do funky stuff
  ratio <- input1 / (input2 + 4)
  funky_output <- input3 * ratio + secret

  return(funky_output)
}

funkier(3, 2, 5, 3)
```

```
## [1] 5.5
```

Now the output of the function is always the same, regardless of the value of other objects in R:

```r
secret <- 100
funkier(3, 2, 5, 3)
```

```
## [1] 5.5
```

The *input parameter* `secret` holds sway here, even though there is also an object with the same name.[1] If we want to try 100, we have to do so *explicitly*:

```r
funkier(3, 2, 5, 100)
```

```
## [1] 102.5
```

When writing your own functions, it may not be obvious that your function depends on external quantities and does not isolate the inputs. In our experience, one of the best ways to detect this issue is to clear the R environment and start from a fresh palette, run the code to create the function, and call the function (perhaps more than once) to ensure that it works as expected. Here is an illustration of what happens when we follow this process with our problematic custom function:

```r
# clear environment
rm(list=ls())

# create function
funky <- function(input1, input2, input3) {

  # do funky stuff
  ratio <- input1 / (input2 + 4)
```

---

[1]To learn more about how R determines which values to use when executing a function, see Section 6.4 of Advance R.

```r
  funky_output <- input3 * ratio + secret

  return(funky_output)
}

# test the function
funky(3, 2, 5)
```

```
## Error in funky(3, 2, 5): object 'secret' not found
```

We get an error because the external quantity is not available. Here is the same process using our corrected function:

```r
# clear environment
rm(list=ls())

# create function
funkier <- function(input1, input2, input3, secret) {

  # do funky stuff
  ratio <- input1 / (input2 + 4)
  funky_output <- input3 * ratio + secret

  return(funky_output)
}


# test the function
funkier(3, 2, 5, secret = 3)
```

```
## [1] 5.5
```

2.2.3 Using Named Arguments

When calling a function (whether it is a built-in function or a custom function that you developed), you can specify which values correspond to which arguments using argument names. Using argument names greatly enhances the readability and flexibility of function calls. When you specify inputs by name, R matches the values to the arguments based on the names rather than the order in which they appear. This feature is particularly useful in complex functions with many optional arguments.

For example, consider the function `one_run()` from 2.2.1:

```r
one_run <- function( N, mn, sd ) {
  vals <- rnorm( N, mean = mn, sd = sd )
  tt <- t.test( vals )
  pvalue <- tt$p.value
```

```
  return(pvalue)
}
```

You could call **one_run()** with *named* arguments in any order:

```
result <- one_run(sd = 0.5, mn = 2, N = 500)
```

In this call, R knows which value to assign to each argument, so we could list the arguments however we like.

Without naming, we would have to specify the arguments in the exact order that they appear in the function definition:

```
result <- one_run( 500, 2, 0.5 )
```

Without the argument names, this line of code is harder to follow—you have to know more about the design of the function to understand how it is being used in this instance.

Getting in the habit of using named arguments will help you avoid errors. If you pass arguments without naming, and in the wrong order, you can end up with very strange results that are hard to diagnose. Even if you get it right, if someone later changes the function (say by adding a new argument in the middle of the list), your code will suddenly break with no explanation.

2.2.4   Argument Defaults

Default arguments allow you to specify typical values for parameters that a user might not need to change every time they use the function. This can make the function easier to use and less error-prone because the defaults ensure that the function behaves sensibly even when some arguments are not explicitly provided. For example, let us revise the **one_run()** function from above to use default arguments:

```
one_run <- function( N = 10, mn = 0, sd = 1 ) {
  vals <- rnorm( N, mean = mn, sd = sd )
  tt <- t.test( vals )
  pvalue <- tt$p.value
  return(pvalue)
}
```

Now our function has a default for N of 10, for **mn** of 0, and for **s** of 1. This means a user can run the function simply by calling **one_run()** without any inputs. Doing so will generate a p-value from a sample of 10 observations with a mean of zero and a standard deviation of 1.

Once we have our function with defaults, we can call the function while specifying only the inputs that differ from the default values:

```r
bigger_sample <- one_run( N = 50 )
```

The function will use its default values for `mn` and `s`. Using defaults lets the user call the function more succinctly.

Later chapters will have much more to say about the process of writing custom functions, as well as many further illustrations and examples.

2.2.5   Function skeletons

In discussing how to write functions for simulations, we will often present *function skeletons*. By a skeleton, we mean code that creates a function with a specific set of input arguments, but where the body is left partially or fully unspecified. Here is a cursory example of a function skeleton:

```r
run_simulation <- function( N, J, mu, sigma, tau ) {
  # simulate data
  # apply estimation procedure
  # repeat
  # summarize results
  return(results)
}
```

In subsequent chapters, we will use function skeletons to outline the organization of code for simulation studies. The skeleton headers make clear what the inputs to the function need to be. Sometimes, we will leave comments in the body of the skeleton to sketch out the general flow of calculations that need to happen. Depending on the details of the simulation, the specifics of these steps might be quite different, but the general structure will often be quite consistent. Finally, the last line of the skeleton indicates the value that should be returned as output of the function. Thus, skeletons are kind of like Mad Libs, but with R code instead of parts of speech.

2.3   \> (Pipe) dreams

Many of the functions from `tidyverse` packages are designed to make it easy to use them in sequence via the `|>` symbol, or *pipe*.[2] The pipe allows us to *compose* several functions, meaning to write a chain of several functions as a sequence, where the result of each function becomes the first input to the next function. In code written with the pipe, the order of function calls follows like a story book or cake recipe, making it easier to see what is happening at each step in the sequence.

---

[2]The pipe is a relatively recent addition to R's basic syntax. Prior to its inclusion in base R, the `magrittr` package provided—and still provides—a pipe symbol `%>%` that works similarly but has some additional syntactic nuances. We use base R's `|>` because it is always available, even without loading any additional packages. To learn more about the nuanced `%>%` pipe and similar operators, see the magrittr package.

Consider the hypothetical functions `f()`, `g()`, and `h()`, and suppose we want to do a calculation that involves composing all three functions. One way to write this calculation is

```
res1 <- f(my_data, a = 4)
res2 <- g(res1, b = FALSE)
result <- h(res2, c = "hot sauce")
```

We have to store the result of each intermediate step in an object, and it takes a careful read of the code to see that we are using `res1` as input to `g()` and `res2` as input to `h()`.

Alternately, we could try to write all the calculations as one line:

```
result <- h( g( f( my_data, a = 4 ), b = FALSE ), c = "hot sauce" )
```

This is a mess. It takes very careful parsing to see that the `b` argument is called as part of `g()` and the `c` argument is part of h()', and the order in which the functions appear is not the same as the order in which they are calculated.

With the pipe we can write the same calculation as

```
result <-
  my_data |>           # initial dataset
  f(a = 4) |>          # do f() to it
  g(b = FALSE) |>      # then do g()
  h(c = "hot sauce")   # then do h()
```

This addresses the all the issues with our previous attempts: the order in which the functions appear is the same as the order in which they are executed; the additional arguments are clearly associated with the relevant functions; and there is only a single object holding the results of the calculations. Pipes are a very nice technique for writing clear code that is easy for others to follow.[3]

2.4 Recipes versus Patterns

As we will elaborate in subsequent chapters, we follow a modular approach to writing simulations, in which each component of the simulation is represented by its own custom function or its own object in R. This modular approach leads to code that always has the same broad structure and where the process of implementing the simulation follows a set sequence of steps. We start by coding a data-generating process, then write one or more data-analysis methods, then determine how to evaluate the performance of the methods, and finally implement an experimental design to examine the performance of the methods

---

[3]Chapter 3.4 of R for Data Science (2nd edition) provides more discussion and examples of how to use `|>`. Chapter 18 of R for Data Science (1st edition) provides more discussion and examples of how to use `magrittr`'s `%>%`.

across multiple scenarios. Over the next several chapters, we will walk through this process several times.

Although we always follow the same broad process, the case studies that we will present are *not* intended as a cookbook that must be rigidly followed. In our experience, the specific features of a data-generating model, estimator, or research question sometimes require tweaking the template or switching up how we implement some aspect of the simulation. And sometimes, it might just be a question of style or preference. Because of this, we have purposely constructed the examples presented throughout the book to use different variations of our central theme rather than always following the exact same style and structure. We hope that presenting these variants and adaptations will both expand your sense of what is possible and also help you to recognize the core design principles—in other words, to distinguish the forest from the trees. Of course, we would welcome and encourage you to take any of the code verbatim, tweak and adapt it for your own purposes, and use it however you see fit. Adapting a good example is usually much easier than starting from a blank screen.

2.5   Exercises

1. Revise the `one_run()` function to use `|>` instead of storing the simulated sample in `vals`.

2. Modify the `one_run()` function to return a `tibble()` that includes separate columns for the test statistic (called `tt$statistic`), the p-value, and the lower and upper end-points of the confidence interval (called `tt$conf.int`).

3. Modify the `one_run()` function so that the sample of data is generated from a non-central t distribution by substituting R's `rt()` function in place of `rnorm()`. Make sure to modify the arguments (and argument names) of `one_run()` to allow the user to specify the non-centrality and degrees of freedom parameters of the non-central t distribution.

4. The non-central t distribution is usually parameterized in terms of non-centrality parameter δ and degrees of freedom ν, and these parameters determine the mean and spread of the distribution. Specifically, the mean of the non-central t distribution is

$$\mathrm{E}(T) = \delta \times \sqrt{\frac{\nu}{2}} \times \frac{\Gamma((\nu - 1)/2)}{\Gamma(\nu/2)},$$

   where $\Gamma()$ is the gamma function (called `gamma()` in R). Create a version of the `one_run()` function that generates data based on a non-central t distribution, but where the input arguments are `mn` for the mean and `df` for the degrees of freedom. Here is a function skeleton to get started:

```r
one_run <- function( N = 10, mn = 5, df = 4) {

  # generate data from non-central t distribution
  # vals <-

  # calculate one-sample t-test
  tt <- t.test( vals )

  # compile results into a tibble and return
  # res <-

  return(res)
}
```

5. Modify `one_run()` to allow the user to specify a hypothesized value for the population mean, to use when calculating the one-sample t-test results.

Chapter 3

An initial simulation

To begin learning about simulation, a good starting place is to examine a small, concrete example. This example illustrates how simulation involves replicating the data-generating and data-analysis processes, followed by aggregating the results across replications. Our little example encapsulates the bulk of our approach to Monte Carlo simulation, touching on all the main components involved. In subsequent chapters we will look at each of these components in greater detail. But first, let us look at a simulation of a very simple statistical problem.

The one-sample t-test is one of the most basic methods in the statistics literature. It tests a null hypothesis that a population mean of some variable is equal to a specific value by comparing the mean of a sample of data to the hypothesized value. If the sample average is discrepant (very different) from the null value, relative to how uncertain we are about our estimate, then the hypothesis is rejected. The test can also be used to generate a confidence interval for the population mean. If the sample consists of independent observations and the variable is normally distributed in the population, then the confidence interval will have exact coverage, in the sense that 95% intervals will include the population mean in 95 out of 100 tries. But what if the population variable is not normally distributed?

To find out, let us look at the coverage of the t-test's 95% confidence interval for the population mean when the method's normality assumption is violated. *Coverage* is the chance of a confidence interval capturing the true parameter value. To examine coverage, we will simulate many samples from a non-normal population with a specified mean, calculate a confidence interval based on each sample, and see how many of the confidence intervals cover the known true population mean.

Before getting to the simulation, let's look at the data-analysis procedure we will be investigating. Here is the result of conducting a t-test on some fake data,

generated from a normal distribution:

```r
# make fake data
dat <- rnorm( n = 10, mean = 4, sd = 2 )

# conduct the test
tt <- t.test( dat )
tt
```

```
##
##  One Sample t-test
##
## data:  dat
## t = 6.0878, df = 9, p-value = 0.0001819
## alternative hypothesis: true mean is not equal to 0
## 95 percent confidence interval:
##  2.164025 4.723248
## sample estimates:
## mean of x
##  3.443636
```

```r
# examine the confidence interval
tt$conf.int
```

```
## [1] 2.164025 4.723248
## attr(,"conf.level")
## [1] 0.95
```

We generated data with a true (population) mean of 4. Did we capture it? To check, we can use the `findInterval()` function, which checks to see where the first number lies relative to the range given in the second argument. Here is an illustration of the syntax:

```r
findInterval( 1, c(20, 30) )
```

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

```r
findInterval( 25, c(20, 30) )
```

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

```r
findInterval( 40, c(20, 30) )
```

```
## [1] 2
```

The `findInterval()` returns a `1` if the value of the first argument value is in the interval specified in the second argument.

We can apply it to check whether our estimated CI covers the true population mean:

```
findInterval( 4, tt$conf.int )
```

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

In this instance, `findInterval()` is equal to `1`, which means our CI captured the true population mean of 4.

Here is the full code for simulating data, computing the data-analysis procedure, and evaluating the result:

```
# make fake data
dat <- rnorm( n = 10, mean = 4, sd = 2 )

# conduct the test
tt <- t.test( dat )

# evaluate the results
findInterval( 4, tt$conf.int ) == 1
```

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

The above code captures the basic form of a single simulation trial: make the data, analyze the data, decide how well we did. The code also illustrates a good way to figure out the details of a simulation: start by figuring out what a single iteration of the simulation might look like. Starting by mucking about this way also allows us to test and develop our code in an interactive, exploratory fashion. For instance, we can play with `findInterval()` to figure out how to use it to determine whether our confidence interval captured the truth. Once we have arrived at working code for a single iteration, we are in a good position to start writing functions to implement the actual simulation. For now, we have generated data from a normal distribution; we will later revise the code to generate data from a non-normal population distribution.

3.1 Simulating a single scenario

We can estimate the coverage of the confidence interval by repeating the above data-generating and data-analysis processes many, many times. R's `replicate()` function is a handy way to repeatedly call a line of code. Its first input argument is `n`, the number of times to repeat the calculation, followed by `expr`, which is one or more lines of code to be called. We can use `replicate` to repeat our simulation process 1000 times in a row, each time generating a new sample of 10 observations from a normal distribution with mean of 4 and a standard deviation of 2. For each replication, we store the result of using `findInterval()` to check whether the confidence interval includes the population mean of 4.

```
rps <- replicate( 1000, {
  dat <- rnorm( n = 10, mean = 4, sd = 2 )
```

```r
  tt <- t.test( dat )
  findInterval( 4, tt$conf.int )
})

head(rps, 20)
```

```
##  [1] 1 1 1 1 1 1 2 1 1 1 1 1 1 1 1 1 1 1 1 1
```

To see how well we did, we can look at a table of the results stored in `rps` and calculate the proportion of replications that the interval covered the population mean:

```r
table( rps )
```

```
## rps
##   0   1   2
##  27 957  16
```

```r
mean( rps == 1 )
```

```
## [1] 0.957
```

We got about 95% coverage, which is good news. In 27 out of the 1000 replications, the interval was too high (so the population mean was below the interval) and in 16 out of the 1000 replications, the interval was too low (so the population mean was above the interval).

It is important to recognize that this set of simulations results, and our coverage rate of 95.7%, itself has some uncertainty in it. Because we only repeated the simulation 1000 times, what we really have is a *sample* of 1000 independent replications, out of an infinite number of possible simulation runs. Our coverage of 95.7% is an *estimate* of what the true coverage would be, if we ran more and more replications. The source of uncertainty of our estimate is called *Monte Carlo simulation error (MCSE)*. We can actually assess the Monte Carlo simulation error in our simulation results using standard statistical procedures for independent and identically distributed data. Here we use a proportion test to check whether the estimated coverage rate is consistent with a true coverage rate of 95%:

```r
covered <- as.numeric( rps == 1 )
prop.test( sum(covered), length(covered), p = 0.95 )
```

```
##
##  1-sample proportions test with continuity
##  correction
##
## data:  sum(covered) out of length(covered), null probability 0.95
## X-squared = 0.88947, df = 1, p-value =
## 0.3456
```

```
## alternative hypothesis: true p is not equal to 0.95
## 95 percent confidence interval:
##  0.9420144 0.9683505
## sample estimates:
##     p
## 0.957
```

The test indicates that our estimate is consistent with the possibility that the true coverage rate is 95%, just as it should be. Things working out should hardly be surprising. Mathematical theory tells us that the *t*-test is exact for normally distributed population variables, and we generated data from a normal distribution. In other words, all we have found so far is that the confidence intervals follow theory when the assumptions of the method are met.

3.2 A non-normal population distribution

To see what happens when the normality assumption is violated, let us now look at a scenario where the population variable follows a geometric distribution. The geometric distribution is usually written in terms of a probability parameter p, so that the distribution has a mean of $(1 - p)/p$. We will use a geometric distribution with a mean of 4 by setting $p = 1/5$. Here is the population distribution of the variable:
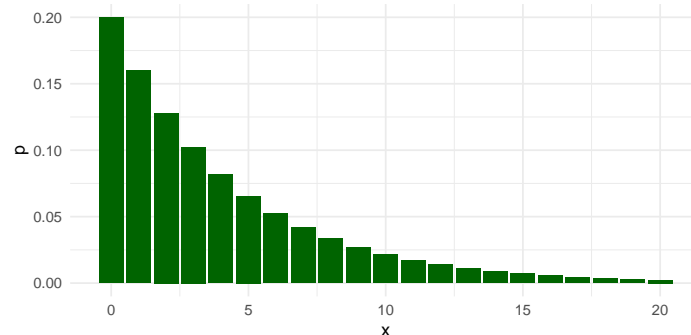
The distribution is highly right-skewed, which suggests that the normal confidence interval might not work very well.

Now let's revise our previous simulation code to use the geometric distribution:

```
rps <- replicate( 1000, {
  dat <- rgeom( n = 10, prob = 1/5 )
  tt <- t.test( dat )
  findInterval( 4, tt$conf.int )
})
table( rps )
```

```
## rps
```

```
##   0   1   2
##   8 892 100
```

Our confidence interval is often entirely too low (such that the population mean is above the interval) and very rarely does our interval fall fully above the population mean. Furthermore, our coverage rate is not the desired 95%:

```
mean( rps == 1 )
```

```
## [1] 0.892
```

To take account of Monte Carlo error, we will again do a proportion test. The following test result calculates a confidence interval for the true coverage rate under the scenario we are examining:

```
covered <- as.numeric( rps == 1 )
prop.test( sum(covered), length(covered), p = 0.95)
```

```
##
##  1-sample proportions test with continuity
##  correction
##
## data:  sum(covered) out of length(covered), null probability 0.95
## X-squared = 69.605, df = 1, p-value <
## 2.2e-16
## alternative hypothesis: true p is not equal to 0.95
## 95 percent confidence interval:
##  0.8707042 0.9102180
## sample estimates:
##     p
## 0.892
```

Our coverage is *too low*; the confidence interval based on the *t*-test misses the the true value more often than it should. We have learned that the *t*-test can fail when applied to non-normal (skewed) data.

3.3 Simulating across different scenarios

So far, we have looked at coverage rates of the confidence interval under a single, specific scenario, with a sample size of 10, a population mean of 4, and a geometrically distributed variable. We know from statistical theory (specifically, the central limit theorem) that the confidence interval should work better if the sample size is big enough. But how big does it have to get? One way to examine this question is to expand the simulation to look at several different scenarios involving different sample sizes. We can think of this as a one-factor experiment, where we manipulate sample size and use simulation to estimate how confidence interval coverage rates change.

To implement such an experiment, we first write our own function that executes the full simulation process for a given sample size:

```
ttest_CI_experiment = function( n ) {

  rps <- replicate( 1000, {
    dat <- rgeom( n = n, prob = 1/5 ) # simulate data
    tt <- t.test( dat )               # analyze data
    findInterval( 4, tt$conf.int )    # evaluate coverage
  })

  coverage <- mean( rps == 1 )        # summarize results

  return(coverage)
}
```

The code inside the body of the function is identical to what we have used above, with the sample size as a function argument, `n`, which enables us to easily run the code for different sample sizes. With our function in hand, we can now run the simulation for a single scenario just by calling it:

```
ttest_CI_experiment(n = 10)
```

```
## [1] 0.885
```

Even though the sample size is still `n = 10`, the simulated coverage rate is a little bit different from what we found previously. That is because there is some Monte Carlo error in each simulated coverage rate.

Our task is now to use this function for several different values of n. We could just do this by copy-pasting and changing the value of `n`:

```
ttest_CI_experiment(n = 10)
```

```
## [1] 0.922
```

```
ttest_CI_experiment(n = 20)
```

```
## [1] 0.91
```

```
ttest_CI_experiment(n = 30)
```

```
## [1] 0.914
```

However, this will quickly get cumbersome if we want to evaluate many different sample sizes. A better approach is to use a mapping function from the `purrr` package.[1] The `map_dbl()` function takes a list of values and calls a function for each value in the list. This accomplishes the same thing as using a `for` loop to

---

[1]Alternately, readers familiar with the `*apply()` family of functions from Base R might prefer to use `lapply()` or `sapply()`, which do essentially the same thing as `purrr::map_dbl()`.

iterate through a list of items (if you happen to be familiar with these), but is more succinct. See Appendix chapter 8.1 for more on `map()`.[2]

To proceed, we first create a list of sample sizes to test out:

```r
ns <- c(10, 20, 30, 40, 60, 80, 100, 120, 160, 200, 300)
```

Now we can use `map_dbl()` to evaluate the coverage rate for each sample size:

```r
coverage_est <- map_dbl( ns, ttest_CI_experiment)
```

This code will run our experiment for each value in `ns`, and then return a vector of the estimated coverage rates for each of the sample sizes.

We advocate for depicting simulation results graphically. To do so, we store the simulation results in a dataset and then create a line plot using a log scale for the horizontal axis:

```r
res <- tibble(
  n = ns,
  coverage = 100 * coverage_est
)

ggplot( res, aes( x = n, y = coverage ) ) +
  geom_hline( yintercept=95, col="red" ) +
  # A reference line for nominal coverage rate
  geom_line() +
  geom_point( size = 4 ) +
  scale_x_log10( breaks = ns, minor_breaks = NULL) +
  labs(
    title="Coverage rates for t-test on exponential data",
    x = "n (sample size)",
    y = "coverage (%)"
  ) +
  coord_cartesian(xlim = c(9,320), ylim=c(85,100), expand = FALSE) +
  theme_minimal()
```

---

[2]You can also check out Section 21.5 of R for Data Science (1st edition), which provides an introduction to mapping.

Coverage rates for t–test on exponential data
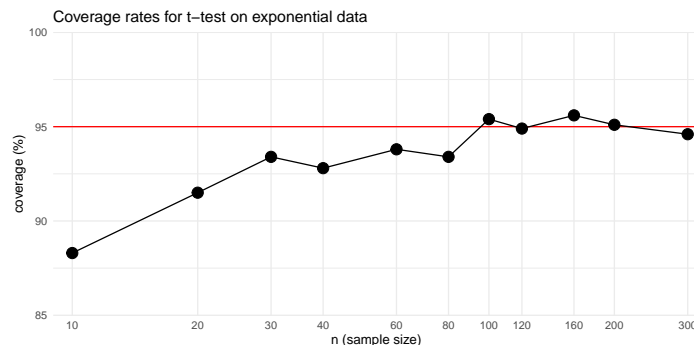
We can see from the graph that the confidence interval's coverage rate improves as sample size gets larger. For sample sizes over 100, the interval appears to have coverage quite close to the nominal 95% level. Although the general trend is pretty clear, the graph is still a bit messy because each point is an *estimated* coverage rate, with some Monte Carlo error baked in.

3.4 Extending the simulation design

So far, we have executed a simple simulation to assess how well a statistical method works in a given circumstance, then expanded the simulation by running a single-factor experiment in which we varied the sample size to see how the method's performance changes. In our example, we found that coverage is below what it should be for small sample sizes, but improves for sample sizes in the 100's.

This example captures all the major steps of a simulation study, which we outlined at the start of Chapter 1. We generated some hypothetical data according to a fully-specified data-generating process: we did both a normal distribution and a geometric distribution, each with a mean of 4. We applied a defined data-analysis procedure to the simulated data: we used a confidence interval based on the t distribution. We assessed how well the procedure worked across replications of the data-generating and data-analysis processes: in this case we focused on the coverage rate of the confidence interval. After creating a function to implement this whole process for a single scenario, we investigated how the performance of the confidence interval changed depending on sample size.

In simulations of more complex models and data-analysis methods, some or all of the steps in the process might have more moving pieces or entail more complex calculations. For instance, we might want to compare the performance of different approaches to calculating a confidence interval. We might also want to examine how coverage rates are affected by other aspects of the data-generating process, such as looking at different population mean values for the geometric distribution—or even entirely different distributions. With such additional layers of complexity, we will need to think systematically about each of the component parts of the simulation. In the next chapter, we introduce an abstract,

general framework for simulations that is helpful for guiding simulation design
and managing all the considerations involved.

3.5   Exercises

1. The simulation function we developed in this chapter uses 1000 repli-
   cations of the data-generating and data-analysis process, which leads
   to some Monte Carlo error in the simulation results. Modify the
   `ttest_CI_experiment()` function to make the number of replications
   an input argument, then re-run the simulation and re-create the graph
   of the results with $R = 10,000$ or even $R = 100,000$. Is the graph more
   regular than the one in the text, above? Use your improved results to
   determine what sample size is large enough to give coverage of at least
   94% (so only 1% off of desired).

2. Modify the `ttest_CI_experiment()` function to make the p parameter
   an input argument. Repeat the one-factor simulation, but use $p = 1/10$
   so that the population mean is $(1 - p)/p = 9$. How do the coverage rates
   change?

More challenging problems

3. Below is a modified version of the `ttest_CI_experiment()` function that
   creates a tibble with lower and upper end-points of the simulated confi-
   dence intervals:

   ```
   lotsa_CIs_experiment = function( n ) {

     lotsa_CIs <- replicate( 1000, {
       # simulate data
       dat <- rgeom( n = n, prob = 1/5)
       # analyze data
       tt <- t.test( dat )
       # return CI
       tibble(lower = tt$conf.int[1], upper = tt.conf.int[2])
     })

     # summarize results
     # <fill in the rest>

     return(coverage)
   }
   ```

   Complete the function by writing code to compute the estimated coverage
   rate and average confidence interval length. Also calculate a 95% confi-
   dence interval for the true coverage rate (you can use `prop.test()` on
   your set of simulation coverage indicators to obtain this, treating your R

simulation replicates as a random sample in its own right). Your modified function should return a one-row tibble with the coverage rate, average confidence interval length, and a CI for the true coverage rate.

4. Modify the `ttest_CI_experiment()` function to include the extensions of the prior problem. Then re-run the simulations with your modified function, obtaining a data frame with each row being a simulation scenario and columns of sample size, estimated coverage, low end of the estimate's confidence interval, and high end of the interval. You will likely want to use `map()` and then `bind_rows()` on your list of results; see Chapter 8.1 for more information about these techniques. Use these data to create a graph that depicts the estimated coverage rates. Try creating a graph that includes the 95% confidence intervals also, so that the Monte Carlo simulation error in the estimated coverage rates is represented in the graph. We recommend using the `ggplot2` function `geom_pointrange()` to represent the confidence intervals.

5. Modify `ttest_CI_experiment()` or `lotsa_CIs_experiment()` so that the user can specify the population mean of the data-generating process. Also let the user specify the number of replications to use. Here is a function skeleton to use as a starting point:

```
ttest_CI_experiment <- function( n, pop_mean, reps) {

  pop_prob <- 1 / (pop_mean + 1)

  # <fill in the rest>

  return(coverage)
}
```

6. Using the modified function from the previous problem, implement a two-factor simulation study for several different values of `n` and several different population means. One way to do this is to run a few simulations with different population means, storing them in a series of datasets, `res1`, `res2`, `res3`, etc. Then use `bind_rows( size1 = res1, ..., .id = "mean" )` to combine the datasets into a single dataset. Make a plot of your results, with `n` on the x-axis, coverage on the y-axis, and different lines for different population means.

Part II

Structure and Mechanics of a Simulation Study

Chapter 4

Structure of a simulation study

Monte Carlo simulation is a very flexible tool that researchers use to study a vast array of different models and topics. Within the realm of methodological research, most simulations share a common structure, nearly always involving the same set of steps or component pieces. In learning to design your own simulations, it is very useful to recognize the core components that most simulation studies share. Identifying these components will help you to organize your work and structure the coding tasks involved in writing a simulation.

In this chapter, we outline the component structure of a methodological simulation study, highlighting the four steps involved in a simulation of a single scenario and the three additional steps involved in multifactor simulations. We then describe a strategy for implementing simulations that mirrors the same component structure, where each step in the simulation is represented by a separate function or object. We call this strategy **_tidy, modular simulation_**. Finally, we show how the tidy, modular simulation strategy informs the structure and organization of code for a simulation study, walking through basic code skeletons (cf. 2.2.5) for each of the steps in a single-scenario simulation.

4.1   General structure of a simulation

The four main steps involved in a simulation study, introduced in Chapter 1, are summarized in the top portion of Table 4.1.

Table 4.1:   Steps in the Simulation Process

	Step	Description
1	**Generate**	Generate a sample of artificial data based on a specific statistical model or data-generating process.
2	**Analyze**	Apply one or more data-analysis procedures, estimators, or workflows to the artificial data.
3	**Repeat**	Repeat steps (1) & (2) R times, recording R sets of results.
4	**Summarize**	Assess the performance of the procedure across the R replications.
5	**Design**	Specify a set of conditions to examine
6	**Execute**	Run the simulation for each condition in the design.
7	**Synthesize**	Compare performance across conditions.

In the simple t-test example presented in Chapter 3, we put each of these steps into action with R code:

- We used the geometric distribution as a data-generating process;
- We used the confidence interval from a one-sample t-test as the data-analysis procedure;
- We repeatedly simulated the confidence intervals with R's `replicate()` function; and
- We summarized the results by estimating the fraction of the intervals that covered the population mean.

We also saw that it was helpful to wrap all of these steps up into a single function, so that we could run the simulation across multiple sample sizes.

These four initial steps are common and shared across nearly all simulations. In our first example, each of the steps was fairly simple, sometimes involving only a single line of code. More generally, each of the steps might be quite a bit more complex. The data-generating process might involve a more complex model with multiple variables or multilevel structure. The data analysis procedure might involve solving a multidimensional optimization problem to get parameter estimates, or might involve a data analysis workflow with multiple steps or contingencies. Further, we might use more than one metric for summarizing the results across replications and describing the performance of the data analysis

procedure. Because each of the four steps involves its own set of choices, it will useful to recognize them as distinct from one another.

In methodological research projects, we usually want to examine simulation results across an array of different conditions that differ not only in terms of sample size, but also in other parameters or features of the data-generating process. Running a simulation study across multiple conditions entails several further steps, which are summarized in the bottom portion of Table 4.1. We will first need to specify the factors and specific conditions to be examined in our experimental design. We will then need to execute the simulation for each of the conditions and store all the results for further analysis. Finally, we will need to find ways to synthesize or make sense of the main patterns in the results across all of the conditions in the design.

Just as with the first four steps, it is useful to recognize these further steps as distinct from one another, each involving its own set of choices and techniques. The design step requires choosing which parameters and features of the data-generating process to vary, as well as which specific values to use for each factor that is varied. Executing a simulation might require a lot of computing power, especially if the simulation design has many conditions or the data analysis procedure takes a long time to compute. How to effectively implement the execution step will therefore depend on the computing requirements and available resources. Finally, many different techniques can be used to synthesizing findings from a multifactor simulation. Which ones are most useful will depend on your research questions and the choices you make in each of the preceeding steps.

4.2   Tidy, modular simulations

It is apparent from Table 4.1 that writing a simulation in R involves a large space of possibilities and will requiring making a bunch of decisions. Considering the number of choices to be made, it is critical to stay organized and to approach the process systematically. Recognizing the components of a simulation is the starting point. Next is to see how to translate the components into R code.

In our own methodological work, we have found it very useful to always follow the same approach to writing code for a simulation. We call this approach *tidy, modular simulation.* It involves two simple principles:

1. Implement each component of a simulation as a distinct function or object.
2. Store all results in rectangular data sets.

Writing separate functions for each component step of a simulation has several benefits. The first is the practical benefit of turning the coding process from a monolithic (and potentially daunting) activity into a set of smaller, discrete tasks. This lets us focus on one task at a time and makes it easier to see progress. Second, following this principle makes for code that is easier to read, test, and

debug. Rather than having to scan through an entire code file to understand how the data analysis procedure is implemented, we can quickly identify the function that implements it, then focus on understanding the workings of that function. Likewise, if another researcher wanted to test out the data analysis procedure on a dataset of their own, they could do so by running the corresponding function rather than having to dissect an entire script. Third, writing separate code for each component makes it possible to tweak the code or swap out pieces of the simulation, such as by adding additional estimation methods or trying out a data-generating process involving different distributional assumptions. We already saw this in Chapter 3, where we modified our initial data-generating process to use a geometric distribution rather than a normal distribution. In short, following the first principle makes for simpler, more robust code that is easier to navigate, easier to test, and easier to extend.

The second principle of tidy, modular simulation is to store all results in rectangular datasets, such as the base R `data.frame` object or the tidyverse `tibble` object.[1] This principle applies to any and all output, including the simulated data from Step 1, the results of data analysis procedures from Step 2, full sets of replicated simulation results from Step 3, and summarized results from Step 4. A primary benefit of following this principle is that it facilitates working with the output of each stage in the simulation process. If you are comfortable using R to analyze real data, you you can use the same skills and tools to examine simulation output as long as it is in tabular form. Many of the data processing and data analysis tools available in R work with—or even require—rectangular datasets. Thus, using rectangular datasets makes it easier to inspect, summarize, and visualize the output.

4.3   Skeleton of a simulation study

The principles of tidy simulation imply that code for a simulation study should usually follow the same broad outline and organization of Table 4.1, with custom functions for each step in process. We will describe the outlines of simulation code using function skeletons to illustrate the inputs and outputs of each component. These skeletons skip over all the specific details, so that we can see the structure more clearly. We will first examine the structure of the code for simulating one specific scenario, then consider how to extend the code to systematically explore a variety of scenarios, as in a multifactor simulation.

In code skeletons, the structure of the first four steps in a simulation looks like this:

```r
# Generate (data-generating process)

generate_data <- function( model_params ) {
```

---

[1] Wickham (2014) provides a broader introduction to the concept of tidy data in the context of data-analysis tasks.

```r
  # stuff
  return(data)
}

# Analyze (data-analysis procedure)

analyze <- function( data ) {
  # stuff
  return(one_result)
}

# Repeat

one_run <- function( model_params ) {
  dat <- generate_data( model_params )
  one_result <- analyze(dat)
  return(one_result)
}

results <- replicate(R, one_run( params ))

# Summarize (calculate performance measures)

assess_performance <- function( results, model_params ) {
  # stuff
  return(performance_measures)
}

assess_performance(results, model_params)
```

The code above shows the full skeleton of a simulation. It involves four functions, where the outputs of one function get used as inputs in subsequent functions. We will now look at the inputs and outputs of each function to see how they align with the four steps in the simulation process. Subsequent chapters examine each piece in much greater detail—putting meat on the bones of each function skeleton, to torture our metaphor—and discuss specific statistical issues and programming techniques that are useful for designing each component.

Besides illustrating the skeletal framework of a simulation, readers might find it useful to use it as a template from which to start writing their own code. The simhelpers package includes the function create_skeleton(), which will open a new R script that contains a template for a simulation study, with sections corresponding to each component:

```r
simhelpers::create_skeleton()
```

The template that appears is a slightly more elaborate version of the code above,

with the main difference being that it also includes some additional lines of code to wire the pieces together for a multifactor simulation. Starting from this template, you will already be on the road to writing a tidy, modular simulation.

4.3.1   Data-Generating Process

The first step in a simulation is specifying a data-generating process. This is a hypothetical model for how data might arise, involving measurements or observations of one or more variables. The bare-bones skeleton of a data-generating function looks like the following:

```
generate_data <- function( model_params ) {
  # stuff
  return(data)
}
```

The function takes as input a set of model parameter values, denoted here as `model_params`. Based on those model parameters, the function generates a hypothetical dataset as output. Generating our own data based on a model allows us to know what the answer is (e.g., the true population mean or the true average effect of an intervention), so that we have benchmark against which to compare the results of a data analysis procedure that generates noisy estimates of the true value.

In practice, `model_params` will usually not be just one input but rather multiple arguments. These arguments might include inputs such as the population mean for a variable, the standard deviation of a distribution of treatment effects, or a parameter controlling the degree of skewness in the population distribution. Many data-generating processes involving multiple variables, such as the response variable and predictor variables in a regression model. In such instances, the inputs of `generate_data()` might also include parameters that determine the degree of dependence or correlation between variables. Further, the `generate_data()` inputs will also usually include arguments relating to the sample size and structure of the hypothetical dataset. For instance, in a simulation of a multilevel dataset where individuals are nested within clusters, the inputs might include an arguments to specify the total number of clusters and the average number of individuals per cluster. We discuss the inputs and form of the data-generating function further in Chapter 6.

4.3.2   Data Analysis Procedure

The second step in a simulation is specifying a data analysis procedure or set of procedures. The bare-bones skeleton of a data-generating function looks like the following:

```
analyze <- function( data ) {
  # stuff
```

```
  return(one_result)
}
```

The function should take a single dataset as input and produce a set of estimates or results (e.g., point estimates, standard errors, confidence intervals, p-values, predictions, etc.). Because we will be using the function to analyze hypothetical datasets simulated from the data-generating process, the `analyze()` function needs to work with `data` inputs that are produced by the `generate_data()` function. Thus, the code in the body of `analyze()` can assume that `data` will include relevant variables with specific names.

Inside the body of the function, `analyze()` includes code to carry out a data analysis procedure. This might involve generating a confidence interval, as in the example from Chapter 3. In another context, it might involve estimating an average growth rate along with a standard error, given a dataset with longitudinal repeated measurements from multiple individuals. In still another context, it might involve generating individual-level predictions from a machine learning algorithm. In simulations that involve comparing multiple analysis methods, we might write an `analyze()` function for each of the methods of interest, or (generally less preferred because it is less modular) we might write one function that does the calculations for all of the methods together.

A well-written estimation method should, in principle, work not only on a simulated, hypothetical dataset but also on a real empirical dataset that has the same format (i.e., appropriate variable names and structure). Because of this, the inputs of the `analyze()` function should not typically include any information about the parameters of the data-generating process. To be realistic, the code for our simulated data-analysis procedure should not make use of anything that the analyst could not know when analyzing a real dataset. Thus, `analyze()` has an argument for the sample dataset but not for `model_params`. We discuss the form and content of the data analysis function further in Chapter 7.

4.3.3 Repetition

The third step in a simulation is to repeatedly evaluate the data-generating process and data analysis procedure. In practice, this amounts to repeatedly calling `generate_data()` and then calling `analyze()` on the result. Here is the skeleton from our simulation template:

```
one_run <- function( model_params ) {
  dat <- generate_data( model_params )
  one_result <- analyze(dat)
  return(one_result)
}

results <- simhelpers::repeat_and_stack(R, one_run( params ))
```

We first create a helper function called `one_run()`, which takes `model_params` as input. Inside the body of the function, we call the `generate_data()` function to simulate a hypothetical dataset. We pass this dataset to `analyze()` and return a small dataset containing the results of the data-analysis procedure. The `one_run()` method is like a coordinator or dispatcher of the system: it generates the data, calls all the evaluation methods we want to call, combines all the results, and hands them back for recording. Making a helper method such as `one_run()` can be useful because it facilitates debugging.

Once we have the `one_run()` helper function, we need a way to call it repeatedly. As with many things in R, there are a variety of different ways to do something over and over. In the above skeleton, we use the `repeat_and_stack()` function from `simhelpers`.[2] In the first argument, we specify the number of times to repeat the process. In the second argument, we specify an expression that evaluates `one_run()` for specified values of the model parameters stored in `params`. The `repeat_and_stack()` function then evaluates the expression repeatedly, `R` times in all, and then stacks up all of the replications into a big dataset, with one or more rows per replication.[3]

We go into further detail about how to approach running the simulation process in Chapter 8. Among other things, we will illustrate how to use the `bundle_sim()` function from the `simhelpers` package to automate the process of coding this step, thereby avoiding the need to write a `one_run()` helper function.

4.3.4   Performance summaries

The fourth step in a simulation is to summarize the distribution of simulation results across replications. Here is the skeleton from our simulation template:

```r
assess_performance <- function( results, model_params ) {
  # stuff
```

---

[2]In the example from Chapter 3, we used the `replicate()` function from base R to repeat the process of generating and analyzing data. This function is a fine alternative to the `repeat_and_stack()` approach demonstrated in the skeleton. The only drawback is that it requires some further work to combine the results across replications. Here is a different version of the skeleton, which uses `replicate()` instead of `repeat_and_stack()`:

```r
results_list <- replicate(n = R, expr = {
  dat <- generate_data( params )
  one_result <- analyze(dat)
  return(one_result)
}, simplify = FALSE)

results <- purrr::list_rbind(results_list)
```

This version of the skeleton does not create a `one_run()` helper function, but instead puts the code from the body of `one_run()` directly into the `expr` argument of `replicate()`. To learn about other ways of repeatedly evaluating the simulation process, see Appendix 8.1.

[3]If you would prefer the output as a list rather than a stacked dataset, set `repeat_and_stack()`'s optional argument `stack = FALSE`.

```
  return(performance_measures)
}

assess_performance(results, params)
```

The `assess_performance()` function takes `results` as input. `results` should be a dataset containing all of the replications of the data-generating and analysis process. In contrast to the `analyze()` function, `assess_performance()` also needs to know the true parameter values of the data-generating process, so it needs to have `model_params` as its other input. The function then uses both of these inputs to calculate performance measures and returns a summary of the performance measures in a dataset.

Performance measures are the metrics or criteria used to assess the performance of a statistical method across repeated samples from the data-generating process. For example, we might want to know how close an estimator gets to the target parameter, on average. We might want to know if a confidence interval captures the true parameter the right proportion of the time, as in the simulation from Chapter 3. Performance is defined in terms of the sampling distribution of estimators or analysis results, across an infinite number of replications of the data-generating process. In practice, we use many replications of the process, but still only a finite number. Consequently, we actually *estimate* the performance measures and need to attend to the Monte Carlo error in the estimates. We discuss the specifics of different performance measures and assessment of Monte Carlo error in Chapter 9.

4.3.5 Multifactor simulations

Thus far, we have sketched out the structure of a modular, tidy simulation for a single context. In our t-test case study, for example, we might ask how well the t-test works when we have $n = 100$ units and the observations follow geometric distribution. However, we rarely want to examine a method only in a single context. Typically, we want to explore how well a procedure works across a range of different contexts. If we choose conditions in a structured and thoughtful manner, we will be able to examine broad trends and potentially make more general claims about the behaviors of the data-analysis procedures under investigation. Thus, it is helpful to think of simulations as akin to a designed experiment: in seeking to understand the properties of one or more procedures, we test them under a variety of different scenarios to see how they perform, then seek to identify more general patterns that hold beyond the specific scenarios examined. This is the heart of simulation for methodological evaluation.

To implement a multifactor simulation, we will follows the same principles of modular, tidy simulation. In particular, we will take the code developed for simulating a single context and bundle it into a function that can be evaluated for any and all scenarios of interest. Simulation studies often follow a full factorial

design, in which each level of a factor (something we vary, such as sample size, true treatment effect, or residual variance) is crossed with every other level. The experimental design then consists of sets of parameter values (including design parameters, such as sample sizes), and these too can be represented in an object, distinct from the other components of the simulation. We will discuss multiple-scenario simulations in Part III (starting with Chapter 11), after we more fully develop the core concepts and techniques involved in simulating a single context.

4.4   Exercises

1. Look back at the *t*-test simulation presented in Chapter 3. The code presented there did not entirely follow the formal structure outlined in this chapter. Revise the code by creating separate functions for each of four components in the simulation skeleton. Using the functions, re-run the simulation and recreate one or more graphs from the exercises in the previous chapter.

Chapter 5

Case Study: Heteroskedastic ANOVA

In this chapter, we present another detailed example of a simulation study to demonstrate how to put the principles of tidy, modular simulation into practice. To illustrate the process of programming a simulation, we reconstruct the simulations from Brown and Forsythe (1974). We will also use this case study as a recurring example in some of the following chapters.

Brown and Forsythe (1974) studied methods for null hypothesis testing in studies that measure a characteristic X on samples from each of several groups. They consider a population consisting of G separate groups, with population means $\mu_1, ..., \mu_G$ and population variances $\sigma_1^2, ..., \sigma_G^2$ for the characteristic X. A researcher obtains samples of size $n_1, ..., n_G$ from each of the groups and takes measurements of the characteristic for each sampled unit. Let x_{ig} denote the measurement from unit i in group g, for $i = 1, ..., n_g$ for each $j = 1, ..., G$. The researcher's goal is to use the sample data to test the hypothesis that the population means are all equal

$$H_0 : \mu_1 = \mu_2 = \cdots = \mu_G.$$

If the population *variances* were all equal (so $\sigma_1^2 = \sigma_2^2 = \cdots = \sigma_G^2$), we could use a conventional one-way analysis of variance (ANOVA) to conduct this test. However, one-way ANOVA might not work well if the variances are not equal. The question is then: what are best practices for testing the null of equal group means, allowing for the possibility that variances could differ across groups?

To tackle this question, Brown and Forsythe evaluated two different hypothesis testing procedures, developed by James (1951) and Welch (1951), both of which avoid the assumption that all groups have equal equality of variances. Brown and Forsythe also evaluated the conventional one-way ANOVA F-test

Table 5.1: Simulation scenarios explored by Brown and Forsythe (1974)

Scenario	Groups	Sample Sizes	Standard Deviations
A	4	4,4,4,4	1,1,1,1
B	4		1,2,2,3
C	4	4,8,10,12	1,1,1,1
D	4		1,2,2,3
E	4		3,2,2,1
F	4	11,11,11,11	1,1,1,1
G	4		1,2,2,3
H	4	11,16,16,21	1,1,1,1
I	4		3,2,2,1
J	4		1,2,2,3
K	6	4,4,4,4,4,4	1,1,1,1,1,1
L	6		1,1,2,2,3,3
M	6	4,6,6,8,10,12	1,1,1,1,1,1
N	6		1,1,2,2,3,3
O	6		3,3,2,2,1,1
P	6	6,6,6,6,6,6	1,1,2,2,3,3
Q	6	11,11,11,11,11,11	1,1,2,2,3,3
R	6	16,16,16,16,16,16	1,1,2,2,3,3
S	6	21,21,21,21,21,21	1,1,2,2,3,3
T	10	20,20,20,20,20,20,20,20,20,20	1,1,1.5,1.5,2,2,2.5,2.5,3,3

as a benchmark, even though this procedure maintains the assumption of equal variances. They also proposed and evaluated a new procedure of their own devising.[1] Their simulation involved comparing the performance of these different hypothesis testing procedures (the methods) under a range of conditions (different data generating processes) with different sample sizes and different degrees of heteroskedasticity. They looked at the different scenarios shown as Table 5.1, varying number of groups, group size, and amount of variation within each group. In all, there are a total of 20 scenarios, covering conditions with between 10 and 6 groups.

When evaluating hypothesis testing procedures, there are two main performance metrics of interest: type-I error rate and power. The type-I error rate is the rate at which a test rejects the null hypothesis when the null hypothesis is actually true. To apply a hypothesis testing procedure, one has to specify a desired, or nominal, type-I error rate, often denoted as the α-level. For a specified α, a valid or well-calibrated test should have an actual type-I error rate less than or equal to the nominal level, and ideally should be very close to nominal. Power is

---

[1] This latter piece makes Brown and Forsythe's study a prototypical example of a statistical methodology paper: find some problem that current procedures do not perfectly solve, invent something to do a better job, and then do simulations and/or math to build a case that the new procedure is better.

Table 5.2: Portion of "Table 1" reproduced from Brown and Forsythe (1974)

Scenario	ANOVA F test			B & F's F* test			Welch's test			James' test		
	10%	5%	1%	10%	5%	1%	10%	5%	1%	10%	5%	1%
A	10.2	4.9	0.9	7.8	3.4	0.5	9.6	4.5	0.8	13.3	7.9	2.4
B	12.0	6.7	1.7	8.9	4.1	0.7	10.3	4.7	0.8	13.8	8.1	2.7
C	9.9	5.1	1.1	9.5	4.8	1.0	10.8	5.7	1.6	12.1	6.7	2.1
D	5.9	3.0	0.6	10.3	5.7	1.4	9.8	4.9	0.9	10.8	5.6	1.3
E	21.9	14.4	5.6	11.0	6.2	1.8	11.3	6.5	2.0	12.9	7.7	2.9
F	10.1	5.1	1.0	9.8	5.7	1.5	10.0	5.0	0.9	10.6	5.5	1.1
G	11.4	6.3	1.8	10.7	5.7	1.5	10.1	5.0	1.1	10.6	5.4	1.3
H	10.3	4.9	1.1	10.3	5.1	1.0	10.2	5.0	1.0	10.5	5.3	1.2
I	17.3	10.8	3.9	11.1	6.2	1.8	10.5	5.5	1.2	10.9	5.8	1.3
J	7.3	4.0	1.0	11.5	6.5	1.8	10.6	5.4	1.1	10.9	5.6	1.1
K	9.6	4.9	1.0	7.3	3.4	0.4	11.4	6.1	1.4	14.7	9.5	3.8

how often a test correctly rejects the null when it is indeed false. It is a measure of how sensitive a method is to violations of the null.

Brown and Forsythe estimated error rates and power for nominal α-levels of 1%, 5%, and 10%. Table 1 of their paper reports the simulation results for type-I error (labeled as "size"). Our Table 5.2 reports some of their results with respect to Type I error. For a well-calibrated hypothesis testing method, the reported numbers should be very close to the desired alpha levels, as listed at the top of the table. We can compare the four tests to each other across each row, where each row is a specific scenario defined by a specific data generating process. Looking at ANOVA, for example, we see some scenarios with very elevated rates. For instance, in Scenario E, the ANOVA F-test has 21.9% rejection when it should only have 10%. In contrast, the ANOVA F works fine under scenario A, which is what one would expect because all the groups have the same variance. Brown and Forsythe's choice of scenarios here illustrates a broader design principle: to provide a full picture of the performance of a method or set of methods, it is wise to always evaluate them under conditions where we expect things to work, as well as conditions where we expect them to not work well.

To replicate the Brown and Forsythe simulation, we will first write functions to generate data for a specified scenario and evaluate data of a given structure. We will then use these functions to evaluate the hypothesis testing procedures in a specific scenario with a particular set of parameters (e.g., sample sizes, number of groups, and so forth). We will then scale up to execute the simulations for a range of scenarios that vary the parameters of the data-generating model, just as reported in Brown and Forsythe's paper.

5.1   The data-generating model

In the heteroskedastic one-way ANOVA simulation, there are three sets of parameter values: population means, population variances, and sample sizes. Rather than attempting to write a general data-generating function immediately, it is often easier to write code for a specific case first and then use that code as a starting point for developing a function. For example, say that we have four groups with means of 1, 2, 5, 6; variances of 3, 2, 5, 1; and sample sizes of 3, 6, 2, 4:

```r
mu <- c(1, 2, 5, 6)
sigma_sq <- c(3, 2, 5, 1)
sample_size <- c(3, 6, 2, 4)
```

Following Brown and Forsythe (1974), we will assume that the measurements are normally distributed within each sub-group of the population. The following code generates a vector of group id's and a vector of simulated measurements:

```r
N <- sum(sample_size) # total sample size
G <- length(sample_size) # number of groups

# group id factor
group <- factor(rep(1:G, times = sample_size))

# mean for each unit of the sample
mu_long <- rep(mu, times = sample_size)

# sd for each unit of the sample
sigma_long <- rep(sqrt(sigma_sq), times = sample_size)

# See what we have?
tibble( group = group, mu = mu_long, sigma = sigma_long )
```

```
## # A tibble: 15 x 3
##    group    mu sigma
##    <fct> <dbl> <dbl>
##  1 1         1  1.73
##  2 1         1  1.73
##  3 1         1  1.73
##  4 2         2  1.41
##  5 2         2  1.41
##  6 2         2  1.41
##  7 2         2  1.41
##  8 2         2  1.41
##  9 2         2  1.41
## 10 3         5  2.24
## 11 3         5  2.24
```

```
## 12 4          6  1
## 13 4          6  1
## 14 4          6  1
## 15 4          6  1
```

Now we have the pieces needed to generate a small dataset consisting of group memberships and the measured characteristic:

```
# Now make our data
x <- rnorm(N, mean = mu_long, sd = sigma_long)
dat <- tibble(group = group, x = x)
dat
```

```
## # A tibble: 15 x 2
##     group       x
##     <fct>   <dbl>
##  1 1        1.24
##  2 1        3.07
##  3 1       -0.681
##  4 2        2.43
##  5 2        2.50
##  6 2        2.15
##  7 2        0.612
##  8 2        0.860
##  9 2        2.09
## 10 3        1.56
## 11 3        5.08
## 12 4        5.68
## 13 4        5.66
## 14 4        5.92
## 15 4        4.38
```

We have followed the strategy of first constructing a dataset with parameters for each observation in each group, making heavy use of base R's rep() function to repeat values in a list. We then called rnorm() to generate N observations in all. This works because rnorm() is *vectorized*; if you give it a vector (or vectors) of parameter values, it will generate each subsequent observation according to the next entry in the vector. As a result, the first x value is simulated from a normal distribution with mean mu_long[1] and standard deviation sd_long[1], the second x is simulated using mu_long[2] and sd_long[2], and so on.

As usual, there are many different and legitimate ways of doing this in R. For instance, instead of using rep() to do it all at once, we could generate observations for each group separately, then stack the observations into a dataset. Do not worry about trying to writing code the "best" way—especially when you are initially putting a simulation together. If you can find a way to accomplish your task at all, then that's often enough (and you should feel good about it!).

5.1.1   Now make a function

Because we will need to generate datasets over and over, we will wrap our code in a function. The inputs to the function will be the parameters of the model that we specified at the very beginning: the set of population means `mu`, the population variances `sigma_sq`, and sample sizes `sample_size`. We make these quantities arguments of the data-generating function so that we can make datasets of different sizes and shapes:

```r
generate_ANOVA_data <- function(mu, sigma_sq, sample_size) {

  N <- sum(sample_size)
  G <- length(sample_size)

  group <- factor(rep(1:G, times = sample_size))
  mu_long <- rep(mu, times = sample_size)
  sigma_long <- rep(sqrt(sigma_sq), times = sample_size)

  x <- rnorm(N, mean = mu_long, sd = sigma_long)
  sim_data <- tibble(group = group, x = x)

  return(sim_data)
}
```

The function is simply the code we built previously, all bundled up. We developed the function by first writing code to make the data-generating process to work once, the way we want, and only then turning the final code into a function for later reuse.

Once we have turned the code into a function, we can call it to get a new set of simulated data. For example, to generate a dataset with the same parameters as before, we can do:

```r
sim_data <- generate_ANOVA_data(
  mu = mu,
  sigma_sq = sigma_sq,
  sample_size = sample_size
)

str(sim_data)
```

```
## tibble [15 x 2] (S3: tbl_df/tbl/data.frame)
##  $ group: Factor w/ 4 levels "1","2","3","4": 1 1 1 2 2 2 2 2 2 3 ...
##  $ x    : num [1:15] 0.777 2.115 1.31 1.848 3.041 ...
```

To generate one with population means of zero in all the groups, but the same group variances and sample sizes as before, we can do:

```r
sim_data_null <- generate_ANOVA_data(
  mu = c( 0, 0, 0, 0 ),
  sigma_sq = sigma_sq,
  sample_size = sample_size
)

str(sim_data)
```

```
## tibble [15 x 2] (S3: tbl_df/tbl/data.frame)
##  $ group: Factor w/ 4 levels "1","2","3","4": 1 1 1 2 2 2 2 2 2 3 ...
##  $ x    : num [1:15] 0.777 2.115 1.31 1.848 3.041 ...
```

Following the principles of tidy, modular simulation, we have written a function that returns a rectangular dataset for further analysis. Also note that the dataset returned by `generate_ANOVA_data()` only includes the variables `group` and `x`, but not `mu_long` or `sd_long`. This is by design. Including `mu_long` or `sd_long` would amount to making the population parameters available for use in the data analysis procedures, which is not something that happens when analyzing real data.

5.1.2 Cautious coding

In the above, we built some sample code, and then bundled it into a function by literally cutting and pasting the initial work we did into a function skeleton. In the process, we shifted from having variables in our workspace with different names to using those variable names as parameters in our function call.

Developing code in this way is not without hazards. In particular, after we have created our function, our workspace is left with a variable `mu` in it and our function also has a parameter named `mu`. Inside the function, R will use the parameter `mu` first, but this is potentially confusing. Another potential source of confusion are lines such as `mu = mu`, which means "set the function's parameter called `mu` to the variable called `mu`." These are different things (with the same name).

Once you have built a function, one way to check that it is working properly is to comment out the initial code (or delete it), clear out the workspace (or restart R), and then re-run the code that uses the function. If things still work, then you can be somewhat confident that you have successfully bundled your code into the function. Once you bundle your code, you can also do a search and replace to change the variable names inside your function to something more generic, to better clarify the distinction betwen object names and argument names.

5.2   The hypothesis testing procedures

Brown and Forsythe considered four different hypothesis testing procedures for heteroskedastic ANOVA, but we will focus on just two of the tests for now. We start with the conventional one-way ANOVA that mistakenly assumes homoskedasticity. R's `oneway.test` function will calculate this test automatically:

```r
sim_data <- generate_ANOVA_data(
  mu = mu,
  sigma_sq = sigma_sq,
  sample_size = sample_size
)

anova_F <- oneway.test(x ~ group, data = sim_data, var.equal = TRUE)
anova_F
```

```
##
##  One-way analysis of means
##
## data:  x and group
## F = 8.9503, num df = 3, denom df = 11,
## p-value = 0.002738
```

We can use the same function to calculate Welch's test by setting `var.equal = FALSE`:

```r
Welch_F <- oneway.test(x ~ group, data = sim_data, var.equal = FALSE)
Welch_F
```

```
##
##  One-way analysis of means (not assuming
##  equal variances)
##
## data:  x and group
## F = 22.321, num df = 3.0000, denom df =
## 3.0622, p-value = 0.01399
```

The main results we need here are the p-values of the tests, which will let us assess Type-I error and power for a given nominal α-level. The following function takes simulated data as input and returns as output the p-values from the one-way ANOVA test and Welch test:

```r
ANOVA_Welch_F <- function(data) {
  anova_F <- oneway.test(x ~ group, data = data, var.equal = TRUE)
  Welch_F <- oneway.test(x ~ group, data = data, var.equal = FALSE)

  result <- tibble(
    ANOVA = anova_F$p.value,
    Welch = Welch_F$p.value
```

```
  )

  return(result)
}
```

```
ANOVA_Welch_F(sim_data)
```

```
## # A tibble: 1 x 2
##     ANOVA   Welch
##     <dbl>   <dbl>
## 1 0.00274 0.0140
```

Following our tidy, modular simulation principles, this function returns a small dataset with the p-values from both tests. Eventually, we might want to use this function on some real data. Our estimation function does not care if the data are simulated or not; we call the input `data` rather than `sim_data` to reflect this.

As an alternative to this function, we could instead write code to implement the ANOVA and Welch tests ourselves. This has some potential advantages, such as avoiding any extraneous calculations that `oneway.test` does, which take time and slow down our simulation. However, there are also drawbacks to doing so, including that writing our own code takes *our* time and opens up the possibility of errors in our code. For further discussion of the trade-offs, see Chapter A.3, where we do implement these tests by hand and see what kind of speed-ups we can obtain.

5.3 Running the simulation

We now have functions that implement steps 2 and 3 of the simulation. Given some parameters, `generate_ANOVA_data` produces a simulated dataset and, given some data, `ANOVA_Welch_F` calculates p-values two different ways. We now want to know which way is better, and by how much. To answer this question, we will need to repeat the chain of generate-and-analyze calculations a bunch of times. To facilitate repetition, we first put the components together into a single function:

```
one_run = function( mu, sigma_sq, sample_size ) {
  sim_data <- generate_ANOVA_data( mu = mu, sigma_sq = sigma_sq, sample_size = sample_size )
  ANOVA_Welch_F(sim_data)
}
```

```
one_run( mu = mu, sigma_sq = sigma_sq, sample_size = sample_size )
```

```
## # A tibble: 1 x 2
##     ANOVA Welch
##     <dbl> <dbl>
```

```
## 1 0.0167 0.107
```

This function implements a single simulation trial by generating artificial data and then analyzing the data, ending with a tidy dataset that has results for the single run.

We next call `one_run()` over and over; see Appendix 8.1 for some discussion of options. The following uses `repeat_and_stack()` from `simhelpers` to evaluate `one_run()` 4 times and then stack the results into a single dataset:

```
library(simhelpers)

sim_data <- repeat_and_stack(4,
  one_run( mu = mu, sigma_sq = sigma_sq, sample_size = sample_size)
)
sim_data
```

```
## # A tibble: 4 x 2
##      ANOVA   Welch
##      <dbl>   <dbl>
## 1 0.0262   0.0125
## 2 0.00451  0.0698
## 3 0.00229  0.0380
## 4 0.0108   0.0423
```

Voila! We have simulated p-values!

5.4   Summarizing test performance

We now have all the pieces in place to reproduce the results from Brown and Forsythe (1974). We first focus on calculating the actual type-I error rate of these tests—that is, the proportion of the time that they reject the null hypothesis of equal means when that null is actually true—for an α-level of .05. To evaluate the type-I error rate, we need to simulate data from a process where the population means are indeed all equal. Arbitrarily, let's start with $G = 4$ groups and set all of the means equal to zero:

```
mu <- rep(0, 4)
```

In the fifth row of Table 1 (Scenario E in our Table 5.1), Brown and Forsythe examine performance for the following parameter values for sample size and population variance:

```
sample_size <- c(4, 8, 10, 12)
sigma_sq <- c(3, 2, 2, 1)^2
```

With these parameter values, we can use `map_dfr` to simulate 10,000 p-values:

```
p_vals <- repeat_and_stack(10000,
  one_run(
    mu = mu,
    sigma_sq = sigma_sq,
    sample_size = sample_size
  )
)
```

We can estimate the rejection rates by summarizing across these replicated p-values. The rule is that the null is rejected if the *p*-value is less than α. To get the rejection rate, we calculate the proportion of replications where the null is rejected:

```
sum(p_vals$ANOVA < 0.05) / 10000
```

```
## [1] 0.1391
```

This is equivalent to taking the mean of the logical conditions:

```
mean(p_vals$ANOVA < 0.05)
```

```
## [1] 0.1391
```

We get a rejection rate that is much larger than $\alpha = .05$. We have learned that the ANOVA F-test does not adequately control Type-I error under this set of conditions.

```
mean(p_vals$Welch < 0.05)
```

```
## [1] 0.0697
```

The Welch test does much better, although it appears to be a little bit in excess of 0.05.

Note that these two numbers are quite close (though not quite identical) to the corresponding entries in Table 1 of Brown and Forsythe (1974). The difference is due to the fact that both Table 1 and are results are actually *estimated* rejection rates, because we have not actually simulated an infinite number of replications. The estimation error arising from using a finite number of replications is called *simulation error* (or *Monte Carlo error*). In Chapter 9, we will look more at how to estimate and control the Monte Carlo simulation error in performance measures.

So there you have it! Each part of the simulation is a distinct block of code, and together we have a modular simulation that can be easily extended to other scenarios or other tests. The exercises at the end of this chapter ask you to extend the framework further. In working through them, you will get to experience first-hand how the modular code that we have started to develop is easier to work with than a single, monolithic block of code.

Table 5.3: Portion of "Table 2" reproduced from Brown and Forsythe (1974)

Variances	Means	Brown's F	B & F's F*	Welch's W
1,1,1,1	0,0,0,0	4.9	5.1	5.0
	1,0,0,0	68.6	67.6	65.0
3,2,2,1	0,0,0,0	NA	6.2	5.5
	1.3,0,0,1.3	NA	42.4	68.2

5.5   Exercises

The following exercises involve exploring and tweaking the above simulation code we have developed to replicate the results of Brown and Forsythe (1974).

1. Table 1 from Brown and Forsythe reported rejection rates for $\alpha = .01$ and $\alpha = .10$ in addition to $\alpha = .05$. Calculate the rejection rates of the ANOVA F and Welch tests for all three α-levels and compare to the table.

2. Try simulating the Type-I error rates for the parameter values in the first two rows of Table 1 of the original paper. Use 10,000 replications. How do your results compare to the report results?

3. In the primary paper, Table 1 is about Type I error and Table 2 is about power. A portion of Table 2 follows:

   In the table, the sizes of the four groups are 11, 16, 16, and 21, for all the scenarios. Try simulating the **power levels** for a couple of sets of parameter values from Table 5.3. Use 10,000 replications. How do your results compare to the results reported in the Table?

4. Instead of making `ANOVA_Welch_F` return a single row with the columns for the p-values, one could instead return a dataset with one row for each test. The "long" approach is often nicer when evaluating more than two methods, or when each method returns not just a p-value but other quantities of interest. For our current simulation, we might also want to store the F statistic, for example. The resulting dataset would then look like the following:

```
ANOVA_Welch_F_long(sim_data)
```

```
## # A tibble: 2 x 3
##   method Fstat  pvalue
##   <chr>  <dbl>   <dbl>
## 1 ANOVA   8.46 0.00338
## 2 Welch  14.3  0.0241
```

   Modify `ANOVA_Welch_F()` to return output in this format, update your simulation code, and then use `group_by()` plus `summarise()` to calculate rejection rates of both tests. `group_by()` is a method for dividing your

data into distinct groups and conducting an operation on each. The classic form of this would be something like the following:

```
sres <-
  res %>%
  group_by( method ) %>%
  summarise( rejection_rate = mean( pvalue < 0.05 ) )
```

5. The `onewaytests` package in R includes functions for calculating Brown and Forsythe's F^* test and James' test for differences in population means. Modify the data analysis function `ANOVA_Welch_F` (or, better yet, `ANOVA_Welch_F_long` from Exercise 4) to also include results from these hypothesis tests. Re-run the simulation to estimate the type-I error rate of all four tests under Scenarios A and B of Table 5.1.

Chapter 6

Data-generating processes

As we saw in Chapter 4, the first step of a simulation is creating artificial data based on some process where we know (and can control) the truth. This step is what we call the data generating process (DGP). Think of it as a recipe for cooking up artificial data, which can be applied over and over, any time we're hungry for a new dataset. Like a good recipe, a good DGP needs to be complete—it cannot be missing ingredients and it cannot omit any steps. Unlike cooking or baking, however, DGPs are usually specified in terms of a statistical model, or a set of equations involving constants, parameter values, and random variables. More complex DGPs, such as those for hierarchical data or other latent variable models, will often involve a series of several equations that describe different dimensions or levels of the model, which need to be followed in sequence to produce an artificial dataset.

In this chapter, we will look at how to instantiate a DGP as an R function (or perhaps a set of functions). Designing DGPs and implementing them in R code involves making choices about what aspects of the model we want to be able to control and how to set up the parameters of the model. We start by providing a high-level overview of DGPs and discussing some of the choices and challenges involved in designing them. We then demonstrate how to write R functions for DGPs. In the remainder, we present detailed examples involving a hierarchical DGP for generating data on students nested within schools and an item response theory DGP for generating data on responses to individual test items.

6.1 Examples

Before diving in, it is helpful to consider a few examples that we will return to throughout this and subsequent chapters.

6.1.1   Example 1: One-way analysis of variance

We have already seen one example of a DGP in the ANOVA example from Chapter 5. Here, we consider observations on some variable X drawn from a population consisting of G groups, where group g has population mean μ_g and population variance σ_g^2 for $g = 1, ..., G$. A simulated dataset consists of n_g observations from each group $g = 1, ..., G$, where X_{ig} is the measurement for observation i in group g. The statistical model for these data can be written as follows:

$$X_{ig} = \mu_g + \epsilon_{ig}, \quad \text{with} \quad \epsilon_{ig} \sim N(0, \sigma_g^2)$$

for $i = 1, ..., n_g$ and $g = 1, ..., G$. Alternately, we could write the model as

$$X_{ig} \sim N(\mu_g, \sigma_g^2).$$

6.1.2   Example 2: Bivariate Poisson model

As a second example, suppose that we want to understand how the usual Pearson sample correlation coefficient behaves with non-normal data and also to investigate how the Pearson correlation relates to Spearman's rank correlation coefficient. To look into such questions, one DGP we might entertain is a bivariate Poisson model, which is a distribution for a pair of counts, C_1, C_2, where each count follows a Poisson distribution and where the pair of counts may be correlated. We will denote the expected values of the counts as μ_1 and μ_2 and the Pearson correlation between the counts as ρ.

To simulate a dataset based on this model, we would first need to choose how many observations to generate. Call this sample size N. One way to generate data following a bivariate Poisson model is to generate *three* independent Poisson random variables for each of the N observations:

$$Z_0 \sim Pois\left(\rho\sqrt{\mu_1\mu_2}\right)$$
$$Z_1 \sim Pois\left(\mu_1 - \rho\sqrt{\mu_1\mu_2}\right)$$
$$Z_2 \sim Pois\left(\mu_2 - \rho\sqrt{\mu_1\mu_2}\right)$$

and then combine the pieces to create two dependent observations:

$$C_1 = Z_0 + Z_1$$
$$C_2 = Z_0 + Z_2.$$

An interesting feature of this model is that the range of possible correlations is constrained: only positive correlations are possible and, because each of the independent pieces must have a non-negative mean, the maximum possible correlation is $\sqrt{\frac{\min\{\mu_1,\mu_2\}}{\max\{\mu_1,\mu_2\}}}$.

6.1.3   Example 3: Hierarchical linear model for a cluster-randomized trial

Cluster-randomized trials are randomized experiments where the unit of randomization is a *group* of individuals, rather than the individuals themselves.

For example, suppose we have a collection of schools and the students within them. A cluster-randomized trial involves randomizing the *schools* into treatment or control conditions and then measuring an outcome such as academic performance on the multiple students within the schools. Typically, researchers will be interested in the extent to which average outcomes differ across schools assigned to different conditions, which captures the impact of the treatment relative to the control condition. We will index the schools using $j = 1, ..., J$ and let n_j denote the number of students observed in school j. Say that Y_{ij} is the outcome measure for student i in school j, for $1 = 1, ..., n_j$ and $j = 1, ..., J$, and let Z_j be an indicator equal to 1 if school j is assigned to the treatment condition and otherwise equal to 0.

A widely used approach for estimating impacts from cluster-randomized trials is heirarchical linear modeling (HLM). One way to write an HLM is in two parts. First, we consider a regression model that describes the distribution of the outcomes across students within school j:

$$Y_{ij} = \beta_{0j} + \epsilon_{ij}, \qquad \epsilon_{ij} \sim N(0, \sigma_\epsilon^2),$$

where β_{0j} is the average outcome across students in school j. Second, we allow that the school-level average outcomes differ by a treatment effect γ_1 and that, for schools within each condition, the average outcomes follow a normal distribution with variance σ_u^2. We can write these relationships as a regression equation for the school-specific average outcome:

$$\beta_{0j} = \gamma_0 + \gamma_{10} Z_j + u_{0j}, \quad u_{0j} \sim N(0, \tau^2),$$

where γ_0 is the average outcome among schools in the control condition.

If we only consider the first stage of this model, it looks a bit like the one-way ANOVA model from the previous example: in both cases, we have multiple observations from each of several groups.
The main distinction is that the ANOVA model treats the G groups as a fixed set, whereas the HLM treats the set of J schools as sampled from a larger population of schools and includes a regression model describing the variation in the school-level average outcomes.

6.2 Components of a DGP

A DGP involves a statistical model with parameters and random variables, but it also often includes further details as well, beyond those that we would consider to be part of the model as we would use it for analyzing real data. In statistical analysis of real data, we often use models that describe only *part* of the distribution of the data, rather than its full, multivariate distribution. For instance, when conducting a regression analysis, we are analyzing the distribution of an outcome or response variable, conditional on a set of predictor variables. In other words, we take the predictor variables as *given* or *fixed*, rather than

modeling their distribution. When using an item response theory (IRT) model, we use responses to a set of items to estimate individual ability levels, given the set of items on the test. We do not (usually) model the items themselves. In contrast, if we are going to *generate* data for simulating a regression model or IRT model, we need to specify distributions for these additional features (the predictors in a regression model, the items in an IRT model); we can no longer just take them as given.

In designing and discussing DGPs, it is helpful to draw distinctions between the components of the focal statistical model and the remaining components of the DGP that are taken as given when analyzing real data. A first relevant distinction is between structural features, covariates, and outcomes (or more generally, endogenous quantities):

- **Structural features** are quantities, such as the per-group sample sizes in the one-way ANOVA example, that describe the structure of a dataset but do not enter directly into the focal statistical model. When analyzing real data, we usually take the structural features as they come, but when simulating data, we will need to make choices about the structural features. For instance, in the HLM example involving students nested within schools, the number of students in each school is a structural feature. To simulate data based on HLM, we will need to make choices about the number of schools and the distribution of the number of students in each school (e.g., we might specify that school sizes are uniformly distributed between specified minimum and maximum sizes), even though we do not have to consider these quantities when estimating a hierarchical model on real data.

- **Covariates** are variables in a dataset that we typically take as given when analyzing real data. For instance, in the one-way ANOVA example, the group assignments of each observation is a covariate. In the HLM example, covariates would include the treatment indicators $Z_1, ..., Z_J$. In a more elaborate version of the HLM, they might also include variables such as student demographic information, measures of past academic performance, or school-level characteristics such as the school's geographic region or treatment assignment. When analyzing real data, we condition on these quantities, but when specifying a DGP, we will need to make choices about how they are distributed (e.g., we might specify that students' past academic performance is normally distributed).

- **Outcomes and endogenous quantities** are the variables whose distribution is described by the focal statistical model. In the one-way ANOVA example, the outcome variable consists of the measurements X_{ig} for $i = 1, ..., n_g$ and $g = 1, ..., G$. In the bivariate Poisson model, the outcomes consist of the component variables Z_1, Z_2, Z_3 and the observed counts C_1, C_2 because all of these quantities follow distributions that are specified as part of the focal model. The focal statistical model specifies the distribution of these variables, and we will be interested in estimating the parameters controlling their distribution.

Note that the focal statistical model only determines this third component of the DGP. The focal model consists of the equations describing what we would aim to estimate when analyzing real data. In contrast, the full statistical model also includes additional elements specify how to generate the structural features and covariates—the pieces that are taken as given when analyzing real data. Table 6.1 contrasts the role of structural features, covariates, and outcomes in real data analysis versus in simulations.

Table 6.1: Real Data Analysis versus Simulation

Component	Real world	Simulation world
Structural features	We obtain data of a given sample size, sizes of clusters, etc.	We specify sample sizes, we specify how to generate cluster sizes
Covariates	Data come with covariates	We specify how to generate covariates
Outcomes	Data come with outcome variables	We generate outcome data based on a focal model
Parameter estimation	We estimate a statistical model to learn about the unknown parameters	We estimate a statistical model and compare the results to the true parameters

For a given DGP, the full statistical model might involve distributions for structural features, distributions for covariates, and distributions for outcomes given the covariates. Each of these distributions will involve parameters that control the properties of the distribution (such as the average and degree of variation in a variable). We think of these parameters as falling into one of three categories: focal, auxiliary, or design.

- **Focal** parameters are the quantities that we care about and seek to estimate in real data analysis. These are typically parts of the focal statistical model, such as the population means $\mu_1, ..., \mu_G$ in the one-way ANOVA model, the correlation between counts ρ in the bivariate Poisson model, or the treatment effect γ_1 in the HLM example.

- **Auxiliary** parameters are the other quantities that go into the focal statistical model or some other part of the DGP, which we might not be substantively interested in when analyzing real data but which nonetheless affect the analysis. For instance, in the one-way ANOVA model, we would consider the population variances $\sigma_1^2, ..., \sigma_G^2$ to be auxiliary if we are not interested in investigating how they vary from group to group. In the bivariate Poisson model we might consider the average counts μ_1 and μ_2 to be auxiliary parameters.

- **Design** parameters are the quantities that control how we generate structural features of the data. For instance, in a cluster-randomized trial,

the fraction of schools assigned to treatment is a design parameter that can be directly controlled by the researchers. Additional design parameters might include the minimum and maximum number of students per school. Typically, in a real data analysis, we would not directly estimate such parameters because we take the distribution of structural features as given.

It is evident from this discussion that DGPs can involve *many* moving parts. One of the central challenges in specifying DGPs is that the performance of estimation methods will generally be affected by the *full* statistical model—including the design parameters and distribution of structural features and covariates—even though they are not part of the focal model.

6.3   A statistical model is a recipe for data generation

Once we have decided on a full statistical model and written it down in mathematical terms, we need to translate it into code. A function that implements a data-generating model should have the following form:

```r
generate_data <- function(
  focal_parameters, auxiliary_parameters, design_parameters
) {

  # generate pseudo-random numbers and use those to make some data

  return(sim_data)
}
```

The function takes a set of parameter values as input, simulates random numbers and does calculations, and produces as output a set of simulated data. Typically, the inputs will consist of multiple parameters, and these will include not only the focal model parameters, but also the auxiliary parameters, sample sizes, and other design parameters. The output will typically be a dataset, mimicking what one would see in an analysis of real data. In some cases, the output data might be augmented with some other latent quantities (normally unobserved in the real world) that can be used later to assess whether an estimation procedure produces results that are close to the truth.

We have already seen an example of a complete DGP function in the case study on one-way ANOVA (see Section 5.1). In this case study, we developed the following function to generate data for a single outcome from a set of G groups:

```r
generate_ANOVA_data <- function(mu, sigma_sq, sample_size) {

  N <- sum(sample_size)
  G <- length(sample_size)
```

```r
  group <- factor(rep(1:G, times = sample_size))
  mu_long <- rep(mu, times = sample_size)
  sigma_long <- rep(sqrt(sigma_sq), times = sample_size)

  x <- rnorm(N, mean = mu_long, sd = sigma_long)
  sim_data <- tibble(group = group, x = x)

  return(sim_data)
}
```

This function takes both the focal model parameters (`mu`, `sigma_sq`) and other design parameters that one might not think of as parameters per-se (`sample_size`). When simulating, we have to specify quantities that we take for granted when analyzing real data.

How would we write a DGP function for the bivariate Poisson model? The equations in Section 6.1 give us the recipe, so it just a matter of re-expressing them in code. For this model, the only design parameter is the sample size, N; the sole focal parameter is the correlation between the variates, ρ; and the auxiliary parameters are the expected counts μ_1 and μ_2. Our function should have all four of these quantities as inputs and should produce as output a dataset with two variables, C_1 and C_2. Here is one way to implement the model:

```r
r_bivariate_Poisson <- function(N, rho, mu1, mu2) {

  # covariance term, equal to E(Z_3)
  EZ3 <- rho * sqrt(mu1 * mu2)

  # Generate independent components
  Z1 <- rpois(N, lambda = mu1 - EZ3)
  Z2 <- rpois(N, lambda = mu2 - EZ3)
  Z3 <- rpois(N, lambda = EZ3)

  # Assemble components
  dat <- data.frame(
    C1 = Z1 + Z3,
    C2 = Z2 + Z3
  )

  return(dat)
}
```

Here we generate 5 observations from the bivariate Poisson with $\rho = 0.5$ and $\mu_1 = \mu_2 = 4$:

```r
r_bivariate_Poisson(5, rho = 0.5, mu1 = 4, mu2 = 4)
```

```
##   C1 C2
## 1  4  4
## 2  2  2
## 3  2  1
## 4  5  6
## 5  2  3
```

6.4 Plot the artificial data

The whole purpose of writing a DGP is to produce something that can be treated just as if it were real data. Considering that is our goal, we should act like it and engage in data analysis processes that we would apply whenever we analyze real data. In particular, it is worthwhile to create one or more plots of the data generated by a DGP, just as we would if we were exploring a new real dataset for the first time. This exercise can be very helpful for catching problems in the DGP function (about which more below). Beyond just debugging, constructing graphic visualizations can be a very effective way to *study* a model and strengthen your understanding of how to interpret its parameters.

In the one-way ANOVA example, it would be conventional to visualize the data with box plots or some other summary statistics for the data from each group. For exploratory graphics, we prefer plots that include representations of the raw data points, not just summary statistics. The figure below uses a density ridge-plot, filled in with points for each observation in each group. The plot is based on a simulated dataset with 50 observations in each of five groups.
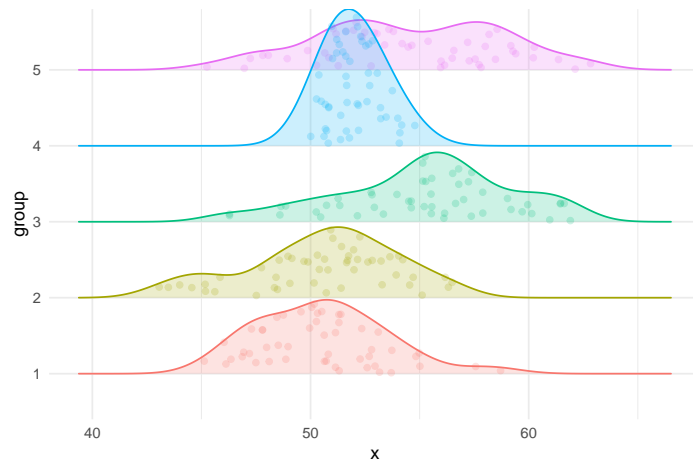
Figure 6.1: Densities of five heteroskedastic groups for the one-way ANOVA example.

Here is a plot of 30 observations from the bivariate Poisson distribution with

means $\mu_1 = 10, \mu_2 = 7$ and correlation $\rho = .65$ (points are jittered slightly to avoid over-plotting):
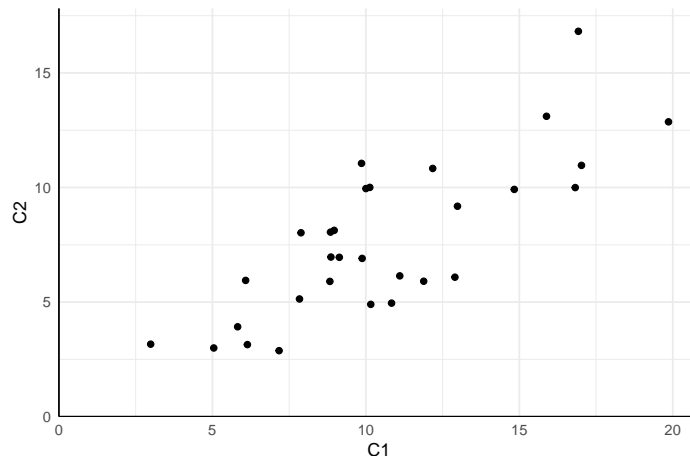
Figure 6.2: $N = 30$ observations from the bivariate Poisson distribution with $\mu_1 = 10, \mu_2 = 7, ho = .65$.

Plots like these are useful for building intuitions about a model. For instance, we can inspect 6.2 to get a sense of the order of magnitude and range of the observations, as well as the likelihood of obtaining multiple observations with identical counts. Depending on the analysis procedures we will apply to the dataset, we might even create plots of transformations of the dataset, such as a histogram of the differences $C_2 - C_1$ or a scatterplot of the rank transformations of C_1 and C_2.

6.5   Check the data-generating function

An important part of programming in R—especially when writing custom functions—is finding ways to test and check the correctness of your code. Just writing a data-generating function is not enough. It is also *critical* to test whether the output it produces is correct. How best to do this will depend on the particulars of the DGP being implemented.

For many DGPs, a broadly useful strategy is to generate a very large sample of data—one so large that the sample distribution should very closely resemble the population distribution. One can then test whether features of the sample distribution closely align with corresponding parameters of the population model.

For the heteroskedastic ANOVA problem, one basic thing we can do is check that the simulated data from each group follows a normal distribution. In the following code, we simulate very large samples from each of the four groups, and

check that the means and variances agree with the input parameters:

```r
mu <- c(1, 2, 5, 6)
sigma_sq <- c(3, 2, 5, 1)

check_data <- generate_ANOVA_data(
  mu = mu,
  sigma_sq = sigma_sq,
  sample_size = rep(10000, 4)
)

chk <-
  check_data %>%
  group_by( group ) %>%
  dplyr::summarise(
    n = n(),
    mean = mean(x),
    var = var(x)
  ) %>%
  mutate(mu = mu, sigma2 = sigma_sq) %>%
  relocate( group, n, mean, mu, var, sigma2 )
chk
```

```
## # A tibble: 4 x 6
##   group       n  mean    mu   var sigma2
##   <fct> <int> <dbl> <dbl> <dbl>  <dbl>
## 1 1     10000 0.988     1  2.97      3
## 2 2     10000 1.99      2  1.99      2
## 3 3     10000 5.02      5  5.00      5
## 4 4     10000 5.98      6  0.993     1
```

It seems we are recovering our parameters.

We can also make some diagnostic plots to assess whether we have normal data (using QQ plots, where we expect a straight line if the data are normal):

```r
ggplot( check_data ) +
  aes( sample = x, color = group ) +
  facet_wrap( ~ group ) +
  stat_qq() + stat_qq_line()
```
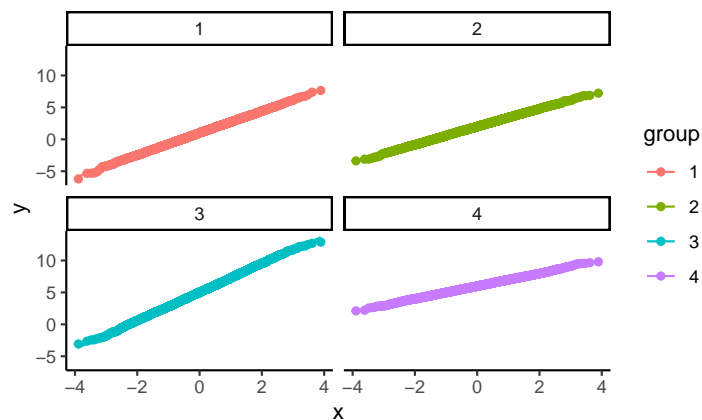
This diagnostic looks good too. Here, these checks may seem a bit silly, but most bugs are silly—at least once you find them! In models that are even a little bit more complex, it is quite easy for small things such as a sign error to slip into your code. Even simple checks such as these can be quite helpful in catching such bugs.

6.6   Example: Simulating clustered data

Writing code for a complicated DGP can feel like a daunting task, but if you first focus on a recipe for how the data is generated, it is often not too bad to then convert that recipe into code. We now illustrate this process with a detailed case study involving a more complex data-generating process Recent literature on multisite trials (where, for example, students are randomized to treatment or control within each of a series of sites) has explored how variation in the strength of effects across sites can affect how different data-analysis procedures behave (e.g., Miratrix et al., 2021; Bloom et al., 2016). In this example, we are going to extend this work to explore best practices for estimating treatment effects in cluster randomized trials. In particular, we will investigate what happens when the treatment impact for each school is related to the size of the school.

6.6.1   A design decision: What do we want to manipulate?

In designing a simulation study, we need to find a DGP that will allow us to address the specific questions we are interested in investigating. For instance, in the one-way ANOVA example, we wanted to see how different degrees of within-group variation impacted the performance of several hypothesis-testing procedures. We therefore needed a data generation process that allowed us to control the extent of within-group variation.

To figure out what DGP to use for simulating data from a cluster-randomized trial, we need to consider how we are going to use those data in our simulation study. Because we are interested in understanding what happens when school-

specific effects are related to school size, we will need data with the following features:

a) observations for students in each of several schools;
b) schools are different sizes and have different mean outcomes;
c) school-specific treatment effects correlate with school size; and
d) schools are assigned to different treatment conditions.

A given dataset will consist of observations for individual students in schools, with each student having a school id, a treatment assignment (shared for all in the school), and an outcome. A good starting point for building a DGP is to first sketch out what a simulated dataset should look like. For this example, we need data like the following:

schoolID	Z	size	studentID	Y
1	1	24	1	3.6
1	1	24	3	1.0
1	etc	etc	etc	etc
1	1	24	24	2.0
2	0	32	1	0.5
2	0	32	2	1.5
2	0	32	3	1.2
etc	etc	etc	etc	etc

When running simulations, it is good practice to look at simple scenarios along with complex ones. This lets us not only identify conditions where some aspect of the DGP is important, but also verify that the feature does *not* matter under scenarios where we know it should not. Given this principle, we land on the following points:

- We need a DGP that lets us generate schools that are all the same size or that are all different sizes.
- Our DGP should allow for variation in the school-specific treatment effects.
- We should have the option to generate school-specific effects that are related or unrelated to school size.

6.6.2   A model for a cluster RCT

DGPs are expressed and communicated using mathematical models. In developing a DGP, we often start by considering the model for the outcomes (along with its focal parameters), which covers some but not all of the steps in the full recipe for generating data. It is helpful to write down the equations for the outcome model and then note what further quantities need to be generated (such as structural features and covariates). Then we can consider how to generate these quantities with auxiliary models.

Section 6.1.3 introduced a basic HLM for a cluster-randomized trial. This model had two parts, starting with a model for our student outcome:

$$Y_{ij} = \beta_{0j} + \epsilon_{ij} \text{ with } \epsilon_{ij} \sim N(0, \sigma_\epsilon^2)$$

where Y_{ij} is the outcome for student i in site j, β_{0j} is the average outcome in site j, and ϵ_{ij} is the residual error for student i in site j. The model was completed by specifying how the site-specific outcomes vary as a function of treatment assignment:

$$\beta_{0j} = \gamma_0 + \gamma_1 Z_j + u_j, \quad u_j \sim N(0, \sigma_u^2).$$

This model has a constant treatment effect: if a school is assigned to treatment, then all outcomes in the cluster are raised by the amount γ_1. But we also want to allow the size of impact to vary by school size. This suggests we will need to elaborate the model to include a treatment-by-size interaction term.

One approach for allowing the school-specific impacts to depend on school size is to introduce school size as a predictor, as in

$$\beta_{0j} = \gamma_0 + \gamma_1 Z_j + \gamma_2 \left(Z_j \times n_j \right) + u_j.$$

A drawback of this approach is that changing the average size of the schools will change the average treatment impact. A more interpretable approach is to allow treatment effects to depend on the *relative* school sizes. To do this, we can define a covariate that describes the deviation in the school size relative to the average size. Thus, let

$$S_j = \frac{n_j - \bar{n}}{\bar{n}},$$

where $\bar{n}$ is the overall average school size. Using this covariate, we then revise our equation for our site j to:

$$\beta_{0j} = \gamma_0 + \gamma_1 Z_j + \gamma_2 \left(Z_j \times S_j \right) + u_j.$$

If γ_2 is positive, then bigger schools will have larger treatment impacts. Because S_j is centered at 0, the overall average impact across schools will be simply γ_1. (If S_j was not centered at zero, then the overall average impact would be some function of γ_1 and γ_2.)

Putting all of the above together, we now have an HLM to describe the distribution of outcomes conditional on the covariates and structural features:

$$\begin{aligned} Y_{ij} &= \beta_{0j} + \epsilon_{ij} & \epsilon_{ij} &\sim N(0, \sigma_\epsilon^2) \\ \beta_{0j} &= \gamma_0 + \gamma_1 Z_j + \gamma_2 Z_j S_j + u_j & u_j &\sim N(0, \sigma_u^2) \end{aligned}$$

Substituting the second equation into the first leads to a single equation for generating the student-level outcomes (or what is called the reduced form of the HLM):

$$Y_{ij} = \gamma_0 + \gamma_1 Z_j + \gamma_2 Z_j S_j + u_j + \epsilon_{ij}$$

The parameters of this focal model are the mean outcome among control schools (γ_0), the average treatment impact (γ_1), the site-size by treatment interaction term (γ_2), the amount of school-level variation (σ_u^2), and the amount of within-school variation (σ_ϵ^2).

There are several ways that we could elaborate this model further. For one, we might want to include a main effect for S_j, so that average outcomes in the absence of treatment are also dependent on school size. For another, we might revise the model to allow for school-to-school variation in treatment impacts that is not explained by school size. For simplicity, we do not build in these further features, but see the exercises at the end of the chapter.

So far we have a mathematical model analogous to what we would write if we were *analyzing* the data. To *generate* data, we also need a way to generate the structural features and covariates involved in the model. First, we need to know the number of clusters (J) and the sizes of the clusters (n_j, for $j = 1, ..., J$). For illustrative purposes, we will generate size sizes from a uniform distribution with average school size $\bar{n}$ and a fixed parameter α that controls the degree of variation in school size. Mathematically,

$$n_j \sim \text{Unif}\left[(1 - \alpha)\bar{n}, (1 + \alpha)\bar{n}\right].$$

Equivalently, we could generate site sizes by taking

$$n_j = \bar{n}(1 + \alpha U_j), \quad U_j \sim unif(-1, 1).$$

For instance, if $\bar{n} = 100$ and $\alpha = 0.25$ then schools would range in size from 75 to 125. This specification is nice because it is simple, with just two parameters, both of which are easy to interpret: $\bar{n}$ is the average school size and α is the degree of variation in school size.

To round out the model, we also need to define how to generate the treatment indicator, Z_j. To allow for different treatment allocations, we will specify a proportion p of clusters assigned to treatment. Because we are simulating a cluster-randomized trial, we do this by drawing a simple random sample (without replacement) of $p \times J$ schools out of the total sample of J schools, then setting $Z_j = 1$ for these schools and $Z_j = 0$ for the remaining schools. We will denote this process as $Z_1, ..., Z_J \sim SRS(p, J)$, where SRS stands for simple random sample.

Now that we have an auxiliary model for school sizes, let us look again at our treatment impact heterogeneity term:

$$\gamma_2 Z_j S_j = \gamma_2 Z_j \left(\frac{n_j - \bar{n}}{\bar{n}}\right) = \gamma_2 \alpha Z_j U_j,$$

where $U_j \sim \text{Unif}(-1, 1)$ is the uniform variable used to generate n_j. Because we have standardized by average school size, the importance of the covariate does not change as a function of average school size, but rather as a function of the

relative variation parameter α. Setting up a DGP with standardized quantities will make it easier to interpret simulation results, especially if we are looking at results from multiple scenarios with different parameter values. To the extent feasible, we want the parameters of the DGP to change only one feature of the data, so that it is easier to isolate the influence of each parameter.

6.6.3   From equations to code

When sketching out the equations for the DGP, we worked from the lowest level of the model (the students) to the higher level (schools) and then to the auxiliary models for covariates and structural features. For writing code to based on the DGP, we will proceed in the opposite direction, from auxiliary to focal and from the highest level to the lowest. First, we will generate the sites and their features:

- Generate school sizes
- Generate school-level covariates
- Generate school-level random effects

Then we will generate the students inside the sites:

- Generate student residuals
- Add everything up to generate student outcomes

The mathematical model gives us the details we need to execute with each of these steps.

Here is the skeleton of a DGP function with arguments for each of the parameters we might want to control, including defaults for each (see A.2 for more on function defaults):

```
gen_cluster_RCT <- function(
    J = 30,
    n_bar = 10,
    alpha = 0,
    p = 0.5,
    gamma_0 = 0, gamma_1 = 0, gamma_2 = 0,
    sigma2_u = 0, sigma2_e = 1
) {

  # generate schools sizes
  # Code (see below) goes here
}
```

Note that the inputs to this function are a mix of *model parameters* (`gamma_0`, `gamma_1`, `gamma_2`, representing coefficients in regressions), *auxilary parameters* (`sigma2_u`, `sigma2_e`, `alpha`, `n_bar`), and *design parameters* (`J`, `p`) that directly inform data generation. We set default arguments (e.g., `gamma_0=0`) so that we can ignore aspects of the DGP that we do not care about for the moment.

Inside the model, we will have a block of code to generate the variables pertaining to schools, and then another to generate the variables pertaining to students.

We first make the schools:

```r
n_min <- round( n_bar * (1 - alpha) )
n_max <- round( n_bar * (1 + alpha) )
nj <- sample( n_min:n_max, J, replace = TRUE )

# Generate average control outcome for all schools
# (the random effects)
u0j <- rnorm( J, mean = 0, sd = sqrt(sigma2_u) )

# randomize schools (proportion p to treatment)
Zj <- ifelse( sample( 1:J ) <= J * p, 1, 0)

# Calculate schools intercepts
S_j <- (nj - n_bar) / n_bar
beta_0j <- gamma_0 + gamma_1 * Zj + gamma_2 * Zj * S_j + u0j
```

The code is a literal translation of the math we did before. Note the line with `sample(1:J) <= J*p`; this is a simple trick to generate a 0/1 indicator for control and treatment conditions.

There is also a serious error in the above code (serious in that the code will run and look fine in many cases, but not always do what we want); we leave it as an exercise (see below) to find and fix it.

Next, we use the site characteristics to generate the individual-level variables:

```r
# Make individual site membership
sid <- as.factor( rep( 1:J, nj ) )

# Generate the individual-level errors and outcome
N <- sum( nj )
e <- rnorm( N, mean = 0, sd = sqrt(sigma2_e) )
Y <- beta_0j[sid] + e

# Bundle into a dataset
dd <- data.frame(
  sid = sid,
  Z = Zj[ sid ],
  Yobs = Y
)
```

A key piece here is the `rep()` function that takes a list and repeats each element of the list a specified number of times. In particular, `rep()` repeats each number $(1, 2, \ldots, J)$, the corresponding number of times as listed in `nj`. Putting the code

above into the function skeleton will produce a complete DGP function (view the complete function here). We can then call the function as so:

```
dat <- gen_cluster_RCT(
  J=3, n_bar = 5, alpha = 0.5, p = 0.5,
  gamma_0 = 0, gamma_1 = 0.2, gamma_2 = 0.2,
  sigma2_u = 0.4, sigma2_e = 1
)

dat
```

```
##     sid Z       Yobs
## 1    1 1   2.3263686
## 2    1 1   2.0202277
## 3    1 1   3.5850632
## 4    1 1   0.9581332
## 5    1 1   2.6183761
## 6    1 1   0.3198559
## 7    2 0  -2.2305376
## 8    2 0   1.0479261
## 9    2 0  -0.6256389
## 10   2 0   1.0891353
## 11   2 0  -0.6051252
## 12   2 0  -0.3099363
## 13   2 0  -0.9828624
## 14   2 0  -0.5571326
## 15   3 0   0.1203995
## 16   3 0   1.7086978
## 17   3 0   0.1213685
```

With this function, we can control the average size of the clusters (`n`), the number of clusters (`J`), the proportion treated (`p`), the average outcome in the control group (`gamma_0`), the average treatment effect (`gamma_1`), the site size by treatment interaction (`gamma_2`), the amount of cross site variation (`sigma2_u`), the residual variation (`sigma2_e`), and the amount of site size variation (`alpha`). The next step is to test the code, making sure it is doing what we think it is. In fact, it is not–there is a subtle bug that only appears under some specifications of the parameters; see the exercises for more on diagnosing and repairing this error.

6.6.4 Standardization in the DGP

One difficulty with the current implementation of the model is that the magnitude of the different parameters are inter-connected. For instance, raising or lowering the within-school variance (σ_u^2) will increase the overall variation in Y, and therefore affect our the interpretation of the treatment effect parameters, because a given value of γ_1 will be less consequential if there is more

overall variation. We can fix this issue by standardizing the model parameters. Standardization will allow us to reduce the set of parameters we might want to manipulate and will ensure that varying the remaining parameters only affects one aspect of the DGP.

For a continuous, normally distributed outcome variable, a common approach to scaling is to constrain the overall variance of the outcome to a fixed value, such as 1 or 100. The magnitude of the other parameters of the model can then be interpreted relative to this scale. Often, we can also constrain the mean of the outcome to a fixed value, such as setting $\gamma_0 = 0$ without affecting the interpretation of the other parameters.

With the current model, the variance of the outcome across students in the control condition is

$$
\begin{aligned}
\mathrm{Var}(Y_{ij}|Z_j = 0) &= \mathrm{Var}(\beta_{0j} + \epsilon_{ij}|Z_j = 0) \\
&= \mathrm{Var}(\gamma_0 + \gamma_1 Z_j + \gamma_2 Z_j S_j + u_j + \epsilon_{ij}|Z_j = 0) \\
&= \mathrm{Var}(\gamma_0 + u_j + \epsilon_{ij}) \\
&= \sigma_u^2 + \sigma_\epsilon^2.
\end{aligned}
$$

To ensure that the total variance is held constant, we can redefine the variance parameters in terms of the intra-class correlation (ICC). The ICC is defined as

$$
ICC = \frac{\sigma_u^2}{\sigma_u^2 + \sigma_\epsilon^2}.
$$

The ICC measures the degree of between-group variation as a proportion of the total variation of the outcome. It plays an important role in power calculations for cluster-randomized trials. If we want the total variance of the outcome to be 1, we need to set $\sigma_u^2 + \sigma_\epsilon^2 = 1$, which the implies that $ICC = \sigma_u^2$, and $\sigma_\epsilon^2 = 1 - ICC$. Thus, we can call our DGP function as follows:

```
ICC <- 0.3
dat <- gen_cluster_RCT(
  J = 30, n_bar = 20, alpha = 0.5, p = 0.5,
  gamma_0 = 0, gamma_1 = 0.3, gamma_2 = 0.2,
  sigma2_u = ICC, sigma2_e = 1 - ICC
)
```

Manipulating the ICC rather than separately manipulating σ_u^2 and σ_ϵ^2 will let us change the degree of between-group variation without affecting the overall scale of the outcome.

A further consequence of setting the overall scale of the outcome to 1 is that the parameters controlling the treatment impact can now be interpreted as standardized mean difference effect sizes. The standardized mean difference for a treatment impact is defined as the average impact over the standard deviation

of the outcome among control observations.[1] Letting δ denote the standardized mean difference parameter,

$$\delta = \frac{E(Y|Z_j = 1) - E(Y|Z_j = 0)}{SD(Y|Z_j = 0)} = \frac{\gamma_1}{\sqrt{\sigma_u^2 + \sigma_\epsilon^2}}$$

Because we have constrained the total variance, γ_1 is equivalent to δ. This equivalence holds for any value of γ_0, so we do not have to worry about manipulating γ_0 in the simulations—we can simply leave it at its default value.

6.7 Sometimes a DGP is all you need

We have introduced the data-generating process as only the first step in developing a simulation study. Indeed, there are many more considerations to come, which we will describe in subsequent chapters. However, this first step is still very useful in its own right, even apart from the other components of a simulation. Sometimes, a data-generating function is all you need to learn about a statistical model.

Writing data-generating functions is a very effective way to *study* a statistical model, such as a model that you might be learning about in a course or through self-study. Writing code based on a model is a much more *active* process than listening to a lecture or reading a book or paper. Coding requires you to make the mathematical notation tangible and can help you to notice details of the model that might be easily missed through listening or reading alone.

Suppose we are taking a first course psychometrics and have just been introduced to item response theory (IRT) models for binary response items. Our instructor has just laid out a bunch of notation:

- We have data from a sample of N individuals, each of whom responds to a set of M test items.
- We let $X_{im} = 1$ if respondent i answers item m correctly, with $X_{im} = 0$ otherwise, for $i = 1, ..., N$ and $m = 1, ..., M$.
- We imagine that each respondent has a latent ability θ_i on whatever domain the test measures.

Now our instructor starts dropping models on us, and puts up a slide showing the equation for a three-parameter IRT model:

$$Pr(X_{im} = 1) = \gamma_m + (1 - \gamma_m)g\left(\alpha_m[\theta_i - \beta_m]\right),$$

where $g(x)$ is the cumulative logistic curve: $g(x) = e^x/(1 + e^x)$. The instructor explains that α_m is discrimination parameter that can take any real value, β_m is a difficulty parameter that has to be greater than zero, and γ_m is a guessing

---

[1]An alternative definition is based on the pooled standard deviation, but this is usually a bad choice if one suspects treatment variation. More treatment variation should not reduce the effect size for the same absolute average impact.

parameter between 0 and 1. They also explain that the guessing parameter
is often hard to estimate and so might get treated as fixed and known, based
on the number of response options on the item. For instance, if all the items
have four options, then we might take $\gamma_m = \frac{1}{4}$ for $m = 1, ..., M$. Finally, they
explain that the ability parameters are assumed to follow a standard normal
distribution, so $\theta_i \sim N(0, 1)$ in the population.

What is this madness? It certainly is a lot of notation to follow. To make sense
of all the moving pieces, let's try simulating from the model using more-or-less
arbitrary parameters. To begin, we will need to pick a test length M and a
sample size N. Let's use $N = 7$ participants and $M = 4$ items for starters:

```
N <- 7
M <- 4
```

The θ_i distribution seems like the next-simplest part of the model, so let's gen-
erate some ability parameters:

```
thetas <- rnorm(N)
```

Now we need sets of parameters $\alpha_m, \beta_m, \gamma_m$ for every item $m = 1, ..., M$. Where
do we get these?

For a particular fixed-length test, the set of item parameters would depend on
the features of the actual test questions. But we are not (yet) dealing with
actual testing data, so we will need to make up an auxiliary model for these
parameters. Perhaps we could just simulate some values? Arbitrarily, let's
draw the difficulty parameters from a normal distribution with mean $\mu_\alpha = 0$
and standard deviation $\tau_\alpha = 1$. The discrimination parameters have to be
greater than zero, and values near $\beta_m = 1$ make the model simplify (in other
words, if $\beta_1 = 1$ then we can drop the parameter from the model), so let's draw
them from a gamma distribution with mean $\mu_\beta = 1$ and standard deviation
$\tau_\beta = 0.2$. This decision requires a bit of work: gamma distributions are usually
parameterized in terms of shape and rate, not mean and standard deviation.
A bit of poking on Wikipedia gives us the answer, however: shape is equal to
$\mu_\beta^2 \tau_\beta^2 = 0.2^2$ and rate is equal to $\mu_\beta \tau_\beta^2 = 0.2^2$. Finally, we imagine that all the
test questions have four possible responses, and therefore set $\gamma_m = \frac{1}{4}$ for all the
items, just like the instructor suggested. Each item requires three numbers; the
easiest way to generate them is to let them all be independent of each other, so
we do that. With that, let's make up some item parameters:

```
alphas <- rnorm(M, mean = 0, sd = 1.5)         # difficulty parameters
betas <- rgamma(M, shape = 0.2^2, rate = 0.2^2)  # discrimination parameters
gammas <- rep(1 / 4, M)                         # guessing parameters
```

A three-parameter IRT model describes the probability that a given respondent
with ability θ_i answers each of the items on the test correctly. To generate
data based on the model, we need to produce scores on every item for every
respondent, leading to a matrix of N respondents by M items. To simplify this

calculation, we write a function to compute the item probabilities for a single respondent:

```r
r_scores <- function(theta_i, alphas, betas, gammas, M) {
  pi_i <- gammas + (1 - gammas) * plogis(alphas * (theta_i - betas))
  scores <- rbinom(M, size = 1, prob = pi_i)
  names(scores) <- paste0("q",1:M)
  return(scores)
}

r_scores(thetas[1], alphas = alphas, betas = betas,
         gammas = gammas, M = M)
```

```
## q1 q2 q3 q4
##  0  1  0  1
```

The first line of the function calculates the probability of correctly answering all M items, and stores the result in a vector `pi_i`. In the next line, we simulate binary outcomes by flipping coins with the specified vector of probabilities. Finally, we assign names to each item so that we can keep track of which score is for which item. Now, using the `map()` function, we can run the function for every one of our respondents:

```r
map_dfr(
  thetas, .f = r_scores,
  alphas = alphas, betas = betas, gammas = gammas, M = M
)
```

```
## # A tibble: 7 x 4
##      q1    q2    q3    q4
##   <int> <int> <int> <int>
## 1     0     0     1     0
## 2     1     1     0     0
## 3     1     0     0     0
## 4     1     1     1     1
## 5     0     0     0     1
## 6     1     0     1     1
## 7     0     1     0     0
```

To make it easier to generate datasets with different characteristics, we bundle the above code chunks into a single data-generating function. To do so, we have to decide what the input parameters should be. We know we need to at least specify N and M. We made assumptions about the item parameters, but we had to specify means and standard deviations for the difficulty and discrimination parameter distributions, so it is natural to allow those to be inputs also. Our data-generating function will then be

```r
r_3PL_IRT <- function(
    N, M = 4,
    diff_M = 0, diff_SD = 1,
    disc_M = 1, disc_SD = 0.2,
    item_options = 4
) {
  # generate ability parameters
  thetas <- rnorm(N)

  # generate item parameters
  alphas <- rnorm(M, mean = diff_M, sd = diff_SD)
  betas <- rgamma(M,
                  shape = disc_M^2 * disc_SD^2,
                  rate = disc_M * disc_SD^2)
  gammas <- rep(1 / item_options, M)

  # simulate item responses
  test_scores <- map_dfr(
   thetas, .f = r_scores,
    alphas = alphas, betas = betas, gammas = gammas, M = M
  )

  # calculate total score
  test_scores$total <- rowSums(test_scores)

  return(test_scores)
}

r_3PL_IRT(N = 7, M = 4)
```

```
## # A tibble: 7 x 5
##      q1    q2    q3    q4 total
##   <int> <int> <int> <int> <dbl>
## 1     1     1     0     0     2
## 2     1     1     1     1     4
## 3     1     1     1     0     3
## 4     1     1     1     1     4
## 5     1     1     1     0     3
## 6     1     1     1     1     4
## 7     1     1     1     1     4
```

Now let's look at a much larger sample of participants, with a longer test that includes $M = 12$ items:

```r
test_scores <- r_3PL_IRT(N = 10000, M = 12)
```

Having written a function for the 3-parameter logistic IRT model makes it easy

to explore properties of the model. For instance, we can easily visualize the distribution of the total scores on the test:

```
ggplot(test_scores, aes(total)) +
  geom_bar() +
  scale_x_continuous(limits = c(0,12.5), breaks = seq(0,12,2))
```
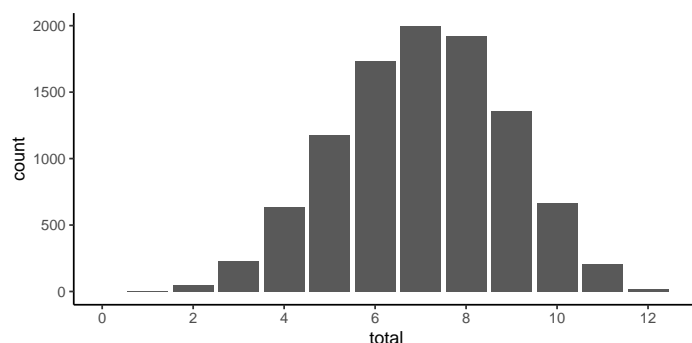

Looking at item variation, we can examine the probability of correctly responding to each of the items by computing sample means for each item:

```
test_scores %>%
  summarise(across(starts_with("q"), mean))
```

```
## # A tibble: 1 x 12
##       q1    q2    q3    q4    q5    q6    q7    q8
##    <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl>
## 1 0.628  0.62 0.629 0.256 0.539 0.620 0.624 0.620
## # i 4 more variables: q9 <dbl>, q10 <dbl>,
## #   q11 <dbl>, q12 <dbl>
```

The percentage of correct responses varies from 25.6% to 63.3. What are the correlations between individual items and the total score? Let's check:

```
test_scores %>%
  summarise(across(starts_with("q"), ~ cor(.x, total)))
```

```
## # A tibble: 1 x 12
##       q1    q2     q3    q4    q5    q6    q7    q8
##    <dbl> <dbl>  <dbl> <dbl> <dbl> <dbl> <dbl> <dbl>
## 1 0.154 0.386 0.0195 0.227 0.445 0.411 0.386 0.421
## # i 4 more variables: q9 <dbl>, q10 <dbl>,
## #   q11 <dbl>, q12 <dbl>
```

Note that simulating a new dataset will produce different results for these summaries because generating each dataset entails sampling a new set of items (with different difficulty and discrimination).

Writing a DGP function makes it possible to study a model through exploration,

simply by examining datasets generated by wiggling the model parameters up or down. For instance, we could look at what happens to the distribution of total scores if the items covered a much broader range of difficulties (higher τ_α) or are mis-calibrated to be too difficult ($\mu_\tau > 0$). What if the items had varying numbers of response options, so the guessing parameters differ? Are there item parameter values that will produce highly unrealistic distributions of total scores? Exercises 6.9.11, 6.9.12, and 6.9.13 ask you to further explore these questions.

Overall, implementing the model as a data-generating function has allowed us to explore the model in a more active way than simply reading about it or listening to a lecture. We have a more visceral feel about how the different parameters would create variation in our data—and it would be easy to tweak those parameters to see how things changed to learn even more.

6.8   More to explore

This chapter has introduced the core components of a data-generating process and demonstrated how to move from formulating a full data-generating model to implementing the model in R code. Our main aim has been to provide enough scaffolding for you to get started with simulating from and exploring a variety of models. The exercises below will give you further practice in developing, testing, and extending DGP functions. Of course, we have not covered every consideration and challenge that arises when writing DGPs for simulations— there is *much* more to explore!

We will cover some further challenges in subsequent chapters. Yet more challenges will surely arise as you apply simulations in your own work. Even though such challenges might not align with the examples or contexts that we have covered here, the concepts and principles that we have introduced should allow you to reason about potential solutions. In doing so, we encourage you adopt the attitude of a chef in a test kitchen by trying out your ideas with code. In the kitchen, there is often no way to know how a dish will turn out until you actually bake it and taste it. Likewise, in developing a DGP, the best way to understand and evaluate a DGP is to write it out in code and explore the datasets that you can produce with it.

6.9   Exercises

6.9.1   The Welch test on a shifted-and-scaled t distribution

The shifted-and-scaled t-distribution has parameters μ (mean), σ (scale), and ν (degrees of freedom). If T follows a student's t-distribution with ν degrees of freedom, then $S = \mu + \sigma T$ follows a shifted-and-scaled t-distribution.

The following function will generate random draws from this distribution. We

additionally scale by $(\nu - 2)/\nu$ to achieve the target standard deviation (a t-distribution has a variance of $\nu/(\nu - 2)$).

```r
r_tss <- function(n, mean, sd, df) {
  mean + sd * sqrt( (df-2)/df ) * rt(n = n, df = df)
}


r_tss(n = 8, mean = 3, sd = 2, df = 5)
```

```
## [1]  0.02822602  3.87035901  4.51376755
## [4]  3.02447410 -0.26265918  2.29642811
## [7]  1.16346358  7.59634125
```

1. Modify the Welch simulation's `simulate_data()` function to generate data from shifted-and-scaled t-distributions rather than from normal distributions. Include the degrees of freedom as an input argument. Simulate a dataset with low degrees of freedom and plot it to see if you see a few outliers.

2. Now generate more data and calculate the means and standard deviations to see if they are correctly calibrated (i.e., generate a big dataset to ensure you get reliable mean and standard deviation estimates). Check `df` equal to 500, 5, 3, and 2.

3. Once you are satisfied you have a correct DGP function, re-run the Type-I error rate calculations from the prior exercises in Section 5.5 using a t-distribution with 5 degrees of freedom. Do the results change substantially?

6.9.2 Plot the bivariate Poisson

In Section 6.3, we provided an example of a DGP function for the bivariate Poisson model. We demonstrated a plot of data simulated from this function in 6.4. Create a similar plot but for a much larger sample size of $N = 1000$.

With such a large dataset, it will likely be hard to distinguish individual observations because of over-plotting. Create a better visual representation of the same simulated dataset, such as a heatmap or a contour plot.

6.9.3 Check the bivariate Poisson function

Although we presented a DGP function for the bivariate Poisson model, we have not demonstrated how to check that the function is correct—we're leaving that to you! Write some code to verify that the function `r_bivariate_Poisson()` is working properly. Do this by generating a very large sample (say $N = 10^4$ or 10^5) and verifying the following:

- The sample means of C_1 and C_2 align with the specified population means.

- The sample variances of C_1 and C_2 are close to the specified population means (because for a Poisson distribution $\mathbb{E}(C_p) = \mathbb{V}(C_p)$ for $p = 1, 2$).
- The sample correlation aligns with the specified population correlation.
- The observed counts C_1 and C_2 follow Poisson distributions.

6.9.4   Add error-catching to the bivariate Poisson function

In Section 6.1, we noted that the bivariate Poisson function as we described it can only produce a constrained range of correlations, which a maximum value that depends on the ratio of μ_1 to μ_2. Our current implementation of the model does not handle this aspect of the model very well:

```
r_bivariate_Poisson(5, rho = 0.6, mu1 = 4, mu2 = 12)
```

```
## Warning in rpois(N, lambda = mu1 - EZ3): NAs
## produced
```

```
##   C1 C2
## 1 NA 11
## 2 NA 11
## 3 NA 13
## 4 NA 15
## 5 NA  9
```

For this combination of parameter values, $\rho \times \sqrt{\mu_1 \mu_2}$ is larger than μ_1, which leads to simulated values for C_1 that are all missing. That makes it pretty hard to compute the correlation between C_1 and C_2.

Please help us fix this issue! Revise `r_bivariate_Poisson()` so that it checks for allowable values of ρ. If the user specifies a combination of parameters that does not make sense, make the function throw an error (using R's `stop()` function).

6.9.5   A bivariate negative binomial distribution

One potential limitation of the bivariate Poisson distribution described above is that the variances of the counts are necessarily equal to the means (i.e., unit dispersion). This limitation is inherited from the univariate Poisson distributions that each variate follows. Just as with the corresponding univariate distributions, one way to relax this limitation is to consider distributions with marginals that are negative binomial rather than Poisson, thereby allowing for overdispersion. Cho et al. (2023) describes one type of bivariate negative binomial distribution and provides a method for constructing a bivariate negative binomial distribution by using latent, gamma-distributed components. Their algorithm involves first generating components from gamma distributions with specified

shape and scale parameters:

$$Z_0 \sim \Gamma\left(\alpha_0, \beta\right)$$
$$Z_1 \sim \Gamma\left(\alpha_1, \beta\right)$$
$$Z_2 \sim \Gamma\left(\alpha_2, \beta\right)$$

for $\alpha_0, \alpha_1, \alpha_2 > 0$ and $\beta > 0$. They then simulate independent Poisson random variables as

$$C_1 \sim Pois\left(Z_0 + Z_1\right)$$
$$C_2 \sim Pois\left(\delta(Z_0 + Z_2)\right).$$

The resulting count variables follow marginal negative binomial distributions with moments

$$\mathbb{E}(C_1) = (\alpha_0 + \alpha_1)\beta \qquad \mathbb{V}(C_1) = (\alpha_0 + \alpha_1)\beta(\beta + 1)$$
$$\mathbb{E}(C_2) = (\alpha_0 + \alpha_2)\beta\delta \qquad \mathbb{V}(C_2) = (\alpha_0 + \alpha_2)\beta\delta(\beta\delta + 1)$$
$$\mathrm{Cov}(C_1, C_2) = \alpha_0\beta^2\delta.$$

The correlation between C_1 and C_2 is thus

$$\mathrm{cor}(C_1, C_2) = \frac{\alpha_0}{\sqrt{(\alpha_0 + \alpha_1)(\alpha_0 + \alpha_2)}} \frac{\beta\sqrt{\delta}}{\sqrt{(\beta + 1)(\beta\delta + 1)}}.$$

1. Write a DGP function that implements this distribution.

2. Write some code to check that the function produces data where each variate follows a negative binomial distribution and where the correlation agrees with the formula given above.

3. Consider parameter values that produce $\mathbb{E}(C_1) = \mathbb{E}(C_2) = 10$ and $\mathbb{V}(C_1) = \mathbb{V}(C_2) = 15$. What are the minimum and maximum possible correlations between C_1 and C_2?

6.9.6 Another bivariate negative binomial distribution

Another model for generating bivariate counts with negative binomial marginal distributions is by using Gaussian copulas. Here is a mathematical recipe for this distribution, which will produce counts with marginal means μ_1 and μ_2 and marginal variances $\mu_1 + \mu_1^2/p_1$ and $\mu_2 + \mu_2^2/p_2$. Start by generating variates from a bivariate standard normal distribution with correlation ρ:

$$\begin{pmatrix} Z_1 \\ Z_2 \end{pmatrix} \sim N\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 & \rho \\ \rho & 1 \end{bmatrix} \right)$$

Now find $U_1 = \Phi(Z_1)$ and $U_1 = \Phi(Z_1)$, where $\Phi()$ is the standard normal cumulative distribution function (called `pnorm()` in R). Then generate the counts by evaluating U_1 and U_2 with the negative binomial quantile function, $F_{NB}^{-1}(x|\mu, p)$

with mean parameters μ and size parameter p (this function is called `qnbinom()` in R):

$$C_1 = F_{NB}^{-1}(U_1|\mu_1, p_1) \qquad C_2 = F_{NB}^{-1}(U_2|\mu_2, p_2).$$

The resulting counts will be correlated, but the correlation will not be equal to ρ.

1. Write a DGP function that implements this distribution.

2. Write some code to check that the function produces data where each variate follows a negative binomial distribution

3. Use the function to create a graph showing the population correlation between the observed counts as a function of ρ. Use $\mu_1 = \mu_2 = 10$ and $p_1 = p_2 = 20$. How does the range of correlations compare to the range from Exercise 6.9.5?

6.9.7   Plot the data from a cluster-randomized trial

Run `gen_cluster_RCT()` with parameter values of your choice to produce data from a simulated cluster-randomized trial. Create a plot of the data that illustrates how student-level observations are nested within schools and how schools are assigned to different treatment conditions.

6.9.8   Checking the Cluster RCT DGP

1. What is the variance of the outcomes generated by the model for the cluster-randomized trial if there are no treatment effects? (Try simulating data to check!) What other quick checks can you run on this DGP to make sure it is working correctly?

2. In `gen_cluster_RCT()` we have the following line of code to generate the number of individuals per site.

```
nj <- sample( n_min:n_max, J, replace=TRUE )
```

   This code has an error. Generate a variety of datasets where you vary `n_min`, `n_max` and `J` to discover the error. Then repair the code. Checking your data generating process across a range of scenarios is extremely important.

6.9.9   More school-level variation

The DGP for the cluster-randomized trial allows for school-level treatment impact variation, but only to the extent that the variation is explained by school size. How could you modify your simulation to allow for school-level treatment impact variation that is not related to school size? Implement this change and generate some data to show how it works.

6.9.10 Cluster-randomized trial with baseline predictors

Extend the DGP for the cluster-randomized trial to include an individual-level covariate X that is correlated with the outcome. Do this by modifying the model for student-level outcomes as

$$Y_{ij} = \beta_{0j} + \beta_1 X_{ij} + \epsilon_{ij}.$$

Keep the same β_1 for all sites. To implement this model as a DGP, you will have to decide how to generate X_{ij}.

1. Use words and equations to explain your auxiliary model for X_{ij}.
2. Implement the model by modifying `gen_cluster_RCT()` accordingly.
3. Use your implementation to find the unconditional variance of the outcome, $\text{Var}(Y|Z_j = 0)$, when $\beta_1 = 0.6$.

6.9.11 3-parameter IRT datasets

A challenge that arises with the IRT model described in Section 6.7 is that the data are generated using *random parameters* (the person ability parameters $\theta_1, ..., \theta_N$ and item characteristics $\alpha_m, \beta_m, \gamma_m$ for $m = 1, ..., M$) that we simulated from auxiliary models. When applying IRT models to actual test data, the analyst's goal will usually involve estimating at least some of these parameters: either using the model for *scoring* by estimating latent ability parameters or for *calibration* by estimating the item characteristics. But each time we generate a new dataset with `r_3PL_IRT()`, those latent parameters will change.

In order to understand how well an estimation procedure will perform on data generated by our function, we will need to keep track of the parameter values, even though those values will not be known in real data analysis contexts. Suppose that our main interest is in understanding how well we can recover the item characteristics.

1. Modify `r_3PL_IRT()` to return a list containing two datasets. The first entry in the list should be a dataset with the person-by-item responses, just as in the original function. The second entry in the list should be an $M \times 3$ dataset containing the item parameters.

2. An alternative strategy for implementing the three-parameter IRT DGP is to write two functions instead of one: a function to simulate a set of M item parameters and a function to simulate the person-by-item responses. Complete the following function skeletons to implement this strategy. Demonstrate how to use the functions to simulate a dataset.

```r
r_3PL_items <- function(
  M,
  diff_M = 0, diff_SD = 1,
  disc_M = 1, disc_SD = 0.2,
  item_options = 4
```

```
) {
  # Code here
  return(item_parameter_data)
}

r_3PL_data <- function( N, item_data ) {
  # Generate item responses
  return(response_data)
}
```

3. Describe the benefits and limitations of the two approaches you have implemented.

4. For your preferred strategy, modify your function(s) to also return the latent person ability parameters.

6.9.12   Check the 3-parameter IRT DGP

For one of the DGPs you wrote in Exercise 6.9.11, write code to check that the function is working properly. What features of the model will you check?

6.9.13   Explore the 3-parameter IRT model

Use the modified DGP function(s) you wrote for Exercise 6.9.11 to explore the model. Simulate data and create visualizations to answer the following questions.

1. What happens to the distribution of total scores if the items covered a very broader range of difficulties (higher τ_α)?
2. What happens if the items are mis-calibrated to be too difficult ($\mu_\tau > 0$)?
3. What if the items had varying numbers of response options, so the guessing parameters differ?
4. Find at least one combination of parameter values that will produce very extreme or unrealistic distributions of total scores.

6.9.14   Random effects meta-regression

Meta-analysis involves working with quantitative findings reported by previous studies on a particular topic, in the form of effect size estimates and their standard errors, to generate integrative summaries and identify patterns in the findings that might not be evident from any previous study considered in isolation. One model that is widely used in meta-analysis is the random effects meta-regression, which relates the effect sizes to known characteristics of the studies that are encoded in the form of predictors. Consider a collection of K studies. Let T_i denote an effect size estimate and s_i denote its standard error for study i. Let x_i be a quantitative predictor variable that represents some

characteristic of study i (such as its year of publication). The random effects meta-regression model assumes

$$T_i = \beta_0 + \beta_1 x_i + u_i + e_i,$$

where $u_i \sim N(0, \tau^2)$ and $e_i \sim N(0, s_i^2)$. In this model, β_0 corresponds to the expected effect size when $x_i = 0$ and β_1 describes the expected difference in effect size per one unit difference in x_i. The first error u_i corresponds to the heterogeneity in the effect sizes above and beyond the variation explained by x_i, and the second error e_i corresponds to the sampling error, which we assume has known variance s_i^2.

1. Of the variables in the random effects meta-regression model, which are structural features, which are covariates, and which are outcomes? Of the parameters described above, which would you classify as focal, which as auxiliary, and which as design parameters?

2. In addition to the focal model described above, what further assumptions or auxiliary models will be needed in order to simulate data for a random effects meta-regression? Propose an auxiliary model for any needed quantities.

3. Using your proposed auxiliary model, write a function to generate data for a random effects meta-regression. Demonstrate your function by creating a plot based on a simulated dataset with $K = 30$ effect sizes.

4. Write code to check the properties of your data-generating function.

6.9.15   Meta-regression with selective reporting

Vevea and Hedges (1995) proposed a meta-regression model that allows for the possibility that not all primary study results are published. They assume that primary study results are generated according to the random effects meta-regression model described in Exercise 6.9.14, but then only a subset of results are observed, where the probability of being included is a function of the result's one-sided p-value for the null hypothesis $H_0 : \delta \leq 0$ against alternative $H_A : \delta > 0$. Let $p_i = 1 - \Phi(T_i/s_i)$ be the one-sided p-value for study result i, where $Phi()$ is the standard normal cumulative distribution (`pnorm()` in R). In one version of the selection model, the selection probability follows a piece-wise constant distribution with

$$\Pr(T_i \text{ is observed}) = \begin{cases} 1 & \text{if} \quad 0 \leq p_i < .025 \\ \lambda_1 & \text{if} \quad .025 \leq p_i < .500 \\ \lambda_2 & \text{if} \quad .500 \leq p_i < 1 \end{cases}$$

for selection probabilities $0 \leq \lambda_1 \leq 1$ and $0 \leq \lambda_2 \leq 1$.

1. Modify your data-generating function from Exercise 6.9.14 to follow the Vevea-Hedges selection model. Ensure that the new data-generating function returns a total of K primary study results.

2. Use the new function to generate a large number of effect size estimates, all with $s_i = 0.35$, using parameters $\beta_0 = 0.1$, $\beta_1 = 0.0$, $\tau = 0.1$, $\lambda_1 = 0.5$, and $\lambda_2 = 0.2$. Plot the distribution of observed effect size estimates.

3. Create several further plots using different values for λ_1 and λ_2. How do these parameters affect the shape of the distribution?

4. Use the `selmodel()` function from the `metafor` package to estimate the Vevea-Hedges selection model based on one of your simulated datasets. (See Exercise 7.5.7 for example syntax.) How do the estimates compare to the model parameters you've specified?

Chapter 7

Data analysis procedures

The overall aims of many simulation studies have to do with understand how a particular data-analysis procedure works or comparing the performance of multiple, competing procedures. Thus, the data-analysis procedure or procedures are the central object of study. Depending on the research question, the data-analysis procedure might be very simple—as simple as just computing a sample correlation–or it might involve a combination of several components. For example, the procedure might entail first computing a diagnostic test for heteroskedasticity and then, depending on the outcome of the test, applying either a conventional formula or a heteroskedasticity-robust formula for standard errors. As another example, a data-analysis procedure might involve using multiple imputation for missingness on key variables, then fitting a statistical model, and then generating predicted values based on the model. Also depending on the research question, we might need to create *several* functions that implement different estimation procedures to be compared.

In this chapter, we demonstrate how to implement data-analysis procedures in the form of R functions, which we call *estimation functions*, so that their performance can eventually be evaluated by repeatedly applying them to artificial data. We start by describing the high-level design of an estimation function, and illustrate with some simple examples. We then discuss approaches for writing simulations that compare multiple data analysis procedures. Next, we describe strategies for validating the coded-up estimation functions before running a full simulation. Finally, we examine methods for handling common computational problems with estimation functions, such as handling non-convergence when using maximum likelihood estimation.

7.1   Writing estimation functions

In the abstract, a function that implements an estimation procedure should have
the following form:

```r
estimate <- function(data) {

  # calculations/model-fitting/estimation procedures

  return(estimates)
}
```

The function takes a dataset as input, fits a model or otherwise calculates an es-
timate, possibly with associated standard errors and so forth, and returns these
quantities as output. The estimates could be point estimates of parameters,
standard errors, confidence intervals, p-values, predictions, or other quantities.
The calculations in the body of the function should be set up to use datasets
that have the same structure (i.e., same dimensions, same variable names) as
the output of the corresponding function for generating simulated data. How-
ever, in principle, we should also be able to run the estimation function on real
data as well.

In Chapter 5 we wrote a function called `ANOVA_Welch_F()` for computing p-
values from two different procedures for testing equality of means in a het-
eroskedastic ANOVA:

```r
ANOVA_Welch_F <- function(data) {
  anova_F <- oneway.test(x ~ group, data = data, var.equal = TRUE)
  Welch_F <- oneway.test(x ~ group, data = data, var.equal = FALSE)

  result <- tibble(
    ANOVA = anova_F$p.value,
    Welch = Welch_F$p.value
  )

  return(result)
}
```

Apply this function to a simulated dataset returns two p-values, one for the
usual ANOVA F test (which assumes homoskedasticity) and one for Welch's
heteroskedastic F test:

```r
sim_data <- generate_ANOVA_data(
  mu = c(1, 2, 5, 6),
  sigma_sq = c(3, 2, 5, 1),
  sample_size = c(3, 6, 2, 4)
)
ANOVA_Welch_F(sim_data)
```

```
## # A tibble: 1 x 2
##     ANOVA   Welch
##     <dbl>   <dbl>
## 1 0.000293 0.0179
```

Our `ANOVA_Welch_F()` function is designed to work with the output of `generate_ANOVA_data()` in that it assumes that the grouping variable is called `group` and the outcome is called `x`. Relying on this assumption would be a poor choice if we were designing a function as part of an R package or for general-purpose use. However, because the primary use of the function is for simulation, it is reasonable to assume that the input data will always have appropriate variable names.

In Chapter 6, we looked at a data-generating function for a bivariate Poisson distribution, an example of a non-normal bivariate distribution. We might use such a distribution to understand the behavior of Pearson's sample correlation coefficient and its normalizing transformation, known as Fisher's z-transformation, which is equivalent to the hyperbolic arc-tangent function (`atanh()` in R). When the sample measurements follow a bivariate normal distribution, Fisher's z-transformed correlation is very close to normally distributed and its standard error is simply $1/\sqrt{N-3}$, and thus independent of the correlation. This makes z-transformation very useful for computing confidence intervals, which can then be back-transformed to the Pearson-r scale.

In this problem, a simple estimation function would take a dataset with two variables as input and compute the sample correlation and its z-transformation, compute confidence intervals for z, and then back-transform the confidence interval end-points. Here is an implementation of these calculations:

```r
r_and_z <- function(data) {

  r <- cor(data$C1, data$C2)
  z <- atanh(r)
  se_z <- 1 / sqrt(nrow(data) - 3)
  ci_z <- z + c(-1, 1) * qnorm(.975) * se_z
  ci_r <- tanh(ci_z)

  tibble( r = r, z = z, CI_lo = ci_r[1], CI_hi = ci_r[2] )
}
```

To check that the function returns a result of the expected form, we generate a small dataset using the `r_bivariate_Poisson()` function developed in the last chapter, then apply our estimation function to the result:

```r
Pois_dat <- r_bivariate_Poisson(40, rho = 0.5, mu1 = 4, mu2 = 4)
r_and_z(Pois_dat)
```

```
## # A tibble: 1 x 4
##       r     z CI_lo CI_hi
```

```
##    <dbl> <dbl> <dbl> <dbl>
## 1 0.557 0.628 0.296 0.740
```

Although it is a little cumbersome to do so, we could also apply the estimation function to a real dataset. Here is an example, which calculates the correlation between ratings of judicial integrity and familiarity with the law from the `USJudgeRatings` dataset (which is included in base R). For the function to work on this dataset, we first need to rename the relevant variables.

```
data(USJudgeRatings)

USJudgeRatings %>%
  dplyr::select(C1 = INTG, C2 = FAMI) %>%
  r_and_z()
```

```
## # A tibble: 1 x 4
##       r     z CI_lo CI_hi
##   <dbl> <dbl> <dbl> <dbl>
## 1 0.869  1.33 0.769 0.927
```

The function returns a valid result—a quite strong correlation!

It is a good practice to test out a newly-developed estimation function on real data as a check that it is working as intended. This type of test ensures that the estimation function is not using information outside of the dataset, such as by using known parameter values to construct an estimate. Applying the function to a real dataset demonstrates that the function implements a procedure that could actually be applied in real data analysis contexts.

7.2 Including Multiple Data Analysis Procedures

Many simulations involve head-to-head comparisons between more than one data-analysis procedure. As a design principle, we generally recommend writing different functions for each estimation method one is planning on evaluating. Doing so makes it easier to add in additional methods as desired or to focus on just a subset of methods. Writing separate function also leads to a code base that is flexible and useful for other purposes (such as analyzing real data). Finally (repeating one of our favorite mantras), separating functions makes debugging easier because it lets you focus attention on one thing at a time, without worrying about how errors in one area might propagate to others.

To see how this works in practice, we will return to the case study from Section 6.6, where we developed a data-generating function for simulating a cluster-randomized trial with student-level outcomes but school-level treatment assignment. Our data-generating process allowed for varying school sizes and heterogeneous treatment effects, which might be correlated with school size. Several

different procedures might be used to estimate an overall average effect from a clustered experiment, including:

- Estimating a multi-level regression model (also known as a hierarchical linear model),
- Estimating an ordinary least squares (OLS) regression model and applying cluster-robust standard errors, or
- Averaging the outcomes by school, then estimating a linear regression model on the mean outcomes.

All three of these methods are widely used and have some theoretical guarantees supporting their use. Education researchers tend to be more comfortable using multi-level regression models, whereas economists tend to use OLS with clustered standard errors.

We next develop estimation functions for each of these procedures. We analyze as we expect would be done in practice; even though we generated data with a school size covariate, we do not include it in our estimation functions. Each function needs to produce a point estimate, standard error, and p-value for the average treatment effect. To have data to practice on, we generate a sample dataset using a revised version of `gen_cluster_RCT()`, which corrects the bug discussed in Exercise 6.9.8:

```
dat <- gen_cluster_RCT(
  J=16, n_bar = 30, alpha = 0.8, p = 0.5,
  gamma_0 = 0, gamma_1 = 0.2, gamma_2 = 0.2,
  sigma2_u = 0.4, sigma2_e = 0.6
)
```

For the multi-level modeling strategy, there are several different existing packages that we could use. We will implement an estimator using the popular `lme4` package, along with the `lmerTest` function for computing a p-value for the average effect. Here is a basic implementation:

```
analysis_MLM <- function( dat ) {

  M1 <- lme4::lmer( Yobs ~ 1 + Z + (1 | sid), data = dat )
  M1_test <- lmerTest::as_lmerModLmerTest(M1)
  M1_summary <- summary(M1_test)$coefficients

  tibble(
    ATE_hat = M1_summary["Z","Estimate"],
    SE_hat = M1_summary["Z","Std. Error"],
    p_value = M1_summary["Z", "Pr(>|t|)"]
  )
}
```

The function fits a multi-level model with a fixed coefficient for the treatment indicator and random intercepts for each school. To get a p-value for the treat-

ment coefficient, we have to convert the model into an `lmerModLmerTest` object
and then pass it through `summary()`. The function outputs only the statistics
in which we are interested.

Our function makes use of the `lme4` and `lmerTest` packages. Rather than
assuming that these packages will be loaded, we call relevant functions using
the package name as a prefix, as in `lme4::lmer()`. This way, we can run the
function even if we have not loaded the packages in the global environment.
This approach is also preferable to loading packages inside the function itself
(e.g., with `require(lme4)`) because calling the function does not change which
packages are loaded in the global environment.

Here is a function implementing OLS regression with cluster-robust standard
errors:

```r
analysis_OLS <- function( dat, se_type = "CR2" ) {

  M2 <- estimatr::lm_robust(
    Yobs ~ 1 + Z, data = dat,
    clusters = sid,  se_type = se_type
  )

  tibble(
    ATE_hat = M2$coefficients[["Z"]],
    SE_hat = M2$std.error[["Z"]],
    p_value = M2$p.value[["Z"]]
  )
}
```

To get cluster-robust standard errors, we use the `lm_robust()` function from the
`estimatr()` package, again calling only the relevant function using the package
prefix rather than loading the whole package. A novel aspect of this estimation
function is that it includes an additional intput argument, `se_type`, which allows
us to control the type of standard error calculated by `lm_robust()`. Adding this
option would let us use the same function to compute (and compare) different
types of clustered standard errors for the average treatment effect estimate. We
set a default option of `"CR2"`, just like the default of `lm_robust()`.

Sometimes an analytic procedure involves multiple steps. For example, aggre-
gation estimator first involves collapsing the data to a school-level dataset, and
then analyzing at the school level. This is fine: we just wrap all the steps in a
single estimation function: from the point of view of *using* the function, it is a
single call, no matter how complicated the process inside. Here is the code for
the aggregate-then-analyze approach:

```r
analysis_agg <- function( dat, se_type = "HC2" ) {

  datagg <- dplyr::summarise(
```

```r
    dat,
    Ybar = mean( Yobs ),
    n = n(),
    .by = c(sid, Z)
  )

  stopifnot( nrow( datagg ) == length(unique(dat$sid) ) )

  M3 <- estimatr::lm_robust(
    Ybar ~ 1 + Z, data = datagg,
    se_type = se_type
  )

  tibble(
    ATE_hat = M3$coefficients[["Z"]],
    SE_hat = M3$std.error[["Z"]],
    p_value = M3$p.value[["Z"]]
  )
}
```

Note the `stopifnot` command: it will throw an error if the condition is not true. This `stopifnot` ensures we do not have both treatment and control students within a single school–if we did, we would have more aggregated values than school ids due to the grouping! Putting *assert statements* in your code like this is a good way to guarantee you are not introducing weird and hard-to-track errors. A `stopifnot` statement halts your code as soon as something goes wrong, rather than letting that initial wrongness flow on to further work, creating odd results that are hard to understand. Here we are protecting ourselves from strange results if, for example, we messed up our DGP code to have treatment not nested within school, or we were using data that did not actually come from a cluster randomized experiment. See Section 19.4 for more.

All of our functions produce output in the same format:

```r
analysis_MLM( dat )
```

```
## # A tibble: 1 x 3
##   ATE_hat SE_hat p_value
##     <dbl>  <dbl>   <dbl>
## 1  -0.111  0.323   0.737
```

```r
analysis_OLS( dat )
```

```
## # A tibble: 1 x 3
##   ATE_hat SE_hat p_value
##     <dbl>  <dbl>   <dbl>
## 1  -0.177  0.307   0.576
```

```r
analysis_agg( dat )
```

```
## # A tibble: 1 x 3
##   ATE_hat SE_hat p_value
##     <dbl>  <dbl>   <dbl>
## 1 -0.0818  0.339   0.813
```

Ensuring that the output of all the functions is structured in the same way will make it easy to keep the results organized once we start running multiple iterations of the simulation. If each estimation method returns a dataset with the same variables, we can simply stack the results on top of each other. Here is a function that bundles all the estimation procedures together:

```r
estimate_Tx_Fx <- function(
    data,
    CR_se_type = "CR2", agg_se_type = "HC2"
) {

  dplyr::bind_rows(
    MLM = analysis_MLM( data ),
    OLS = analysis_OLS( data, se_type = CR_se_type),
    agg = analysis_agg( data, se_type = agg_se_type),
    .id = "estimator"
  )

}
```

```r
estimate_Tx_Fx(dat)
```

```
## # A tibble: 3 x 4
##   estimator ATE_hat SE_hat p_value
##   <chr>       <dbl>  <dbl>   <dbl>
## 1 MLM        -0.111  0.323   0.737
## 2 OLS        -0.177  0.307   0.576
## 3 agg       -0.0818  0.339   0.813
```

This is a common coding pattern for simulations that involve multiple estimation procedures. Each procedure is expressed in its own function, then these are assembled together in a single function so that they can all easily be applied to the same dataset. Stacking the results row-wise will make it easy to compute performance measures for all methods at once. The benefit of stacking will become even more evident once we are working across multiple replications of the simulation process, as we will in Chapter 8.

7.3 Validating an Estimation Function

Just as with data-generating functions, it is critical to verify the accuracy of an implemented estimation function. If an estimation function involves a known procedure that has been implemented in R or one of its contributed packages, then a straightforward way to do this is to compare your implementation to another existing implementation. For estimation functions that involve multi-step procedures or novel methods, other approaches to verification may be needed, which rely more on statistical theory.

7.3.1 Checking against existing implementations

For our Welch test function, we can check the output of `ANOVA_Welch_F()` against the built-in `oneway.test` function. Let's do that with a fresh set of data:

```r
sim_data <- generate_ANOVA_data(
  mu = c(1, 2, 5, 6),
  sigma_sq = c(3, 2, 5, 1),
  sample_size = c(3, 6, 2, 4)
)

aov_results <- oneway.test(x ~ factor(group), data = sim_data,
                           var.equal = FALSE)
aov_results
```

```
##
##  One-way analysis of means (not assuming
##  equal variances)
##
## data:  x and factor(group)
## F = 28.367, num df = 3.0000, denom df =
## 3.3253, p-value = 0.007427
```

```r
Welch_results <- ANOVA_Welch_F(sim_data)
all.equal(aov_results$p.value, Welch_results$Welch)
```

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

We use `all.equal()` because it will check equality up to a tolerance in R, which can avoid some perplexing errors due to rounding.

For the bivariate correlation example, we can check the output of `r_and_z()` against R's built-in `cor.test()` function:

```r
Pois_dat <- r_bivariate_Poisson(15, rho = 0.6, mu1 = 14, mu2 = 8)

my_result <- r_and_z(Pois_dat) |> subset(select = -z)
my_result
```

```
## # A tibble: 1 x 3
##       r   CI_lo CI_hi
##   <dbl>   <dbl> <dbl>
## 1 0.503 -0.0125 0.807
```

```
R_result <- cor.test(~ C1 + C2, data = Pois_dat)
R_result <- tibble(r = R_result$estimate[["cor"]],
                   CI_lo = R_result$conf.int[1],
                   CI_hi = R_result$conf.int[2])
R_result
```

```
## # A tibble: 1 x 3
##       r   CI_lo CI_hi
##   <dbl>   <dbl> <dbl>
## 1 0.503 -0.0125 0.807
```

```
all.equal(R_result, my_result)
```

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

This type of test is even more useful here because `r_and_z()` uses our own implementation of the confidence interval calculations, rather than relying on R's built-in functions as we did with `ANOVA_Welch_F()`.

7.3.2 Checking novel procedures

Simulations are usually an integral part of projects to develop novel statistical methods. Checking estimation functions in such projects presents a challenge: if an estimation procedure truly is new, how do you check that your code is correct? Effective methods for doing so will vary from problem to problem, but an over-arching strategy is to use theoretical results about the performance of the estimator to check that your implementation works as expected. For instance, we might work out the algebraic properties of an estimator for a special case and then check that the result of the estimation function agrees with our algebra. For some estimation problems, we might be able to identify theoretical properties of an estimator when applied to a very large sample of data and when the model is correctly specified. If we can find results about large-sample behavior, then we can test an estimation function by applying it to a very large sample and checking whether the resulting estimates are very close to specified parameter values. We illustrate each of these approaches using our functions for estimating treatment effects from cluster-randomized trials.

We start by testing an algebraic property. With each of the three methods we have implemented, the treatment effect estimator is a difference between the weighted average of the outcomes from students in each treatment condition; the only difference between the estimators is in what weights are used. In the special case where all schools have the same number of students, the weights used by all three methods end up being the same: all three methods allocate equal weight to

each school. Therefore, we know that there should be no difference between the three point estimates. Furthermore, a bit of algebra will show that the cluster-robust standard error from the OLS approach will end up being identical to the robust standard error from the aggregation approach. If there are also equal numbers of schools assigned to both conditions, then the standard error from the multilevel model will also be identical to the other standard errors.

Let's verify that our estimation functions produce results that are consistent with these theoretical properties. To do so, we will need to generate a dataset with equal cluster sizes, setting $\alpha = 0$:

```
dat <- gen_cluster_RCT(
  J=12, n_bar = 30, alpha = 0, p = 0.5,
  gamma_0 = 0, gamma_1 = 0.2, gamma_2 = 0.2,
  sigma2_u = 0.4, sigma2_e = 0.6
)
table(dat$sid) # verify equal-sized clusters
```

```
##
##  1  2  3  4  5  6  7  8  9 10 11 12
## 30 30 30 30 30 30 30 30 30 30 30 30
```

```
estimate_Tx_Fx(dat)
```

```
## # A tibble: 3 x 4
##   estimator ATE_hat SE_hat p_value
##   <chr>       <dbl>  <dbl>   <dbl>
## 1 MLM        -0.525  0.366   0.183
## 2 OLS        -0.525  0.366   0.183
## 3 agg        -0.525  0.366   0.183
```

All three methods yield identical results. Now let's try equal school sizes but unequal allocation to treatment:

```
dat <- gen_cluster_RCT(
  J=12, n_bar = 30, alpha = 0, p = 2 / 3,
  gamma_0 = 0, gamma_1 = 0.2, gamma_2 = 0.2,
  sigma2_u = 0.4, sigma2_e = 0.6
)
estimate_Tx_Fx(dat)
```

```
## # A tibble: 3 x 4
##   estimator ATE_hat SE_hat p_value
##   <chr>       <dbl>  <dbl>   <dbl>
## 1 MLM         0.189  0.547   0.737
## 2 OLS         0.189  0.413   0.663
## 3 agg         0.189  0.413   0.657
```

As expected, all three point estimators match, but the SE from the multilevel

model is a little bit discrepant from the others.

We can also use large-sample theory to check the multilevel modeling estimator. If the model is correctly specified, then *all* the parameters of the model should be accurately estimated if the model is fit to a very large sample of data. To check this property, we will need access to the full model output, not just the selected results returned by `analysis_MLM()`. One way to handle this is to make a small tweak to the estimation function, adding an option to control whether to return the entire model or just selected results. Here is the tweaked function:

```r
analysis_MLM <- function( dat, all_results = FALSE) {

  M1 <- lme4::lmer( Yobs ~ 1 + Z + (1 | sid), data = dat )
  M1_test <- lmerTest::as_lmerModLmerTest(M1)

  if (all_results) {
    return(summary(M1_test))
  }

  M1_summary <- summary(M1_test)$coefficients

  tibble(
    ATE_hat = M1_summary["Z","Estimate"],
    SE_hat = M1_summary["Z","Std. Error"],
    p_value = M1_summary["Z", "Pr(>|t|)"]
  )
}
```

Setting `all_results` to `TRUE` will return the entire function; keeping it at the default value of `FALSE` will return the same output as the other functions. Now let's apply the estimation function to a very large dataset, with variation in cluster sizes. We set `gamma_2 = 0` so that the estimation model is correctly specified:

```r
dat <- gen_cluster_RCT(
  J=5000, n_bar = 20, alpha = 0.9, p = 2 / 3,
  gamma_0 = 2, gamma_1 = 0.30, gamma_2 = 0,
  sigma2_u = 0.4, sigma2_e = 0.6
)

analysis_MLM(dat, all_results = TRUE)
```

```
## Linear mixed model fit by REML. t-tests use
##   Satterthwaite's method [lmerModLmerTest]
## Formula: Yobs ~ 1 + Z + (1 | sid)
##    Data: dat
##
## REML criterion at convergence: 242678
```

```
##
## Scaled residuals:
##     Min      1Q  Median      3Q     Max
## -4.3080 -0.6581  0.0007  0.6594  4.2134
##
## Random effects:
##  Groups   Name        Variance Std.Dev.
##  sid      (Intercept) 0.3972   0.6302
##  Residual             0.6030   0.7765
## Number of obs: 98772, groups:  sid, 5000
##
## Fixed effects:
##              Estimate Std. Error        df
## (Intercept) 2.017e+00  1.636e-02 4.969e+03
## Z           2.838e-01  2.003e-02 4.964e+03
##             t value Pr(>|t|)
## (Intercept)  123.29   <2e-16 ***
## Z             14.17   <2e-16 ***
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Correlation of Fixed Effects:
##   (Intr)
## Z -0.817
```

The intercept and treatment effect coefficient estimates are very close to their true parameter values, as are the estimated school-level variance and student-level residual variance. This all gives some assurance that the `analysis_MLM()` function is working properly.

Of course, it is important to bear in mind that these tests are only partial verifications. With the algebraic test, we have only checked that the functions seem to be working properly for scenarios with equal school sizes, but they still might have errors that only appear when school sizes vary. Likewise, `analysis_MLM()` seems to be working properly for very large datasets, but our test does not rule out the possibility of bugs that only crawl out when J is small. Our large-sample test also relies on the correctness of the `gen_cluster_RCT()` function; if we had seen a discrepancy between parameters and estimates from the multi-level model, it could have been because of a problem with the data-generation function rather than with the estimation function.

These limitations are typical of what can be accomplished through tests based on theoretical results, because theoretical results typically only hold under specific conditions. After all, if we had comprehensive theoretical results, we would not need to simulate anything in the first place! Nonetheless, it is good to work through such tests to the extent that relevant theory is available for the problem

you are studying.

7.3.3   Checking with simulations

Checking, debugging, and revising should not be limited to when you are initially developing estimation functions. It often happens that later steps in the process of conducting a simulation will reveal problems with the code for earlier steps. For instance, once you have run the data-generating and estimation steps repeatedly, calculated performance summaries, and created some graphs of the results, you might find an unusual or anomolous pattern in the performance of an estimator. This might be a legitimate result—perhaps the estimator really does behave weirdly or not work well—or it might be due to a problem in how you implemented the estimator or data-generating process. When faced with an unusual pattern, we recommend revisiting the estimation code to double check for bugs and also thinking further about what might lead to the anomoly. Further exploration might lead you to a deeper understanding of how a method works and perhaps even an idea for how to improve the estimator or refine the data-generating process.

A good illustration of this process comes from one of Luke's past research projects (see Pashley et al. (2024)), in which he and other co-authors were working on a way to improve Instrumental Variable (IV) estimation using post-stratification. The method they studied involved grouping units based on a covariate that predicts compliance status, then calculating estimates within each group, then summarizing the estimates across groups. They used simulations to see whether this method would improve the accuracy of the overall summary effect estimate. In the first simulation, the estimates were full of NAs and odd results because the estimation function failed to account for what happens in groups of observations where the number of compliers was estimated to be zero. After repairing that problem and re-running everything, the simulation results still indicated serious and unexpected bias, which turned out to be due to an error in how the estimation function implemented the step of summarizing estimates across groups. After again correcting and re-running, the simulation results showed that the gains in accuracy from this new method were minimal, even when the groups were formed based on a variable that was almost perfectly predictive of compliance status. Eventually, we understood that the groups with very few compliers produced such unstable estimates that they spoiled the overall average estimate. This inspired us to revise our estimation strategy and introduce a method that dropped or down-weighted strata with few compliers, which ultimately helped us to strengthen the contribution of our work.

As this experience highlights, simulations seldom follow a single, well-defined trajectory. The point of conducting simulations is to help us, as researchers, learn about estimation methods so that we can analyze real data better. What we learn from simulation gives us a better understanding of the methods (potentially including a better understanding of theoretical results), leading to ideas about better methods to create new scenarios to explore in further simulations.

Of course, at some point one needs to step off this merry-go-round, write up the findings, cook dinner, and clean the bathroom. But, just like many other research endeavors, simulations follow a highly iterative process.

7.4 Handling errors, warnings, and other hiccups

Especially when working with more advanced estimation methods, it is possible that your estimation function will fail, throw an error, or return something uninterpretable for certain input datasets. For instance, maximum likelihood estimation often requires iterative, numerical optimization algorithms that sometimes fail to converge. This might happen rarely enough that it takes a while to even notice that it is a problem, but even quite rare things can occur when you run simulations with many thousands of repetitions. Less dire but still annoying, your estimation function might generate warnings, which can pile up if you are running many repetitions. In some cases, such warnings might also signal that the estimator produced a bad result, and it may not be clear whether we should retain this result (or include it in overall performance assessments). After all, the function tried to warn us that something is off!

Errors and warnings in estimation functions pose two problems, one purely technical and one conceptual. On a technical level, R functions stop running if they hit errors (though not warnings), so we need ways to handle the errors in order to get our simulations up and running. On a conceptual level, we need to decide how to use the information contained in errors and warnings, whether that be by further elaborating the estimation procedures to address different contingencies or by evaluating the performance of the estimators in a way that appropriately accounts for errors. We consider each of the problems here, then revisit the conceptual considerations in Chapter 9.

7.4.1 Capturing errors and warnings

Some estimation functions will require complicated or stochastic calculations that can sometimes produce errors. Intermittent errors can really be annoying and time-consuming if not addressed. To protect yourself, it is good practice to anticipate potential errors, preventing them from stopping code execution and allowing your simulations to keep running. We will demonstrate some techniques for error-handling using tools from the `purrr` package.

For illustrative purposes, consider the following error-prone function that sometimes returns what we want, sometimes returns `NaN` due to taking the square root of a negative number, and sometimes crashes completely because `broken_code()` does not exist:

```
my_complex_function = function( param ) {
```

```r
    vals = rnorm( param, mean = 0.5 )
    if ( sum( vals ) > 5 ) {
        broken_code( 4 )
    } else {
        sqrt( sum( vals ) * sign( vals )[[1]] )
    }
}
```

Running it produces some results and an occasional warning, and some errors:

```r
set.seed(3)
my_complex_function( 1 )
```

```
## [1] 0.6796568
```

```r
my_complex_function( 10 )
```

```
## [1] 2.132087
```

```r
my_complex_function( 5 )
```

```
## Warning in sqrt(sum(vals) * sign(vals)[[1]]):
## NaNs produced
```

```
## [1] NaN
```

Running it many times produces warnings, then an error:

```r
resu <- replicate(20, my_complex_function( 7 ))
```

```
## Warning in sqrt(sum(vals) * sign(vals)[[1]]):
## NaNs produced
## Warning in sqrt(sum(vals) * sign(vals)[[1]]):
## NaNs produced
```

```
## Error in broken_code(4): could not find function "broken_code"
```

The `purrr` package includes a function called `safely` that makes it easy to trap errors. To use it, we feed the estimation function into `safely()` to create a new version:

```r
my_safe_function <- safely( my_complex_function, otherwise = NA )
my_safe_function( 7 )
```

```
## $result
## [1] 2.175561
##
## $error
## NULL
```

The safe version of the function returns a list with two entries: the result (or NULL if there was an error), and the error message (or NULL if there was no

error). `safely()` is an example of a *functional* (or an *abverb*), which takes a function and returns a new function that does something slightly different. We include `otherwise = NA` so we always get a result, rather than a `NULL` when there is an error.

We can use the safe function repeatedly and it will always return a result:

```
resu <- replicate(20, my_safe_function( 7 ), simplify = FALSE)
```

```
## Warning in sqrt(sum(vals) * sign(vals)[[1]]):
## NaNs produced
## Warning in sqrt(sum(vals) * sign(vals)[[1]]):
## NaNs produced
## Warning in sqrt(sum(vals) * sign(vals)[[1]]):
## NaNs produced
## Warning in sqrt(sum(vals) * sign(vals)[[1]]):
## NaNs produced
## Warning in sqrt(sum(vals) * sign(vals)[[1]]):
## NaNs produced
```

```
resu <- transpose( resu )
unlist(resu$result)
```

```
##  [1] 1.3870195 0.5638654        NA 1.6995292
##  [5]        NA        NA       NaN 2.2121710
##  [9]        NA       NaN       NaN 1.8801925
## [13]       NaN 1.9154618       NaN        NA
## [17] 2.2245636        NA        NA 0.8854747
```

The `transpose()` function takes a list of lists, and reorganizes them to give you a list of all the first elements, a list of all the second elements, etc. This is very powerful for wrangling data, because then we can make a tibble with list columns as so:

```
tb <- tibble( result = unlist( resu$result ), error = resu$error )
head( tb, n = 4 )
```

```
## # A tibble: 4 x 2
##   result error
##    <dbl> <list>
## 1  1.39  <NULL>
## 2  0.564 <NULL>
## 3 NA     <smplErrr>
## 4  1.70  <NULL>
```

The `purrr` package includes several other functionals that are useful for handling errors and warnings. The `possibly()` wrapper will try to run a function and will return a specified value in the event of an error:

```
my_possible_function <- possibly( my_complex_function, otherwise = NA )
my_possible_function( 7 )
```

```
## [1] 1.506734
```

```
rs <- replicate(20, my_possible_function( 7 ))
```

```
## Warning in sqrt(sum(vals) * sign(vals)[[1]]):
## NaNs produced
## Warning in sqrt(sum(vals) * sign(vals)[[1]]):
## NaNs produced
## Warning in sqrt(sum(vals) * sign(vals)[[1]]):
## NaNs produced
```

```
rs
```

```
##  [1]         NA 0.7023915 0.9495728         NA
##  [5]         NA 1.8784947 0.9838187         NA
##  [9]         NA 1.7676572 1.4809897         NA
## [13] 2.1019082         NA       NaN       NaN
## [17] 1.8629289 1.3467997       NaN 1.3017348
```

It works as a simpler version of `safely()`, which does not record error messages.

The `quietly` functional leads to results that are bundled together with any console output, warnings, and messages, rather than printing anything to the console:

```
my_quiet_function <- quietly( my_complex_function )
```

```
my_quiet_function( 1 )
```

```
## $result
## [1] 0.1724504
##
## $output
## [1] ""
##
## $warnings
## character(0)
##
## $messages
## character(0)
```

This can be especially useful to reduce extraneous printing in a simulation, which can slow down code execution more than you might expect. However, `quietly()` does not trap errors:

```
rs <- replicate(20, my_quiet_function( 7 ))
```

```
## Error in broken_code(4): could not find function "broken_code"
```

Double-wrapping your function will handle both errors and warnings, but the structure it produces gets a bit complicated:

```
my_safe_quiet_function <- quietly( safely( my_complex_function, otherwise = NA ) )
my_safe_quiet_function(7)
```

```
## $result
## $result$result
## [1] NA
##
## $result$error
## <simpleError in broken_code(4): could not find function "broken_code">
##
##
## $output
## [1] ""
##
## $warnings
## character(0)
##
## $messages
## character(0)
```

Even though the result is a bit of a mess, this structure provides all the pieces that we need to do further calculations on the result (when available), along with errors, warnings, and other output.

To see how this works in practice, we will adapt our `analysis_MLM()` function, which makes use of `lmer()` for fitting a multilevel model. Currently, the estimation function sometimes prints messages to the console:

```
set.seed(101012)  # (I picked this to show a warning.)
dat <- gen_cluster_RCT( J = 50, n_bar = 100, sigma2_u = 0 )
mod <- analysis_MLM(dat)
```

```
## boundary (singular) fit: see help('isSingular')
```

Wrapping `lmer()` with `quietly()` makes it possible to catch such output and store it along with other results, as in the following:

```
quiet_lmer <- quietly(lme4::lmer)
qmod <- quiet_lmer( Yobs ~ 1 + Z + (1|sid), data=dat )
qmod
```

```
## $result
## Linear mixed model fit by REML ['lmerMod']
## Formula: Yobs ~ 1 + Z + (1 | sid)
##    Data: ..2
```

```
## REML criterion at convergence: 14026.44
## Random effects:
##  Groups    Name        Std.Dev.
##  sid       (Intercept) 0.0000
##  Residual              0.9828
## Number of obs: 5000, groups:  sid, 50
## Fixed Effects:
## (Intercept)              Z
##   -0.013930      -0.008804
## optimizer (nloptwrap) convergence code: 0 (OK) ; 0 optimizer warnings; 1 lme4 warni
##
## $output
## [1] ""
##
## $warnings
## character(0)
##
## $messages
## [1] "boundary (singular) fit: see help('isSingular')\n"
```

However, the `lmerTest` package does not like the structure of the results, and
produces an error:

```
lmerTest::as_lmerModLmerTest(qmod$result)
```

```
## Error in lmerTest::as_lmerModLmerTest(qmod$result): Unable to extract deviance funct
```

We can side-step this by combining `as_lmerModLmerTest()` and `lmer()` into a
single function. While we are at it, we also layer on `summary()`. To do so, we
use the `compose()` functional from `purrr`, which takes a list of functions and
wraps them into one:

```
lmer_with_test <- purrr::compose(
  summary,
  lmerTest::as_lmerModLmerTest,
  lme4::lmer
)
```

The resulting `lmer_with_test()` function acts as if we were calling `lmer()`,
then feeding the result into `as_lmerModLmerTest()`, then feeding the result
into `summary()`. We then wrap the combination function with `safely()` and
`quietly()`:

```
quiet_safe_lmer <- purrr::quietly(purrr::safely(lmer_with_test))
```

Now we can use our suitably quieted and safe function in a new version of the
estimation function:

```r
analysis_MLM_safe <- function( dat, all_results = FALSE ) {

  M1 <- quiet_safe_lmer( Yobs ~ 1 + Z + (1 | sid), data=dat )

  if (all_results) {
    return(M1)
  }

  message <- ifelse( length( M1$message ) > 0, M1$message, NA_character_ )
  warning <- ifelse( length( M1$warning ) > 0, M1$warning, NA_character_ )
  error <- ifelse( length( M1$result$error) > 0, M1$result$error$message, NA_character_ )

  tibble(
    ATE_hat = M1$result$result$coefficients["Z","Estimate"],
    SE_hat = M1$result$result$coefficients["Z","Std. Error"],
    p_value = M1$result$result$coefficients["Z", "Pr(>|t|)"],
    message = message,
    warning = warning,
    error = error
  )
}
```

This quiet version runs without extraneous messages:

```r
mod <- analysis_MLM_safe(dat)
mod
```

```
## # A tibble: 1 x 6
##     ATE_hat SE_hat p_value message     warning error
##       <dbl>  <dbl>   <dbl> <chr>        <chr>   <chr>
## 1 -0.00880 0.0278   0.751 "boundary~ <NA>     <NA>
```

Now we have the estimation results along with any diagnostic information from messages or warnings. Storing this information will let us evaluate what proportion of the time there was a warning or message, run additional analyses on the subset of replications where there was no such warning, or even modify the estimation procedure to take the diagnostics into account.

7.4.2 Adapting estimation procedures for errors and warnings

So far, we have seen techniques for handling technical hiccups that occur when data analysis procedures do not always produce results. But how do we account for the absence of results in a simulation? In Chapter 9, we will delve into the conceptual issues with summarizing the performance of methods that do not always provide an answer. One of the best solutions to such problems still concerns the formulation of estimation functions, and so we introduce it here.

That solution is to *re-define the estimator* to include contingencies for handling lack of results.

Consider a data analyst who was planning to apply a fancy statistical model to their data, but then finds that the model does not converge. What would that analyst do in practice (besides cussing and taking a snack break)? Rather than giving up entirely, they would probably think of an alternative analysis and attempt to apply it, perhaps by simplifying the model in some way. To the extent that we can anticipate such possibilities, we can build these error-contingent alternative analyses into our estimation function.

To illustrate, let's look at an error (a not-particularly-subtle one) that can crop up in the cluster-randomized trial example when clusters are very small:

```
set.seed(65842)
tiny_dat <- gen_cluster_RCT( J = 10, n_bar = 2, alpha = 0.5)
analysis_MLM_safe(tiny_dat)
```

```
## # A tibble: 1 x 3
##   message warning error
##   <chr>   <chr>   <chr>
## 1 <NA>    <NA>     number of levels of each groupi~
```

```
table(tiny_dat$sid)
```

```
##
##  1  2  3  4  5  6  7  8  9 10
##  1  1  1  1  1  1  1  1  1  1
```

The error occurs because all 10 simulated schools include a single student, making it impossible to estimate a random-intercepts multilevel model. A natural fall-back analysis here would be to estimate an ordinary least squares regression analysis.

Suppose that our imaginary analyst is not especially into nuance, and so will fall back onto ordinary least squares whenever the multilevel model produces an error. We can express this logic in our estimation function by first catching the error thrown by `lmer()` and then running an OLS regression in the event an error is thrown:

```
analysis_MLM_contingent <- function( dat, all_results = FALSE ) {

  M1 <- quiet_safe_lmer( Yobs ~ 1 + Z + (1 | sid), data=dat )

  if (all_results) {
    return(M1)
  }

  if (!is.null(M1$result$result)) {
```

```r
    # If lmer() returns a result
    res <- tibble(
      ATE_hat = M1$result$result$coefficients["Z","Estimate"],
      SE_hat = M1$result$result$coefficients["Z","Std. Error"],
      p_value = M1$result$result$coefficients["Z", "Pr(>|t|)"],
    )
  } else {
    # If lmer() errors, fall back on OLS
    M_ols <- summary(lm(Yobs ~ Z, data = dat))
    res <- tibble(
      ATE_hat = M_ols$coefficients["Z","Estimate"],
      SE_hat = M_ols$coefficients["Z", "Std. Error"],
      p_value = M_ols$coefficients["Z","Pr(>|t|)"]
    )
  }

  # Store original messages, warnings, errors
  res$message <- ifelse( length( M1$message ) > 0, M1$message, NA_character_ )
  res$warning <- ifelse( length( M1$warning ) > 0, M1$warning, NA_character_ )
  res$error <- ifelse( length( M1$result$error) > 0, M1$result$error$message, NA_character_ )

  return(res)
}
```

We still store the messages, warnings, and errors from the initial `lmer()` fit so that we can keep track of how often errors occur. The function now returns an treatment effect estimate even if `lmer()` errors:

```r
analysis_MLM_contingent(tiny_dat)
```

```
## # A tibble: 1 x 6
##    ATE_hat SE_hat p_value message warning error
##      <dbl>  <dbl>   <dbl> <chr>   <chr>   <chr>
## 1    0.400  0.603   0.525 <NA>    <NA>    number o~
```

Of course, we can easily anticipate the conditions under which this particular error will occur: all we need to do is check whether all the clusters are single observations. Because it is easily anticipated, a better strategy for handling this error is to check *before* fitting the multilevel model and proceeding accordingly in the event that the clusters are all singletons. Exercise 7.5.5 asks you to implement this approach and further refine this contingent analysis strategy.

Adapting estimation functions to address errors can be an effective—and often very interesting—strategy for studying the performance of estimation methods. Rather than studying the performance of a data-analysis method that is only sometimes well-defined, we shift to studying a stylized cognitive model for the analyst's decision-making process, which handles contingencies that might crop

up whether analyzing simulated data or real empirical data. Of course, studying such a model is only interesting to the extent that the decision-making process it implements is a plausible representation of what an analyst might actually do in practice.

The adaptive estimation approach does lead to more complex estimation functions, which entail implementing multiple estimation methods and a set of decision rules for applying them. Often, the set of contingencies that need to be handled will not be immediately obvious, so you may find that you need to build and refine the decision rules as you learn more about how they work. Running an estimation procedure over multiple, simulated datasets is an excellent (if aggravating!) way to identify errors and edge cases. We turn to procedures for doing so in the next chapter.

7.5   Exercises

7.5.1   More Heteroskedastic ANOVA

In the classic simulation by Brown and Forsythe (1974), they not only looked at the performance of the homoskedastic ANOVA-F test and Welch's heteroskedastic-F test, they also proposed their own new hypothesis testing procedure.

1. Write a function that implements the Brown-Forsythe F* test (the BFF* test!) as described on p. 130 of Brown and Forsythe (1974), using the following code skeleton:

```r
BF_F <- function( data ) {

  # fill in the guts here

  return(pval)
}
```

   Run the following code to check that your function produces a result:

```r
sim_data <- generate_ANOVA_data(
  mu = c(1, 2, 5, 6),
  sigma_sq = c(3, 2, 5, 1),
  sample_size = c(3, 6, 2, 4)
)
BF_F( sim_data )
```

2. Try calling your `BF_F` function on a variety of datasets of different sizes and shapes, to make sure it works. What kinds of datasets should you test out?

3. Add the BFF* test into the output of `Welch_ANOVA_F()` by calling your

`BF_F()` function inside the body of `Welch_ANOVA_F()`.

4. The `onewaytests` package implements a variety of different hypothesis testing procedures for one-way ANOVA. Validate your `Welch_ANOVA_F()` function by comparing the results to the output of the relevant functions from `onewaytests`.

7.5.2 Contingent testing

In the one-way ANOVA problem, one approach that an analyst might think to take is to conduct a preliminary significance test for heterogeneity of variances (such as Levene's test or Bartlett's test), and then report the p-value from the homoskedastic ANOVA F test if variance heterogeneity is not detected but the p-value from the BFF* test if variance heteogeneity is detected. Modify the `Welch_ANOVA_F()` function to return the p-value from this contingent BFF* test in addition to the p-values from the (non-contingent) ANOVA-F, Welch, and BFF* tests. Include an input option that allows the user to control the α level of the preliminary test for heterogeneity of variances, as in the following skeleton.

```
Welch_ANOVA_F <- function( data , pre_alpha = .05) {
  # preliminary test for variance heterogeneity
  # compute non-contingent F tests for group differences
  # compute contingent test
  # compile results
  return(result)
}
```

7.5.3 Check the cluster-RCT functions

Section 7.2 presented functions implementing several different strategies for estimating an average treatment effect from a cluster-randomized trial. Write some code to validate these functions by comparing their output to the results of other tools for doing the same calculation. Use one or more datasets simulated with `gen_cluster_RCT()`. For each of these tests, you will need to figure out the appropriate syntax by reading the package documentation.

1. For `analysis_MLM()`, check the output by fitting the same model using `lme()` from the `nlme()` package or `glmmTMB()` from the package of the same name.

2. For `analysis_OLS()`, check the output by fitting the linear model using the base R function `lm()`, then computing standard errors using `vcovCL()` from the `sandwich` package. Also compare the output to the results of feeding the fitted model through `coef_test()` from the `clubSandwich` package.

3. For `analysis_agg()`, check the output by aggregating the data to the

school-level, fitting the linear model using `lm()`, and computing standard errors using `vcovHC()` from the `sandwich` package.

7.5.4 Extending the cluster-RCT functions

Exercise 6.9.10 from Chapter 6 asked you to extend the data-generating function for the cluster-randomized trial to include generating a student-level covariate, X, that is predictive of the outcome. Use your modified function to generate a dataset.

1. Modify the estimation functions from Section 7.2 to use models that include the covariate as a predictor.

2. Further extend the functions to include an input argument for the set of predictors to be included in the model, as in the following skeleton for the multi-level model estimator:

```
analysis_MLM <- function(dat, predictors = "Z") {

}

analysis_MLM( dat )
analysis_MLM( dat, predictors = c("Z","X"))
analysis_MLM( dat, predictors = c("Z","X", "X:Z"))
```

   Hint: Check out the `reformulate()` function, which makes it easy to build formulas for different sets of predictors.

7.5.5 Contingent estimator processing

In Section 7.4.2 we developed a version of `analysis_MLM()` that fell back on OLS regression in the event that `lmer()` produced any error. The implementation that we demonstrated is not especially smart. For one, it does not anticipate that the error will occur. For another, if we are using this function as one of several estimation strategies, it will require fitting the OLS regression multiple times. Can you fix these problems?

1. Revise `analysis_MLM_contingent()` so that it checks whether all clusters are single observations *before* fitting the multilevel model. Handle event the contingency where all clusters are singletons by skipping the model-fitting step, returning `NA` values for the point estimator, standard error, and p-value, and returning an informative message in the `error` variable. Test that the function is working as expected.

2. Revise `estimate_Tx_Fx()` to use your new version of `analysis_MLM_contingent()`. The revised function will sometimes return `NA` values for the `MLM` results. To implement the strategy of falling-back on OLS regression, add some code that replaces any `NA` values with corresponding results of `analysis_OLS()`. Test that the function is working as expected.

7.5.6 Estimating 3-parameter item response theory models

Exercise 6.9.11 asked you to write a data-generating function for the 3-parameter IRT model described in described in Section 6.7. Use your function to generate a large dataset. Using functions from the {ltm}, {mirt}, or {TAM} packages, *estimate* the parameters of the 3-parameter IRT model based on the simulated dataset.

1. Write a function to *estimate* a 3-parameter IRT model and return a dataset containing estimates of the item characteristics $(\alpha_m, \beta_m, \gamma_m)$.

2. Add an option to the function to allow the user to specify known values of γ_m.

3. Create a graphic showing how the item parameter estimates compare to the true item characteristics.

4. Write a function or set of functions to apply 1-parameter, 2-parameter, and 3-parameter models and return datasets containing the person ability estimates $\theta_1, ..., \theta_N$ and corresponding standard errors of measurement.

7.5.7 Meta-regression with selective reporting

Exercise 6.9.15 asked you to write a data-generating function for the Vevea and Hedges (1995) selection model. The {metafor} package includes a function for fitting this model (as well as a variety of other selection models). Here is an example of the syntax for estimating this model, using a dataset from the {metadat} package:

```r
library(metafor)
data("dat.assink2016", package = "metadat")

# rename variables and tidy up
dat <-
  dat.assink2016 %>%
  mutate( si = sqrt(vi) ) %>%
  rename( Ti = yi, s_sq = vi, Xi = year )

# fit a random effects meta-regression model
rma_fit <- rma.uni(yi = Ti, sei = si, mods = ~ Xi, data = dat)
# fit two-step selection model
selmodel(rma_fit, type = "step", steps = c(.025, .500))
```

```
##
## Mixed-Effects Model (k = 100; tau^2 estimator: ML)
##
## tau^2 (estimated amount of residual heterogeneity): 0.2314 (SE = 0.0500)
## tau (square root of estimated tau^2 value):         0.4810
```

```
##
## Test for Residual Heterogeneity:
## LRT(df = 1) = 349.3718, p-val < .0001
##
## Test of Moderators (coefficient 2):
## QM(df = 1) = 42.1433, p-val < .0001
##
## Model Results:
##
##           estimate      se     zval     pval
## intrcpt     0.4149  0.1013   4.0942  <.0001
## Xi         -0.0782  0.0120  -6.4918  <.0001
##             ci.lb    ci.ub
## intrcpt     0.2163   0.6135  ***
## Xi         -0.1018  -0.0546  ***
##
## Test for Selection Model Parameters:
## LRT(df = 2) = 1.7814, p-val = 0.4104
##
## Selection Model Results:
##
##                        k  estimate      se      zval
## 0      < p <= 0.025   59    1.0000     ---       ---
## 0.025 < p <= 0.5      23    0.6990  0.2307   -1.3049
## 0.5   < p <= 1        18    0.5027  0.2743   -1.8132
##                            pval    ci.lb    ci.ub
## 0      < p <= 0.025        ---      ---      ---
## 0.025 < p <= 0.5        0.1919   0.2470   1.1511
## 0.5   < p <= 1          0.0698   0.0000   1.0403   .
##
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

The `selmodel()` function can also be used to fit selection models in which one or both of the selection parameters are fixed to user-specified values. For example:

```
# Fixing lambda_1 = 0.5, lambda_2 = 0.2
fix_both <- selmodel(rma_fit, type = "step", steps = c(.025, .500),
                     delta = c(1, 0.5, 0.2))

# Fixing lambda_1 = 0.5, estimating lambda_2
fix_one <- selmodel(rma_fit, type = "step", steps = c(.025, .500),
                    delta = c(1, 0.5, NA))
```

1. Write an estimation function that fits the selection model and returns estimates, standard errors, and confidence intervals for each of the model parameters $(\beta_0, \beta_1, \tau, \lambda_1, \lambda_2)$.

2. The `selmodel()` fitting function sometimes returns errors, as in the following example:

```
dat_sig <- dat %>% filter(Ti / si > 0)
rma_pos <- rma.uni(yi = Ti, sei = si, mods = ~ Xi, data = dat_sig)
# fit two-step selection model
sel_fit <- selmodel(rma_pos, type = "step", steps = c(.025, .500))

## Warning: One or more intervals do not contain any
## observed p-values.

## Warning: One or more 'delta' estimates are (almost) equal to their lower or upper bound.
## Treat results with caution (or consider adjusting 'delta.min' and/or 'delta.max').
```

Modify your estimation function to catch and return warnings such as these. Write code demonstrating that the function works as expected.

3. The `selmodel()` throws warnings when the dataset contains no observations with p_i in one of the specified intervals. Modify your estimation function to set the selection probability for an interval to $\lambda_1 = 0.1$ if there are no p_i values between .025 and .500 and to set $\lambda_2 = 0.1$ if there are no p_i values larger than .500. Write code demonstrating that the function works as expected.

Chapter 8

Running the Simulation Process

In the prior two chapters we saw how to write functions that generate data according to a particular model and functions that implement data-analysis procedures on simulated data. The next step in a simulation involves putting these two pieces together, running the DGP function and the data-analysis function repeatedly to obtain results (in the form of point estimates, standard errors, confidence intervals, p-values, or other quantities) from many replications of the whole process.

As with most things R-related, there are many different techniques that can be used to repeat a set of calculations over and over. In this chapter, we demonstrate several techniques for doing so. We then explain how to ensure reproducibility of simulation results by setting the seed used by R's random number generator.

8.1   Repeating oneself

Suppose that we want to simulate Pearson's correlation coefficient calculated based on a sample from the bivariate Poisson function. We saw a DGP function for the bivariate Poisson in Section 6.3, and an estimation function in Section 7.1. To produce a simulated correlation coefficient, we need to run these two functions in turn:

```
dat <- r_bivariate_Poisson( N = 30, rho = 0.4, mu1 = 8, mu2 = 14 )
r_and_z(dat)
```

```
## # A tibble: 1 x 4
##        r     z CI_lo CI_hi
##    <dbl> <dbl> <dbl> <dbl>
```

```
## 1 0.533 0.595 0.214 0.750
```

To execute a simulation with these components, we need to repeat this set of calculations over and over. R has many different functions for doing exactly this. As one of many alternatives, the `simhelpers` package includes a function called `repeat_and_stack()`, which can be used to evaluate an arbitrary expression many times over. We can use it to generate five replications of our correlation coefficient:

```r
library(simhelpers)
repeat_and_stack(
  n = 5,
  {
    dat <- r_bivariate_Poisson( N = 30, rho = 0.4, mu1 = 8, mu2 = 14 )
    r_and_z(dat)
  },
  id = "rep",
  stack = TRUE
)
```

```
##           r         z       CI_lo      CI_hi rep
## 1 0.6406898 0.7593429   0.3645711 0.8132451   1
## 2 0.2165457 0.2200290  -0.1558849 0.5350714   2
## 3 0.5664693 0.6423085   0.2590719 0.7696643   3
## 4 0.4534481 0.4890323   0.1113731 0.6994524   4
## 5 0.5044732 0.5552884   0.1762338 0.7317497   5
```

The first argument specifies the number of times to repeat the calculation. The second argument is an R expression that will be evaluated. The expression is wrapped in curly braces (`{}`) because it involves more than a single line of code. Including the option `id = "rep"` returns a dataset that includes a variable called `rep` to identify each replication of the process. Setting the option `stack = TRUE` will stack up the output of each expression into a single tibble, which will facilitate later calculations on the results. Setting this option is not necessary because it is `TRUE` by default; setting `stack = FALSE` will return the results in a list rather than a tibble (try this for yourself to see!).

There are many other functions that work very much like `repeat_and_stack()`, including the base-R function `replicate()` and the now-deprecated function `rerun()` from {purrr}. The functions in the `map()` family from {purrr} can also be used to do the same thing as `repeat_and_stack()`. See Appendix A.1 for more discussion of these alternatives.

8.2   One run at a time

A slightly different technique for running multiple replications of a process is to first write a function that executes a single run of the simulation, and then

repeatedly evaluate that single function. For instance, here is a function that stitches together the two steps in the bivariate-Poisson correlation simulation:

```
one_bivariate_Poisson_r <- function(N, rho, mu1, mu2) {
  dat <- r_bivariate_Poisson( N = N, rho = rho, mu1 = mu1, mu2 = mu2 )
  res <- r_and_z(dat)
  return(res)
}
```

Calling the function produces a nicely formatted set of results:

```
one_bivariate_Poisson_r(N = 30, rho = 0.4, mu1 = 8, mu2 = 14)
```

```
## # A tibble: 1 x 4
##       r     z CI_lo CI_hi
##   <dbl> <dbl> <dbl> <dbl>
## 1 0.571 0.650 0.266 0.773
```

We can then evaluate the function over and over using `repeat_and_stack()`:

```
repeat_and_stack(
  n = 5,
  one_bivariate_Poisson_r( N = 30, rho = 0.4, mu1 = 8, mu2 = 14 ),
  id = "rep"
)
```

```
##           r         z        CI_lo     CI_hi rep
## 1 0.6920971 0.8519697  0.44204893 0.8423369   1
## 2 0.4639223 0.5022978  0.12445393 0.7061652   2
## 3 0.5054484 0.5565974  0.17750188 0.7323572   3
## 4 0.3102351 0.3208056 -0.05632999 0.6030973   4
## 5 0.2699476 0.2768073 -0.10005206 0.5743583   5
```

This technique of wrapping the data-generating function and estimation function inside of another function might strike you as a bit cumbersome because the wrapper is only two lines of code and writing it requires repeating many of the function argument names when calling the data-generating function (`N = N, rho = rho`, etc.). However, the wrapper technique can be useful for more complicated simulations, such as those that involve comparison of multiple estimation methods.

Consider the cluster-randomized experiment case study presented in Section 6.6 and 7.2. In this simulation, we are interested in comparing the performance of three different estimation methods: a multi-level model, a linear regression with clustered standard errors, and a linear regression on the data aggregated to the school level. A single replication of the simulation entails generating a dataset and then applying three different estimation functions to it. Here is a function that takes our simulation parameters and runs a single trial of the full process:

```r
one_run <- function(
  n_bar = 30, J = 20, gamma_1 = 0.3, gamma_2 = 0.5,
  sigma2_u = 0.20, sigma2_e = 0.80, alpha = 0.75
) {

  dat <- gen_cluster_RCT(
    n_bar = n_bar, J = J, gamma_1 = gamma_1, gamma_2 = gamma_2,
    sigma2_u = sigma2_u, sigma2_e = sigma2_e, alpha = alpha
  )
  MLM <- analysis_MLM( dat )
  LR <- analysis_OLS( dat )
  Agg <- analysis_agg( dat )

  bind_rows( MLM = MLM, LR = LR, Agg = Agg, .id = "method" )
}
```

We have added a bunch of defaults to our function, so that we can run it without having to remember all the various input parameters. When we call the function, we get a nicely structured table of results:

```r
one_run( n_bar = 30, J = 20, alpha=0.5 )
```

```
## # A tibble: 3 x 4
##   method ATE_hat SE_hat p_value
##   <chr>    <dbl>  <dbl>   <dbl>
## 1 MLM      0.506  0.255  0.0630
## 2 LR       0.474  0.261  0.0881
## 3 Agg      0.511  0.255  0.0609
```

We organize the output in a tibble to make it easier to do subsequent data processing and analysis. The results for each method are organized in separate lines. For each method, we record the impact estimate, its estimated standard error, and a nominal *p*-value. Note how the `bind_rows()` method can take naming on the fly, and give us a column of `method`, which will be very useful for keeping track of which results come from which estimation.

Once we have a function to execute a single run, we can produce multiple results using `repeat_and_stack()`:

```r
R <- 1000
ATE <- 0.30
runs <- repeat_and_stack(R,
                         one_run( n_bar = 30, J=20, gamma_1 = ATE ),
                         id = "runID")
saveRDS( runs, file = "results/cluster_RCT_simulation.rds" )
```

Setting `id = "runID"` lets us keep track of which iteration number produced which result. Once our simulation is complete, we save our results to a file so

that we can avoid having to re-run the full simulation if we want to explore the results in some future work session.

We now have results for each of our estimation methods applied to each of 1000 generated datasets. The next step is to evaluate how well the estimators did. For example, we will want to examine questions about bias, precision, and accuracy of the three point estimators. In Chapter 9, we will look systematically at ways to quantify the performance of estimation methods.

8.2.1 Reparameterizing

In Section 6.6.4, we discussed how to index the DGP of the cluster-randomized experiment using an intra-class correlation (ICC) instead of using two separate variance components. This type of re-parameterization can be handled as part of writing a wrapper function for executing the DGP and estimation procedures. Here is a revised version of `one_run()`, which also renames some of the more obscure model parameters using terms that are easier to interpret:

```r
one_run <- function(
  n_bar = 30, J = 20, ATE = 0.3, size_coef = 0.5,
  ICC = 0.4, alpha = 0.75
) {
  stopifnot( ICC >= 0 && ICC < 1 )

  dat <- gen_cluster_RCT(
    n_bar = n_bar, J=J, gamma_1 = ATE, gamma_2 = size_coef,
    sigma2_u = ICC, sigma2_e = 1-ICC, alpha = alpha
  )

  MLM = analysis_MLM( dat )
  LR = analysis_OLS( dat )
  Agg = analysis_agg( dat )

  bind_rows( MLM = MLM, LR = LR, Agg = Agg, .id = "method" )
}
```

Note the `stopifnot`: it is wise to ensure our parameter transforms are all reasonable, so we do not get unexplained errors or strange results later on. It is best if your code fails as soon as possible! Otherwise debugging can be quite hard.

Controlling how we use the foundational elements such as our data generating code is a key technique for making the higher level simulations sensible and more easily interpretable. In the revised `one_run()` function, we transform the `ICC` input parameter into the parameters used by `gen_cluster_RCT()` so as to maintain the effect size interpretation of our simulation. We have not modified `gen_cluster_RCT()` at all: instead, we specify the parameters of the DGP function in terms of the parameters we want to directly control in the

simulation. Here we have put our entire simulation into effect size units, and are now providing "knobs" to the simulation that are directly interpretable.

8.3   Bundling simulations with `simhelpers`

The techniques that we have demonstrated for repeating a set of calculations each involve a very specific coding pattern, which will often have the same structure even if the details of the data-generating model or the names of the input parameters are very different from the examples we have presented. The `simhelpers` package provides a function `bundle_sim()` that abstracts this common pattern and allows you to automatically stitch together (or "bundle") a DGP function and an estimation function, so that they can be run once or multiple times. Thus, `bundle_sim()` provides a convenient alternative to writing your own `one_run()` function for each simulation, thereby saving a bit of typing (and avoiding an opportunity for bugs to creep into your code).

`bundle_sim()` takes a DGP function and an estimation function as inputs and gives us back a new function that will run a simulation using whatever parameters we give it. Here is a basic example, which creates a function for simulating Pearson correlation coefficients with a bivariate Poisson distribution:

```
sim_r_Poisson <- bundle_sim(f_generate = r_bivariate_Poisson,
                            f_analyze = r_and_z,
                            id = "rep")
```

If we specify the optional argument `id = "rep"`, the function will include a variable called `rep` with a unique identifier for each replication of the simulation process. We can use the newly created function like so:

```
sim_r_Poisson( 4, N = 30, rho = 0.4, mu1 = 8, mu2 = 14)
```

```
##           r         z      CI_lo     CI_hi rep
## 1 0.4584003 0.4952841  0.1175430 0.7026316   1
## 2 0.2136916 0.2170364 -0.1588034 0.5329322   2
## 3 0.4675940 0.5069866  0.1290674 0.7085081   3
## 4 0.6562349 0.7861718  0.3876033 0.8221341   4
```

To create this simulation function, `bundle_sim()` examined `r_bivariate_Poisson()`, figured out what its input arguments are, and made sure that the simulation function includes the same input arguments. You can see the full set of arguments for `sim_r_Poisson()` by evaluating it with `args()`:

```
args(sim_r_Poisson)
```

```
## function (reps, N, rho, mu1, mu2, seed = NA_integer_)
## NULL
```

In addition to the expected arguments from `r_bivariate_Poisson()`, the function has some additional inputs. Its first argument is `reps`, which controls the

number of times that the simulation process will be evaluated. Its last argument is `seed`, which we will discuss in Section 8.4.

The `bundle_sim()` function requires specifying a DGP function and a *single* estimation function, with the data as the first argument. For our cluster-randomized experiment example, we would then need to use our `estimate_Tx_Fx()` function that organizes all of the estimators (see Chapter 7.2). We then use `bundle_sim()` to create a function for running an entire simulation:

```r
sim_cluster_RCT <- bundle_sim( gen_cluster_RCT, estimate_Tx_Fx, id = "runID" )
```

We can call the newly created function like so:

```r
sim_cluster_RCT( 2,
                 n_bar = 30, J = 20, gamma_1 = ATE,
                 sigma2_u = 0.3, sigma2_e = 0.7 )
```

```
##   estimator    ATE_hat     SE_hat     p_value runID
## 1       MLM 1.0718041 0.3464600 0.009834928     1
## 2       OLS 0.8725333 0.3581403 0.041659400     1
## 3       agg 1.1574631 0.4486484 0.018880161     1
## 4       MLM 0.3975797 0.2379827 0.111564711     2
## 5       OLS 0.4656465 0.2686438 0.111156240     2
## 6       agg 0.3142312 0.2140596 0.159372293     2
```

Again, `bundle_sim()` produces a function with input names that exactly match the inputs of the DGP function that we give it. It is not possible to re-parameterize or change argument names, as we did with `one_run()` in Section 8.2.1. See Exercise 8.5.3 for further discussion of this limitation.

To use the simulation function in practice, we call it by specifying the number of replications desired (which we have stored in `R`) and any relevant input parameters.

```r
runs <- sim_cluster_RCT( R,
                         n_bar = 30, J = 20, gamma_1 = ATE,
                         sigma2_u = 0.3, sigma2_e = 0.7 )
saveRDS( runs, file = "results/cluster_RCT_simulation.rds" )
```

The `bundle_sim()` function is just a convenient way to create a function that pieces together the steps in the simulation process, which is especially useful when the component functions include many input parameters. The function has several further features, which we will demonstrate in subsequent chapters.

8.4   Seeds and pseudo-random number generators

In prior chapters, we have used built-in functions to generate random numbers and also written our own data-generating functions that produce artificial data following a specific random process. With either type of function, re-running it with the exact same input parameters will produce different results. For instance, running the `rchisq` function with the same set of inputs will produce two different sequences of χ^2 random variables:

```r
c1 <- rchisq(4, df = 3)
c2 <- rchisq(4, df = 3)
rbind(c1, c2)
```

```
##        [,1]     [,2]     [,3]     [,4]
## c1 2.859183 2.925194 9.362208 2.502835
## c2 3.495920 5.326844 1.008615 2.359409
```

If you run the same code as above, you will get different results from these. Likewise, running the bivariate Poisson function from Section 6.3 or the `sim_r_Poisson()` function from Section 8.3 multiple times will produce different datasets:

```r
dat_A <- r_bivariate_Poisson(20, rho = 0.5, mu1 = 4, mu2 = 7)
dat_B <- r_bivariate_Poisson(20, rho = 0.5, mu1 = 4, mu2 = 7)
identical(dat_A, dat_B)
```

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

```r
sim_A <- sim_r_Poisson( 10, N = 30, rho = 0.4, mu1 = 8, mu2 = 14)
sim_B <- sim_r_Poisson( 10, N = 30, rho = 0.4, mu1 = 8, mu2 = 14)
identical(sim_A, sim_B)
```

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

Of course, this is the intended behavior of these functions, but it has an important consequence that needs some care and attention. Using functions like `rchisq()`, `r_bivariate_Poisson()`, or `r_bivariate_Poisson()` in a simulation study means that the results will not be fully reproducible.

When using DGP functions for simulations, it is useful to be able to exactly control the process of generating random numbers. This is much more feasible than it sounds: Monte Carlo simulations are random, at least in theory, but computers are deterministic. When we use R to generate what we have been referring to as "random numbers," the functions produce what are actually *pseudo-random* numbers. Pseudo-random numbers are generated from chains of mathematical equations designed to produce sequences of numbers that appear random, but actually follow a deterministic sequence. Each subsequent random number is a calculated by starting from the previously generated value (i.e., the

current state of the random number generator), applying a complicated function, and storing the result (i.e., updating the state). The numbers returned by the generator form a chain that, ideally, cycles through an extremely long list of values in a way that looks stochastic and unpredictable.

The state of the pseudo-random number generator is shared across different functions that produce pseudo-random numbers, so it does not matter if we are generating numbers with `rnorm()` or `rchisq()` or `r_bivariate_Poisson()`. Each time we ask for a random number from the generator, its state is updated. Functions like `rnorm()` and `rchisq()` all call the low-level generator and then transform the result to be of the correct distribution.

Because the generator is actually deterministic, we can control its output by specify a starting value or initial state, In R, the state of the random number generator can be controlled by setting what its known as the seed. The `set.seed()` function allows us to specify a seed value, so that we can exactly reproduce a calculation. For example,

```r
set.seed(6)
c1 <- rchisq(4, df = 3)
set.seed(6)
c2 <- rchisq(4, df = 3)
rbind(c1, c2)
```

```
##         [,1]    [,2]     [,3]     [,4]
## c1 2.575556 0.93847 8.062264 3.685932
## c2 2.575556 0.93847 8.062264 3.685932
```

Similarly, we can set the seed and run a series of calculations involving multiple functions that make use of the random number generator:

```r
# First time
set.seed(6)
c1 <- rchisq(4, df = 3)
dat_A <- r_bivariate_Poisson(20, rho = 0.5, mu1 = 4, mu2 = 7)

# Exactly reproduce the calculations
set.seed(6)
c2 <- rchisq(4, df = 3)
dat_B <- r_bivariate_Poisson(20, rho = 0.5, mu1 = 4, mu2 = 7)

bind_rows(A = r_and_z(dat_A), B = r_and_z(dat_B), .id = "Rep")
```

```
## # A tibble: 2 x 5
##   Rep       r     z  CI_lo CI_hi
##   <chr> <dbl> <dbl>  <dbl> <dbl>
## 1 A     0.299 0.308 -0.165 0.655
## 2 B     0.299 0.308 -0.165 0.655
```

The `bundle_sim()` function demonstrated in Section 8.3 creates a function for repeating the process of generating and analyzing data. By default, the function it produces includes an argument `seed`, which allows the user to set a seed value before repeatedly evaluating the DGP function and estimation function. By default, the `seed` argument is `NULL` and so the current seed is not modified. Specifying an integer-valued seed will make the results exactly reproducible:

```
sim_A <- sim_r_Poisson( 10, N = 30, rho = 0.4, mu1 = 8, mu2 = 14,
                        seed = 25)
sim_B <- sim_r_Poisson( 10, N = 30, rho = 0.4, mu1 = 8, mu2 = 14,
                        seed = 25)
identical(sim_A, sim_B)
```

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

In practice, it is a good idea to always set seed values for your simulations, so that you (or someone else) can exactly reproduce the results. Attending to reproducibility allows us to easily check if we are running the same code that generated a set of results. For instance, try running the previous blocks of code on your machine; if you set the seed to the same value as we did, you should get identical output.

Setting seeds is also very helpful for debugging. Suppose we had an error that showed up in one of a thousand replications, causing the simulation to crash sometimes. If we set a seed and find that the code crashes, we can debug and then rerun the simulation. If it now runs without error, we know we fixed the problem. If we had not set the seed, we would not know if we were just getting (un)lucky, and avoiding the error by chance.

8.5   Exercises

8.5.1   Welch simulations

In the prior chapter's exercises, you made a new `BF_F` function for the Welch simulation. Now incorporate the `BF_F` function into the `one_run()` function, and use your revised function to generate simulation results for this additional estimator.

8.5.2   Compare sampling distributions of Pearson's correlation coefficients

1. Use `sim_r_Poisson()` to generate 5000 replications of the Fisher-z-transformed correlation coefficient under a bivariate Poisson distribution with $\rho = 0.7$ for a sample of $N = 40$ observations. You pick the remaining parameters.

2. Create a bundled simulation function by combining the data-generating function from Exercise 6.9.5 or 6.9.6 with the `r_and_z()` estimation func-

tion. Run the function to generate 5000 replications of the Fisher-z-transformed correlation coefficient under a bivariate negative binomial distribution, with the same parameter values as above.

3. Create a plot that shows both sampling distributions, making it easy to compare the distributions.

8.5.3 Reparameterization, redux

In Section 8.2.1, we illustrated how the `one_run()` simulation wrapper function could be tweaked in order to reparameterize the model in terms of a single intra-class correlation rather than two variance parameters. But what if you want to avoid having to write your own simulation wrapper and instead use `bundle_sim()`? Revise `gen_cluster_RCT()` to accomplish the reparameterization, then bundle it with `analyze_data()`.

8.5.4 Fancy clustered RCT simulations

In Exercise 6.9.10, your task was to write a data-generating function for a cluster-randomized trial that includes a baseline covariate. Then in Exercise 7.5.4, your task was to create an estimation function that could be applied to data from such a trial.

1. Now, using your work from these exercises, create a bundled simulation function that combines the data-generating function and the estimation function. Ensure that the estimation function returns average treatment effect estimates both with and without controlling for the baseline covariate.

2. Use the resulting function to simulate results from 1000 replications of a cluster-randomized trial, each analyzed two ways (with and without covariate adjustment).

3. Create a plot that shows the sampling distribution of each average treatment effect estimator in a way that makes it easy to compare the distributions.

Chapter 9

Performance criteria

Once we have run our simulation, we have a pile of results to sort through. Given these results, the question is now: how do we assess how well our evaluated analysis procedures worked? In this chapter, we look at a variety of **performance criteria** that can answer this question. Once we have a set performance criteria, we can also compare multiple estimators to each other by seeing which have better performance.

Performance criteria are generally assessments of how an analytic strategy behaves on average if you repeat the experimental process an infinite number of times. For example, the bias of an estimator in a given scenario is how far off, on average, the estimator would be from the true parameter value if you repeated the experiment an infinite number of times.

Although we cannot generally work out the exact performance of our analysis procedure in full mathematical detail, our set of simulation results do constitute a (typically large) *sample* of how well things will tend to worked out given the specified scenario. We can then use that sample to *estimate* the performance criteria of interest. For example, when we wanted to know what percent of the time we would reject the null hypothesis (for a given, specified situation) we estimated that by seeing how often we rejected in 1000 trials.

Now, because we have only a sample of trials rather than the full distribution, our estimates of performance are merely estimates. In other words, they can be wrong, just due to random chance. We can describe how wrong with the **Monte Carlo standard error (MCSE)**. The MCSE is the standard error of our estimate of performance due to the simulation only having a finite number of trials. Just as with statistical uncertainty when analyzing data, we can estimate our MCSE and even use them to generate confidence intervals for our performance estimates. The MCSE is *not* related to the estimators or analytic procedures being evaluated; the MCSE is a function of how much simulation we can do. In a simulation study, we could, in theory, know *exactly* how well

we would do for a given context, if we ran an infinite number of simulations; the MCSE tells us how far we are from this ideal, given how many simulation trials we actually ran. Given a desired MCSE, we could similarly determine how many replications were needed to ensure our performance estimates have a desired level of precision.

9.1   Different kinds of performance

There are several classes of performance criteria we might be interested in, depending on what we are evaluating. In particular, we can as how well we are We talk through them in the following sections after giving a high-level overview.

Point Estimation. Point estimation is when we try to measure the size of an estimand such as an actual average treatment effect γ_1. Estimation has two major components, the point estimator and the uncertainty estimator. We generally evaluate both the *actual* properties of the point estimator and the performance of the *estimated* properties of the point estimator.

For the point estimate, we generally need to know our target *estimand*, which is the "right answer" that we are trying to estimate in our scenario. Continuing our running example of exploring best practices for analyzing a cluster randomized experiment, we might want to assess how well our estimate of the treatment effect $\hat{\gamma}_1$ does for the *estimand* of the site-average treatment effect, γ_1, for example.

Given our estimate $\hat{\gamma}_1$ and our estimand γ_1, we can ask whether we will get the right answer on average (if not, we have *bias*). We can also ask how variable our estimate will tend to be (this is estimating the *variance* or *true standard error* of our estimator). For estimation, we generally are concerned with two things: bias and variance. An estimator is biased if it would generally give estimates that are systematically higher (or lower) than the parameter being estimated in a given scenario. The variance of an estimator is a measure of how much the estimates vary from trial to trial. The variance is the true standard error, squared. We can ask how far off the truth we are likely to be on average (this is the *root mean squared error*). These are its actual properties.

Uncertainty Estimation. Point estimates also usually come with estimates of uncertainty: when we estimate the average treatment effect, we will also get an estimated standard error, $\widehat{SE}$, that tells us how far we are likely to be from our target. We need to understand the properties of $\widehat{SE}$ as well. We can ask whether our standard error estimator tends to be too large or too small, when compared to the true standard error. We can also assess whether the estimated standard error is usually accurate, or unstable across our simulation scenarios.

Inference. Inference is when we do hypothesis testing, asking whether there is evidence for some sort of effect, or asking whether there is evidence that some coefficient is greater than or less than some specified value. In particular, for

our example, to know if there is evidence that there is an average treatment effect at all we would test the null of $H_0 : \gamma_1 = 0$. We would then

For inference, we first might ask whether our methods are valid, i.e., ask whether the methods work correctly when we test for a treatment effect when there is none. For example, we might wonder whether using multilevel models could open the door to inference problems if we had model misspecification, such as in a scenario where the residuals had some non-normal distribution. These sorts of questions are questions of validity.

Also for inference, we might ask which method is better for detecting an effect when there is one. Here, we want to know how our estimators perform in circumstances with a non-zero average treatment effect. Do they reject the null often, or rarely? How much does using aggregation decrease (or increase?) our chances of rejection? These are questions about power.

Confidence Intervals. Finally, we might want to know how well confidence intervals based on our methods work. Do the intervals capture the true estimands with the desired level of accuracy, across the simulation trials? Are the intervals for one method generally shorter or longer than those of another?

Final thoughts. Inference and estimation are clearly highly related–if we have a good estimate of the treatment effect and it is not zero (this is estimation), then we are willing to say that there is a treatment effect (this is inference)–but depending on the framing, the way you would set up a simulation to investigate the behavior of your estimators could be different. For example, if you were interested in inference, you might want to know how often you would reject the null hypothesis of no treatment effect—if just focused on estimation, you may not have a simulation that looks at this question of validity as directly.

In the above, we discussed how to assess the performance of a single procedure, but in general we often have different methods for obtaining some estimate, and want to know which is best. For example, we want to identify which estimation strategy (aggregation, linear regression, or multilevel modeling) we should generally use when analyzing cluster randomized trial data—this is comparison. The goals for a simulation comparing different approaches should be to identify whether the strategies are different, when and how one is superior to the other, and what the salient differences are driven by. To fully understand the trade-offs and benefits, we will generally need to compare the different approaches with respect to a variety of metrics of success.

9.2   Assessing a Point Estimator

Assessing the actual properties of a point estimator is generally fairly simple. For a given scenario, repeatedly generate data and estimate effects. Then take summary measures such as the mean and standard deviation of these repeated trials' estimates to estimate the actual properties of the estimator via Monte

Carlo. Given sufficient simulation trials, we can obtain arbitrarily accurate measures.

The most common measures of an estimator are the bias, variance, and mean squared error. For example, we can ask what the *actual* variance (or standard error) of our estimator is. We can ask if our estimator is biased. We can ask what the overall $RMSE$ (root mean squared error) of our estimator is.

To be more formal, consider an estimator T that is targeting a parameter θ. We call the targeted parameter the *estimand*. In most cases, to run our simulation we set the estimand θ and then generate a (typically large) series of datasets where θ is the true target. We then analyze each dataset, obtaining a sample of estimates $T_1, ..., T_R$, all of the target θ. With this approach, we know θ, but in some cases our estimand is not one of the data generation parameters; we then have to obtain θ in some other manner. See below for further discussion and an example of this

With our target θ and our estimates T_r in hand, we first assess whether our estimator is biased by comparing the mean of our R estimates,

$$\bar{T} = \frac{1}{R} \sum_{r=1}^{R} T_r \ ,$$

to θ. The bias of our estimator is

$$bias = \bar{T} - \theta.$$

We can also ask how variable our estimator is, by calculating the variance of our R estimates

$$S_T^2 = \frac{1}{R-1} \sum_{r=1}^{R} \left(T_r - \bar{T} \right)^2.$$

Importantly, the square root of S_T^2, S_T is the true standard error of our estimator (up to Monte Carlo simulation uncertainty). The true SE S_T is more interpretable due to being on the same metric as our initial estimates.

Finally, the Root Mean Square Error (RMSE) is a combination of the above two measures:

$$RMSE = \left\{ \frac{1}{R} \sum_{r=1}^{R} (T_r - \theta)^2 \right\}^{1/2}.$$

Often people talk about the MSE (Mean Squared Error)–this is just the RMSE squared. Just like the true SE is versus the variance, the RMSE is more interpretable than the MSE.

An important relationship connecting these three measures is

$$RMSE^2 = bias^2 + variance = bias^2 + SE^2.$$

It is important to clarify an important point: the *true standard error* of an estimator $\widehat{\gamma_1}$ is the standard deviation of $\widehat{\gamma_1}$ across multiple datasets. In practice, we never know this value, but in a simulation we can obtain it as the standard deviation of our simulation trial estimates. Generally, when people say "Standard Error" they actually mean *estimated* Standard Error, $(\widehat{SE})$, obtained when we use empirical data to estimate the SE. In general research, we often neglect to monitor that the standard errors themselves are estimates of a true parameter, and thus have their own uncertainty. For assessing actual properties in a simulation, by contrast, we can actually have the true standard error (up to Monte Carlo simulation error), along with our set of estimates.

For absolute assessments of performance, an estimator with low bias, low variance, and thus low RMSE is desired. For comparisons of relative performance, an estimator with lower RMSE is usually preferable to an estimator with higher RMSE; if two estimators have comparable RMSE, then the estimator with lower bias would usually be preferable.

It is important to recognize that the above performance measures depend on the scale of the parameter. For example, if our estimators are measuring a treatment impact in dollars, then our bias, SE, and RMSE are all in dollars. The variance and MSE would be in dollars squared, which is why we take their square roots to put them back on an intepretable dollars scale.

Often the scale of the outcome is irrelevant in our simulations. This is especially the case if we are comparing one estimator to the other. To ease interpretation, we might want to assess estimators relative to the baseline variation. To achieve this, we can generate data so the outcome has unit variance (i.e., we generate *standardized data*). Then the bias, median bias, and root mean-squared error would all be in standard deviation units.

By contrast, a nonlinear change of scale of a parameter can lead to nonlinear changes in performance. For instance, suppose that θ is a measure of the proportion of time that a behavior occurs. A natural way to transform this parameter would be to put it on the log-odds (logit) scale. However, because of the nonlinear aspect of the logit,

$$\text{Bias}\left[\text{logit}(T)\right] \neq \text{logit}\left(\text{Bias}[T]\right), \qquad \text{RMSE}\left[\text{logit}(T)\right] \neq \text{logit}\left(\text{RMSE}[T]\right),$$

and so on. This is fine, but one should be aware that this can happen and do it on purpose.

9.2.1 Comparing the Performances of the Cluster RCT Estimation Procedures

Given our simulation results generated in the last chapter, we next assess the bias, standard error, and RMSE of our three different estimators of the ATE. These performance criteria address these primary questions:

- Is the estimator systematically off? (bias)

- Is it precise? (standard error)
- Does it predict well? (RMSE)

Let us see how the three estimators compare on these criteria.

Are the estimators biased? Bias is with respect to a target estimand. Here we assess whether our estimates are systematically different from the γ_1 parameter we used to generate the data (this is the ATE parameter, which we had set to 0.30).

```
runs %>%
  group_by( method ) %>%
  summarise(
    mean_ATE_hat = mean( ATE_hat ),
    bias = mean( ATE_hat - ATE )  )
```

```
## # A tibble: 3 x 3
##   method mean_ATE_hat    bias
##   <chr>         <dbl>   <dbl>
## 1 Agg           0.306 0.00561
## 2 LR            0.390 0.0899
## 3 MLM           0.308 0.00788
```

Linear regression, with a bias of about 0.09 effect size units, appears about ten times as biased as the other estimators. There is no evidence of major bias for Agg or MLM. This is because the linear regression is targeting the person-average average treatment effect. Our data generating process makes larger sites have larger effects, so the person average is going to be higher since those larger sites will count more. Our estimand, by contrast, is the site average treatment effect, i.e., the simple average of each site's true impact, which our DGP has set to 0.30. The Agg and MLM methods, by contrast, estimate this site-average effect, putting them in line with our DGP.

If we had instead decided our target estimand was the person average effect, then we would see linear regression as unbiased, and Agg and MLM as biased; it is important to think carefully about what the estimators are targeting, and report bias with respect to a clearly articulated goal.

Which method has the smallest standard error? The true Standard Error is simply how variable a point estimator is, and is calculated as the standard deviation of the point estimates for a given estimator. The Standard Error reflects how stable our estimates are across datasets that all came from the same data generating process. We calculate the standard error, and also the relative standard error using linear regression as a baseline:

```
true_SE <- runs %>%
  group_by( method ) %>%
  summarise(
    SE = sd( ATE_hat )
```

```
  )
true_SE %>%
  mutate( per_SE = SE / SE[method=="LR"] )
```

```
## # A tibble: 3 x 3
##    method     SE per_SE
##    <chr>  <dbl>  <dbl>
## 1 Agg    0.168  0.916
## 2 LR     0.183  1
## 3 MLM    0.168  0.916
```

These standard errors are all what we would be trying to estimate with a standard error estimator in a normal data analysis. The other methods appear to have SEs about 8% smaller than Linear Regression.

Which method has the smallest Root Mean Squared Error?

So far linear regression is not doing well: it has more bias and a larger standard error than the other two. We can assess overall performance by combining these two quantities with the RMSE:

```
runs %>%
  group_by( method ) %>%
  summarise(
    bias = mean( ATE_hat - ATE ),
    SE = sd( ATE_hat ),
    RMSE = sqrt( mean( (ATE_hat - ATE)^2 ) )
  ) %>%
  mutate( per_RMSE = RMSE / RMSE[method=="LR"] )
```

```
## # A tibble: 3 x 5
##    method    bias     SE   RMSE per_RMSE
##    <chr>    <dbl>  <dbl>  <dbl>    <dbl>
## 1 Agg    0.00561 0.168  0.168    0.823
## 2 LR     0.0899  0.183  0.204    1
## 3 MLM    0.00788 0.168  0.168    0.823
```

We also include SE and bias as reference.

RMSE is a way of taking both bias and variance into account, all at once. For Agg and MLM, the RMSE is basically the standard error; this makes sense as they are not biased. For LR, the combination of bias plus increased variability gives a higher RMSE. That said, clearly the standard error dominates the bias term (note how RMSE and SE are more similar than RMSE and bias). This is especially the case as RMSE is the square root of the bias and standard errors *squared*; this makes difference between them even more extreme. Overall, Agg and MLM have RMSEs around 16% smaller than LR–this seems notable.

9.2.2 Estimands Not Represented By a Parameter

In our Cluster RCT example, we focused on the estimand of the ATE as captured by our model parameter γ_1. But say we were interested in the person-average effect. This is not represented by any number in our data generating process, so we would have to calculate it and then compare all of our estimates to it.

We offer two ways of doing this. The first is to simply generate a massive dataset, and then average across it to get a good estimate of the true person-average effect. If our dataset is big enough, then the uncertainty in this estimate will be negligible compared to the uncertainty in our simulation.

Here we try this:

```r
dat = gen_cluster_RCT( n_bar = 30, J=100000,
                       gamma_1 = 0.3, gamma_2 = 0.5,
                       sigma2_u = 0.20, sigma2_e = 0.80,
                       alpha = 0.75  )
ATE_person = mean( dat$Yobs[dat$Z==1] ) - mean( dat$Yobs[dat$Z==0] )
ATE_person
```

```
## [1] 0.3919907
```

Note our estimate of the person-average effect of 0 is about what we would expect given the bias we saw earlier for the linear model!

With respect to the `ATE_person` estimand, the bias and RMSE of our estimators will shift, but SE will stay the same:

```r
runs %>%
  group_by( method ) %>%
  summarise(
    bias = mean( ATE_hat - ATE_person ),
    SE = sd( ATE_hat ),
    RMSE = sqrt( mean( (ATE_hat - ATE_person)^2 ) )
  ) %>%
  mutate( per_RMSE = RMSE / RMSE[method=="LR"] )
```

```
## # A tibble: 3 x 5
##   method      bias     SE  RMSE per_RMSE
##   <chr>      <dbl>  <dbl> <dbl>    <dbl>
## 1 Agg     -0.0864  0.168 0.189     1.03
## 2 LR      -0.00212 0.183 0.183     1
## 3 MLM     -0.0841  0.168 0.188     1.02
```

For the person-weighted estimand, Agg and MLM are biased, and LR is unbiased. RMSE is now a tension between bias and reduced variance. Overall, Agg and MLM are 4% worse than LR in terms of RMSE, because they have lower SEs but more bias.

The second method of calculating `ATE_person` would be to record the true person average effect of the dataset with each simulation iteration, and then average those at the end. This is in effect generating our massive dataset in pieces; the overall average of our dataset-specific `ATE_person`s gives our population person-weighted ATE. To do this we would need to modify our `gen_cluster_RCT()` DGP code to track this additional information. We might have, for example

```
tx_effect = gamma_1 + gamma_2 * (nj-n_bar)/n_bar
beta_0j = gamma_0 + Zj * tx_effect + u0j
```

and then we would return `tx_effect` as well as `Yobs` and `Z` as a column in our dataset. This is similar to directly calculating *potential outcomes*, as discussed in Chapter 21.

Once we modified our DGP code, we *also* need to modify our analysis functions to record this information. We might have, for example:

```
analyze_data = function( dat ) {
  MLM = analysis_MLM( dat )
  LR = analysis_OLS( dat )
  Agg = analysis_agg( dat )
  res <- bind_rows( MLM = MLM, LR = LR, Agg = Agg,
              .id = "method" )
  res$ATE_person = mean( dat$tx_effect )
  return( res )
}
```

Now when we run our simulation, we would have a column which is the true person average treatment effect for each dataset. We could then take the average of those across our datasets to estimate the true person average treatment effect in the population, and then compare our point estimators to that value.

Clearly, an estimand that is not represented by a parameter is more difficult to work with, but it is not impossible. The key is to be clear as to what you are trying to estimate: the performance of an estimator depends on the estimand the estimator is compared to.

9.3   Assessing a Standard Error Estimator

Statistics is perhaps more about assessing how good an estimate is than making an estimate in the first place. This translates to simulation studies: in our simulation we can know an estimator's actual properties, but if we were to use this estimator in practice we would have to also estimate its associated standard error, and generate confidence intervals and so forth using this standard error estimate. To understand if this would work in practice, we would need to evaluate not only the behavior of the estimator itself, but the behavior of these associated things. In other words, we generally not only want to know whether

our point estimator is doing a good job, but we usually want to know whether we are able to get a good standard error for that point estimator as well.

To do this we first compare the expected value of $\widehat{SE}$ (estimated with the average $\widehat{SE}$ across our simulation trials) to the actual SE. This tells us whether our uncertainty estimates are *biased*. We could also examine the standard deviation of $\widehat{SE}$ across trials, which tells us whether our estimates of uncertainty are relatively stable. We finally could examine whether there is correlation between $\widehat{SE}$ and the actual error (e.g., $|T - \theta|$). Good estimates of uncertainty should predict error in a given context (especially if calculating conditional estimates); see Sundberg (2003).

For the first assessment, we usually assess the quality of a standard error estimator with a relative performance criteria, rather than an absolute one, meaning we compare the estimated standard error to the true standard error as a ratio.

For an example, suppose that in our simulation we are examining the performance of a point-estimator T for a parameter θ along with an estimator $\widehat{SE}$ for the standard error of T. In this case, we likely do not know the true standard error of T, for our simulation context, prior to the simulation. However, we can use the variance of T across the replications (S_T^2) to directly estimate the true sampling variance $\mathrm{Var}(T) = SE^2(T)$. The *relative bias* of $\widehat{SE}^2$ would then be estimated by $RB = \bar{V}/S_T^2$, where $\bar{V}$ is the average of $\widehat{SE}^2$ across simulation runs. Note that a value of 1 for relative bias corresponds to exact unbiasedness of the variance estimator. The relative bias measure is a measure of *proportionate* under- or over-estimation. For example, a relative bias of 1.12 would mean the standard error was, on average, 12% too large. We discuss relative performance measures further in Section 9.6.1.

9.3.1   Why Not Assess the Estimated SE directly?

We typically see assessment of $\widehat{SE}^2$, not $\widehat{SE}$. In other words, we typically work with assessing whether the variance estimator is unbiased, etc., rather than the standard error estimator. This comes out of a few reasons. First, in practice, so-called unbiased standard errors usually are not in fact actually unbiased (see the delightfully titled section 11.5, "The Joke Is on Us: The Standard Deviation Estimator is Biased after All," in Westfall and Henning (2013) for further discussion). For linear regression, for example, the classic standard error estimator is an unbiased *variance* estimator, meaning that we have a small amount of bias due to the square-rooting because:

$$E[\sqrt{V}] \neq \sqrt{E[V]}.$$

Variance is also the component that gives us the classic bias-variance breakdown of $MSE = Variance + Bias^2$, so if we are trying to assign whether an overall

MSE is due to instability or systematic bias, operating in this squared space may be preferable.

That being said, to put things in terms of performance criteria humans understand, it is usually nicer to put final evaluation metrics back into standard error units. For example, saying there is a 10% reduction in the standard error is more meaningful (even if less impressive sounding) than saying there is a 19% reduction in the variance.

9.3.2   Assessing SEs for Our Cluster RCT Simulation

To assess whether our estimated SEs are about right, we can look at the average *estimated* (squared) standard error and compare it to the true standard error. Our standard errors are *inflated* if they are systematically larger than they should be, across the simulation runs. We can also look at how stable our standard error estimates are, by taking the standard deviation of our standard error estimates. We interpret this quantity relative to the actual standard error to get how far off, as a percent of the actual standard error, we tend to be.

```
runs %>% group_by( method ) %>%
  summarise(
    SE = sd( ATE_hat ),
    mean_SEhat = sqrt( mean( SE_hat^2 ) ),
    infl = 100 * mean_SEhat / SE,
    sd_SEhat = sd( SE_hat ),
    stability = 100 * sd_SEhat / SE )
```

```
## # A tibble: 3 x 6
##   method    SE mean_SEhat  infl sd_SEhat stability
##   <chr> <dbl>      <dbl> <dbl>    <dbl>     <dbl>
## 1 Agg   0.168      0.174  104.   0.0232      13.8
## 2 LR    0.183      0.185  101.   0.0309      16.8
## 3 MLM   0.168      0.174  104.   0.0232      13.8
```

The SEs for Agg and MLM appear to be a bit conservative on average. (3 or 4 percentage points too big).

The last column (`stability`) shows how variable the standard error estimates are relative to the true standard error. 50% would mean the standard error estimates can easily be off by 50% of the truth, which would not be particularly good. Here we see the linear regression is more unstable than the other methods (cluster-robust standard errors are generally known to be a bit unstable, so this is not too surprising). It is a bad day for linear regression.

9.4   Assessing an Inferential Procedure (Hypothesis Testing)

When hypothesis tests are used in practice, the researcher specifies a null (e.g., no treatment effect), collects data, and generates a *p*-value, which is a measure of how extreme the observed data are from what we would expect to naturally occur, if the null were true. When we assess a method for hypothesis testing, we are therefore typically concerned with two aspects: *validity* and *power*.

9.4.1   Validity

Validity revolves around whether we erroneously reject a true null more than we should. Put another way, we say an inference method is valid if it has no more than an α chance of rejecting the null, when it is true, when we are testing at the α level. This means if we used this method 1000 times, where the null was true for all of those 1000 times, we should not see more than about 1000α rejections (so, 50, if we were using the classic $\alpha = 0.05$ rule).

To assess validity we would therefore specify a data generating process where the null is in fact true. We then, for a series of such data sets with a true null, conduct our inferential processes on the data, record the *p*-value, and score whether we reject the null hypothesis or not.

We might then test our methods by exploring more extreme data generation processes, where the null is true but other aspects of the data (such as outliers or heavy skew) make estimation difficult. This allows us to understand if our methods are robust to strange data patterns in finite sample contexts.

The key concept for validity is that the date we generate, no matter how we do it, must be data with a true null. The check is always then to see if we reject the null more than we should.

9.4.2   Power

Power is, loosely speaking, how often we notice an effect when one is there. Power is a much more nebulous concept than validity, because some effects (e.g. large effects) are clearly easier to notice than others. If we are comparing estimators to each other, the overall chance of noticing is less of a concern, because we are typically interested in relative performance. That being said, in order to generate data for a power evaluation, we have to generate data where there is something to detect. In other words, we need to commit to what the alternative is, and this can be a tricky business.

Typically, we think of power as a function of sample size or effect size. Therefore, we will typically examine a sequence of scenarios with steadily increasing sample size or effect size, estimating the power for each scenario in the sequence.

We then, for each sample in our series, estimate the power by the same process

as for validity, above. When assessing validity, we want rejection rates to be low, below α, and when assessing power we want them to be as high as possible. But the simulation process itself, other than the data generating process, is exactly the same.

9.4.3 The Rejection Rate

To put some technical terms to this framing, for both validity and power assessment the main performance criterion is the **rejection rate** of the hypothesis test. When the data are simulated from a model in which the null hypothesis being tested is true, then the rejection rate is equivalent to the **Type-I error rate** of the test. When the data are simulated from a model in which the null hypothesis is false, then the rejection rate is equivalent to the **power** of the test (for the given alternate hypothesis represented by the DGP). Ideally, a testing procedure should have actual Type-I error equal to the nominal level α (this is the definition of validity), but such exact tests are rare.

There are some different perspectives on how close the actual Type-I error rate should be in order to qualify as suitable for use in practice. Following a strict statistical definition, a hypothesis testing procedure is said to be **level-α** if its actual Type-I error rate is *always* less than or equal to α. Among a set of level-α tests, the test with highest power would be preferred. If looking only at null rejection rates, then the test with Type-I error closest to α would usually be preferred. A less stringent criteria is sometimes used instead, where type I error would be considered acceptable if it is within 50% of the desired α.

Often, it is of interest to evaluate the performance of the test at several different α levels. A convenient way to calculate a set of different rejection rates is to record the simulated p-values and then calculate from those. To illustrate, suppose that P_r is the p-value from simulation replication k, for $k = 1, ..., R$. Then the rejection rate for a level-α test is defined as $\rho_\alpha = \Pr(P_r < \alpha)$ and estimated as, using the recorded p-values,

$$r_\alpha = \frac{1}{R} \sum_{r=1}^{R} I(P_r < \alpha).$$

For a null DGP, one can also plot the emperical cumulative density function of the p-values; a valid test should give a $45°$ line as the p-values should be standard uniform in distribution.

9.4.4 Inference in our Cluster RCT Simulation

For our scenario, we generated data with an actual treatment effect. Without further simulation, we therefore could only assess power, not validity. This is easily solved! We simply rerun our simulation code that we made last chapter with `simhelpers`, but with setting `ATE = 0`.

```r
set.seed( 404044 )
runs_val <- sim_function( R, n_bar = 30, J = 20, gamma_1 = 0 )
saveRDS( runs_val, file = "results/cluster_RCT_simulation_validity.rds" )
```

Assessing power and validity is exactly the same calculation: we see how often we have a p-value less than 0.05. For power we have:

```r
runs %>% group_by( method ) %>%
  summarise( power = mean( p_value <= 0.05 ) )
```

```
## # A tibble: 3 x 2
##   method power
##   <chr>  <dbl>
## 1 Agg    0.376
## 2 LR     0.503
## 3 MLM    0.383
```

For validity:

```r
runs_val %>% group_by( method ) %>%
  summarise( power = mean( p_value <= 0.05 ) )
```

```
## # A tibble: 3 x 2
##   method power
##   <chr>  <dbl>
## 1 Agg    0.051
## 2 LR     0.059
## 3 MLM    0.048
```

The power when there is an effect (for this specific scenario) is not particularly high, and the validity is around 0.05, as desired.

Linear regression has notabily higher power... but this may be in part due to the invalidity of the test (note the rejection rate is around 6%, rather than the target of 5%). The elevated power is also likely due to the upward bias in estimation. As discussed above, LR is targeting the person-average impact which, in this case, is not 0 even under our null because we have kept our impact heterogeniety parameter to its default of $\gamma_2 = 0.2$, meaning we have treatment variation around 0. We could run our simulation with truly null effects to see if the false rejection rate goes down.

9.5   Assessing Confidence Intervals

Some estimation procedures result in confidence intervals (or sets) which are ranges of values that should contain the true answer with some specified degree of confidence. For example, a normal-based confidence interval is a combination of an estimator and its estimated uncertainty.

We typically score a confidence interval along two dimensions, **coverage rate** and **average length**. To calculate coverage rate, we score whether each interval "captured" the true parameter. A success is if the true parameter is inside the interval. To calculate average length, we record each confidence interval's length, and then average across simulation runs. We say an estimator has good properties if it has good coverage, i.e. it is capturing the true value at least $1-\alpha$ of the time, and if it is generally short (i.e., the average length of the interval is less than the average length for other methods).

Confidence interval coverage is simultaneously evaluating the estimators in terms of how well they estimate (precision) and their inferential properties. We have combined inference and estimation.

Suppose that the confidence intervals are for the target parameter θ and have coverage level β. Let A_r and B_r denote the lower and upper end-points of the confidence interval from simulation replication r, and let $W_r = B_r - A_r$, all for $r = 1, ..., R$. The coverage rate ω_β and average length $E(W)$ criteria are then as defined in the table below.

Criterion	Definition	Estimate
Coverage	$\omega_\beta = \Pr(A \leq \theta \leq B)$	$\frac{1}{R} \sum_{r=1}^{R} I(A_r \leq \theta \leq B_r)$
Expected length	$E(W) = E(B - A)$	$\bar{W} = \bar{B} - \bar{A}$

Just as with hypothesis testing, a strict statistical interpretation would deem a hypothesis testing procedure acceptable if it has actual coverage rate greater than or equal to β. If multiple tests satisfy this criterion, then the test with the lowest expected length would be preferable. Some analysts prefer to look at lower and upper coverage separately, where lower coverage is $\Pr(A \leq \theta)$ and upper coverage is $\Pr(\theta \leq B)$.

9.5.1 Confidence Intervals in our Cluster RCT Example

For our CRT simulation, we first have to calculate confidence intervals, and then assess coverage. We could have used methods such as `confint()` in the estimation approaches; this would be preferred if we wanted more accurately calculated confidence intervals that used t-distributions and so forth to account for the moderate number of clusters.

But if we want to use normal assumption confidence intervals we can calculate them post-hoc:

```
runs %>% mutate( CI_l = ATE_hat - 1.96*SE_hat,
                 CI_h = ATE_hat + 1.96*SE_hat,
                 covered = CI_l <= ATE & ATE <= CI_h,
                 width = CI_h - CI_l ) %>%
```

```
group_by( method ) %>%
summarise( coverage = mean( covered ),
           width = mean( width ))
```

```
## # A tibble: 3 x 3
##   method coverage width
##   <chr>     <dbl> <dbl>
## 1 Agg       0.942 0.677
## 2 LR        0.908 0.717
## 3 MLM       0.943 0.677
```

Our coverage is about right for Agg and MLM, and around 5 percentage points too low for LR. Linear regression is taking a hit from the bias term. The CIs of LR are a bit wider than the other methods due to the estimated SEs being slightly larger.

9.6   Additional Thoughts on Measuring Performance

In this section we provide some additional thoughts on performance measures. We first discuss relative vs. absolute criteria some more, then touch on robust measures of performance. We finally summarize the measures we discuss in this chapter.

9.6.1   Selecting Relative vs. Absolute Criteria

We have primarily examined performance estimators for point estimators using absolute criteria, focusing on measures like bias directly on the scale of the outcome. In contrast, for evaluation things such as estimated standard errors, which are always positive and scale-dependent, it often makes sense to use relative criteria, i.e., criteria calculated as proportions of the target parameter (T/θ) rather than as differences $(T - \theta)$. We typically apply absolute criteria to point estimators and relative criteria to standard error estimators (we are setting aside, for the moment, the relative criteria of a measure from one estimation procedure to another, as we saw earlier when we compared the SEs to a baseline SE of linear regression for the cluster randomized trial simulation. So how do we select when to use what?

As a first piece of guidance, establish whether we expect the performance (e.g., bias, standard error, or RMSE) of a point estimate to depend on the magnitude of the estimand. For example, if we are estimating some mean θ, and we generate data where $\theta = 100$ vs where $\theta = 1000$ (or any other arbitrary number), we would not generally expect the value of θ to change the magnitude of bias, variance, or MSE. On the other hand, these different θs would have a large impact on the *relative* bias and *relative* MSE. (Want smaller relative bias? Just

add a million to the parameter!) For these sorts of "location parameters" we generally use absolute measures of performance.

That being said, a more principled approach for determining whether to use absolute or relative performance criteria depends on assessing performance for *multiple* values of the parameter. In many simulation studies, replications are generated and performance criteria are calculated for several different values of a parameter, say $\theta = \theta_1, ..., \theta_p$. Let's focus on bias for now, and say that we've estimated (from a large number of replications) the bias at each parameter value. We present two hypothetical scenarios, A and B, in the figures below.
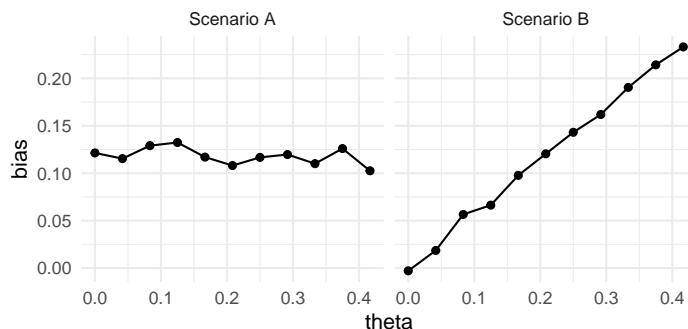
If the absolute bias is roughly the same for all values of θ (as in Scenario A), then it makes sense to report absolute bias as the summary performance criterion. On the other hand, if the bias grows roughly in proportion to θ (as in Scenario B), then relative bias might be a better summary criterion.

Performance relative to a baseline estimator.

Another relative measure, as we saw earlier, is to calculate performance relative to some baseline. For example, if one of the estimators is the "generic method," we could calculate ratios of the RMSE of our estimators to the baseline RMSE. This can provide a way of standardizing across simulation scenarios where the overall scale of the RMSE changes radically. This could be critical to, for example, examining trends across simulations that have different sample sizes, where we would expect all estimators' performance measures to improve as sample size grows. This kind of relative standardization allows us to make statements such as "Aggregation has standard errors around 8% smaller than linear regression"– which is very interpretable, more interpretable than saying "Aggregation has standard errors around 0.01 smaller than linear regression." In the latter case, we do not know if that is big or small.

While a powerful tool, standardization is not without risks: if you scale relative to something, then higher or lower ratios can either be due to the primary method of interest (the numerator) or due to the behavior of the reference method in the denominator. These relative ratios can end up being confusing to interpret due to this tension.

They can also break when everything is on a constrained scale, like power. If

we have a power of 0.05, and we improve it to 0.10, we have doubled our power, but if it is 0.10 and we increase to 0.15, we have only increased by 50%. Ratios when near zero can be very deceiving.

9.6.2 Robust Measures of Performance

Depending on the model and estimation procedures being examined, a range of different criteria might be used to assess estimator performance. For point estimation, we have seen bias, variance and MSE as the three core measures of performance. Other criteria exist, such as the median bias and the median absolute deviation of T, where we use the median $\tilde{T}$ of our estimates rather than the mean $\bar{T}$.

The usual bias, variance and MSE measures can be sensitive to outliers. If an estimator generally does well, except for an occasional large mistake, these classic measures can return very poor overall performance. Instead, we might turn to quantities such as the median bias (sort all the estimation errors across the simulation scenarios, and take the middle), or the Median Absolute Distance (MAD, where you take the median of the absolute values of the errors, which is an alternative to RMSE) as a measure of performance.

Other robust measures are also possible, such as simply truncating all errors to a maximum size (this is called Windsorizing). This is a way of saying "I don't care if you are off by 1000, I am only going to count it as 10."

9.6.3 Summary of Peformance Measures

We list most of the performance criteria we saw in this chapter in the table below, for reference:

Criterion	Definition	Estimate
Bias	$\mathrm{E}(T) - \theta$	$\bar{T} - \theta$
Median bias	$\mathrm{M}(T) - \theta$	$\tilde{T} - \theta$
Variance	$\mathrm{E}\left[(T - \mathrm{E}(T))^2\right]$	S_T^2
MSE	$\mathrm{E}\left[(T - \theta)^2\right]$	$\left(\bar{T} - \theta\right)^2 + S_T^2$
MAD	$\mathrm{M}\left[|T - \theta|\right]$	$\left[|T - \theta|\right]_{R/2}$
Relative bias	$\mathrm{E}(T)/\theta$	$\bar{T}/\theta$
Relative median bias	$\mathrm{M}(T)/\theta$	$\tilde{T}/\theta$
Relative MSE	$\mathrm{E}\left[(T - \theta)^2\right]/\theta^2$	$\frac{\left(\bar{T} - \theta\right)^2 + S_T^2}{\theta^2}$

- Bias and median bias are measures of whether the estimator is systematically higher or lower than the target parameter.

- Variance is a measure of the **precision** of the estimator—that is, how far it deviates *from its average*. We might look at the square root of this, to assess the precision in the units of the original measure. This is the true SE of the estimator.
- Mean-squared error is a measure of **overall accuracy**, i.e. is a measure how far we typically are from the truth. We more frequently use the root mean-squared error, or RMSE, which is just the square root of the MSE.
- The median absolute deviation (MAD) is another measure of overall accuracy that is less sensitive to outlier estimates. The RMSE can be driven up by a single bad egg. The MAD is less sensitive to this.

9.7 Uncertainty in Performance Estimates (the Monte Carlo Standard Error)

Our performance criteria are defined as average performance across an infinite number of trials. Of course, in our simulations we only run a finite number of trials, and estimate the performance criteria with the sample of trials we generate. For example, if we are assessing coverage across 100 trials, we can calculate what fraction rejected the null for that 100. This is an *estimate* of the true coverage rate. Due to random chance, we might see a higher, or lower, proportion rejected than what we would see if we ran the simulation forever.

To account for estimation uncertainty we want associated uncertainty estimates to go with our point estimates of performance. We want to, in other words, treat our simulation results as a dataset in its own right. (And yes, this is quite meta!)

Once we frame the problem in these terms, it is relatively straightforward to calculate standard errors for most of the performance critera because we have an independent and identically distributed set of measurements. We call these standard errors Monte Carlo Simulation Errors, or MCSEs. For some of the performance criteria we have to be a bit more clever, as we will discuss below.

We list MCSE expressions for many of our straightforward performance measures on the following table. In reading the table, recall that, for an estimator T, we have S_T being the standard deviation of T across our simulation runs (i.e., our estimated true Standard Error). We also have

- Sample skewness (standardized): $g_T = \dfrac{1}{RS_T^3} \sum_{r=1}^{R} \left(T_r - \bar{T}\right)^3$

- Sample kurtosis (standardized): $k_T = \dfrac{1}{RS_T^4} \sum_{r=1}^{R} \left(T_r - \bar{T}\right)^4$

Criterion for T	MCSE
Bias $(T - \theta)$	$\sqrt{S_T^2/R}$
Variance (S_T^2)	$S_T^2 \sqrt{\dfrac{k_T - 1}{R}}$
MSE	see below
MAD	-
Power & Validity (r_α)	$\sqrt{r_\alpha (1 - r_\alpha)/R}$
Coverage (ω_β)	$\sqrt{\omega_\beta (1 - \omega_\beta)/R}$
Average length $(\mathrm{E}(W))$	$\sqrt{S_W^2/R}$

The MCSE for the MSE is a bit more complicated, and does not quite fit on our table:

$$\widehat{MCSE}(\widehat{MSE}) = \sqrt{\frac{1}{R}\left[S_T^4(k_T - 1) + 4S_T^3 g_T\left(\bar{T} - \theta\right) + 4S_T^2\left(\bar{T} - \theta\right)^2\right]}.$$

For relative quantities with respect to an estimand, simply divide the criterion by the target estimand. E.g., for relative bias T/θ, the standard error would be

$$SE\left(\frac{T}{\theta}\right) = \frac{1}{\theta} SE(T) = \sqrt{\frac{S_T^2}{R\theta^2}}.$$

For square rooted quantities, such as the SE for the true SE (square root of the Variance) or the RMSE (square root of MSE) we can use the Delta method. The Delta method says (with some conditions), that if we assume $X \sim N(\phi, V)$, then we can approximate the distribution of $g(X)$ for some continuous function $g(\cdot)$ as

$$g(X) \sim N\left(g(\phi),\ g'(\phi)^2 \cdot V\right),$$

where $g'(\phi)$ is the derivative of $g(\cdot)$ evaluated at ϕ. In other words,

$$SE(g(\hat{X})) \approx g'(\theta) \times SE(\hat{X}).$$

For estimation, we plug in $\hat{\theta}$ and our estimate of $SE(\hat{X})$ into the above. Back to the square root, we have $g(x) = \sqrt{(x)}$ and $g'(x) = 1/2\sqrt{(x)}$. This gives, for example, the estimated MCSE of the SE as

$$\widehat{SE}(\widehat{SE}) = \widehat{SE}(S_T^2) = \frac{1}{2S_T^2}\widehat{SE}(S_T^2) = \frac{1}{2S_T^2} S_T^2 \sqrt{\frac{k_T - 1}{R}} = \frac{1}{2}\sqrt{\frac{k_T - 1}{R}}.$$

9.7.1 MCSE for Relative Variance Estimators

Estimating the MCSE of the relative bias or relative MSE of a (squared) standard error estimator, i.e., of $E(\widehat{SE^2} - SE^2)/SE^2)$ or $\widehat{MSE}/MSE$, is complicated by the appearance of an estimated quantity, SE^2 or MSE, in the denominator of the ratio. This renders the simple division approach from above

unusable, technically speaking. The problem is we cannot use our clean expressions for MCSEs of relative performance measures since we are not taking the uncertainty of our denominator into account.

To properly assess the overall MCSE, we need to do something else. One approach is to use the *jackknife* technique. Let $\bar{V}_{(j)}$ and $S^2_{T(j)}$ be the average squared standard error estimate and the true variance estimate calculated from the set of replicates **that excludes replicate** j, for $j = 1, ..., R$. The relative bias estimate, excluding replicate j would then be $\bar{V}_{(j)}/S^2_{T(j)}$. Calculating all R versions of this relative bias estimate and taking the variance of these R versions yields the jackknife variance estimator:

$$MCSE\left(\frac{\widehat{SE}^2}{SE^2}\right) = \frac{1}{R}\sum_{j=1}^{R}\left(\frac{\bar{V}_{(j)}}{S^2_{T(j)}} - \frac{\bar{V}}{S^2_T}\right)^2.$$

This would be quite time-consuming to compute if we did it by brute force. However, a few algebra tricks provide a much quicker way. The tricks come from observing that

$$\bar{V}_{(j)} = \frac{1}{R-1}\left(R\bar{V} - V_j\right)$$

$$S^2_{T(j)} = \frac{1}{R-2}\left[(R-1)S^2_T - \frac{R}{R-1}\left(T_j - \bar{T}\right)^2\right]$$

These formulas can be used to avoid re-computing the mean and sample variance from every subsample. Instead, you calculate the overall mean and overall variance, and then do a small adjustment with each jackknife iteration. You can even implement this with vector processing in R!

9.7.2 Calculating MCSEs With the `simhelpers` Package

The `simhelper` package is designed to calculate MCSEs (and the performance metrics themselves) for you. It is easy to use: take this set of simulation runs on the Welch dataset:

```
library( simhelpers )
data( welch_res )
welch <- welch_res %>%
  filter( method == "t-test" ) %>%
  dplyr::select( -method, -seed, -iterations )

welch

## # A tibble: 8,000 x 8
##       n1    n2 mean_diff     est    var p_val
##    <dbl> <dbl>     <dbl>   <dbl>  <dbl> <dbl>
## 1    50    50         0  0.0258 0.0954 0.934
```

```
## 2    50     50         0   0.00516 0.0848 0.986
## 3    50     50         0  -0.0798  0.0818 0.781
## 4    50     50         0  -0.0589  0.102  0.854
## 5    50     50         0   0.0251  0.118  0.942
## 6    50     50         0  -0.115   0.106  0.725
## 7    50     50         0   0.157   0.115  0.645
## 8    50     50         0  -0.213   0.121  0.543
## 9    50     50         0   0.509   0.117  0.139
## 10   50     50         0  -0.354   0.0774 0.206
## # i 7,990 more rows
## # i 2 more variables: lower_bound <dbl>,
## #   upper_bound <dbl>
```

We can calculate performance metrics across all the range of scenarios. Here is the rejection rate:

```
welch_sub = filter( welch, n1 == 50, n2 == 50, mean_diff==0 )
calc_rejection(welch_sub, p_val)
```

```
##   K_rejection rej_rate rej_rate_mcse
## 1        1000    0.048   0.006759882
```

And coverage:

```
calc_coverage(welch_sub, lower_bound, upper_bound, mean_diff)
```

```
## # A tibble: 1 x 5
##   K_coverage coverage coverage_mcse width
##        <int>    <dbl>         <dbl> <dbl>
## 1       1000    0.952       0.00676  1.25
## # i 1 more variable: width_mcse <dbl>
```

Using `tidyverse` it is easy to process across scenarios (more on experimental design and multiple scenarios later):

```
welch %>% group_by(n1,n2,mean_diff) %>%
  summarise( calc_rejection( p_values = p_val ) )
```

```
## # A tibble: 8 x 6
## # Groups:   n1, n2 [2]
##      n1    n2 mean_diff K_rejection rej_rate
##   <dbl> <dbl>     <dbl>       <int>    <dbl>
## 1    50    50       0          1000    0.048
## 2    50    50       0.5        1000    0.34
## 3    50    50       1          1000    0.876
## 4    50    50       2          1000    1
## 5    50    70       0          1000    0.027
## 6    50    70       0.5        1000    0.341
## 7    50    70       1          1000    0.904
```

```
## 8    50    70        2           1000    1
## # i 1 more variable: rej_rate_mcse <dbl>
```

9.7.3 MCSE Calculation in our Cluster RCT Example

We can check our MCSEs for our performance measures to see if we have enough simulation trials to give us precise enough estimates to believe the differences we reported earlier. In particular, we have:

```r
library( simhelpers )
runs$ATE = ATE
runs %>%
  summarise( calc_absolute( estimates = ATE_hat,
                            true_param = ATE,
                            criteria = c("bias","stddev", "rmse")) ) %>%
  dplyr::select( -K_absolute ) %>%
  knitr::kable(digits=3)
```

bias	bias_mcse	stddev	stddev_mcse	rmse	rmse_mcse
0.034	0.003	0.178	0.002	0.181	0.003

We see the MCSEs are quite small relative to the linear regression bias term and all the SEs (`stddev`) and RMSEs: we have simulated enough runs to see the gross trends identified. We have *not* simulated enough to for sure know if MLM and Agg are not slightly biased. Given our MCSEs, they could have true bias of around 0.01 (two MCSEs).

9.8 Exercises

1. Continuing the exercises from the prior chapters, estimate rejection rates of the BFF* test for the parameter values in the fifth line of Table 1 of Brown and Forsythe (1974).

2. Implement the jackknife as described above in code. Check your answers against the `simhelpers` package for the built-in `t_res` dataset:

```r
library( simhelpers )
calc_relative(data = t_res, estimates = est, true_param = true_param)
```

```
## # A tibble: 1 x 7
##   K_relative rel_bias rel_bias_mcse rel_mse
##        <int>    <dbl>         <dbl>   <dbl>
## 1       1000     1.00        0.0128   0.163
## # i 3 more variables: rel_mse_mcse <dbl>,
## #   rel_rmse <dbl>, rel_rmse_mcse <dbl>
```

3. As foreground to the following chapters, can you explore multiple scenarios for the cluster RCT example to see if the trends are common? First write

a function that takes a parameter, runs the entire simulation, and returns the results as a small table. You pick which parameter, e.g., average treatment effect, `alpha`, or whatever you like), that you wish to vary. Here is a skeleton for the function:

```
my_simulation <- function( my_param ) {
  # call the sim_function() simulation function from the end of last
  # chapter, setting the parameter you want to vary to my_param

  # Analyze the results, generating a table of performance metrics,
  # e.g., bias or coverage. Make sure your analysis is a data frame,
  # like we saw earlier this chapter.

  # Return results
}
```

Then use code like the following to generate a set of results measured as a function of a varying parameter:

```
vals = seq( start, stop, length.out = 5 )
res = map_df( vals, my_simulation )
```

The above code will give you a data frame of results, one column for each performance measure. Finally, you can use this table and plot the performance measure as a function of the varying parameter.

Chapter 10

Project: Cronbach Alpha

In this section we walk through a case study of Cronbach Alpha to give an extended "project," or series of exercises, that walk you through writing a complete simulation starting with the filling out of the code skeleton we get from `simhelpers`'s `create_skeleton()` package.

10.1 Background

Cronbach's α coefficient is commonly reported as a measure of the internal consistency among a set of test items. Consider a set of p test items with population variance-covariance matrix $\Phi = \left[\phi_{ij}\right]_{i,j=1}^{p}$, where ϕ_{ij} is the covariance of item i and item j on the test, across all students taking the test. This population variance-covariance matrix describes how our p test items co-vary.

Cronback's α is, under this model, defined as

$$\alpha = \frac{p}{p-1}\left(1 - \frac{\sum_{i=1}^{p}\phi_{ii}}{\sum_{i=1}^{p}\sum_{j=1}^{p}\phi_{ij}}\right).$$

Given a sample of size n, the usual estimate of α is obtained by replacing the population variances and covariances with corresponding sample estimates. Letting s_{ij} denote the sample covariance of items i and j

$$A = \frac{p}{p-1}\left(1 - \frac{\sum_{i=1}^{p}s_{ii}}{\sum_{i=1}^{p}\sum_{j=1}^{p}s_{ij}}\right).$$

If we assume that the items follow a multivariate normal distribution, then A corresponds to the maximum likelihood estimator of α.

Our goal is to examine the properties of our estimator A when the set of P items is *not* multi-variate normal, but rather follows a multivariate t distribution with v degrees of freedom. For simplicity, we shall assume that the items have common variance and have a **compound symmetric** covariance matrix, such that $\phi_{11} = \phi_{22} = \cdots = \phi_{pp} = \phi$ and $\phi_{ij} = \rho\phi$. In this case we can simplify our expression for α to

$$\alpha = \frac{p\rho}{1 + \rho(p-1)}.$$

In particular, we are interested in whether A is a biased estimator for α, when we have items that are not multi-variate normal. We are also interested in the standard error of A, and how that changes as features of our DGP change. Finally, we have a corresponding asymptotic variance estimator to get estimated standard errors for A, and we want to know if this variance estimator has generally good properties as well.

10.2   Getting started

First create the skeleton of our simulation. We will then walk through filling in all the pieces.

```r
library( simhelpers )
create_skeleton()
```

10.3   The data-generating function

The first two sections in the skeleton are about the data-generating model:

```r
rm(list = ls())


#----------------------------------------------------------
# Set development values for simulation parameters
#----------------------------------------------------------

# What are your model parameters?
# What are your design parameters?


#----------------------------------------------------------
# Data Generating Model
#----------------------------------------------------------

dgm <- function(model_params) {

  return(dat)
```

```
}
```

```
# Test the data-generating model - How can you verify that it is correct?
```

We need to create and test a function that takes model parameters (and sample sizes and such) as inputs, and produces a simulated dataset. The following function generates a sample of n observations of p items from a multivariate t-distribution with a compound symmetric covariance matrix, intra-class correlation ρ, and v degrees of freedom:

```
# model parameters
alpha <- 0.73 # true alpha
df <- 12 # degrees of freedom

# design parameters
n <- 50 # sample size
p <- 6 # number of items


library(mvtnorm)

r_mvt_items <- function(n, p, alpha, df) {
  icc <- alpha / (p - alpha * (p - 1))
  V_mat <- icc + diag(1 - icc, nrow = p)
  X <- rmvt(n = n, sigma = V_mat, df = df)
  colnames(X) <- LETTERS[1:p]
  X
}
```

Note how we translate the target α to ICC for our DGP; we will see this type of translation more later on.

We check our method first to see if we get the right kind of data:

```
small_sample <- r_mvt_items(n = 8, p = 3, alpha = 0.73, df = 5)
small_sample
```

```
##                 A           B           C
## [1,]   0.84178327  0.79667212  0.89763338
## [2,]  -0.22368394  0.03461279  0.18828500
## [3,]  -1.04857817  1.57395368 -0.45917554
## [4,]  -0.62138749 -1.71804224  0.07028801
## [5,]   1.01420764  0.82780069  0.27966729
## [6,]  -0.09936605  0.29165411  0.60147379
## [7,]   1.55303030  0.64559263  1.27739829
## [8,]   2.54590497  0.69538104  1.48876612
```

It looks like we have 8 observations of 3 items, as desired.

To check that the function is indeed simulating data following the intended distribution, let's next generate a very large sample of items. We can then verify that the correlation matrix of the items is compound-symmetric and that the marginal distributions of the items follow t-distributions with specified degrees of freedom.

```r
big_sample <- r_mvt_items(n = 100000, p = 4, alpha = 0.73, df = 5)
round(cor(big_sample), 3)
```

```
##       A     B     C     D
## A 1.000 0.403 0.402 0.403
## B 0.403 1.000 0.409 0.403
## C 0.402 0.409 1.000 0.408
## D 0.403 0.403 0.408 1.000
```

Is this what it should look like?

We can also check normality:

```r
qqplot(qt(ppoints(200), df = 5), big_sample[,2], ylim = c(-4,4))
```
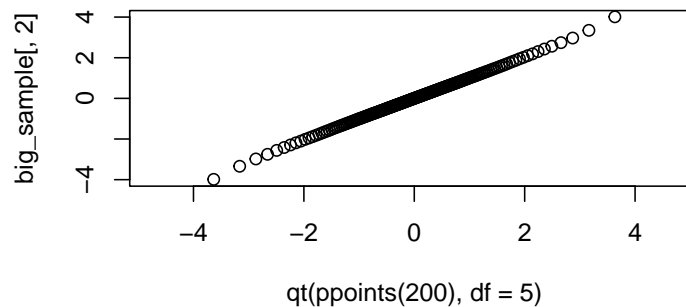

Looks good! A nice straight line.

10.4   The estimation function

The next section of the template looks like this:

```r
#-------------------------------------------------------
# Model-fitting/estimation/testing functions
#-------------------------------------------------------

estimate <- function(dat, design_params) {

  return(result)
}

# Test the estimation function
```

van Zyl, Neudecker, and Nel (2000) demonstrate that, if the items have a compound-symmetric covariance matrix, then the asymptotic variance of A is

$$\text{Var}(A) \approx \frac{2p(1-\alpha)^2}{(p-1)n}.$$

Substituting A in place of α on the right hand side gives an estimate of the variance of A. The following function calculates A and its variance estimator from a sample of data:

```r
estimate_alpha <- function(dat) {
  V <- cov(dat)
  p <- ncol(dat)
  n <- nrow(dat)

  # Calculate A with our formula
  A <- p / (p - 1) * (1 - sum(diag(V)) / sum(V))

  # Calculate our estimate of the variance (SE^2) of A
  Var_A <- 2 * p * (1 - A)^2 / ((p - 1) * n)

  # Pack up our results
  data.frame(A = A, Var = Var_A)
}

estimate_alpha(small_sample)
```

```
##           A       Var
## 1 0.6503423 0.0458477
```

The **psych** package provides a function for calculating α, which can be used to verify that the calculation of A in `estimate_alpha` is correct:

```r
library(psych)
summary(alpha(x = small_sample))$raw_alpha
```

```
## Number of categories should be increased  in order to count frequencies.

##
## Reliability analysis
##   raw_alpha std.alpha G6(smc) average_r S/N ase
##        0.65      0.69    0.79      0.42 2.2 0.2
##   mean   sd median_r
##   0.48 0.74     0.26

## NULL
```

The next step is to evaluate these individual estimates and see how well our estimator A performs.

10.4.1   Exercises (Naive confidence intervals)

1. One way to obtain an approximate confidence interval for α would be to take $A \pm z\sqrt{\mathrm{Var}(A)}$, where $\mathrm{Var}(A)$ is estimated as described above and z is a standard normal critical value at the appropriate level (i.e., $z = 1.96$ for a 95% CI). Extend your simulation to calculate a confidence interval for each simulation round (put this code inside `estimate_alpha()`) and then calculate confidence interval coverage.

Your `estimate_alpha` would then give a result like this:

```
set.seed(40200)
dat = r_mvt_items(n = 50, p = 5, alpha = 0.9, df = 3 )
estimate_alpha(dat)
```

```
##           A           Var   CI_low   CI_high
## 1 0.9425904 0.0001647933 0.916916 0.9682647
```

2. You can calculate confidence intervals with coverage other than 95% by calculating an appropriate number of standard errors, z (usually just taken as 2, as above, for a nominal 95%), with

```
coverage = 0.95
z = qnorm( (1-coverage) / 2, lower.tail = FALSE )
z
```

```
## [1] 1.959964
```

Extend `estimate_alpha()` to allow for a specified coverage by adding a parameter, `coverage`, along with a default of 0.95. Revise the body of `estimate_alpha` to calculate a confidence interval with the specified coverage rate.

10.5   Estimator performance

The next section of the template deals with performance calculations.

```
#--------------------------------------------------------
# Calculate performance measures
# (For some simulations, it may make more sense
# to do this as part of the simulation driver.)
#--------------------------------------------------------

performance <- function(results, model_params) {

  return(performance_measures)
}

# Check performance calculations
```

The `performance()` function takes as input a bunch of simulated data (which we might call `results`) and the true values of the model parameters (`model_params`) and returns as output a set of summary performance measures. As noted in the comments above, for simple simulations it might not be necessary to write a separate function to do these calculations. For more complex simulations, though, it can be helpful to break these calculations out in a function.

To start to get the code working that we would put into this function, it is useful to start with some simulation replicates to practice on. We can generate 1000 replicates using samples of size $n = 40$, $p = 6$ items, a true $\alpha = 0.8$, and $v = 5$ degrees of freedom. We use the `simhelpers repeat_and_stack()` method to do our replication:

```r
one_run <- function( n, p, alpha, df ) {
  dat <- r_mvt_items(n = n, p = p, alpha = alpha, df = df)
  estimate_alpha(dat)
}
true_alpha = 0.7
results = repeat_and_stack( 1000,
                            one_run(40, 6, alpha=true_alpha, df=5) ) %>%
  bind_rows()
```

10.5.1 Exercises (Calculating Performance)

For the Cronbach alpha simulation, we might want to calculate the following performance measures:

1. With the parameters specified above, calculate the bias of A. Also calculate the Monte Carlo standard error (MCSE) of the bias estimate.

2. Estimate the true Standard Error of A.

3. Calculate the mean squared error of A.

4. Calculate the relative bias of the asymptotic variance estimator.

5. Using the work from above, wrap your code in an `alpha_performance()` function that takes the simulation results returned by `run_alpha_sim` and returns a one-row data frame with columns corresponding to the bias, mean squared error, and relative bias of the asymptotic variance estimator.

E.g., a function that behaves like so:

```r
alpha_performance(results, true_alpha)
```

```
##          bias      bias_SE         SE        MSE
## 1 -0.02329445 0.003741931 0.1183302 0.1205433
##     bias_Var
## 1 0.5078144
```

6. Extend your function to add in the MCSEs for the SE and MSE. Code up the skewness and kurtosis values by hand, using the formula in the MCSE section of the performance measure chapter.

7. **(Challenge problem)** Code up a jackknife MCSE function to calculate the MCSE for the relative bias of the asymptotic variance estimator. Use the following template that takes a vector of point estimates and associated standard errors.

```r
jackknife_MCSE <- function( estimates, SEs ) {
  # code
}
```

You would use this function as:

```r
jackknife_MCSE( alpha_reps$A, sqrt( alpha_reps$Var ) )
```

10.6   Replication (and the simulation)

We now have all the components we need to get simulation results, given a set of parameter values. In the next section of the template, we put all these pieces together in a function—which we might call the *simulation driver*—that takes as input 1) parameter values, 2) the desired number of replications, and 3) optionally, a seed value (this allows for reproducability, see Chapter **??**. The function produces as output a single set of performance estimates. Generically, the function looks like this:

```r
#-----------------------------------------------------------
# Simulation Driver - should return a data.frame or tibble
#-----------------------------------------------------------

runSim <- function(iterations, model_params, design_params, seed = NULL) {
  if (!is.null(seed)) set.seed(seed)

  results <- rerun(iterations, {
              dat <- dgm(model_params)
              estimate(dat, design_params)
            }) %>%
    bind_rows()


  performance(results, model_params)
}

# demonstrate the simulation driver
```

The `runSim` function should require very little modification for a new simulation. Essentially, all we need to change is the names of the functions that are called,

so that they line up with the functions we have designed for our simulation. Here's what this looks like for the Cronbach alpha simulation (we pull out the code to replicate into its own method, `one_run()`, which helps with debugging):

```
#--------------------------------------------------------
# Simulation Driver - should return a data.frame or tibble
#--------------------------------------------------------


one_run <- function( n, p, alpha, df ) {
    dat <- r_mvt_items(n = n, p = p, alpha = alpha, df = df)
    estimate_alpha(dat)
}


run_alpha_sim <- function(iterations, n, p, alpha, df, seed = NULL) {

  if (!is.null(seed)) set.seed(seed)

  results <-
    rerun(iterations, one_run(n, p, alpha, df) ) %>%
    bind_rows()

  alpha_performance(results, alpha = alpha)
}
```

10.7 Extension: Confidence interval coverage

However, van Zyl, Neudecker, and Nel (2000) suggest that a better approximation involves first applying a transformation to A (to make it more normal in shape), then calculating a confidence interval, then back-transforming to the original scale (this is very similar to the procedure for calculating confidence intervals for correlation coefficients, using Fisher's z transformation). Let our transformed parameter and estimator be

$$\beta = \frac{1}{2} \ln (1 - \alpha)$$
$$B = \frac{1}{2} \ln (1 - A)$$

and our transformed variance estimator be

$$V^B = \frac{p}{2n(p-1)}.$$

(This expression comes from a Delta method expansion on A.)

An approximate confidence interval for β is given by $[B_L, B_U]$, where

$$B_L = B - z\sqrt{V^B}, \qquad B_U = B + z\sqrt{V^B}.$$

Applying the inverse of the transformation gives a confidence interval for α:

$$[1 - \exp(2B_U),\ 1 - \exp(2B_L)].$$

10.8   A taste of multiple scenarios

In the previous sections, we've created code that will generate a set of performance estimates, given a set of parameter values. We can created a dataset that represents every combination of parameter values that we want to examine. How do we put the pieces together?

If we only had a couple of parameter combinations, it would be easy enough to just call our `run_alpha_sim` function a couple of times:

```
run_alpha_sim(iterations = 100, n = 50, p = 4, alpha = 0.7, df = 5)
```

```
## Warning: `rerun()` was deprecated in
## purrr 1.0.0.
## i Please use `map()` instead.
##   # Previously
##   rerun(100, one_run(n, p,
##   alpha, df))
##
##   # Now
##   map(1:100, ~ one_run(n, p,
##   alpha, df))
## This warning is displayed
## once every 8 hours.
## Call
## `lifecycle::last_lifecycle_warnings()`
## to see where this warning was
## generated.

##          bias    bias_SE        SE        MSE
## 1 -0.01211522 0.01088426 0.1088426 0.1089725
##     bias_Var
## 1 0.4913622
```

```
run_alpha_sim(iterations = 100, n = 100, p = 4, alpha = 0.7, df = 5)
```

```
##          bias    bias_SE        SE        MSE
## 1 -0.0117337 0.00761985 0.0761985 0.07671916
##     bias_Var
```

```
## 1 0.4727169
```

```
run_alpha_sim(iterations = 100, n = 50, p = 8, alpha = 0.7, df = 5)
```

```
##          bias    bias_SE        SE        MSE
## 1 -0.02601087 0.01120983 0.1120983 0.1145292
##    bias_Var
## 1 0.4319068
```

```
run_alpha_sim(iterations = 100, n = 100, p = 8, alpha = 0.7, df = 5)
```

```
##          bias    bias_SE         SE        MSE
## 1 0.007758062 0.006203414 0.06203414 0.06220884
##    bias_Var
## 1 0.5299059
```

But in an actual simulation we will probably have too many different combinations to do this "by hand." The final sections of the simulation template demonstrate two different approaches to doing the calculations for *every* combination of parameter values, given a set of parameter values one wants to explore.

This is discussed further in Chapter @ref(exp_design), but let's get a small taste of doing this now. In particular, the following code will evaluate the performance of A for true values of α ranging from 0.5 to 0.9 (i.e., `alpha_true_seq <- seq(0.5, 0.9, 0.1)`) via `map_df()`:

```
alpha_true_seq <- seq(0.5, 0.9, 0.1)
results <- map_df( alpha_true_seq,
                   run_simulation,
                   R = 100,
                   n = 50, p = 5, df = 5 )
```

How does coverage change for different values of A?

10.8.1 Exercises

1. Show the inverse transform of $B = g(A)$ gives the above expression.

2. Make a new function, `estimate_alpha_xform()` that, given a dataset, calculates a confidence interval for α following the method described above.

3. Using the modified `estimate_alpha_xform()`, generate 1000 replicated confidence intervals for $n = 40$, $p = 6$ items, a true $\alpha = 0.8$, and $v = 5$ degrees of freedom. Using these replicates, calculate the true coverage rate of the confidence interval. Also calculate the Monte Carlo standard error (MCSE) of this coverage rate.

4. Calculate the average length of the confidence interval for α, along with its MCSE.

5. Compare the results of this approach to the more naive approach. Are there gains in performance?

6. *Challenge* Derive the variance expression for the transformed estimator using the Delta method on the variance expression for A coupled with the transform. The Delta method says that:

$$var(f(A)) \approx \frac{1}{f'(\alpha)}(A - \alpha)^2.$$

Part III

Multifactor Simulations

Chapter 11

Designing the multifactor simulation experiment

So far, we have created code that will run a simulation for a single combination of parameter values. In practice, simulation studies typically examine a range of different values, including varying the levels of the true parameter values and perhaps also varying sample sizes, to explore a range of different scenarios. We either want reassurance that our findings are general, or we want to understand what aspects of the context lead to our found results. A single simulation gives us no hint as to either of these questions. It is only by looking across a range of settings that we can fully understand trade-offs, general rules, and limits. Let's now look at the remaining piece of the simulation puzzle: the study's experimental design.

Simulation studies often take the form of **full factorial** designed experiments. In full factorials, each factor (a particular knob a researcher might turn to change the simulation conditions) is varied across multiple levels, and the design includes *every* possible combination of the levels of every factor. One way to represent such a design is as a list of the factors and levels being explored.

For example, for the Cronbach alpha simulation discussed in the prior chapter, we might want to vary:

- the sample size, with values of 50 or 100
- the number of items, with values of 4 or 8
- the true value of alpha, with values ranging from 0.1 to 0.9
- the degrees of freedom of the multivariate t distribution, with values of 5, 10, 20, or 100

The above parameters describe a $2 \times 2 \times 9 \times 4$ factorial design, where each element is the number of options for that factor. This is a four factor experiment, because we have four different things we are varying.

To implement in code, we first save the simulation parameters as a list of factors, each factor having a list of values to explore. We then run a simulation for every possible combination of these values. Here is code that generates all the scenarios we will run given the above design, storing these combinations in a data frame, `params`, that represents the full experimental design:

```
design_factors <- list(
  n = c(50, 100),
  p = c(4, 8),
  alpha = seq(0.1, 0.9, 0.1),
  df = c(5, 10, 20, 100)
)

params <- cross_df(design_factors)
params
```

```
## # A tibble: 144 x 4
##        n     p alpha    df
##    <dbl> <dbl> <dbl> <dbl>
## 1     50     4   0.1     5
## 2    100     4   0.1     5
## 3     50     8   0.1     5
## 4    100     8   0.1     5
## 5     50     4   0.2     5
## 6    100     4   0.2     5
## 7     50     8   0.2     5
## 8    100     8   0.2     5
## 9     50     4   0.3     5
## 10   100     4   0.3     5
## # i 134 more rows
```

See what we get?

Last chapter, we wrote a `run.experiment()` method to run a simulation for a given scenario. The parameters we would pass to `run.experiment()` correspond to the columns of `params`. We have a total of $2 \times 2 \times 9 \times 4 = 144$ rows, each row corresponding to a simulation scenario to explore. With multifactor experiments, it is easy to end up running a lot of experiments!

11.1 Choosing parameter combinations

How do we go about choosing parameter values to examine? Choosing which parameters to use is a central part of good simulation design because the primary limitation of simulation studies is always their *generalizability*. On the one hand, it's difficult to extrapolate findings from a simulation study beyond the set of simulation conditions that were examined. On the other hand, it is often difficult or impossible to examine the full space of all possible parameter values, except

for very simple problems. Even in the relatively straightforward Cronbach alpha simulation, we have four factors, and the last three could, in principle, each take an infinite number of different levels. How can we come up with a defensible set of levels to examine?

The choice of simulation conditions needs to be made in the context of the problem or model that you are studying, so it is a bit difficult to offer valid, decontextualized advice. We provide a few observations all the same:

1. For research simulations, it often is important to be able to relate your findings to previous research. This suggests that you should select parameter levels to make this possible, such as by looking at sample sizes similar to those examined in previous studies. That said, previous simulation studies are not always perfect (actually, there are a lot of really crummy ones out there!), and so prior work should not generally be your sole guide or justification.

2. Generally, it is better to err on the side of being more comprehensive. You learn more by looking at a broader range of conditions, and you can always boil down your results to a more limited set of conditions for purposes of presentation.

3. It is also important to explore breakdown points (e.g., what sample size is too small for a method to work?) rather than focusing only on conditions where a method might be expected to work well. Pushing the boundaries and identifying conditions where estimation methods break will help you to provide better guidance for how the methods should be used in practice.

An important point regarding (2) is that you can be more comprehensive and then have fewer replications per scenario. For example, say you were planning on doing 1000 simulations per scenario, but then you realize there is some new factor that you do not think matters, but that you believe other researchers will worry about. You could add in that factor, say with four levels, and then do 250 simulations per scenario. The total work remains the same.

When analyzing the final simulation you would first verify you do not see trends along this new factor, and then marginalize out that factor in your summaries of results. Marginalizing out a factor (i.e., averaging your performance metrics across the additional factor) is a powerful technique of making a claim about how your methods work *on average* across a *range* of scenarios, rather than for a specific scenario; this comes up in the next chapter on presenting results.

Overall, you generally want to vary parameters that you believe matter, or that you think other people will believe matter. The first is so you can learn. The second is to build your case.

Once you have identified your parameters, you then have to decide on the levels of the parameter you will include in the simulation. There are three strategies you might take:

1. Vary a parameter over as much of its range as you can.
2. Choose parameter levels to represent a realistic practical range. These ranges would ideally be empirically justified based on systematic reviews of prior applications. They may also simply come from ones informal impressions of what is realistic in practice.
3. Choose parameters to emulate an important known application or context.

Of these choices, (1) is the most general—but is also the most computationally intensive. Option (2) focuses attention, ideally, on what is of practical relevance to a practitioner. Option (3) is usually coupled with a subsequent applied data analysis, and in this case the simulation is often used to enrich that analysis. In particular, if the simulation shows the methods work for data with the given form of the target application, people may be more willing to believe the application's findings.

Regardless of how you select your primary parameters, you should also vary nuisance parameters (at least a little) to test the sensitivity of your results to these other aspects. While simulations will (generally) never be fully generalizable, you can certainly make them so they avoid the obvious things a critic might identify as an easy dismissal of your findings.

To recap, as you think about your parameter selection, always keep the following design principles and acknowledgements:

- The primary limitation of simulation studies is **generalizability**.
- Choose conditions that allow you to relate your findings to previous work.
- Err towards being comprehensive. Your goal should be to build an understanding of the major moving parts, and you can always tailor your final presentation of results to give the simplified story, once you find it.
- Explore breakdown points (e.g., what sample size is too small for applying a given method?).

Finally, you should fully expect to add and subtract from your set of simulation factors as you get your initial simulation results! No one ever runs just a single simulation.

11.1.1 Choosing parameters for the Clustered RCT

Extending our case study presented in Section 6.6 to a multifactor simulation, we next design our full experiment.

So far, we have only investigated a single scenario at a time, although our modular approach does make exploring a range of scenarios by re-calling our simulation function relatively straightforward. But how do our findings generalize? When are the different methods differently appropriate? To answer this, we need to extend to a multifactor simulation to *systematically* explore how our three estimators behave across a range of contexts. We begin by identifying some research questions we might have, given our preliminary results.

Regarding bias, in our initial simulation, we noticed that Linear Regression is estimating a person-weighted quantity, and so would be considered biased for the cluster-average ATE. We might next ask, how large is bias in practice, and much does bias change as we change the cluster-size by impact relationship?

For precision, we saw that Linear Regression has a higher standard error. But is this a general finding? If not, are there contexts where linear regression will have a lower standard error than the others?

Again for precision, we originally thought that aggregation would lose information because the little clusters would have the same weight as big clusters, but be more imprecisely estimated. Were we wrong? Or perhaps if cluster size was even more variable, aggregation might do worse and worse.

Finally, the estimated SEs for all three methods all appeared to be good, although they were rather variable, relative to the true SE. We might then ask, are the standard errors always the right size, on average? Will the estimated SEs fall apart (e.g., be way too large or way too small, in general) for some contexts? If so, which ones?

To answer all of these questions we need to more systematically explore the space of models. But we have a lot of knobs to turn. In particular, with our DGP we can generate fake cluster randomized data where we vary any of the following features:

- How much the average impact varies across clusters, and how strongly that is connected to cluster size
- How much the cluster intercepts vary (degree of cross cluster variation)
- How much residual variation there is
- What is the average cluster size and the variation in cluster sizes
- How many clusters do we have
- What proportion of clusters are treated

We cannot easily vary all of these factors without having too many simulations to easily peform. We instead reflect on our research questions, speculate as to what is likely to matter, and then consider varying the following:

- Average cluster size: Does the number of students/cluster matter?
- Number of clusters: Do cluster-robust SEs work with fewer clusters?
- Variation in cluster size: Do varying cluster sizes cause bias or break things?
- Correlation of cluster size and cluster impact: Will correlation cause bias?
- Cross cluster variation: Does the amount of cluster variation matter?

When designing the final factors, it is important to ensure each factor is isolated, in that changing one of them should not change a host of other things that might impact performance. For example, in our case, if we simply added more cross cluster variation by directly increasing the random effects for the clusters, our total variation will also increase. If we then see that a method deteriorates as variation increases, we then have a confound: is it the cross cluster variation

is causing the problem, or is it the total variation? We therefore want to vary cluster variation while controlling total variation; this is why we use the ICC knob discussed in Section 6.6.the section on the data generation process.

Given our research interests and the way we parameterize our DGP, we end up with the following:

```r
crt_design_factors <- list(
  n_bar = c( 20, 80, 320 ),
  J = c( 5, 20, 80 ),
  ATE = c( 0.2 ),
  size_coef = c( 0, 0.2 ),
  ICC = c( 0, 0.2, 0.4, 0.6, 0.8 ),
  alpha = c( 0, 0.5, 0.8 )
)
```

Note our ATE factor only has one level: we could later expand this if we wanted to, but based on theoretical concerns we are fairly confident the ATE will not impact our research questions, so we leave it as it is, picked to capture what is a plausible "realistic" ATE.

11.1.2 Redundant factor combinations

Also note that we have some redundancy. In particular, if `size_coef` is nonzero, but `alpha` is 0, then the cluster size will not impact the cluster average ATE as there is no variation in cluster size. We could drop those factors, which would make our simulation no longer fully crossed. This would save us simulation runs—in essence we are running the same simulation for `alpha=0` two times, once for each `size_coef` value, for each level of `ICC`, `n_bar` and J. We will leave this in as a sanity check to our results, however: we know we should get the same results and if we do not, then we either have uncontrolled uncertainty in our simulation or an error in our coding.

Also, if computation is cheap, then keeping the multifactor structure will make analysis later on much easier. Otherwise our experiment is not balanced, and so when we average performance across some factors to see the effect of others, we can end up with surprising and misleading results.

11.2 Using pmap to run multifactor simulations

To run simulations across all of our factor combinations, we are going to use a very useful method in the `purrr` package called `pmap()`. `pmap()` marches down a set of lists, running a function on each p-tuple of elements, taking the ith element from each list for iteration i, and passing them as parameters to the specified function. `pmap()` then returns the results of this sequence of function calls as a list of results.

Here is a small illustration of `pmap()` in action:

```r
my_function <- function( a, b, theta, scale ) {
    scale * (a + theta*(b-a))
}

args = list( a = 1:3,
             b = 5:7,
             theta = c(0.2, 0.3, 0.7) )
purrr::pmap_dbl(  args, my_function, scale = 10 )
```

```
## [1] 18 32 58
```

One important note is the variable names for the lists being iterated over must correspond exactly to function arguments of the called function. Extra parameters can be passed after the function name; these will also be passed to each function call, but will be the same for all calls. See how `scale` is the same for all calls in the above example.

Just like `map()` or `map2()`, `pmap()` has variants such as `_dbl` or `_df`. These variants automatically stack or convert the list of things returned into a tidier collection (for `_dbl` it will convert to a vector of numbers, for `_df` it will stack the results to make a large dataframe, assuming each thing returned is a little dataframe).

So far, this is great, but it does not quite look like what we want: our factors are stored as a dataframe, not three lists. This is where R gets interesting: in R, the columns of a dataframe are actually stored as a list of vectors or lists (with each of the vectors or lists having the exact same length). This works beautifully with `pmap()`. Witness:

```r
args[[2]]
```

```
## [1] 5 6 7
```

```r
a_df = as_tibble(args)
a_df
```

```
## # A tibble: 3 x 3
##       a     b theta
##   <int> <int> <dbl>
## ## 1     1     5   0.2
## ## 2     2     6   0.3
## ## 3     3     7   0.7
```

```r
a_df[[2]]
```

```
## [1] 5 6 7
```

```r
purrr::pmap_dbl( a_df, my_function, scale = 10)
```

```
## [1] 18 32 58
```

When we pass our data frame `a_df` to `pmap()`, `pmap()` takes it as a list of lists, and therefore does exactly what it did before.

All of this means `pmap()` can run a specified function on each row of a dataset. Continuing the Cronbach Alpha simulation from above, we would have the following:

```
params$iterations <- 500
sim_results <-  params %>%
  mutate(res = pmap(., run_alpha_sim ) )
```

The above code calls our `run_alpha_sim()` method for each row of our list of scenarios we want to explore. Even better, we are storing the results **as a new variable in the same dataset**.

```
sim_results
```

```
## # A tibble: 144 x 6
##           n     p alpha    df iterations res
##       <dbl> <dbl> <dbl> <dbl>      <dbl> <lgl>
## 1     50     4   0.1     5        500 NA
## 2    100     4   0.1     5        500 NA
## 3     50     8   0.1     5        500 NA
## 4    100     8   0.1     5        500 NA
## 5     50     4   0.2     5        500 NA
## 6    100     4   0.2     5        500 NA
## 7     50     8   0.2     5        500 NA
## 8    100     8   0.2     5        500 NA
## 9     50     4   0.3     5        500 NA
## 10   100     4   0.3     5        500 NA
## # i 134 more rows
```

The above code may look a bit peculiar: we are storing a set of dataframes (our result) in our original dataframe. This is actually ok in R: our results will be in what is called a **list-column**, where each element in our list column is the little summary of our simulation results for that scenario. Here is the third scenario, for example:

```
sim_results$res[[3]]
```

```
## [1] NA
```

List columns are neat, but hard to work with. To turn into normal data we can use `unnest()` to expand the `res` variable, replicating the values of the main variables once for each row in the nested dataset:

```
library(tidyr)
sim_results <- unnest(sim_results, cols = res) %>%
  dplyr::select( -iterations )
sim_results
```

```
## # A tibble: 144 x 5
##         n     p alpha    df res
##     <dbl> <dbl> <dbl> <dbl> <lgl>
## 1     50     4   0.1     5 NA
## 2    100     4   0.1     5 NA
## 3     50     8   0.1     5 NA
## 4    100     8   0.1     5 NA
## 5     50     4   0.2     5 NA
## 6    100     4   0.2     5 NA
## 7     50     8   0.2     5 NA
## 8    100     8   0.2     5 NA
## 9     50     4   0.3     5 NA
## 10   100     4   0.3     5 NA
## # i 134 more rows
```

We can put all of this together in a a tidy workflow as follows:

```
sim_results <-
  params %>%
  mutate(res = pmap(., .f = run_alpha_sim)) %>%
  unnest(cols = res)
```

If you like, you can simply use the `simhelpers` package:

```
sim_results <- evaluate_by_row(params, run_alpha_sim)
```

The above code is auto-generated by the `create_skeleton()` method as well. One advantage of `simhelpers` is it is easy to then do the above in parallel; see Section 18.

We finally save our results using tidyverse's `write_csv()`; see "R for Data Science" textbook, 11.5. We first ensure we have a directory by making one via `dir.create()` (see Section 17.3 for more on files):

```
dir.create("results", showWarnings = FALSE )
write_csv( sim_results, file = "results/cronbach_results.csv" )
```

Our simulation results for all our scenarios are now saved!

11.3 When to calculate performance metrics when running multiple simulations

For a single scenario simulation, we repeatedly generate and analyze data, and then assess the performance across the repetitions. When we extend to multi-factor simulations, we have a choice: do we compute performance measures for each simulation scenario as we go (inside) or do we compute all of them after we get all of our individual results (outside)? We discuss the pros and cons of each approach next.

11.3.1 Aggregate as you simulate (inside)

The *inside* approach runs a stand-alone simulation for each scenario of interest. For each combination of factors, we simulate data, assess performance, and return a summary table. We then stack these tables to get the final results.

This approach, which is what we illustrated above, is straightforward: we already have a method to run simulations for a single scenario, and we just repeat it across multiple scenarios and combine the outputs. After the `pmap()` call and the stacking of results, we end up with a dataframe with all our simulations represented, one simulation context per row (or maybe we have bundles of rows for each simulation context, with one row for each method), with the columns being our factors and measured performance outcomes. This table of performance is ideally all we need to write up our results.

With "inside," we do not have much data to store, and it is easier to modularize the simulation code. On the cons side, we have no ability to add new performance measures on the fly or look at the individual estimates. For example, say we wanted to see if the distribution of estimates in a scenario across iterations was right skewed, because we were worried the estimator sometimes broken down and have extreme answers? We might want to make a histogram of the point estimates, or calculate the skew of the estimates as a performance measure. As the individual estimates are lost, we would have no way of doing this without rerunning the entire simulation.

11.3.2 Keep all simulation runs (outside)

In the *outside* approach, when we finish each single scenario we do not calculate the performance, but instead return the entire set of individual estimates as a dataframe, with each row being a method's estimate for a given dataset. The benefit of the outside approach is, given these raw estimates, we can dynamically add or change how we calculate performance measures without re-running the entire simulation. This is especially important if the simulation is time intensive (e.g., if the estimators being evaluated are computationally expensive). With the outside approach, however, we end up with massive amounts of data to store and manipulate.

For our Cronbach simulation, to move from inside to outside, we just take the summarizing step out of `run_alpha_sim()`. E.g.,:

```r
run_alpha_sim_raw <- function(iterations, n, p, alpha, df, coverage = 0.95 ) {

  results <-
    replicate(n = iterations, {
      dat <- r_mvt_items(n = n, p = p, alpha = alpha, df = df)
      estimate_alpha(dat, coverage = coverage)
    }, simplify = FALSE) %>%
    bind_rows()
```

```
  results
}
```

Each call to `run_alpha_sim_raw()` now gives one row per simulation trial:

```
run_alpha_sim_raw( iterations = 4,
                   50, 6, 0.5, 3 )
```

```
##           A       Var_A        CI_L       CI_U
## 1 0.5402995 0.01014358 0.29374115 0.7007831
## 2 0.3867717 0.01805035 0.05786946 0.6008526
## 3 0.4617342 0.01390704 0.17303773 0.6496454
## 4 0.4810237 0.01292815 0.20267301 0.6622008
```

We then save the entire set of estimates, rather than the performance. The primary advantage of the outside approach is we can then generate new performance measures, as they occur to us, later on. The disadvantage is this result file will be R times as many rows as the older file, which can get quite, quite large.

But disk space is cheap! Here we run the same experiment with our more complete storage. Note how the `pmap_df` stacks the multiple rows from each run, giving us everything nicely bundled up:

```
params$res <- params %>%
    pmap( run_alpha_sim_raw, iterations = 500 )
sim_results_full <- unnest( params,
                            cols = res )
write_csv( sim_results_full, "results/cronbach_results_full.csv" )
```

We end up with a lot more rows. Here is the number of rows for the outside vs inside approach:

```
nrow( sim_results_full )
```

```
## [1] 72000
```

```
nrow( sim_results )
```

```
## [1] 144
```

Comparing the file sizes on the disk, one is several k, the other is several megabytes:

```
file.size("results/cronbach_results.csv") / 1024
```

```
## [1] 3.961914
```

```
file.size("results/cronbach_results_full.csv") / 1024
```

```
## [1] 7445.908
```

11.3.3 Getting raw results ready for analysis

If we generated raw results then we need to collapse them by experimental run before calculating performance measures so we can explore the trends across the experiments.

One way to do this is to use `group_by()` and `summarize()` to summrize our raw results.

```
sim_results_full %>%
    group_by( n, p, alpha, df ) %>%
  summarise(
    bias = mean(A - alpha),
    RMSE = sqrt(mean((A - alpha)^2))
  )
```

```
## # A tibble: 144 x 6
## # Groups:   n, p, alpha [36]
##        n     p alpha    df    bias  RMSE
##    <dbl> <dbl> <dbl> <dbl>   <dbl> <dbl>
##  1    50     4   0.1     5 -0.103  0.388
##  2    50     4   0.1    10 -0.0527 0.263
##  3    50     4   0.1    20 -0.0190 0.221
##  4    50     4   0.1   100 -0.0313 0.219
##  5    50     4   0.2     5 -0.0966 0.399
##  6    50     4   0.2    10 -0.0406 0.225
##  7    50     4   0.2    20 -0.0301 0.223
##  8    50     4   0.2   100 -0.0348 0.206
##  9    50     4   0.3     5 -0.0683 0.281
## 10    50     4   0.3    10 -0.0331 0.199
## # i 134 more rows
```

If we want to use our full performance measure function `alpha_performance()` to get additional metrics such as MCSEs, we would *nest* our data into a series of mini-datasets (one for each simulation), and then process each element. As we saw above, nesting collapses a larger dataframe into a dataframe of dataframes:

```
results <- sim_results_full |>
  dplyr::select( -iterations, -seed ) |>
  group_by( n, p, alpha, df ) |>
  nest( .key = "alpha_sims" )
results
```

```
## # A tibble: 144 x 5
## # Groups:   n, p, alpha, df
## #   [144]
##        n     p alpha    df alpha_sims
##    <dbl> <dbl> <dbl> <dbl> <list>
##  1    50     4   0.1     5 <tibble [500 x 4]>
```

```
## 2    100    4   0.1     5 <tibble [500 x 4]>
## 3     50    8   0.1     5 <tibble [500 x 4]>
## 4    100    8   0.1     5 <tibble [500 x 4]>
## 5     50    4   0.2     5 <tibble [500 x 4]>
## 6    100    4   0.2     5 <tibble [500 x 4]>
## 7     50    8   0.2     5 <tibble [500 x 4]>
## 8    100    8   0.2     5 <tibble [500 x 4]>
## 9     50    4   0.3     5 <tibble [500 x 4]>
## 10   100    4   0.3     5 <tibble [500 x 4]>
## # i 134 more rows
```

Note how each row of our nested data has a little dataframe of the individual simulation results, with 500 rows each. Once nested, we can then use `map()` to apply a function to each element of the nested dataframe.

```
results <- results %>%
  mutate( performance = map2( alpha_sims, alpha,
                              alpha_performance ) )
results <- results %>%
  dplyr::select( -alpha_sims ) %>%
  unnest( cols="performance" )
results
```

```
## # A tibble: 576 x 7
## # Groups:   n, p, alpha, df
## #   [144]
##        n     p alpha    df criterion            est
##    <dbl> <dbl> <dbl> <dbl> <chr>              <dbl>
## 1     50     4   0.1     5 alpha bias       -0.103
## 2     50     4   0.1     5 alpha RMSE        0.388
## 3     50     4   0.1     5 V relative bias   0.436
## 4     50     4   0.1     5 coverage          0.826
## 5    100     4   0.1     5 alpha bias       -0.0347
## 6    100     4   0.1     5 alpha RMSE        0.224
## 7    100     4   0.1     5 V relative bias   0.500
## 8    100     4   0.1     5 coverage          0.85
## 9     50     8   0.1     5 alpha bias       -0.0728
## 10    50     8   0.1     5 alpha RMSE        0.333
## # i 566 more rows
## # i 1 more variable: MCSE <dbl>
```

We have built our final performance table *after* running the entire simulation, rather than running it on each simulation scenario in turn.

Now, if we want to add a performance metric, we can simply change `alpha_performance` and recalculate, without running the time-intensive simulations. Being able to re-analyze your results is generally a far easier fix than running all the simulations again. Summarizing during the simulation

vs. after, as we just did, leads to the same set of results. In fact, if we use the same seed, we would *exactly* the same results. The inside vs. outside choice is one of using disk space in exchange for later flexibility.

11.4 Running the Cluster RCT multifactor experiment

We run our cluster RCT simulation using the same code pattern as we used with Cronbach alpha. Because we are not exactly sure what performance metrics we want, we will save our individual results, and then calculate performance metrics on the full data. I.e., we are using the outside approach, not inside.

We first make our table of scenarios:

```
params <-
  cross_df(crt_design_factors) %>%
  mutate(
    seed = 20200320 + 17 * 1:n()
  )
```

To allow reproducibility, we give a different seed for each scenario just to avoid anything confusing about shared randomness across scenarios. We then run the simulation 1000 times each for all our scenarios, and unnest to get our final data:

```
params$res = pmap(params, .f = run_CRT_sim, reps = 1000 )
res = params %>%
  unnest( cols=c(data) )
saveRDS( res, file = "results/simulation_CRT.rds" )
```

Normally we would do this in parallel for speed; we discuss how to do that in Section 18. Even under parallel processing, this simulation took overnight to run. Our final results look like this:

```
res
```

```
## # A tibble: 810,000 x 13
##     n_bar     J   ATE size_coef   ICC alpha  reps
##    <dbl> <dbl> <dbl>     <dbl> <dbl> <dbl> <dbl>
## 1     20     5   0.2         0     0     0  1000
## 2     20     5   0.2         0     0     0  1000
## 3     20     5   0.2         0     0     0  1000
## 4     20     5   0.2         0     0     0  1000
## 5     20     5   0.2         0     0     0  1000
## 6     20     5   0.2         0     0     0  1000
## 7     20     5   0.2         0     0     0  1000
## 8     20     5   0.2         0     0     0  1000
## 9     20     5   0.2         0     0     0  1000
```

```
## 10    20    5  0.2         0    0    0 1000
## # i 809,990 more rows
## # i 6 more variables: seed <dbl>, runID <chr>,
## #   method <chr>, ATE_hat <dbl>, SE_hat <dbl>,
## #   p_value <dbl>
```

We have a lot of rows of data!

11.4.1 Calculating performance metrics

Our next step is to group our results by our simulation factors and calculate all our performance metrics at once. For example, here we calculate our main performance measures by hand:

```r
res <- readRDS( file = "results/simulation_CRT.rds" )

sres <-
  res %>%
  group_by( n_bar, J, ATE, size_coef, ICC, alpha, method ) %>%
  summarise(
    bias = mean(ATE_hat - ATE),
    SE = sd( ATE_hat ),
    RMSE = sqrt( mean( (ATE_hat - ATE )^2 ) ),
    ESE_hat = sqrt( mean( SE_hat^2 ) ),
    SD_SE_hat = sqrt( sd( SE_hat^2 ) ),
    power = mean( p_value <= 0.05 ),
    R = n(),
    .groups = "drop"
  )
```

If we want MCSEs (we do), then we can do that by hand as well, or use the `simhelpers` package as so:

```r
library( simhelpers )
sres <- res %>%
  group_by( n_bar, J, ATE, size_coef, ICC, alpha, method ) %>%
  summarise( calc_absolute( estimates = ATE_hat,
                            true_param = ATE,
                            criteria = c("bias","stddev",
                                         "rmse")),
             calc_relative_var( estimates = ATE_hat,
                                var_estimates = SE_hat^2,
                                criteria = "relative bias" ) ) %>%
  rename( SE = stddev,
          SE_mcse = stddev_mcse ) %>%
  dplyr::select( -K_absolute, -K_relvar ) %>%
  ungroup()
```

```r
colnames( sres )
```

```
##  [1] "n_bar"            "J"
##  [3] "ATE"              "size_coef"
##  [5] "ICC"              "alpha"
##  [7] "method"           "bias"
##  [9] "bias_mcse"        "SE"
## [11] "SE_mcse"          "rmse"
## [13] "rmse_mcse"        "rel_bias_var"
## [15] "rel_bias_var_mcse"
```

11.4.2   Making analyze_data() quiet

If we run our Cluster RCT simulation when there is little cluster variation, we will get a lot of messages and warnings from our MLM estimator. For example, from a single call we get:

```r
res <- analyze_data(dat)
```

```
## boundary (singular) fit: see help('isSingular')
```

When we scale up to our full simulations, these messages and warnings can become a nuisance. To keep track of these issues, we trap messages and warnings using the `quietly()` method of the `purrr` package as so (see Chapter @(#safe_code) for more on capturing warnings and trapping errors):

```r
quiet_lmer = quietly( lmer )

quiet_analyze_data <- function( dat ) {

    # MLM
    M1 <- quiet_lmer( Yobs ~ 1 + Z + (1|sid), data=dat )
    M = M1$result
    message1 = ifelse( length( M1$message ) > 0, 1, 0 )
    warning1 = ifelse( length( M1$warning ) > 0, 1, 0 )

  ...

    # Compile our results
    tibble(
      method = c( "MLM", "LR", "Agg" ),
      ATE_hat = c( est1, est2, est3 ),
      SE_hat = c( se1, se2, se3 ),
      p_value = c( pv1, pv2, pv3 ),
      message = c( message1, 0, 0 ),
      warning = c( warning1, 0, 0 )
    )
```

```
}
```

We now get a note about the message regarding convergence saved in our results:

```
res <- quiet_analyze_data(dat)
res
```

```
## # A tibble: 3 x 7
##   method ATE_hat SE_hat    df p_value message
##   <chr>   <dbl>  <dbl> <dbl>   <dbl>   <dbl>
## 1 MLM    0.235 0.440   20.0   0.599       1
## 2 LR     0.235 0.0467   1     0.125       0
## 3 Agg    0.232 0.0468   1     0.127       0
## # i 1 more variable: warning <dbl>
```

See? No more warnings are printed to the console, but we do see the message as a variable in our results.

11.5 Exercises

11.5.1 Comparing the trimmed mean, median and mean

In this exercise, you will write a simulation to compare different forms of an estimator for estimating the same thing. In particular, you will compare estimation of the center of a symmetric distribution via mean, trimmed mean, and median (so the mean and median are the same). These are the three estimation strategies that we might be comparing in a paper (pretend you "invented" the trimmed mean and want to demonstrate its utility).

To do this, you should break building this simulation evaluation down into lots of functions to show the general framework. This framework can readily be extended to more complicated simulation studies. This extended exercise illustrates how methodologists might compare different strategies for estimation, and is what we might see in the "simulation" section of a stats paper.

For our data-generation function use the scaled t-distribution so the standard deviation will always be 1 but we will have different fatness of tails (high chance of outliers):

```
gen.data = function( n, mu, df0 ) {
    mu + rt( n, df=df0 ) / sqrt( df0 / (df0-2) )
}
```

The variance of a t distribution is $df/(df-2)$, so when we divide our observations by the square root of this, we standardize them so they have unit variance.

1) Verify this generates data with mean `mu` and standard deviation 1 for various `df0` values.

2) Write a method to calculate the mean, trimmed mean, and median of a vector of data. The trimmed mean should trim 10% of the data from each end. The method should return a data frame with the three estimates, with each row being one of our estimators.

3) Verify your method works by analyzing a dataset generated with `gen.data()`. For example, you can generate a dataset of size 100 with `gen.data(100, 0, 3)` and then analyze it.

4) Use `bundle_sim()` to create a simulation function that generates data and then analyzes it. The function should take `n` and `df0` as arguments, and return the estimates from your analysis method. Use `id` to give each simulation run an ID.

5) Run your simulation function for 1000 datasets of size 10, with `mu=0` and `df0=5`. Store the results in a variable called `raw.exps`.

6) Write a function to calculate the RMSE, bias, and standard error for your three estimators, given the results.

7) Make a single function that takes $df0$ and n, and runs a simulation and returns the performances of your three methods.

8) Now make a grid of $n = 10, 50, 250, 1250$ and $df_0 = 3, 5, 15, 30$, and generate results for your multifactor simulation.

9) Make a plot showing how SE changes as a function of sample size for each estimator. Are they different?

Chapter 12

Presenting multifactor simulation results

Once we have our performance measures for each method for each of our simulation scenarios, how do we explore them? For our Cluster RCT simulation, for example, we have 270 different simulation scenarios across our factors. For each scenario we calculate a whole suite of performance measures we might be interested in (e.g., bias, se, rmse, coverage, …), and we have these performance measures for each of our three methods. All these results can be stored as a table with 810 rows (three rows per simulation scenario, with each row corresponding to a specific method) and one column per performance metric. Navigating all of this can feel somewhat overwhelming. How can we understand trends across this complex domain?

Tackling this question is the primary purpose of this chapter. A first principle to keep in mind is that the goal of a simulation study is to provide evidence for a research question. If you keep the research question in mind, it will be easier to stay on track and not get overwhelmed by the many options you have for analysis. This first principle will, for example, help you navigate which performance measures are most important. A second principle is that a good piece of analysis will give you clear understanding of how one or more of your simulation factors matter, in terms of your performance measures of interest.

For your final write-up, you will not want to present everything. A wall of numbers and observations only serves to pummel the reader. Instead, present selected results that clearly illustrate the main findings from the study, along with anything unusual or anomalous. Your presentation will typically be best served with a few well-chosen figures. Then, in the text of your write-up, you might include a few specific numerical comparisons. Do not include too many of these, and be sure to say why the numerical comparisons you include are important.

To form these final exhibits, you will likely have to generate a wide range of results that show different facets of your simulation. These are for you, and will help you deeply understand what is going on. You then try to simplify the story, in a way that is honest and transparent, by curating this full set of figures to your final ones. Some of the remainder will then become supplementary materials that contain further detail to both enrich your main narrative and demonstrate that you are not hiding anything.

Results are by definition a simplified summary of a complex thing. The alert reader will know this, and will thus be suspicious about what you might have left out. To give a great legitimacy bump to your work, you should also provide reproducible code so others could, if so desired, rerun the simulation and conduct your analysis themselves, or perhaps rerun your simulation under different conditions. Even if no one touches your code, the code's existence and availability builds confidence. People will naturally think, "if that researcher is so willing to let me see what they actually did, then they must be fairly confident it does not contain too many horrendous mistakes."

There are three primary tools for presenting simulation results:

1. Tabulation
2. Visualization
3. Modeling

We next walk through these three modes, with a few examples taken from the literature and our own work.

12.1   Tabulation

Traditionally, simulation study results are presented in big tables. In general, we believe tables rarely make the take-aways of a simulation readily apparent. Perhaps tables are fine if...

- they involve only a few numbers, and a few targeted comparisons.
- it is important to report *exact* values for some quantities.

Unfortunately, simulations usually produce lots of numbers, and involve making lots of comparisons. You are going to want to show, for example, the relative performance of alternative estimators, or the performance of your estimators under different conditions for the data-generating model. This means a lot of rows, and a lot of dimensions. Tables can do two dimensions; when you try to cram more than that into a table, no one is particularly well served.

Furthermore, in simulation, exact values for your bias/RMSE/type-I error, or whatever, are not usually of interest. And in fact, we rarely have them due to Monte Carlo simulation error. The tables provide a false sense of security, unless you include uncertainty, which clutters your table even further.

Overall, tables and simulations do not particularly well mix. In particular, if

you are ever tempted into putting your table in landscape mode to get it to fit on the page, think again. It is often more useful and insightful to present results in graphs (Gelman et al., 2002).

To illustrate, consider the following table of simulation results showing the false rejection rate, against an α of 0.10, for an estimator of an average treatment impact. We have two factors of interest, the treatment and control group sizes.

nT	nC	reject
2	2	19
2	4	16
2	10	20
2	50	26
2	500	31
10	2	18
10	4	9
10	10	7
10	50	7
10	500	8
500	2	29
500	4	14
500	10	8
500	50	5
500	500	5

We can see that the rejection rates are often well above 10%, and that if there are few treatment units, the rates are all way too high. Because of the ordering of rows, it is a bit harder to see how the number of control units impacts the rate, and understanding the joint relationship between number of treatment and number of control requires extra thinking. But this is a classic type of table you might see in a paper: the table is a group of tables indexed by one factor, with the second varying within each group.

By contrast, a plot of these exact same numbers (this is an "interaction plot" showing the "interaction" of nT and nC) can make trends much more clear:
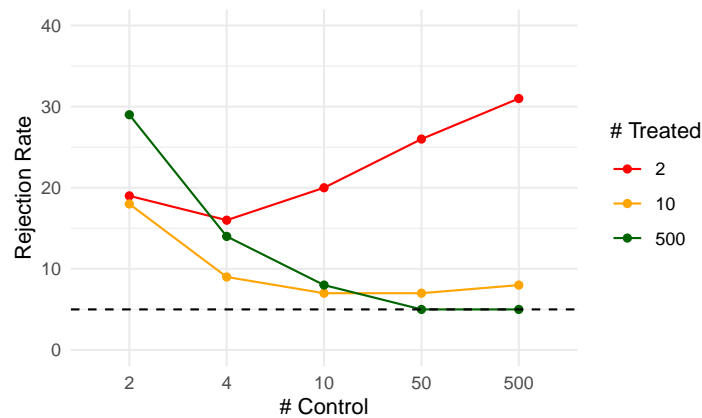
Now we immediately see that only if both nC and nT are above 50 do we achieve anything close to valid tests. Even if nC is 500, we are elevated if nT is only 10. When nT is 2, then increasing nC actually *increases* the rejection rate, meaning larger samples are worse; this is not obvious from looking at the raw table results.

12.1.1 Example: estimators of treatment variation

Tables do have some purpose. For example, tables can be used a bit more effectively to show average performance across a range of simulation scenarios. In general, tables are more plausibly useful for displaying a summary of findings. Do not use them for raw results.

For example, in ongoing work, Miratrix has been studying the performance of a suite of estimators designed to estimate individual treatment effects. To test which estimators perform better or worse than the others, we designed a series of scenarios where we varied the data-generating model by a variety of factors. We then, for each scenario, calculated the relative performance of each estimator to the median of all estimators considered.

We can then ask, do some methods perform better than their peers on average across all scenarios considered? The following table gives an answer to this question: we evaluate each method, averaged across all scenarios, along four metrics: relative bias, relative se, relative rmse, and R^2. To easily see who is good and who is bad, we order the methods from highest average relative RMSE to lowest:

model	bias	se	rmse	sd_bias	sd_se	sd_rmse	R2	sd_R2
BART S	-6	-28	-17	13	14	12	0.40	0.25
CF	-10	-2	-10	14	34	11	0.35	0.19
CF LC	-10	-1	-10	14	33	10	0.34	0.19
LASSO R	2	-21	-10	9	13	10	0.31	0.25
LASSO MCM EA	2	-20	-10	9	13	10	0.31	0.25
LASSO MOM DR	2	-21	-9	9	13	10	0.31	0.25
RF MOM DR	3	-12	-8	15	16	8	0.31	0.20
LASSO T	-1	-10	-6	16	23	9	0.32	0.23
LASSO T INT	-4	19	5	16	55	17	0.28	0.20
LASSO MCM	20	4	8	20	10	8	0.14	0.15
LASSO MOM IPW	20	4	8	20	10	8	0.14	0.15
ATE	47	-60	9	48	7	17	NA	NA
RF T	-22	60	11	17	48	19	0.29	0.13
RF MOM IPW	15	27	12	31	20	13	0.16	0.12
OLS S	-26	87	23	28	83	34	0.31	0.22
BART T	-38	103	25	19	54	22	0.32	0.18
CDML	9	71	31	20	99	46	0.24	0.20

We are summarizing 324 scenarios. The first columns show relative performance. To calculate these values we, for each method m, performance metric Q, and scenario s, calculate $P_{ms} = Q_{ms}/median(Q_{ms})$, and then average the P_{ms} across the scenarios to get $\bar{P}_m$. Each method also has an R^2_{ms} value for each scenario; we simply take the average of these across all scenarios for the penultimate column.

The standard deviation columns show the standard deviation of the performances across the full set of scenarios: they give some sense of how much the relative performance of a method changes from scenario to scenario. Seeing this variation more explicitly might be better done with a visualization; we explore that below.

Overall, the table does give a nice summary of the results, but we still do not feel it makes the results particularly visceral. Visualization can make trends jump out much more clearly. That said, the table *is* showing four performance measures, one of which (the R^2) is on a different scale than the others; this is hard to do with a single visualiztion.

So much for tables.

12.2 Visualization

We believe visualization to be the primary vehicle for communicating simulation results. To illustrate some illustration principles, we next present a series of visualizations, illustrating some different themes behind visualization that we believe are important. In the following chapters we talk about how to get to this final point by iteratively refining a series of plots.

12.2.1   Example 1: Biserial correlation estimation

Our first example, from Pustejovsky (2014), shows the bias of a biserial correlation estimate from an extreme groups design. This simulation was a 4-factor, $96 \times 2 \times 5 \times 5$ factorial design (factors being true correlation for a range of values, cut-off type, cut-off percentile, and sample size). The correlation, with 96 levels, forms the x-axis, giving us nice performance curves. We use line type for the sample size, allowing us to easily see how bias collapses as sample size increases. Finally, the facet grid gives our final factors of cut-off type and cut-off percentile. All our factors, and nearly 5000 explored simulation scenarios, are visible in a single plot.

Source: Pustejovsky, J. E. (2014).
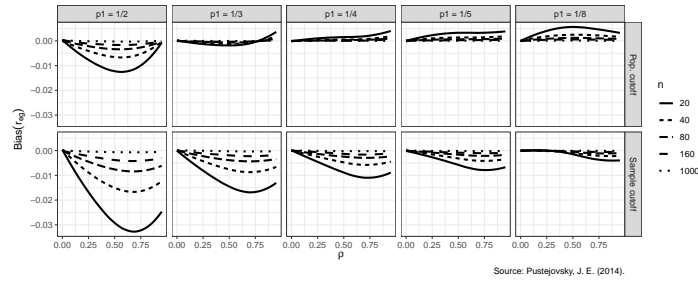
To make this figure, we smoothed the lines with respect to `rho` using `geom_smooth()`. Smoothing is a nice tool for taking some of the simulation jitter out of an analysis to show overall trends more directly.

This style of plotting, with a bunch of small plots, is called "many small multiples" and is beloved by Edward Tufte, who has written extensively on best on information design (see, for example, Tufte and Graves-Morris (1983)). Tufte likes many small multiples, in part, because in a single plot we can display many different variables: here, our facets are organized by two (`p1` and the cutoff approach), and within each facet we have three (our outcome of bias, rho (x-axis), and n (line type)). We have five variables in total; this means we can fully show all combinations of our factors along with an outcome in a four factor experiment!

12.2.2   Example 2:   Variance estimation and Meta-regression

In our next example, from Tipton and Pustejovsky (2015), we explore Type-I error rates of small-sample corrected F-tests based on cluster-robust variance estimation in meta-regression. The simulation aimed to compare 5 different small-sample corrections.

This was another complex experimental design, varying several factors:

- sample size (m)
- dimension of hypothesis (q)
- covariates tested

- degree of model mis-specification

Tipton, E., & Pustejovsky, J. E. (2015)
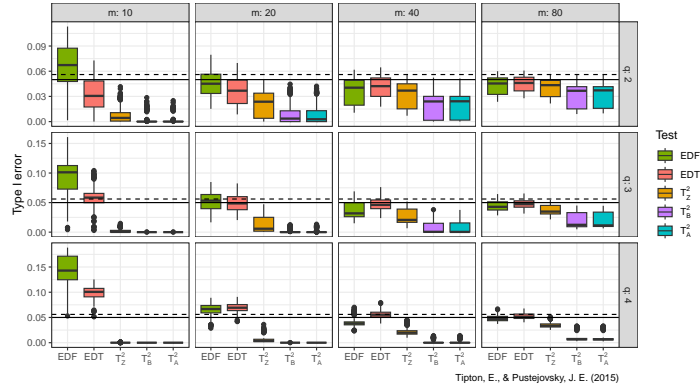
Again using small multiples, we are able to show two of our simulation factors: sample size (m) and dimension of hypothesis (q). The x-axis shows each of our five methods we are comparing. The boxplots are "holding" the other factors, and show the Type-I error rates for the different small-sample corrections across the covariates tested and degree of model misspecification. We add a line at the target 0.05 rejection rate to ease comparison. The reach of the boxes shows how some methods are more or less vulnerable to different types of misspecification. Some estimators (e.g., T_A^2) are clearly hyper-conservitive, with very low rejection rates. Other methods (e.g., EDF), have a range of very high rejection rates when $m = 10$; the degree of rejection rate must depend on model mis-specification and number of covariates tested (the things in the boxes).

12.2.3   Example 3: Heat maps of coverage

For data with many levels of two different factors, one option is to use a heat map. For example, the visualization below shows the coverage of parametric bootstrap confidence intervals for momentary time sampling data. In this simulation study the authors were comparing maximum likelihood estimators to posterior mode (penalized likelihood) estimators of prevalence. We have a 2-dimensional parameter space of prevalence (19 levels) by incidence (10 levels). We also have 12 levels of sample size.

The plot shows the combinations of prevalence and incidence as a grid for each sample size level. We break coverage into ranges of interest, with green being "good" (near 95%) and yellow being "close" (92.5% or above). Blue and purple show conservative (above 95%) coverage. For this kind of plotting to work, we need our MCSE to be small enough that our coverage is estimated precisely enough to show structure. We have two plots, one for each of the methods being compared.
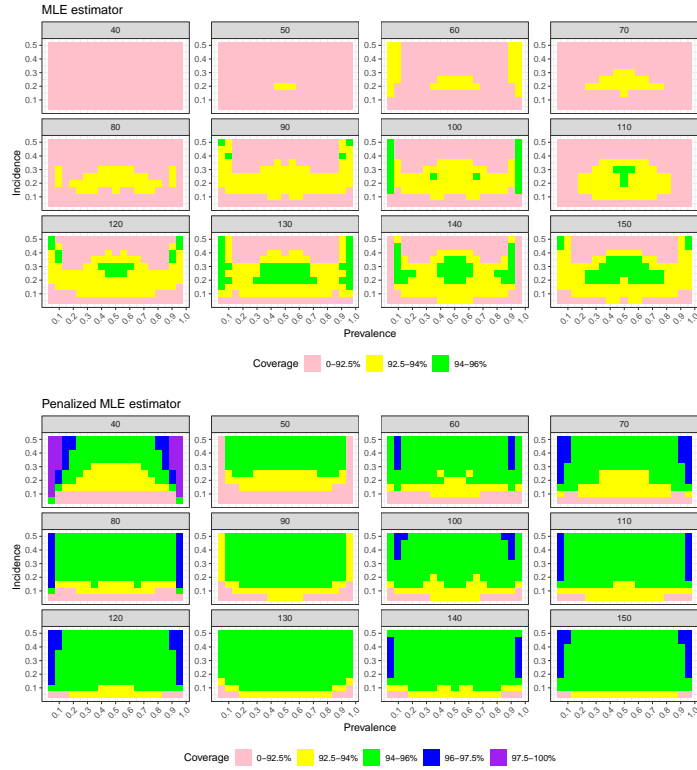
For each plot, we can see clear trends, where coverage degrades for low incidence rates. We are *wrapping* our small multiples by sample size–if you have many levels of a factor you can wrap to show all the levels, which is good, but wrapping does not take advantage of the two-dimensional aspect of having rows and columns of plots (such as we saw with Example 1 and Example 2).

For comparing our two estimators, the prevelance of green in the bottom plot shows generally good behavior for the penalized MLE. The upper plot has less green, showing worse coverage; the improvement of the penalized MLE over the simple MLE is clear. To see this plot in real life, see Pustejovsky and Swan (2015).

## 12.2.4   Example 4: Relative performance of treatment effect estimators

Revisiting the example of different estimators for estimating treatment variation from the table example above, we can try to plot our results.

As a starting point, we can use the same data we used for the table, and just plot the values as bars (after rescaling `R2` by 100 to put it on a similar scale to the other measures):
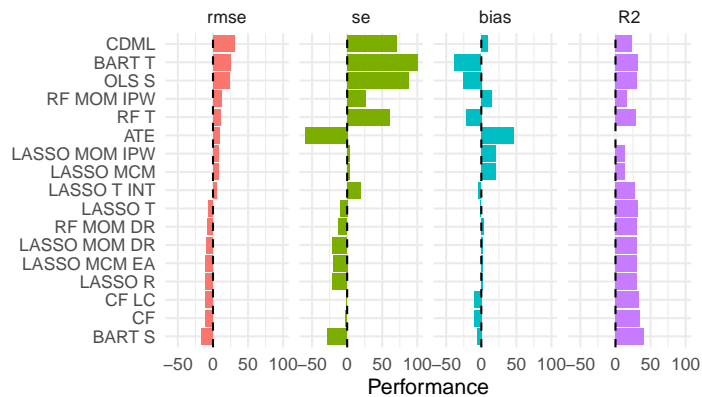
Now we can more visually see how the trends of performance between the different methods correspond. This plot does not, however, show how variation across scenarios might play out. We can extend this plot by plotting boxplots of the actual performances across all scenarios.

In the plot below, we show the range of relative performances for each estimator vs the median, across the simulations. We again order the methods from highest average RMSE to lowest, and plot the average performance across all the simulations as little circles (these would correspond to the bars, above).

Relative performance across all simulation sce

Cropped at 50% and 200%.
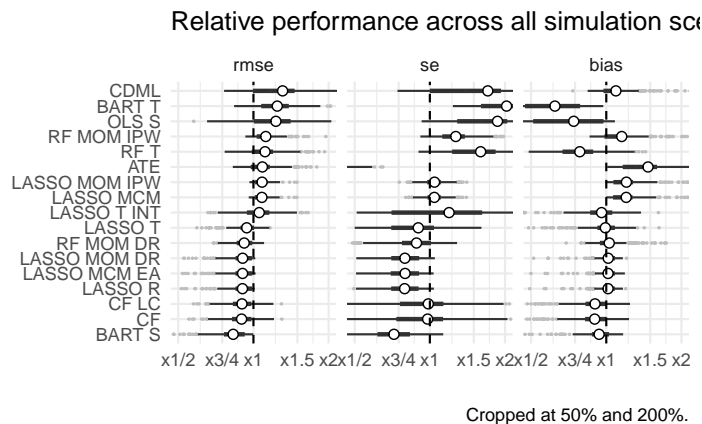
The simulation summarizes performance across 324 scenarios, now showing how much the relative performance can change from scenario to scenario. We truncate extreme values to make the plot more readable and bring focus to central tendencies. We are able to see three performance measures at the same time. The x-axis is on a log scale, again selected to navigate long tails and highlight relative performances. The log scaling also makes the scale of improved performance (less than x1) similar to worse performance (above x1).

We dropped R2 for these plot, since the R2 measure was in percentage points, and, due to estimation uncertainty, included negative values; this was not com-

patible with the log scaling. We have lost something in order to gain something; what plot is best will often be a matter of aesthetic opinion. Pick your plot based on whether it is clearly communicating the message you are trying to get across. (We could also dive into complex plot management, making an R2 plot and adding it to the right of the above plot; we could do this with plot control packages such as `patchwork` or `cowplot`, but we do not do that here.)

12.3 Modeling

Simulations are designed experiments, often with a full factorial structure. The results are datasets in their own right, just as if we had collected data in the wild. We can therefore leverage classic means for analyzing such full factorial experiments. For example, we can regress a performance measure against our factor levels to get the "main effects" of how the different levels impact performance, holding the other levels constant. This type of regression is called a "meta regression" (Kleijnen (1981), Friedman and Pressman (1988), Gilbert and Miratrix (2024)), as we are regressing on already processed results. It also has ties to meta analysis (see, e.g., Borenstein et al. (2021)), where we look for trends across sets of experiments.

In the language of a full factor experiment, we might be interested in the "main effects" and the "interaction effects." A main effect is whether, averaging across the other factors in our experiment, a factor of interest systematically impacts performance. When we look at a main effect, the other factors help ensure our main effect is generalizable: if we see a trend when we average over the other varying aspects, then we can state that our finding is relevant across the host of simulation contexts explored, rather than being an idiosyncratic aspect of a specific and narrow context

If we are comparing multiple methods, we would include the method itself as a factor in our regression. Then the estimated main effects for each method will tell us if a method is, on average, higher or lower than the baseline method, averaging across all the simulation scenarios. The main effect of the simulation factors will tell us if that factor impacts the performance measure on average across the methods considered. We might expect, for example, that for all methods the true standard error goes down as sample size increases.

Meta-regressions would also typically include interactions between method and factor, to see if some factors impact different methods differently. They can also include interactions between simulation factors, which allows us to explore how the impact of a factor can matter more or less, depending on other aspects of the context.

12.3.1 Example 1: Biserial, revisited

For example, consider the bias of the biserial correlation estimates from above. Visually, we see that several factors appear to impact bias, but we might want to

get a sense of how much. In particular, how much does the population vs sample cutoff option matter for bias, across all the simulation factors considered?

We can use ANOVA to decompos the variation in bias into components predicted by various combinations of the simulation factors. Using ANOVA we can identify which factors have negligible/minor influence on the bias of an estimator, and which factors drive the variation we see. We can then summarise our anova table to see the contribution of the various factors and interactions to the total amount of variation in performance:

order	source	eta.sq	eta.sq.part
1	p1	0.21	0.77
1	fixed	0.14	0.70
1	n	0.12	0.67
1	rho	0.02	0.26
2	p1:n	0.18	0.74
2	fixed:n	0.12	0.66
2	rho:fixed	0.03	0.33
2	rho:n	0.02	0.23
2	rho:p1	0.02	0.20
2	p1:fixed	0.02	0.20
3	rho:fixed:n	0.03	0.30
3	rho:p1:n	0.01	0.18
3	p1:fixed:n	0.01	0.17
3	rho:p1:fixed	0.00	0.06
4	rho:p1:fixed:n	0.00	0.06

Here we see which factors are explaining the most variation. E.g., `p1` is explaining 21% of the variation in bias across simulations. The contribution of any of the three- or four-way interactions are fairly minimal, by comparison, and could be dropped to simplify our model.

Modeling summarizes overall trends, and ANOVA allows us to identify what factors are relatively more important for explaining variation in our performance measure. We could fit a regression model or ANOVA model for each performance measure in turn, to understand what drives our results.

12.3.2 Example 2: Comparing methods for cross-classified data

Lee and Pustejovsky (2023) were interested in evaluating how different modeling approaches perform when analyzing cross-classified data structures. To do this they conducted a multi-factor simulation to compare three methods: a method called CCREM, two-way OLS with cluster-robust variance estimation (CRVE), and two-way fixed effects with CRVE. The simulation was complex, involving several factors, so they fit an ANOVA model to understand which factors had the most influence on performance. In particular, they ran *four* multifactor

simulations, each in a different set of conditions. They then used ANOVA to explore how the simulation factors impacted bias within each of these contexts.

One of their tables in the supplementary materials (Table S5.2, see here, page 20, and reproduced below) shows the results of these four ANOVA models, with each column being a simulation context (those being assumptions met, homoscedasticity violated, exogeneity violated, and presence of random slopes), and the rows corresponding to factors manipulated within the simulation. Small, medium, and large effects are marked to make them jump out to the eye.

ANOVA Results on Parameter Bias

Source	Assumptions	Homoscedasticity	Exogeneity	Rand Slope
Method	0.000	0.006	0.995 L	0.000
Effect Size (r)	0.131 M	0.008	0.020 S	0.142 L
Number of Schools (H)	0.014 S	0.113 M	0.188 L	0.001
Students per School (J)	0.016 S	0.016 S	0.747 L	0.110 M
IUCC	0.007	0.007	0.033 S	0.073 M
method × r	0.006	0.006	0.007	0.012 S
method × H	0.004	0.002	0.157 L	0.000
method × J	0.002	0.000	0.878 L	0.010 S
method × IUCC	0.012 S	0.003	0.037 S	0.000
r × H	0.103 M	0.010 S	0.059 S	0.377 L
r × J	0.006	0.024 S	0.008	0.051 S
r × IUCC	0.065 M	0.025 S	0.084 M	0.136 M
H × J	0.002	0.014 S	0.062 M	0.105 M
H × IUCC	0.024 S	0.008	0.034 S	0.137 M
J × IUCC	0.004	0.088 M	0.013 S	0.029 S

Note: (S)mall = .01, (M)edium = .06, (L)arge = .14

We see that when model assumptions are met or only homoscedasticity is violated, choice of method (CCREM, two-way OLS-CRVE, FE-CRVE) has almost no impact on parameter bias ($\eta^2 = 0.000$ to 0.006). However, under an exogeneity violation, method choice has a large effect ($\eta^2 = 0.995$), indicating that some methods (like OLS-CRVE) have much more bias than others. Other factors such as the effect size of the parameter and the number of schools can also show moderate-to-large impacts on bias in several conditions.

The table also shows how an interaction between simulation factors can matter. For example, interactions between method and number of schools, or students per school, can really impact bias under the Exogeniety Violated condition; this means the different methods respond differently as sample size changes.

Overall, the table shows how some aspects of the DGP matter more, and some less.

Using meta regresion can also account for simulation uncertainty in some contexts, which can be especially important when the number of iterations per scenario is low. See Gilbert and Miratrix (2024) for more on this.

Chapter 13

Building good vizualizations

Visualization should nearly always be the first step in analyzing simulation results. In the prior chapter, we saw a series of visualizations that showed overall trends across a variety of examples. Those visualizations were not the initial ones created for those research projects. In practice, making a visualization often requires creating a *bunch* of graphs to look at different aspects of the data. From that pile of graphs, you would then refine ones that communicate the overall results most cleanly, and include those in your main write-up.

In our work, we find we often generate a series of R Markdown reports with comprehensive simulation results targeting our various research questions. These initial documents are then discussed internally by the research team.

In this chapter we discuss a set of common tools that we frequently use to explore our simulation results. In particular, we focus on four essential tools:

1. **Subsetting**: Multifactor simulations can be complex and confusing. Sometimes it is easier to first explore a subset of the simulation results, such as a single factor level.
2. **Many small multiples**: Plot many results in a single plot, with facets to break up the results by simulation factors.
3. **Bundling**: Group the results by a primary factor of interest, and then plotting the performance measure as a boxplot so you can see how much variation there is within that factor level.
4. **Aggregation**: Average the performance measure across some of the simulation factors, so you can see overall trends.

To illustrate these tools, we walk through them using our running example of comparing methods for analyzing a Cluster RCT. We will start with an investigation of bias.

As a reminder, in our Cluster RCT example, we have three methods for estimating the average treatment effect: linear regression of the student-level outcome

onto treatment (with cluster-robust standard errors); aggregation, where we regress the cluster-level average outcome onto treatment (with heteroskedastic robust standard errors); and multilevel modeling with random effects. We want to know if these methods are biased for our defined estimand, which is the cluster-average effect. We have five simulation factors: school size (`n_bar`), number of schools (`J`), the intraclass correlation (`ICC`), the degree of variation in school size (`alpha`), and the relationship between school size and treatment effect (`size_coef`).

Once we go through the core tools, we continue our evaluation of our simulation to show how we can assess various performance metrics of interest (true standard error, RMSE, estimated standard errors, and coverage) using these tools. We do not dive deeply into validity or power; see Chapter 20 for more on these measures.

13.1   Subsetting and Many Small Multiples

As an initial exploration, you can simply filter the simulation results to a single factor level for some nuisance parameter. Generally, with small multiples, it is relatively straightforward to look at *three simulation factors*. This is because, with a facet grid, you can plot five things easily: two for the facets, one for the x-axis, one for color/line type, and one for the y-axis. We usually use two of these for method and outcome, giving three factors to explore.

For example, for our simulation, we might examine an ICC of 0.20 only, taking it as a "reasonable" value that, given our substance matter knowledge, we know is frequently found in empirical data. We might further pick $\bar{n} = 80$, as our middle level for that factor. This leaves three factors, allowing us to plot all of our simulation results. We plot bias as a function of `J`, with different lines for the different methods, and facets for the different levels of `size_coef` and `alpha`.

```r
sres_sub <- sres %>%
  filter( ICC == 0.20, n_bar == 80 )
ggplot( sres_sub, aes( as.factor(J), bias,
                       col=method, pch=method, group=method ) ) +
  facet_grid( size_coef ~ alpha, labeller = label_both ) +
  geom_point() + geom_line() +
  geom_hline( yintercept = 0 ) +
  theme_minimal()
```
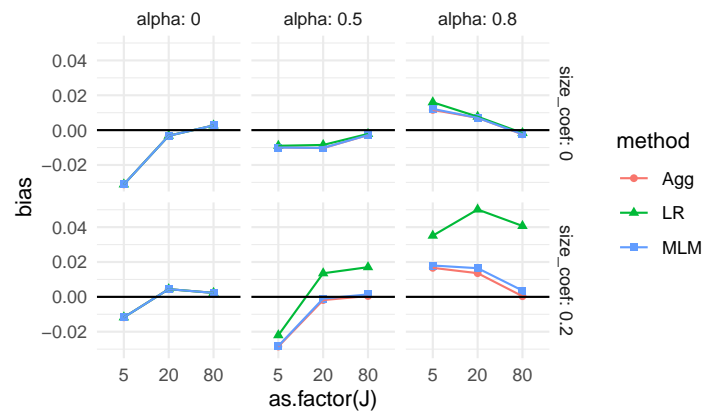
Each point is one of our methods in one of our simulation scenarios. We are looking at the raw results. We connect the points with lines to help us see trends within each of the small multiples. The lines help us visually track which group of points goes with which.

We immediately see that when there is a lot of site variation, and it relates to outcome, linear regression is very different from the other two methods. We also see that when `alpha` is 0 and `size_coef` is 0, we may also have a negative bias. Before we get too excited about this surprising result, we calculate MCSEs to see if this is a real effect or just noise:

```
ggplot( sres_sub, aes( as.factor(J), bias,
                       col=method, pch=method, group=method ) ) +
  facet_grid( size_coef ~ alpha, labeller = label_both ) +
  geom_point( position = position_dodge( width=0.3) ) +
  geom_line(position = position_dodge( width=0.3)) +
  geom_errorbar( aes( ymin = bias - 1.96*bias_mcse,
                      ymax = bias + 1.96*bias_mcse ),
                 position = position_dodge( width=0.3),
                 width = 0 ) +
  geom_hline( yintercept = 0 ) +
  theme_minimal()
```
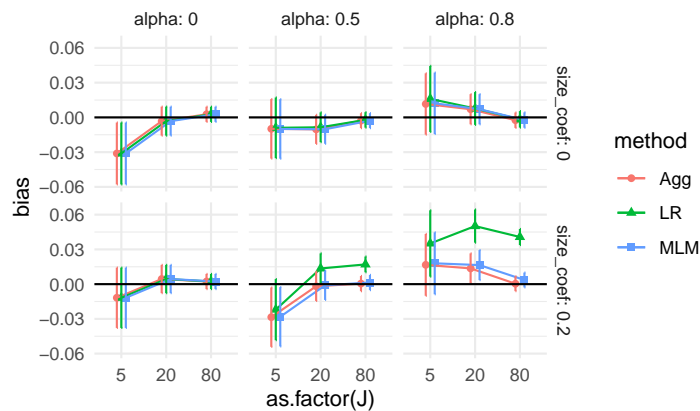
Our confidence intervals exclude zero! Our excitement mounts. We next check all the scenarios with `alpha = 0`, and `size_coef = 0` to see if this is a real effect. We can still plot all our data, as we only have three factors, `ICC`, `J_bar`, and `n_bar`, left to plot.

```
null_sub <- sres %>%
  dplyr::filter( alpha == 0, size_coef == 0 )
ggplot( null_sub, aes( ICC, bias,
                       col=method, pch=method, group=method ) ) +
  facet_grid( J ~ n_bar, labeller = label_both ) +
  geom_point( position = position_dodge( width=0.03) ) +
  geom_line( position = position_dodge( width=0.03) ) +
  geom_errorbar( aes( ymin = bias - 1.96*bias_mcse,
                      ymax = bias + 1.96*bias_mcse ),
                 position = position_dodge( width=0.03),
                 width = 0 ) +
  geom_hline( yintercept = 0 ) +
  theme_minimal()
```
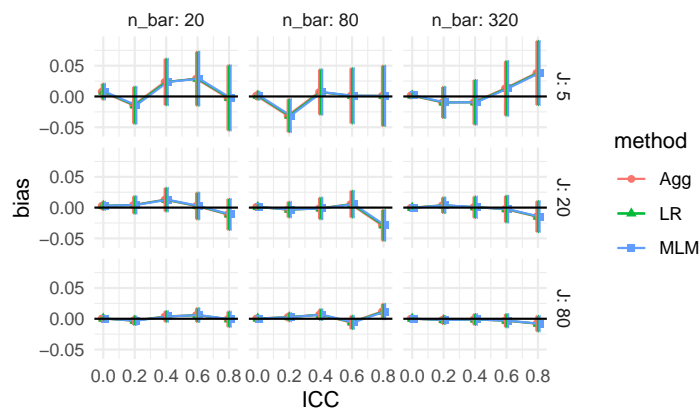

It appears that our `ICC=0.20` and `n_bar=80` scenario was just a fluke. Almost

everything else easily covers 0, and we are not seeing any major trends. Overall we conclude that indeed, when there is no variation, or when the variation does not relate to impact, nothing is particularly biased. Interestingly, we further see that all methods seem to give identical estimates when there is no site variation, regardless of ICC, J, or `n_bar` (that is the easiest explanation of all the estimated biases and associated MCSEs being identical).

Subsetting is a very useful tool, especially when the scope of the simulation feels overwhelming. And as we just saw, it can also be used as a quick validity check: we can subset to a known context where we know nothing exciting should be happening, and then check that indeed nothing is there.

Subsetting allows for a deep dive into a specific context. It also can make it easier to think through what is happening in a complex context. Sometimes we might even just report a subset in our final analysis. In this case, we would consider the other levels as a "sensitivity" analysis vaguely alluded to in our main report and placed elsewhere, such as an online supplemental appendix.

It would be our job, in this case, to verify that our reported findings on the main results indeed were echoed in our other, set-aside, simulation runs. In our case, as we see below, we will see little effect of the ICC on how one model performs relative to another; we thus might be able to safely ignore the ICC factor in our main report.

Subsetting is useful, but if you do want to look at all your simulation results at once, you need to somehow aggregate your results to make them all fit on the plot. We next present bundling, a way of using the core idea of small multiples for showing all of the raw results, but in a semi-aggregated way.

13.2   Bundling

When faced with many simulation factors, we can *bundle* the simulations into groups defined by a selected primary factor of interest, and then plot each bundle with a boxplot of the distribution of a selected performance criteria. Each boxplot shows the central measure of how well an estimator worked across a set of scenarios, along with a sense of how much that performance varied across those scenarios. If the boxes are narrow, then we know that the variation across simulations within the box did not impact performance much. If the boxes are wide, then we know that the factors that vary within the box matter a lot for performance.

With bundling, we generally need a good number of simulation runs per scenario, so that the MCSE in the performance measures does not make our boxplots look substantially more variable (wider) than the truth. (Consider a case where all the scenarios within a box have zero bias; if MCSE were large, we would see a wide boxplot when we should not.)

To illustrate bundling, we group our Cluster RCT results by method, ICC, the

size coefficient (how strong the cluster size to treatment impact relationship is), and alpha (how much the cluster sizes vary). For a specific ICC, size, and alpha, we will put the boxes for the three methods side-by-side to directly compare them:

```
ggplot( sres, aes( as.factor(alpha), bias, col=method, group=paste0(ICC,method) ) ) +
  facet_grid( size_coef ~ ICC, labeller = label_both ) +
  geom_boxplot(coef = Inf) +
  geom_hline( yintercept = 0 ) +
  theme_minimal()
```
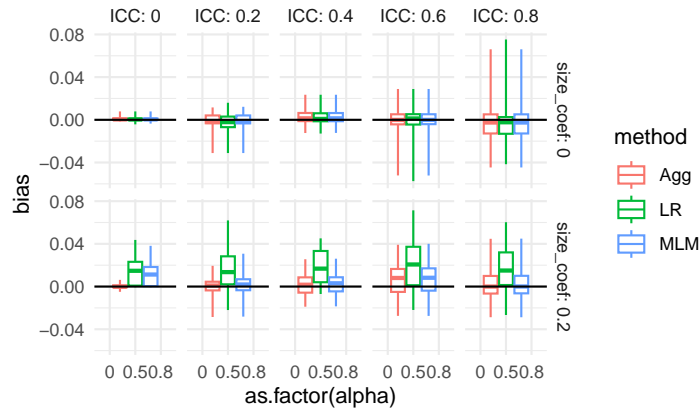

Each box is a collection of simulation trials. E.g., for `ICC = 0.6`, `size_coef = 0.2`, and `alpha = 0.8` each of the three boxes contains 9 scenarios representing the varying level 1 and level 2 sample sizes. Here are the 9 for the Aggregation method:

```
filter( sres,
        ICC == 0.6,
        size_coef == 0.2,
        alpha == 0.8, method=="Agg" ) %>%
  dplyr::select( n_bar:alpha, bias ) %>%
  knitr::kable( digits = 2 )
```

n_bar	J	ATE	size_coef	ICC	alpha	bias
20	5	0.2	0.2	0.6	0.8	0.04
20	20	0.2	0.2	0.6	0.8	0.02
20	80	0.2	0.2	0.6	0.8	-0.01
80	5	0.2	0.2	0.6	0.8	-0.02
80	20	0.2	0.2	0.6	0.8	0.02
80	80	0.2	0.2	0.6	0.8	0.00
320	5	0.2	0.2	0.6	0.8	0.01
320	20	0.2	0.2	0.6	0.8	0.01
320	80	0.2	0.2	0.6	0.8	0.01

Our bias boxplot makes some trends clear. For example, we see that there is virtually no bias for any method when the size coefficient is 0 and the ICC is 0. It is a bit more unclear, but it seems there is also virtually no bias when the size coefficient is 0 regardless of ICC, but the boxes get wider as ICC increases, making us wonder if something else is potentially going on. When alpha is 0 and the size coefficient is 0.2, all methods have a negative bias for most scenarios considered, as all boxes and almost all of the whiskers are below the 0 line (when ICC is 0.6 or 0.8 we may have some instances of 0 or positive bias, if that is not MCSE giving long tails).

The apparent outliers (long tails) for some of the boxplots suggest that the other two factors (cluster size and number of clusters) do relate to the degree of bias. We could try bundling along different aspects to see if that explains these differences:

```
ggplot( sres, aes( as.factor(n_bar), bias, col=method, group=paste0(n_bar,method) ) ) +
  facet_grid( alpha ~  size_coef, labeller = label_both ) +
  geom_boxplot(coef = Inf) +
  geom_hline( yintercept = 0 ) +
  theme_minimal()
```
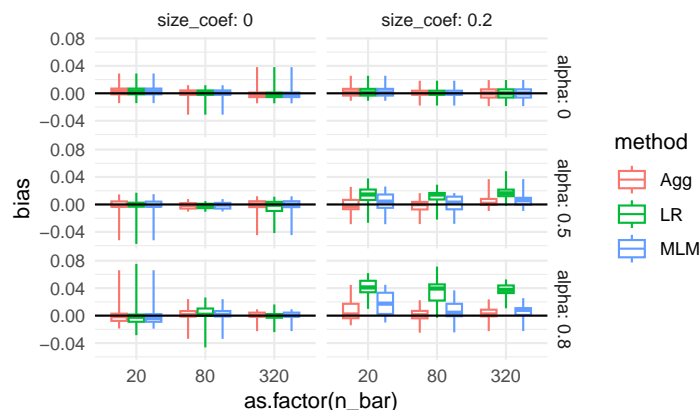

No progress there; we have long tails suggesting something is allowing for large bias in some contexts. This could be MCSE, with some of our bias estimates being large due to random chance. Or it could be some specific combination of factors allows for large bias (e.g., perhaps small sample sizes makes our estimators more vulnerable to bias). In an actual analysis, we would make a note to investigate these anomalies later on.

In general, playing around with factors so that the boxes are generally narrow is a good idea; it means that you have found a representation of the data where the variation within your bundles is less important. This might not always be possible, if all your factors matter; in this case the width of your boxes tells you to what extent the bundled factors matter relative to the factors explicitly present in your plot.

13.3   Aggregation

Boxplots can make seeing trends more difficult, as the eye is drawn to the boxes and tails, and the range of your plot axes can be large due to needing to accommodate the full tails and outliers of your results; this can compress the mean differences between groups, making them look small. Instead of bundling, we can therefore aggregate, where we average all the scenarios within a box to get a single number of average performance. This will show us overall trends rather than individual simulation variation.

When we aggregate, and average over some of the factors, we collapse our simulation results down to fewer moving parts. Aggregation across factors is better than having not having varied those factors in the first place! A performance measure averaged over a factor is a more general answer of how things work in practice than having not varied the factor at all.

For example, if we average across ICC and site variation, and see that our methods had different degrees of bias as a function of J, we would know that the found trend is a general trend across a range of scenarios defined by different ICC and site variation levels, rather than a specific one tied to a single ICC and amount of site variation. Our conclusions would then be more general: if we had not explored more scenarios, we would not have any sense of how general our found trend might be.

That said, if some of our scenarios had no bias, and some had large bias, when we aggregated we would report that there is generally a moderate amount of bias. This would not be entirely faithful to the actual results. If, however, the initial boxplots show results generally in one direction or another, then aggregation will be more faithful to the spirit of the results.

Also, aggregated results can be misleading if you have scaling issues or extreme outliers. With bias, our scale is fairly well set, so we are good. But if we were aggregating standard errors over different sample sizes, then the larger standard errors of the smaller sample size simulations (and the greater variability in estimating those standard errors) would swamp the standard errors of the larger sample sizes. Usually, with aggregation, we want to average over something we believe does not change massively over the marginalized-out factors. To achieve this, we can often average over a relative measure (such as standard error divided by the standard error of some baseline method), which tend to be more invariant and comparable across scenarios.

A major advantage of aggregation over the bundling approach is we can have fewer replications per scenario. If the number of replicates within each scenario is small, then the performance measures for each scenario is estimated with a lot of error; the aggregate, by contrast, will be an average across many more replicates and thus give a good sense of *average* performance. The averaging, in effect, gives a lot more replications per aggregated performance measure.

For our cluster RCT, we might aggregate our bias across our sample sizes as

follows:

```
ssres <-
  sres %>%
  group_by( method, ICC, alpha, size_coef ) %>%
  summarise( bias = mean( bias ),
             n = n() )
```

We now have a single bias estimate for each combination of ICC, alpha, and size_coef; we have collapsed 9 scenarios into one overall scenario that generalizes bias across different sizes of experiment. We can then plot, using many small multiples:

```
ggplot( ssres, aes( ICC, bias, col=method ) ) +
  facet_grid( size_coef ~  alpha, labeller = label_both ) +
  geom_point( alpha=0.75 ) +
  geom_line( alpha=0.75 ) +
  geom_hline( yintercept = 0 ) +
  theme_minimal()
```
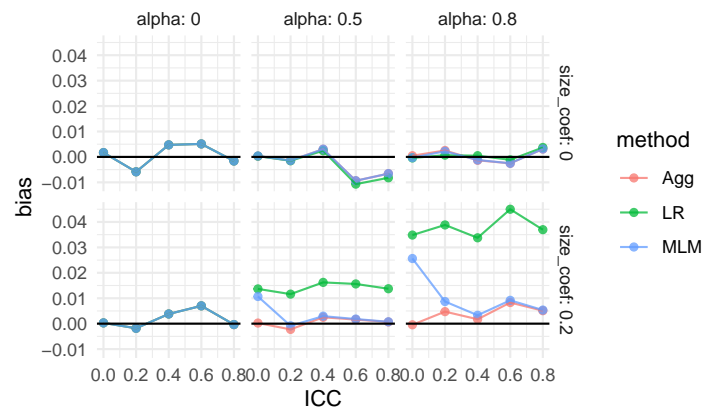

We see more clearly that greater variation in cluster size (alpha) leads to greater bias for the linear regression estimator, but only if the coefficient for size is nonzero (which makes sense given our theoretical understanding of the problem—if size is not related to treatment effect, it is hard to imagine how varying cluster sizes would cause much bias). We are looking at an interaction between our simulation factors: we only see bias for linear regression when cluster size relates to impact and there is variation in cluster size. As ICC increases, we are not seeing any major differences in the pattern of our results We also see that all the estimators have near zero bias when there is no variation in cluster size, with the overplotted lines on the top row of the figure.

If you have many levels of a factor, as we do with ICC, you can let ggplot aggregate directly by taking advantage of the smoothing options:

```r
ggplot( sres, aes( ICC, bias, col=method ) ) +
  facet_grid( alpha ~  size_coef, labeller = label_both ) +
  geom_point( alpha=0.10,
              position = position_dodge(width = 0.04) ) +
  geom_smooth( se=FALSE ) +
  geom_hline( yintercept = 0 ) +
  theme_minimal()
```
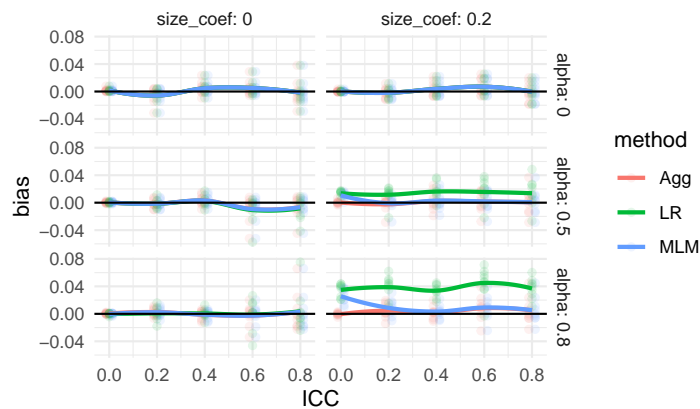

In the above, we let the original points show faintly as well, to give a sense of the variation across simulation trials.

13.3.0.1   A note on how to aggregate

Some performance measures are biased with respect to the Monte Carlo uncertainty. The estimated standard error, for example, is biased; the variance, by contrast, is not. The RMSE is biased, the MSE is not.

When aggregating, therefore, it is often best to aggregate the unbiased performance measures, and then calculate the biased ones from those. For example, to estimate aggregated standard error you might do the following:

```r
agg_perf <- sres %>%
  group_by( ICC, method, alpha, size_coef ) %>%
  summarise( SE = sqrt( mean( SE^2 ) ) )
```

Because bias is linear, you do not need to worry about the bias of the standard error. But if you are looking at the magnitude of bias ($|bias|$), then you can run into issues when the biases are close to zero, if they are measured noisily. In this case, looking at average bias, not average $|bias|$, is safer.

13.4 Assessing true SEs

We just did a deep dive into bias.
Uncertainty (standard errors) is another primary performance criterion of interest.

As an initial exploration, we plot the standard error estimates from our Cluster RCT simulation, using smoothed lines to visualize trends. We use `ggplot`'s `geom_smooth` to aggregate over `size_coef` and `alpha`, which we leave out of the plot. We include individual data points to visualize variation around the smoothed estimates:

```
ggplot( sres, aes( ICC, SE, col=method ) ) +
  facet_grid( n_bar ~  J, labeller = label_both ) +
  geom_jitter( height = 0, width = 0.05, alpha=0.5 ) +
  geom_smooth( se=FALSE, alpha=0.5 ) +
  theme_minimal()
```

```
## `geom_smooth()` using method
## = 'loess' and formula = 'y ~
## x'
```
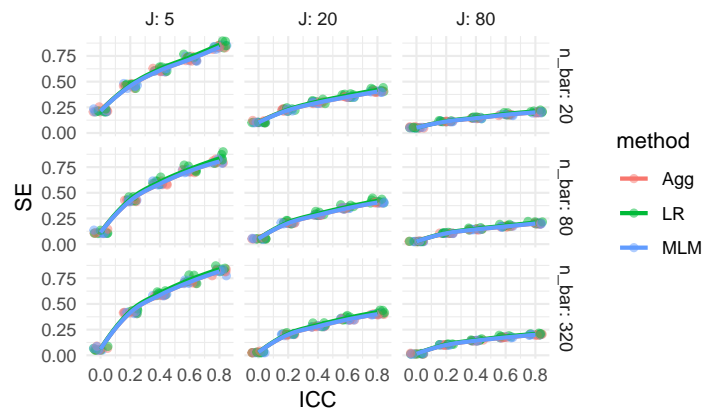

We observe several broad trends in the standard error behavior. First, standard error increases with the intraclass correlation (ICC). This is as expected: greater similarity within clusters reduces the effective sample size. Second, standard error decreases as the number of clusters (J) increases, which reflects the benefit of having more independent units of analysis. In contrast, increasing the cluster size (n_bar) has relatively little effect on the standard error (the rows of our facets look about the same). Lastly, all methods show fairly similar levels of standard error overall.

While we can extract all of these from the figure, the figure is still not ideal for *comparing* our methods. The dominant influence of design features like ICC and sample size obscures our ability to detect meaningful differences between methods. In other words, even though SE changes across scenarios, it's difficult

to tell which method is actually performing better within each scenario.

We can also view the same information using boxplots, effectively "bundling" over the left-out dimensions. We also put `n_bar` in our bundles because maybe it does not matter that much:

```
ggplot( sres, aes( ICC, SE, col=method, group=paste0( ICC, method ) ) ) +
  facet_grid( . ~  J, labeller = label_both ) +
  geom_boxplot( width = 0.2, coef = Inf) +
  scale_x_continuous( breaks = unique( sres$ICC)) +
  theme_minimal()
```
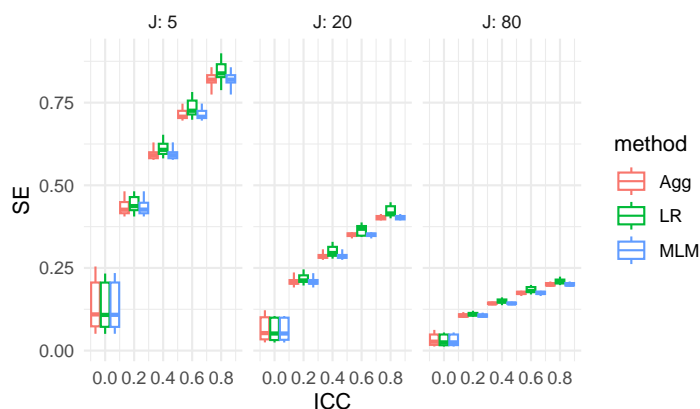

Our plots are still dominated by the strong effects of ICC and the number of clusters (J). When performance metrics like standard error vary systematically with design features, it becomes difficult to compare methods meaningfully across scenarios.

To address this, we shift our focus through standardization. Instead of noting that:

> "All my SEs are getting smaller,"

we want to conclude that:

> "Estimator 1 has systematically higher SEs than Estimator 2 across scenarios."

Simulation results are often driven by broad design effects, which can obscure the specific methodological questions we care about. Standardizing helps bring those comparisons to the forefront. Let's try that next.

#### 13.4.0.1   Standardizing to compare across simulation scenarios

One straightforward strategy for standardization is to compare each method's performance to a designated baseline. In this example, we use Linear Regression (LR) as our baseline.

We focus on the standard error (SE) of each method's estimate, rescaling it relative to LR. We do this by, for each simulation scenario, dividing each method's SE by the SE of LR, to produce `SE.scale`. This relative measure, SE.scale, allows us to examine how much better or worse each method performs in terms of precision under varying conditions.

```
ssres <-
  sres %>%
  group_by( n_bar, J, ATE, size_coef, ICC, alpha ) %>%
  mutate( SE.scale = SE / SE[method=="LR"]) %>%
  ungroup()
```

We can then treat it as a measure like any other. Here we bundle:

```
ggplot( ssres, aes( ICC, SE.scale, col=method,
                    group = interaction(ICC, method) ) ) +
  facet_grid( n_bar ~  J, labeller = label_both ) +
  geom_boxplot( position="dodge", width=0.1 ) +
  scale_y_continuous( labels = scales::percent_format() )
```
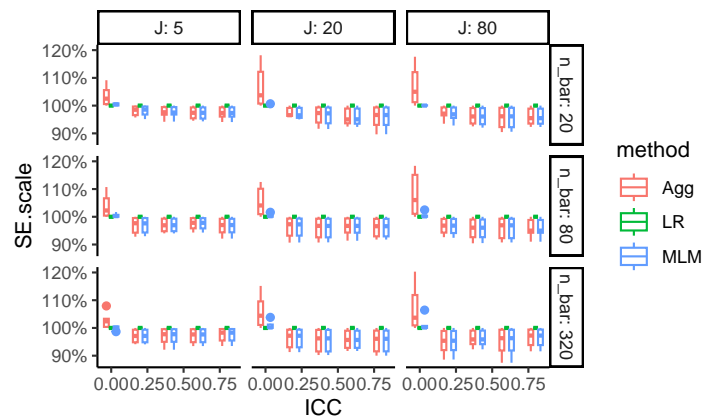

The figure above shows how each method compares to LR across simulation scenarios. We see that Aggregation performs worse than LR when the Intraclass Correlation Coefficient (ICC) is zero. However, when ICC is greater than zero, Aggregation yields improved precision. The Multilevel Model (MLM), in contrast, appears more adaptive. It captures the benefits of aggregation when ICC is high, but avoids the precision cost when ICC is zero. This adaptivity makes MLM appealing in practice when ICC is unknown or variable across contexts.

Although faceting by n_bar and J helps reveal potential interaction effects, it may be more effective to collapse across these variables for a cleaner summary. We are also not seeing how site size variation is impacting these results, and we might think that matters, especially for aggregation.

As a warning regarding Monte Carlo uncertainty: when standardizing results, it is important to remember that uncertainty in the baseline measure (here, LR)

propagates to the standardized values. This should be considered when inter-
preting variability in the scaled results. Uncertaintly for relative performance
is generally tricky to assess.

To clarify the main patterns, we average our SE.scale across simulation settings—
relative performance is on the same scale, so averaging is a natural thing to do.

```
s2 <-
  ssres %>%
  group_by( ICC, alpha, method ) %>%
  summarise( SE.scale = mean( SE.scale ) )

ggplot( s2, aes( ICC, SE.scale, col=method ) ) +
  facet_wrap( ~ alpha ) +
  geom_point() + geom_line() +
  scale_y_continuous( labels = scales::percent_format() ) +
  labs( title = "Average relative SE to Linear Regression",
        y = "Relative Standard Error" )
```
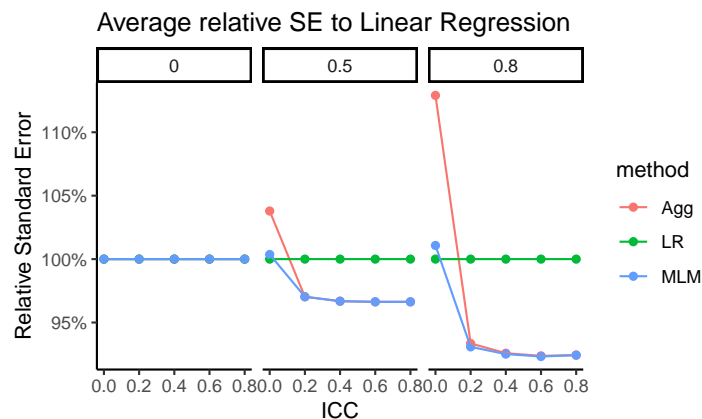

Our aggregated plot of precision of aggregation and MLM relative to Linear
Regression gives a simple story clearly told. The performance of aggregation
improves with ICC. MLM also has benefits over LR, and does not pay much
cost when ICC is low.

We can also visualize the variability in relative standard errors across simula-
tion scenarios using boxplots. This allows us to examine how consistent each
method's performance is under different ICC conditions.

```
ssres %>%
  filter( method != "LR" ) %>%
  ggplot( aes( ICC, SE.scale, col=method,
               group = interaction(ICC, method) ) ) +
  facet_wrap( ~ alpha, nrow=1) +
  geom_hline( yintercept = 1  ) +
```

```
geom_boxplot( position="dodge", width=0.1 ) +
scale_y_continuous( breaks=seq(90, 125, by=5 ) ) )
```
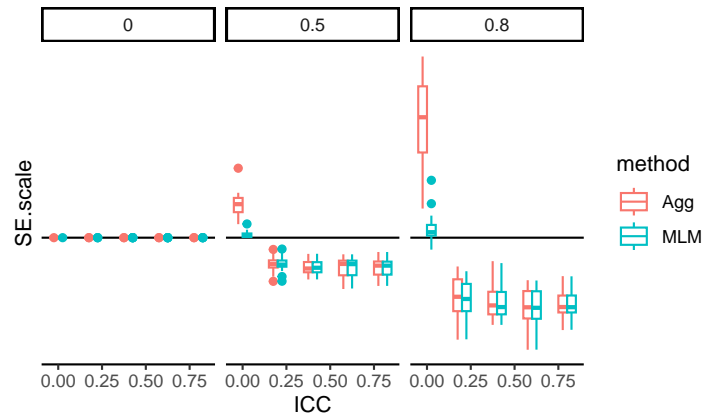

These boxplots show the full distribution of relative standard errors across all simulated scenarios, separated by ICC level. We exclude LR as it is the reference method.

The pattern is clear: when ICC = 0, Aggregation performs worse than LR, and MLM performs about the same. But as ICC increases, Aggregation and MLM both improve, and perform about the same to each other. This highlights the robustness of MLM across diverse conditions.

We might also explore how uncertainty changes with other factors. Here, we see whether cluster size meaningfully helps:

```
sres %>%
  filter( alpha == 0.8, size_coef == 0.2 ) %>%
ggplot( aes( n_bar, SE, col=factor(ICC), group=ICC ) ) +
  facet_grid( J ~ method, labeller = label_both, scales = "free") +
  geom_point() + geom_line()
```
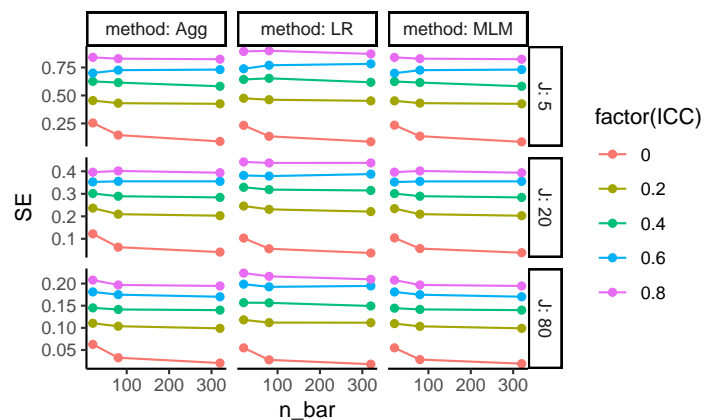
If the ICC is low, cluster size matters. Otherwise, the benefits are much more slim.

13.5   The Bias-SE-RMSE plot

We can also visualize bias and standard error together, along with RMSE, to get a fuller picture of performance. To illustrate, we subset to our biggest scenarios, in terms of sample size, and no ICC:

```r
bsr <- sres %>%
  filter( n_bar == 320, J==80, ICC == 0 )

bsr <- bsr %>%
  dplyr::select( -R, -power, -ESE_hat, -SD_SE_hat ) %>%
  pivot_longer( cols=c("bias","SE","RMSE"),
                names_to = "measure",
                values_to = "value" ) %>%
  group_by( measure, size_coef, method, ICC, alpha ) %>%
  summarise( value = mean( value ),
             n = n() )

bsr$measure = factor( bsr$measure, levels=c("bias", "SE", "RMSE"),
                       labels =c("|bias|", "SE", "RMSE" ) )

ggplot( bsr, aes( alpha, value, col=method )) +
  facet_grid( size_coef ~ measure ) +
  geom_line() + geom_point() +
  labs( y = "", x = "Site Variation" )  +
  geom_hline( yintercept = 0 ) +
  theme( legend.position="bottom",
         legend.direction="horizontal",
         legend.key.width=unit(1,"cm"),
         panel.border = element_blank() )
```
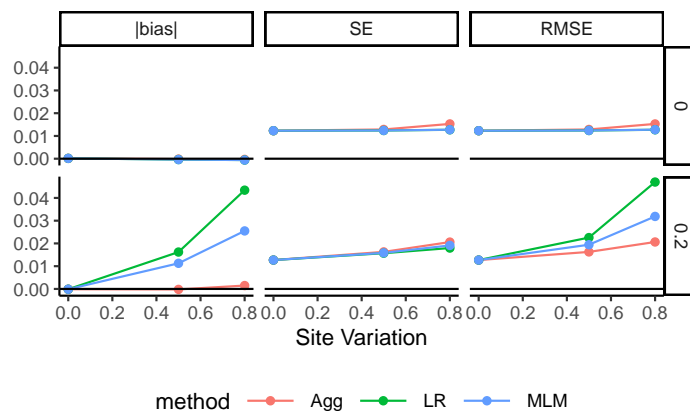
The combination of bias, standard error, and RMSE provides a rich and informative view of estimator performance.

As an illustration, in the above plot, we focus on a specific simulation scenario with n_bar = 320, J = 80, and ICC = 0. The top row represents settings where effect size is independent of cluster size, while the bottom row reflects a correlation between size and effect.

These types of visualizations directly illustrates the canonical relationship:

$$\text{RMSE}^2 = \text{Bias}^2 + \text{SE}^2$$

In the plot we get overall performance (RMSE) clearly decomposed into into its two fundamental components: systematic error (bias) and variability (standard error). Jere we see how bias for LR, for example, is dominant when site variation is high. The differences in SE are not driving differences in overall estimator performance, bias is.

Frankly, this is the kind of diagnostic plot I often wish were included in more applied simulation studies.

13.6 Assessing estimated SEs

So far we have examined the performance of our *point estimators*. We next look at ways to assess our *estimated* standard errors. A good first question is whether they are about the right size, on average, across all the scenarios.

Here it is very important to see if they are *reliably* the right size, so the bundling method is an especially important tool here. We first see if the average estimated SE, relative to the true SE, is usually around 1 across all scenarios:

```
sres <- sres %>%
  mutate( inflate = ESE_hat / SE  )
```

```r
ggplot( sres,
        aes( ICC, inflate, col=method,
             group = interaction(ICC,method) ) ) +
    facet_grid( . ~ J, labeller = label_both) +
  geom_boxplot( position="dodge" ) +
  geom_hline( yintercept=1 ) +
  labs( color="n" ) +
  scale_y_continuous( labels = scales::percent_format() )
```
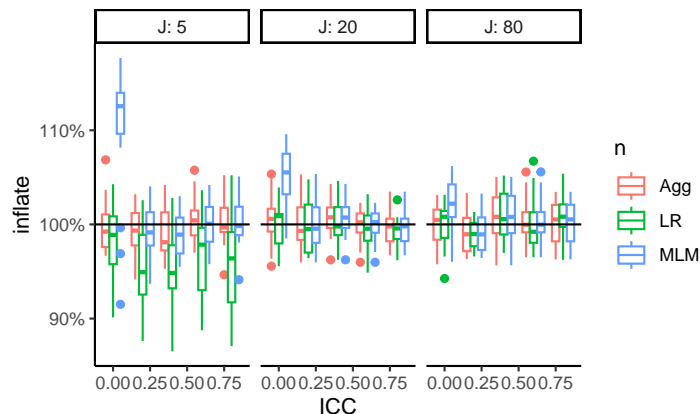

We see that our estimated SEs are about right, on average, across all scenarios. When ICC is 0 and J is small, the MLM SEs are a bit too high. When J is 5, the LR estimator can be a bit low under some circumstances. We can start exploring these trends to dig into why our are wide (suggesting that other factors dictate when the SEs are biased).

We can look at the $J = 80$ to see what MCSEs are like. The `simhelpers` `calc_relative_var()` method gives mcses for relative bias.

```r
se_res <- res %>%
  group_by( n_bar, J, ATE, size_coef, ICC, alpha, method ) %>%
  summarize( calc_relative_var( estimates = ATE_hat,
                     var_estimates = SE_hat^2,
                     criteria = "relative bias" ) )
se_res %>%
  filter( J == 80, n_bar == 80 ) %>%
  ggplot( aes( ICC, rel_bias_var, col=method ) ) +
  facet_grid( size_coef ~ alpha  ) +
  geom_hline( yintercept = 1 ) +
  geom_point( position = position_dodge( width=0.05) ) +
  geom_line( position = position_dodge( width=0.05) ) +
  geom_errorbar( aes( ymin = rel_bias_var - 1.96*rel_bias_var_mcse,
                      ymax = rel_bias_var + 1.96*rel_bias_var_mcse ),
                 position = position_dodge( width=0.05 ),
```

```
                        width = 0 )
```
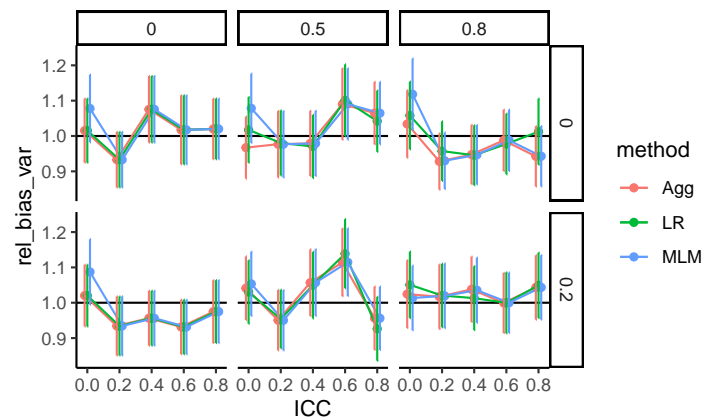

In looking at this plot, we see no real evidence of miscalibration. This makes us think the boxes in the prior plot are wide due to MCSE rather than other simulation factors driving some slight miscalibration in some scenarios when J is high. We might then assume this applies to the $J = 20$ case as well.

Finally, we can look at how stable the estimated SEs are, relative to the actual uncertainty. We calculate the standard deviation of the estimated standard errors and compare that to the standard deviation of the point estimate.

```r
sres <- mutate( sres,
                SD_SE_hat_rat = SD_SE_hat / SE )

ggplot( sres,
        aes( ICC, SD_SE_hat_rat, col=method,
             group = interaction(ICC,method) ) ) +
    facet_grid( . ~ J, labeller = label_both) +
  geom_boxplot( position="dodge" ) +
  labs( color="n" ) +
  scale_y_continuous( labels = scales::percent_format() )
```
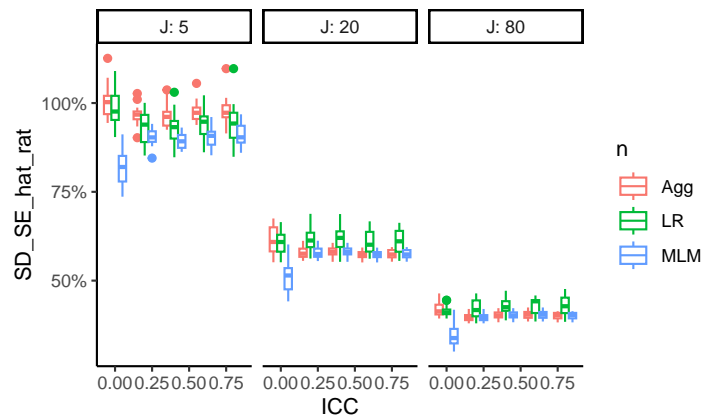
It looks like MLM has more reliably estimated SEs than other methods when ICC is small. Aggregation has more trouble estimating uncertainty when J is small. Finally, LR's SEs are generally more unstable, relative to its performance, when J is larger.

Assessing the stability of standard errors is usually very in the weeds of a performance evaluation. It is a tricky measure: if the true SE is high for a method, then the relative instability will be lower, even if the absolute instability is the same. Thinking through what might be driving what can be difficult, and is often not central to the main purpose of an evaluation.

People often look at confidence interval coverage and confidence interval width, instead, to assess the quality of estimated SEs.

13.7   Assessing confidence intervals

Coverage is a blend of how accurate our estimates are and how good our estimated SEs are. To assess coverage, we first calculate confidence intervals using the estimated effect, estimated standard error, and degrees of freedom. Once we have our calculated t-based intervals, we can average them across runs to get average width and coverage using `simhelpers`. A good confidence interval estimator would be one which is generally relatively short while maintaining proper coverage.

Our calculations are as so:

```
res$df = res$J
res <- mutate( res,
               tstar = qt( 0.975, df=df ),
               CI_low = ATE_hat - tstar*SE_hat,
               CI_high = ATE_hat + tstar*SE_hat,
               width = CI_high - CI_low )
```

```r
covres <- res %>%
  group_by( n_bar, J, ICC, alpha, size_coef, method, ATE ) %>%
  summarise( calc_coverage( lower_bound = CI_low,
                            upper_bound = CI_high,
                            true_param = ATE ) ) %>%
  ungroup()
```

We then look at those simulations with a relationship of site size and impact. We subset to `n_bar = 80`, `size_coef = 0.2` and `alpha = 0.5` to simplify for our initial plot:

```r
c_sub <- covres %>%
  dplyr::filter( size_coef != 0, n_bar == 80, alpha == 0.5 )

ggplot( c_sub, aes( ICC, coverage, col=method, group=method ) ) +
  facet_grid( . ~ J, labeller = label_both ) +
  geom_line() +
  geom_point() +
  geom_errorbar( aes( ymax = coverage + 2*coverage_mcse,
                      ymin = coverage - 2*coverage_mcse ), width=0 ) +
  geom_hline( yintercept = 0.95 )
```
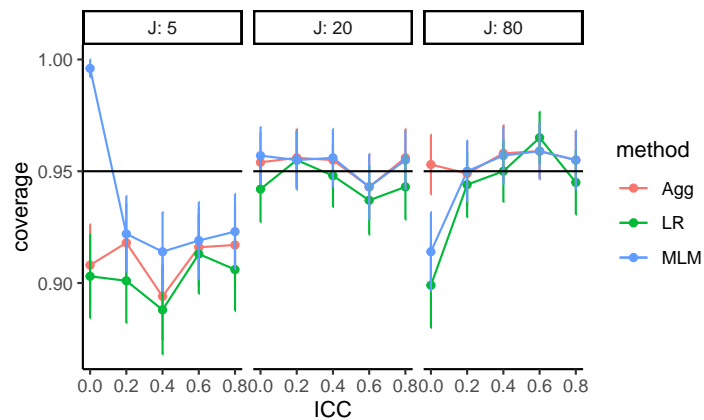

Generally coverage is good unless *J* is low or ICC is 0. Monte Carlo standard errors indicate that, in some settings, the observed coverage is reliably different from the nominal 95%, suggesting issues with estimator bias, standard error estimation, or both. We might want to see if these results are general across other settings (see exercises).

For confidence interval width, we can calculate the average width relative to the width of LR across all scenarios:

```r
covres <- covres %>%
  group_by( n_bar, J, ICC, alpha, size_coef ) %>%
```

```r
  mutate( width_rel = width / width[method=="LR"] ) %>%
  ungroup()

c_agg <- covres %>%
  group_by( ICC, J, alpha, method ) %>%
  summarise( coverage = mean( coverage ),
             coverage_mcse = sqrt( mean( coverage_mcse^2 ) ) / n(),
             width_rel = mean( width_rel ) ) %>%
  filter( method != "LR" )

ggplot( c_agg, aes( ICC, width_rel, col=method, group=method ) ) +
  facet_grid( J ~ alpha ) +
  geom_hline( yintercept = 1 ) +
  geom_line() + geom_point() +
  labs( y = "Relative CI Width",
        title = "Average Relative CI Width to Linear Regression" ) +
  scale_y_continuous( labels = scales::percent_format() )
```
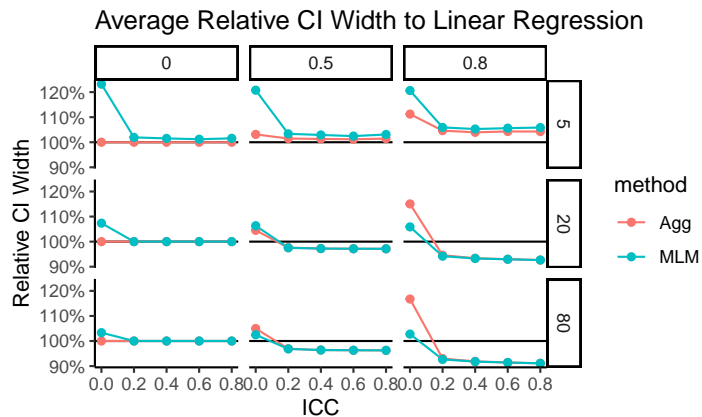

Confidence interval width serves as a proxy for precision. Narrow intervals suggest more precise estimates. We see MLM has wider intervals, relative to LR, when ICC is low. When there is site variation, both Agg and MLM have shorter intervals.

13.8   Exercises

13.8.1   Assessing uncertainty

Select a plot from this chapter that does not have monte carlo standard errors. Add monte carlo standard errors to that selected plot.

13.8.2 Assessing power

Make a plot showing how power changes as J changes. As an extra step, add MCSEs to the plot to assess whether you have a reasonable numbers of replications in the simulation.

13.8.3 Going deeper with coverage

For our cluster RCT, we saw coverage is low in some circumstances. Explore the full set of simulation results, possibly adding your own analyses, to ascertain why coverage is low. Is it due to estimator bias? Unreliably estimated standard errors? Something else? Make a final plot and short write-up that captures how coverage is vulnerable for the three estimators.

Chapter 14

Special Topics on Reporting Simulation Results

In this chapter we cover some special topics on reporting simulation results. We first walk through some examples of how to do regression modeling. We then dive more deeply into what to do when you have only a few iterations per scenario, and then we discuss what to do when you are evaluating methods that sometimes fail to converge or give an answer.

14.1 Using regression to analyze simulation results

In Chapter 12 we saw some examples of using regression and ANOVA to analyze simulation results. We next provide some further in-depth examples that give the code for doing this sort of thing.

14.1.1 Example 1: Biserial, revisited

We first give the code that produced the final ANOVA summary table for the biserial correlation example in Chapter 12. In the visualization there, we saw that several factors appeared to impact bias, but we might want to get a sense of how much. Under modeling of that same chapter, we saw a table that partialed out the variance across several factors so we could see which simulation factors mattered most for bias.

To build that table, we first fit a regression model to see:

```r
options(scipen = 5)
mod = lm( bias ~ fixed + rho + I(rho^2) + p1 + n, data = r_F)
summary(mod, digits=2)
```

```
##
## Call:
## lm(formula = bias ~ fixed + rho + I(rho^2) + p1 + n, data = r_F)
##
## Residuals:
##        Min          1Q      Median          3Q
## -0.0215935 -0.0013608   0.0003823   0.0015677
##        Max
##  0.0081802
##
## Coefficients:
##                      Estimate  Std. Error
## (Intercept)          0.00218473  0.00015107
## fixedSample cutoff  -0.00363520  0.00009733
## rho                 -0.00942338  0.00069578
## I(rho^2)             0.00720857  0.00070868
## p1.L                 0.00461700  0.00010882
## p1.Q                -0.00160546  0.00010882
## p1.C                 0.00081464  0.00010882
## p1^4                -0.00011190  0.00010882
## n.L                  0.00362949  0.00010882
## n.Q                 -0.00103981  0.00010882
## n.C                  0.00027941  0.00010882
## n^4                  0.00001976  0.00010882
##                     t value Pr(>|t|)
## (Intercept)          14.462  < 2e-16 ***
## fixedSample cutoff  -37.347  < 2e-16 ***
## rho                 -13.544  < 2e-16 ***
## I(rho^2)             10.172  < 2e-16 ***
## p1.L                 42.426  < 2e-16 ***
## p1.Q                -14.753  < 2e-16 ***
## p1.C                  7.486 8.41e-14 ***
## p1^4                 -1.028   0.3039
## n.L                  33.352  < 2e-16 ***
## n.Q                  -9.555  < 2e-16 ***
## n.C                   2.568   0.0103 *
## n^4                   0.182   0.8559
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.003372 on 4788 degrees of freedom
## Multiple R-squared:  0.5107, Adjusted R-squared:  0.5096
## F-statistic: 454.4 on 11 and 4788 DF,  p-value: < 2.2e-16
```

The above printout gives main effects for each factor, averaged across other

factors. Because `p1` and `n` are ordered factors, the `lm()` command automatically generates linear, quadradic, cubic and fourth order contrasts for them. We smooth our `rho` factor, which has many levels of a continuous measure, with a quadratic curve. We could instead use splines or some local linear regression if we were worried about model fit for a complex relationship.

The main effects are summaries of trends across contexts. For example, averaged across the other contexts, the "sample cutoff" condition is around 0.004 lower than the population (the baseline condition).

We can also use ANOVA to get a sense of the major sources of variation in the simulation results (e.g., identifying which factors have negligible/minor influence on the bias of an estimator). To do this, we use `aov()` to fit an analysis of variance model:

```
anova_table <- aov(bias ~ rho * p1 * fixed * n, data = r_F)
summary(anova_table)
```

```
##                  Df   Sum Sq  Mean Sq  F value
## rho               1 0.002444 0.002444  1673.25
## p1                4 0.023588 0.005897  4036.41
## fixed             1 0.015858 0.015858 10854.52
## n                 4 0.013760 0.003440  2354.60
## rho:p1            4 0.001722 0.000431   294.71
## rho:fixed         1 0.003440 0.003440  2354.69
## p1:fixed          4 0.001683 0.000421   287.98
## rho:n             4 0.002000 0.000500   342.31
## p1:n             16 0.019810 0.001238   847.51
## fixed:n           4 0.013359 0.003340  2285.97
## rho:p1:fixed      4 0.000473 0.000118    80.87
## rho:p1:n         16 0.001470 0.000092    62.91
## rho:fixed:n       4 0.002929 0.000732   501.23
## p1:fixed:n       16 0.001429 0.000089    61.12
## rho:p1:fixed:n   16 0.000429 0.000027    18.36
## Residuals      4700 0.006866 0.000001
##                  Pr(>F)
## rho              <2e-16 ***
## p1               <2e-16 ***
## fixed            <2e-16 ***
## n                <2e-16 ***
## rho:p1           <2e-16 ***
## rho:fixed        <2e-16 ***
## p1:fixed         <2e-16 ***
## rho:n            <2e-16 ***
## p1:n             <2e-16 ***
## fixed:n          <2e-16 ***
## rho:p1:fixed     <2e-16 ***
```

```
## rho:p1:n       <2e-16 ***
## rho:fixed:n    <2e-16 ***
## p1:fixed:n     <2e-16 ***
## rho:p1:fixed:n <2e-16 ***
## Residuals
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

The advantage here is the multiple levels of our categorical factors get bundled together in our table of results, making a tidier display.

The table in Chapter 12 is a summary of this anova table, which we generate as follows:

```
library(lsr)
etaSquared(anova_table) %>%
  as.data.frame() %>%
  rownames_to_column("source") %>%
  mutate( order = 1 + str_count(source, ":" ) ) %>%
  group_by( order ) %>%
  arrange( -eta.sq, .by_group = TRUE ) %>%
  relocate( order ) %>%
  knitr::kable( digits = 2 )
```

We group the results by the order of the interaction, so that we can see the main effects first, then two-way interactions, and so on. We then sort within each group to put the high importance factors first. The resulting variance decomposition table (see Chapter 12) shows which factors are explaining how much of the variation.

14.1.2 Example 2: Cluster RCT example, revisited

When we have several methods to compare, we can also use meta-regression to understand how these methods change as other simulation factors change. We next continue our running Cluster RCT example.

We first turn our simulation levels (except for ICC, which has several levels) into factors, so R does not assume that sample size, for example, should be treated as a continuous variable:

```
sres_f = sres %>%
  mutate( across( c( n_bar, J, size_coef, alpha ), factor ) )
sres_f$ICC = as.numeric( sres_f$ICC )

# Run the regression
M <- lm( bias ~ (n_bar + J + size_coef + ICC + alpha) * method,
         data = sres_f )
```

```
# View the results
stargazer::stargazer(M, type = "text",
                        single.row = TRUE )
```

```
##
## =================================================
##                         Dependent variable:
##                    -----------------------------
##                                 bias
## -------------------------------------------------
## n_bar80                    -0.003 (0.002)
## n_bar320                   -0.001 (0.002)
## J20                        -0.002 (0.002)
## J80                        -0.002 (0.002)
## size_coef0.2                0.003 (0.002)
## ICC                         0.001 (0.003)
## alpha0.5                   -0.002 (0.002)
## alpha0.8                    0.001 (0.002)
## methodLR                   -0.012*** (0.004)
## methodMLM                   0.001 (0.004)
## n_bar80:methodLR            0.0001 (0.003)
## n_bar320:methodLR          -0.00001 (0.003)
## n_bar80:methodMLM          -0.0005 (0.003)
## n_bar320:methodMLM         -0.001 (0.003)
## J20:methodLR                0.005* (0.003)
## J80:methodLR                0.006* (0.003)
## J20:methodMLM               0.001 (0.003)
## J80:methodMLM               0.001 (0.003)
## size_coef0.2:methodLR      0.016*** (0.002)
## size_coef0.2:methodMLM      0.003 (0.002)
## ICC:methodLR               -0.0003 (0.004)
## ICC:methodMLM              -0.006 (0.004)
## alpha0.5:methodLR           0.006** (0.003)
## alpha0.8:methodLR          0.017*** (0.003)
## alpha0.5:methodMLM          0.001 (0.003)
## alpha0.8:methodMLM          0.003 (0.003)
## Constant                    0.002 (0.003)
## -------------------------------------------------
## Observations                     810
## R2                               0.273
## Adjusted R2                      0.248
## Residual Std. Error        0.014 (df = 783)
## F Statistic            11.283*** (df = 26; 783)
## =================================================
## Note:                  *p<0.1; **p<0.05; ***p<0.01
```

We can quickly generate a lot of regression coefficients, making our meta-regression somewhat hard to interpret. The above model does not even have interactions of the simulation factors–which, given the found interactions from our plots, is a major concern! That said, picking out the significant coefficients is a quick way to obtain a lot of clues as to what is driving performance. E.g., several features interact with the LR method for bias. The other two methods seem less impacted.

14.1.2.1 Using LASSO to simplify the model

We can simplify our model using LASSO regression, to drop coefficients that are less relevant. This requires some work to make our model matrix of dummy variables with all the interactions.

```
library(modelr)
library(glmnet)
```

```
## Loaded glmnet 4.1-9
```

```
# Define formula with all three-way interactions
form <- bias ~ ( n_bar + J + size_coef + ICC + alpha) * method

# Create model matrix
X <- model.matrix(form, data = sres_f)[, -1]  # drop intercept

# Fit LASSO
fit <- cv.glmnet(X, sres_f$bias, alpha = 1)

# Coefficients
coef(fit, s = "lambda.1se") %>%
  as.matrix() %>%
  as.data.frame() %>%
  rownames_to_column("term") %>%
  filter(abs(s0) > 0) %>%
  knitr::kable(digits = 3)
```

term	s0
(Intercept)	0.001
size_coef0.2	0.002
alpha0.8	0.001
size_coef0.2:methodLR	0.008
alpha0.8:methodLR	0.007

When using regression, and especially LASSO, which levels are baseline can impact the final results. Here "Agg" is our baseline method, and so our coefficients are showing how other methods differ from the Agg method. If we selected LR as baseline, then we might suddenly see Agg and MLM as having large coefficients.

One trick is to give dummy variables for all the methods, and overload the `method` factor with the baseline method, so that it is always the first level.

```r
form <- bias ~ 0 + ( n_bar + J + size_coef + ICC + alpha) * method
sres_f$method <- factor(sres_f$method)
vars = c("n_bar", "J", "size_coef", "alpha", "method")
contr.identity <- function(x) {
  n = nlevels(x)
  m <- diag(n)
  rownames(m) <- colnames(m) <- levels(x)


  m
}
contr.identity(sres_f$n_bar)
```

```
##      20 80 320
## 20    1  0   0
## 80    0  1   0
## 320   0  0   1
```

```r
X <- model.matrix(~ 0 + ( n_bar + J + size_coef  + alpha) * method,
                  data = sres_f,
                  contrasts.arg = lapply(sres_f[,vars],
                                         \(x) contr.identity(x)))

colnames(X)
```

```
##  [1] "n_bar20"
##  [2] "n_bar80"
##  [3] "n_bar320"
##  [4] "J5"
##  [5] "J20"
##  [6] "J80"
##  [7] "size_coef0"
##  [8] "size_coef0.2"
##  [9] "alpha0"
## [10] "alpha0.5"
## [11] "alpha0.8"
## [12] "methodAgg"
## [13] "methodLR"
## [14] "methodMLM"
## [15] "n_bar20:methodAgg"
## [16] "n_bar80:methodAgg"
## [17] "n_bar320:methodAgg"
## [18] "n_bar20:methodLR"
## [19] "n_bar80:methodLR"
## [20] "n_bar320:methodLR"
```

```
## [21] "n_bar20:methodMLM"
## [22] "n_bar80:methodMLM"
## [23] "n_bar320:methodMLM"
## [24] "J5:methodAgg"
## [25] "J20:methodAgg"
## [26] "J80:methodAgg"
## [27] "J5:methodLR"
## [28] "J20:methodLR"
## [29] "J80:methodLR"
## [30] "J5:methodMLM"
## [31] "J20:methodMLM"
## [32] "J80:methodMLM"
## [33] "size_coef0:methodAgg"
## [34] "size_coef0.2:methodAgg"
## [35] "size_coef0:methodLR"
## [36] "size_coef0.2:methodLR"
## [37] "size_coef0:methodMLM"
## [38] "size_coef0.2:methodMLM"
## [39] "alpha0:methodAgg"
## [40] "alpha0.5:methodAgg"
## [41] "alpha0.8:methodAgg"
## [42] "alpha0:methodLR"
## [43] "alpha0.5:methodLR"
## [44] "alpha0.8:methodLR"
## [45] "alpha0:methodMLM"
## [46] "alpha0.5:methodMLM"
## [47] "alpha0.8:methodMLM"
```

Now do the LASSO on this colinear mess:

```r
fit <- cv.glmnet(X, sres_f$bias, alpha = 1)
coef(fit, s = "lambda.1se") %>%
  as.matrix() %>%
  as.data.frame() %>%
  rownames_to_column("term") %>%
  filter(abs(s0) > 0) %>%
  knitr::kable(digits = 3)
```

term	s0
(Intercept)	0.003
size_coef0	-0.002
size_coef0.2	0.000
alpha0.8	0.001
size_coef0.2:methodLR	0.008
alpha0.8:methodLR	0.007

We can also extend to allow for pairwise interactions of simulation factors:

```
form2 <- bias ~ ( n_bar + J + size_coef + ICC + alpha)^2 * method
```

Interestingly, we get basically the same result:

term	s0
(Intercept)	0.002
size_coef0.2:alpha0.8	0.002
size_coef0.2:methodLR	0.002
size_coef0.2:alpha0.8:methodLR	0.021

14.1.2.2 Fitting models to each method

We know each method responds differently to the simulation factors, so we could fit three models, one for each method, and compare them.

```
meth = c( "LR", "MLM", "Agg" )
models <- map( meth, function(m) {
  M <- lm( bias ~ (n_bar + J + size_coef + ICC + alpha)^2,
      data = sres_f %>% filter( method == m ) )
  tidy( M )
} )
models <- models %>% set_names(meth) %>%
  bind_rows( .id = "model" )

m_res <- models %>%
  dplyr::select( model, term, estimate ) %>%
  pivot_wider( names_from="model", values_from="estimate" )

m_res %>%
  knitr::kable( digits = 2 )
```

term	LR	MLM	Agg
(Intercept)	0.01	0.00	0.01
n_bar80	-0.01	-0.01	-0.01
n_bar320	0.00	0.00	0.00
J20	-0.01	0.00	-0.01
J80	-0.01	0.00	0.00
size_coef0.2	0.00	0.01	0.00
ICC	0.01	0.02	0.01
alpha0.5	-0.01	-0.01	-0.01
alpha0.8	-0.01	0.00	0.00
n_bar80:J20	0.01	0.01	0.01
n_bar320:J20	0.00	0.00	0.00
n_bar80:J80	0.01	0.01	0.01
n_bar320:J80	0.00	0.00	0.00
n_bar80:size_coef0.2	0.00	0.00	0.00
n_bar320:size_coef0.2	0.00	0.00	0.00
n_bar80:ICC	0.00	0.00	0.00
n_bar320:ICC	-0.01	0.00	-0.01
n_bar80:alpha0.5	0.00	0.00	0.00
n_bar320:alpha0.5	0.00	0.00	0.01
n_bar80:alpha0.8	0.00	0.00	0.00
n_bar320:alpha0.8	0.00	0.00	0.00
J20:size_coef0.2	0.00	0.00	0.00
J80:size_coef0.2	0.00	0.00	-0.01
J20:ICC	-0.01	-0.02	-0.01
J80:ICC	0.00	-0.01	0.00
J20:alpha0.5	0.01	0.01	0.01
J80:alpha0.5	0.01	0.01	0.01
J20:alpha0.8	0.02	0.01	0.01
J80:alpha0.8	0.01	0.00	0.00
size_coef0.2:ICC	0.01	-0.01	0.01
size_coef0.2:alpha0.5	0.02	0.00	0.00
size_coef0.2:alpha0.8	0.04	0.01	0.00
ICC:alpha0.5	-0.01	-0.01	-0.01
ICC:alpha0.8	0.00	-0.01	0.00

Of course, this is a hard to read table. We could instead plot, or use LASSO to simplify.

```
m_resL <- m_res %>%
  pivot_longer( -term,
                names_to = "model", values_to = "estimate" ) %>%
  mutate( term = factor(term, levels = unique(term)) ) %>%
  mutate( has_nbar = str_detect(term, "n_bar" ),
          has_J = str_detect(term, "J"),
```

```
        has_size_coef = str_detect(term, "size_coef"),
        has_ICC = str_detect(term, "ICC"),
        has_alpha = str_detect(term, "alpha") )

ggplot( m_resL,
        aes( x = term, y = estimate,
             fill = model, group = model ) ) +
  facet_wrap( ~ has_nbar, scales="free_y" ) +
  geom_bar( stat = "identity", position = "dodge" ) +
  coord_flip()
```
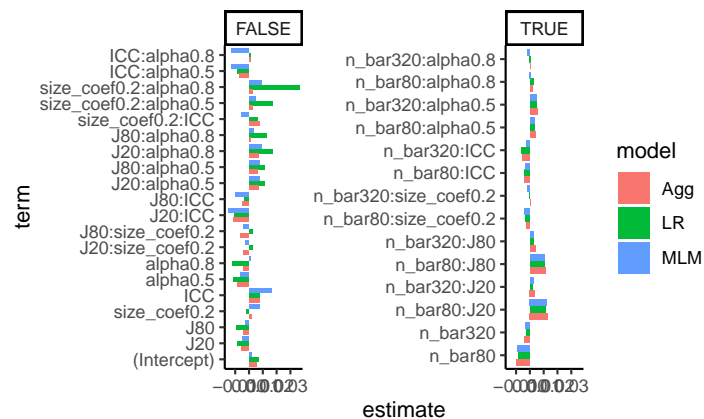

Here we see how LR stands out, but also how MLM stands out under different simulation factor combinations. Staring at this provides some understanding of how the methods are similar, and dissimilar.

For another example we turn to the standard error. Here we regress $log(SE)$ onto the coefficients, and we rescale ICC to be on a 5 point scale to control it's relative coeffceint size to the dummy variables. We regress $log(SE)$ and then exponentiate the coefficients to get the relative change in SE. We can then interpret an exponentiated coefficient of, 0.64 for MLM for `n_bar80` as a 36% reduction of the standard error when we increase n_bar from the baseline of 20 to 80.

Here we make a plot like above, but with these relative changes:
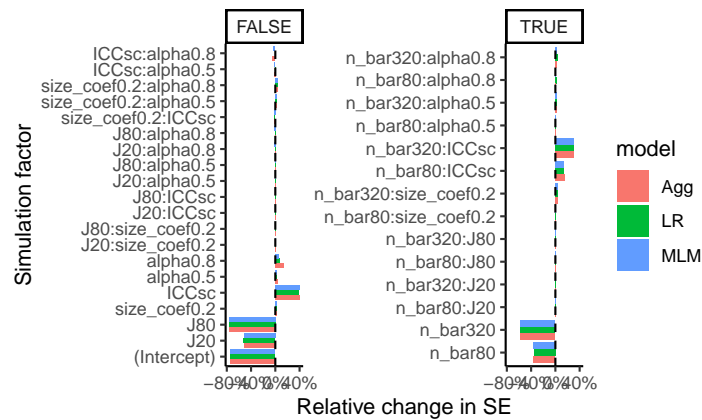
This clearly shows that the methods are basically the same in terms of uncertainty estimation. We also see some interesting trends, such as the impact of `n_bar` declines when ICC is higher (see the interaction terms at rigth of plot).

## 14.2 Using regression trees to find important factors

Sometimes with more complex experiments, where the various factors are interacting with each other in strange ways, it can be a bit tricky to decipher what is running what. Another tool one might use to explore is to fit a regression tree on the simulation results.

```
source( here::here( "code/create_analysis_tree.R" ) )
```

```
## Loading required package: rpart
```

```
set.seed(4344443)
create_analysis_tree( sres_f,
                      outcome = "bias",
                      predictor_vars = c("method", "n_bar", "J",
                                         "size_coef", "ICC", "alpha"),
                      tree_title = "Cluster RCT Bias Analysis Tree" )
```

Cluster RCT Bias Analysis Tree
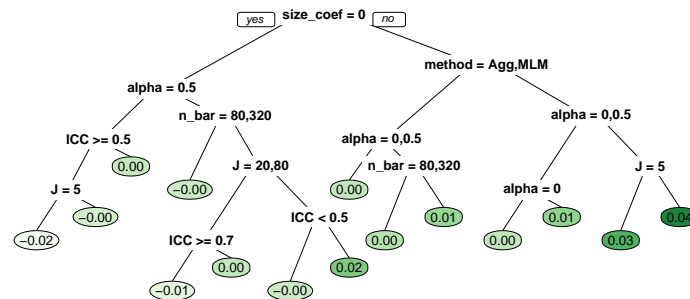
We will not walk through the tree code, but you can review it here. This function is a wrapper of the `rpart` package.

The default pruning is based on a cross-fitting evaluation, and our sample size is not too terribly high (just the number of simulation scenarios fit). Rerunning the code with a different seed can give a different tree. In general, it might be worth forcibly simplifying the tree. Trees are built greedily, so forcibly trimming often gives you the big things. For example:

```
create_analysis_tree( sres_f,
                      outcome = "bias",
                      predictor_vars = c("method", "n_bar", "J",
                                         "size_coef", "ICC", "alpha"),
                      tree_title = "Smaller Cluster RCT Bias Analysis Tree" )
```

Smaller Cluster RCT Bias Analysis Tree
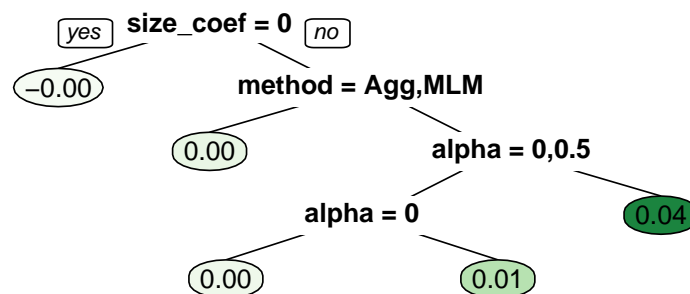
A very straightforward story: if `size_coef` is not 0, we are using LR, and alpha is large, then we have large bias.

We can also zero in on specific methods to understand how they engage with the simulation factors, like so:

```
create_analysis_tree( filter( sres_f, method=="LR" ),
                      outcome = "bias",
                      min_leaves = 4,
                      predictor_vars = c("n_bar", "J",
                                        "size_coef", "ICC", "alpha"),
                      tree_title = "Drivers of Bias for LR method" )
```

Drivers of Bias for LR method
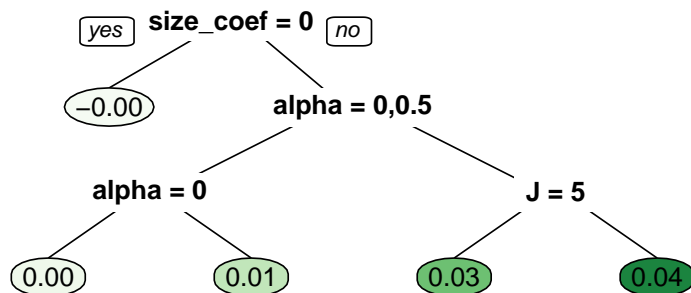
We force more leaves to get at some more nuance. We again immediately see, for the LR method, that bias is large when we have non-zero size coefficient *and* large alpha value. Then, when *J* is small, bias is even larger.

Generally we would not use a tree like this for a final reporting of results, but they can be important tools for *understanding* your results, which leads to how to make and select more conventional figures for final reporting.

14.3   Analyzing results with few iterations per scenario

When your simulation iterations are expensive to run (i.e., when each model fitting takes several minutes), then running thousands of iterations for many scenarios may no longer be computationally feasible. In this case you will have very noisy estimates of estimator performance.

For a given scenario, if the methods being evaluated are substantially different, then even with a few iterations you may be able to demonstrate what you need to, but in general the Monte Carlo Standard Errors (MCSEs) may be so large that you will have a hard time telling if something is going on, or if it is just noise in the simulation itself.

One tool to handle this is aggregation: if you use visualization methods that average across scenarios, those averages will have more precise estimates of (average) performance. Do not, by contrast, trust the bundling approaches–the MCSEs will make your boxes wider, and give the impression that there is more

variation across scenarios than there really is.

Regression approaches can be particularly useful: the regressions will effectively average performance across scenario, and give summaries of overall trends. You can even fit random effects regression, specifically accounting for the noise in the scenario-specific performance measures. For more on this approach see Gilbert and Miratrix (2024).

14.3.1 Example: ClusterRCT with only 100 replicates per scenario

In the prior chapter we analyzed the results of our cluster RCT simulation with 1000 replicates per scenario. But say we only had 100 per scenario. Using the prior chapter as a guide, we recreate some of the plots to show how MCSE can distort the picture of what is going on.

First, we look at our single plot of the raw results. Before we plot, however, we calculate MCSEs and add them to the plot as error bars.

```
sres_sub <- sres %>%
  filter( n_bar == 320, J == 20 ) %>%
  mutate( bias.mcse = SE / sqrt( R ) )
ggplot( sres_sub, aes( as.factor(alpha), bias,
                       col=method, pch=method, group=method ) ) +
  facet_grid( size_coef ~ ICC, labeller = label_both ) +
  geom_point() +
  geom_errorbar( aes( ymin = bias - 2*bias.mcse,
                      ymax = bias + 2*bias.mcse ),
                 width = 0 ) +
  geom_line() +
  geom_hline( yintercept = 0 ) +
  theme_minimal()
```
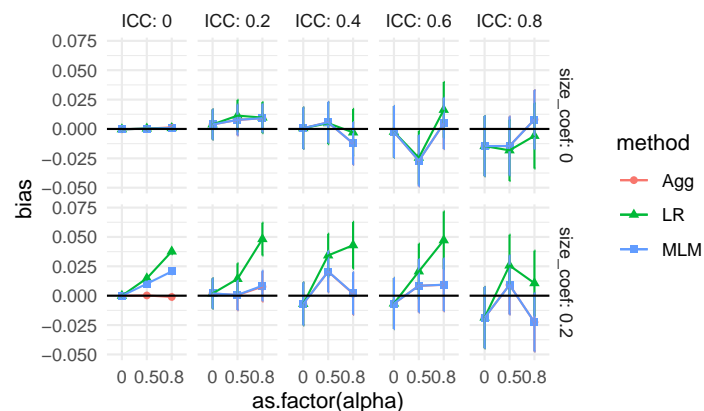

Aggregation should smooth out some of our uncertainty. When we aggregate

across 9 scenarios, our number of replicates goes from 100 to 900; our MCSEs should be about a third the size. Here is our aggregated bias plot:

```r
sres_sub2 <- sres %>%
  mutate( bias.mcse = SE / sqrt( R ) ) %>%
  group_by( n_bar, J ) %>%
  summarise( bias = mean( bias ),
             bias.mcse = sqrt( mean( bias.mcse^2 )) / sqrt(n()),
             .groups = "drop" )

ggplot( sres_sub, aes( as.factor(alpha), bias,
                       col=method, pch=method, group=method ) ) +
  facet_grid( size_coef ~ ICC, labeller = label_both ) +
  geom_point() +
  geom_errorbar( aes( ymin = bias - 2*bias.mcse,
                      ymax = bias + 2*bias.mcse ),
                 width = 0 ) +
  geom_line() +
  geom_hline( yintercept = 0 ) +
  theme_minimal()
```
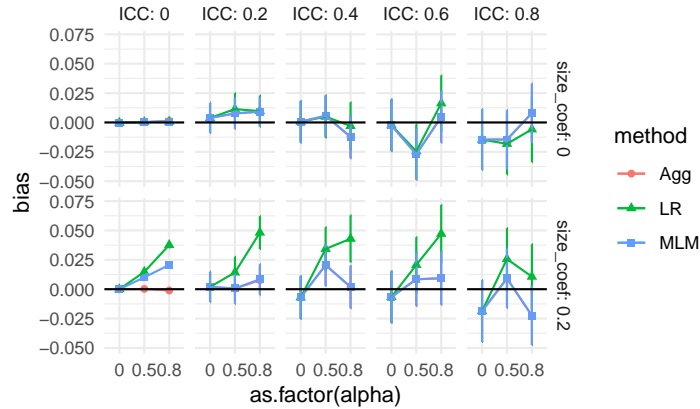

To get aggregate MCSE, we aggregate our scenario-specific MCSEs as follows:

$$MCSE_{agg} = \sqrt{\frac{1}{K^2} \sum_{k=1}^{K} MCSE_k^2}$$

where $MCSE_i$ is the Monte Carlo Standard Error for scenario i, and k is the number of scenarios. Assuming a collection of estimates are independent, the overall SE^2 of the average is the average SE^2 divided by K.

Even with the additional replicates per point, we see noticable noise in our plot. Note how our three methods track each other up and down in the zero-bias scenarios, giving a sense of a shared bias in some cases. This is because all

methods are analyzing the same set of datasets; they have shared uncertainty. This uncertainty can be deceptive. It can also be a boon: if we are explicitly comparing the performance of one method vs another, the shared uncertainty can be subtracted out, similar to having a blocked experiment Gilbert and Miratrix (2024).

Here we fit a multilevel model to the data.

```r
library(lme4)
sub_res = filter( res, runID <= 100 ) %>%
  mutate( error = ATE_hat - ATE,
          simID = paste0( n_bar, "_", J, "_", size_coef, "_", ICC, "_", alpha ),
          J = as.factor(J),
          n_bar = as.factor(n_bar),
          alpha = as.factor(alpha),
          size_coef = as.factor(size_coef) )

M <- lmer( error ~ method*(J + n_bar + ICC + alpha + size_coef) + (1|runID) + (1|simID),
           data = sub_res )
arm::display(M)
```

```
## lmer(formula = error ~ method * (J + n_bar + ICC + alpha + size_coef) +
##     (1 | runID) + (1 | simID), data = sub_res)
##                      coef.est coef.se
## (Intercept)          -0.09     0.05
## methodLR             -0.02     0.05
## methodMLM             0.00     0.05
## J20                   0.05     0.04
## J80                   0.04     0.04
## n_bar80               0.06     0.04
## n_bar320              0.04     0.04
## ICC                  -0.03     0.06
## alpha0.5             -0.01     0.04
## alpha0.8              0.04     0.04
## size_coef0.2          0.04     0.03
## methodLR:J20          0.01     0.04
## methodMLM:J20         0.00     0.04
## methodLR:J80          0.02     0.04
## methodMLM:J80         0.00     0.04
## methodLR:n_bar80      0.01     0.04
## methodMLM:n_bar80     0.00     0.04
## methodLR:n_bar320     0.00     0.04
## methodMLM:n_bar320    0.00     0.04
## methodLR:ICC         -0.01     0.06
## methodMLM:ICC        -0.01     0.06
## methodLR:alpha0.5     0.00     0.04
## methodMLM:alpha0.5    0.00     0.04
```

```
## methodLR:alpha0.8       0.01      0.04
## methodMLM:alpha0.8      0.00      0.04
## methodLR:size_coef0.2   0.01      0.03
## methodMLM:size_coef0.2  0.00      0.03
##
## Error terms:
##  Groups    Name         Std.Dev.
##  simID     (Intercept) 0.19
##  runID     (Intercept) 0.02
##  Residual              0.33
## ---
## number of obs: 2430, groups: simID, 270; runID, 3
## AIC = 2046.9, DIC = 1712.4
## deviance = 1849.6
```

We can look at the random effects:

```
ranef_vars <- as.data.frame(VarCorr(M)) %>%
  dplyr::select(grp = grp, sd = vcov) %>%
  mutate( sd = sqrt(sd),
          ICC = sd^2 / sum(sd^2 ) )


knitr::kable(ranef_vars, digits = 2)
```

grp	sd	ICC
simID	0.19	0.24
runID	0.02	0.00
Residual	0.33	0.75

The above model is a multilevel model that allows us to estimate how bias varies with method and simulation factor, while accounting for the uncertainty in the simulation. The random variation for `simID` captures unexplained variation due to the interactions of the simulation factors. We see a large value, indicating that many interactions are present, and our main effects are not fully capturing all trends.

14.4   What to do with warnings in simulations

Sometimes our analytic strategy might give some sort of warning (or fail altogether). For example, from the cluster randomized experiment case study we have:

```
set.seed(101012)  # (I picked this to show a warning.)
dat <- gen_cluster_RCT( J = 50, n_bar = 100, sigma2_u = 0 )
mod <- lmer( Yobs ~ 1 + Z + (1|sid), data=dat )


## boundary (singular) fit: see help('isSingular')
```

We have to make a deliberate decision as to what to do about this:

- Keep these "weird" trials?
- Drop them?

Generally, when a method fails or gives a warning is something to investigate in its own right. Ideally, failure would not be too common, meaning we could drop those trials, or keep them, without really impacting our overall results. But one should at least know what one is ignoring.

If you decide to drop them, you should drop the entire simulation iteration including the other estimators, even if they worked fine! If there is something particularly unusual about the dataset, then dropping for one estimator, and keeping for the others that maybe didn't give a warning, but did struggle to estimate the estimand, would be unfair: in the final performance measures the estimators that did not give a warning could be being held to a higher standard, making the comparisons between estimators biased.

If your estimators generate warnings, you should calculate the rate of errors or warning messages as a performance measure. Especially if you drop some trials, it is important to see how often things are acting peculuarly.

As discussed earlier, the main tool for doing this is the `quietly()` function:

```
quiet_lmer = quietly( lmer )
qmod <- quiet_lmer( Yobs ~ 1 + Z + (1|sid), data=dat )
qmod
```

```
## $result
## Linear mixed model fit by REML ['lmerModLmerTest']
## Formula: ..1
##    Data: ..2
## REML criterion at convergence: 14026.44
## Random effects:
##  Groups   Name        Std.Dev.
##  sid      (Intercept) 0.0000
##  Residual             0.9828
## Number of obs: 5000, groups:  sid, 50
## Fixed Effects:
## (Intercept)            Z
##    -0.013930     -0.008804
## optimizer (nloptwrap) convergence code: 0 (OK) ; 0 optimizer warnings; 1 lme4 warnings
##
## $output
## [1] ""
##
## $warnings
## character(0)
##
```

```
## $messages
## [1] "boundary (singular) fit: see help('isSingular')\n"
```

You then might have, in your analyzing code:

```r
analyze_data <- function( dat ) {

    M1 <- quiet_lmer( Yobs ~ 1 + Z + (1|sid), data=dat )
    message1 = ifelse( length( M1$message ) > 0, 1, 0 )
    warning1 = ifelse( length( M1$warning ) > 0, 1, 0 )

    # Compile our results
    tibble( ATE_hat = coef(M1)["Z"],
            SE_hat = se.coef(M1)["Z"],
            message = message1,
            warning = warning1 )
}
```

Now you have your primary estimates, and also flags for whether there was a convergence issue. In the analysis section you can then evaluate what proportion of the time there was a warning or message, and then do subset analyses to those simulation trials where there was no such warning.

For example, in our cluster RCT running example, we know that ICC is an important driver of when these convergence issues might occur, so we can explore how often we get a convergence message by ICC level:

```r
res %>%
  group_by( method, ICC ) %>%
  summarise( message = mean( message ) ) %>%
  pivot_wider( names_from = "method", values_from="message" )
```

```
## Warning: There were 15 warnings in
## `summarise()`.
## The first warning was:
## i In argument: `message =
##   mean(message)`.
## i In group 1: `method =
##   "Agg"` `ICC = 0`.
## Caused by warning in `mean.default()`:
## ! argument is not numeric or logical: returning NA
## i Run
##   `dplyr::last_dplyr_warnings()`
##   to see the 14 remaining
##   warnings.
```

```
## # A tibble: 5 x 4
##     ICC   Agg    LR   MLM
##   <dbl> <dbl> <dbl> <dbl>
```

```
## 1   0       NA    NA    NA
## 2   0.2     NA    NA    NA
## 3   0.4     NA    NA    NA
## 4   0.6     NA    NA    NA
## 5   0.8     NA    NA    NA
```

We see that when the ICC is 0 we get a lot of convergence issues, but as soon as we pull away from 0 it drops off considerably. At this point we might decide to drop those runs with a message or keep them. In this case, we decide to keep. It should not matter much, except possibly when ICC = 0, and we know the convergence issues are driven by trying to estimate a 0 variance, and thus is in some sense expected. Furthermore, we know people using these methods would likely ignore these messages, and thus we are faithfully capturing how these methods would be used in practice. We might eventually, however, want to do a separate analysis of the ICC = 0 context to see if the MLM approach is actually falling apart, or if it is just throwing warnings.

Chapter 15

Case study: Comparing different estimators

In a previous exercise (See Exercise 11.5.1), you wrote a simulation to compare the mean, median, and trimmed mean for estimating the same thing. This exercise is analogous to what we often are doing in a paper: pretend we have "invented" the trimmed mean and want to demonstrate its utility.

In this chapter, we walk through a deeper analysis of the results from such a simulation. In this simulation we have three factors: sample size, a degrees of freedom to control the thickness of the tails (thicker tails means higher chance of outliers), and a degree of skew (how much the tails tend to the right vs. the left). For our data-generation function we use a scaled skew t-distribution so the standard deviation will always be 1 and the mean will always be 0 while we change the fatness of the tails. See the attached code file for the simulation. Our final multi-factor simulation results look like this (we ran 1000 trials per scenario):

```
results = read_rds( here::here( "results/skewed_t_simulation.rds" ) )
results
```

```
## # A tibble: 144 x 8
##          n   df0  skew      seed estimator   RMSE
##      <dbl> <dbl> <dbl>     <dbl> <chr>       <dbl>
## 1      10     3     0  42242459 mean        0.323
## 2      10     3     0  42242459 median      0.246
## 3      10     3     0  42242459 trim.mean   0.246
## 4      10     3    10  42242476 mean        0.333
## 5      10     3    10  42242476 median      0.303
## 6      10     3    10  42242476 trim.mean   0.246
## 7      10     5     0  42242493 mean        0.320
```

```
##  8    10    5     0 42242493 median    0.304
##  9    10    5     0 42242493 trim.mean 0.290
## 10    10    5    10 42242510 mean      0.327
## # i 134 more rows
## # i 2 more variables: bias <dbl>, SE <dbl>
```

Our first question is how sample size impacts our different estimators' precision. We plot:

```
ns = unique( results$n )
ggplot( results, aes(x=n, y=SE, col=estimator) ) +
        facet_grid( skew ~ df0 ) +
        geom_line() + geom_point() +
        scale_x_log10( breaks=ns )
```
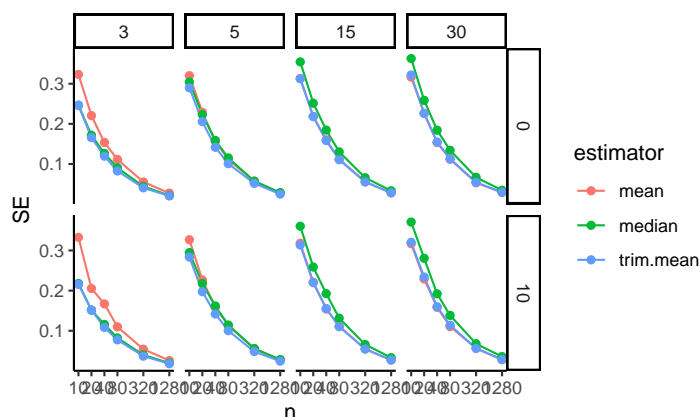

The above doesn't show differences clearly because all the SEs goes to zero as n increases. One move when we see heavy trends like this is to log our outcome, or otherwise rescale. The logging version shows differences are relatively constant given changing sample size.

```
ggplot( results, aes(x=n, y=SE, col=estimator) ) +
  facet_grid( skew ~ df0 ) +
  geom_line() + geom_point() +
  scale_x_log10( breaks=ns ) +
  scale_y_log10()
```
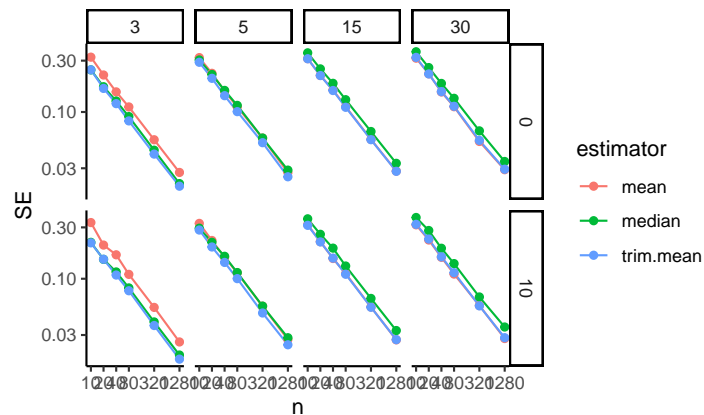
One step better would be to rescale using our knowledge of standard errors. If we scale by the square root of sample size, we should get horizontal lines. We now clearly see the trends.

```
results <- mutate( results, scaleSE = SE * sqrt(n) )
```

```
ggplot( results, aes(x=n, y=scaleSE, col=estimator) ) +
  facet_grid( skew ~ df0 ) +
    geom_line() + geom_point() +
    scale_x_log10( breaks=ns )
```
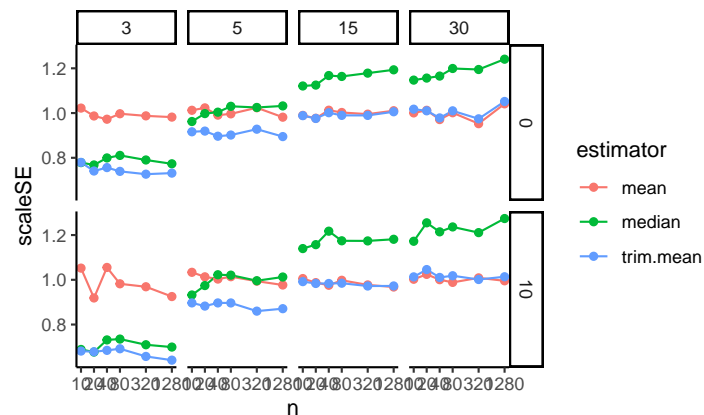

Overall, the scaled error of the mean is stable across the different distributions. The trimmed mean is a real advantage when the degrees of freedom are small (note the blue line is far below the red line on the left hand plot): we are cropping outliers that destabilize our estimate which leads to great wins. As the distribution grows more normal (i.e., as the degrees of freedom increases), this is no longer an advantage and the trimmed mean gets closer to the mean in terms of performance. We might think we should be penalized slightly by having dropped 10% of our data, making the standard errors slightly larger: if this is the case, then it is not large as the MCSE swamps it (the red and blue

line are basically overlapping).

The median is not able to take advantage of the nuances of the individual observations in the data because it is entirely determined by the middle value. When outliers cause real concern, this cost is minimal. When outliers are not a concern, the median is just worse.

Overall, we see for precision, the trimmed mean seems an excellent choice: in the presence of outliers it is far more stable than the mean, and when there are no outliers the cost of using it is small.

In terms of thinking about designing simulation studies, we see clear visual displays of simulation results can tell very clear stories. Eschew complicated tables with lots of numbers.

15.1 Bias-variance tradeoffs

We just looked at the precision of our three estimators, but we do not take into account bias. In our data generating processes, our median is not the same as the mean. As a diagnostic we can generate large datasets for each value of our simulation parameters, and compare the mean and median:

```r
source( "case_study_code/trimmed_mean_simulation.R" )
```

```
## Loading required package: stats4
```

```
##
## Attaching package: 'sn'
```

```
## The following object is masked from 'package:psych':
##
##      tr
```

```
## The following object is masked from 'package:lubridate':
##
##      dst
```

```
## The following object is masked from 'package:stats':
##
##      sd
```

```r
vals = expand.grid( df0 = unique( results$df0 ),
                    skew = unique( results$skew ) )
vals$n = 1000000
res <- pmap_df( vals, \(n,df0,skew) {
  d <- gen.data(n,df0,skew)
  tibble( df0=df0, skew=skew,
          mean = mean(d),
          median = median(d),
          sd = sd(d) )
```

```
  } )
knitr::kable( res, digits=2 )
```

df0	skew	mean	median	sd
3	0	0	0.00	1.00
5	0	0	0.00	1.00
15	0	0	0.00	1.00
30	0	0	0.00	1.00
3	10	0	-0.25	1.07
5	10	0	-0.25	1.00
15	10	0	-0.21	1.00
30	10	0	-0.20	1.00

Our trimmed estimator now has a cost: trimming could cause bias. The more extreme trimmed estimator, the median, would in fact be systematically off by a lot under the skewed scenarios.

Our trimming, etc., is *biased* if we think of our goal as estimating the mean: we tend to cut extreme right tail values, but there are no extreme left tail values to cut. But if the trimmed estimators are much more stable, we might still wish to use them.

Before we just looked at the SE. But we actually want to know the standard error, bias, and overall error (RMSE). Can we plot all these on a single plot? Yes we can! To plot, we first gather our outcomes to make a long form dataframe of results:

```
res2 = pivot_longer( results, cols = c( RMSE, bias, SE ),
                        names_to="Measure",
                        values_to="value" )
res2 = mutate( res2,
                Measure = factor( Measure, levels=c("bias", "SE","RMSE" )))
```

And then we plot, making a facet for each outcome of interest. We need to bundle because we have a lot of factors (one now being measure). We first look at boxplots:

```
ns = unique( res2$n )
ggplot( res2, aes(x=as.factor(n), y=value, col=estimator ) ) +
    facet_grid( skew ~ Measure ) +
    geom_hline( yintercept=0, col="darkgrey" ) +
  geom_boxplot( position = "dodge" ) +
    labs( y="" )
```
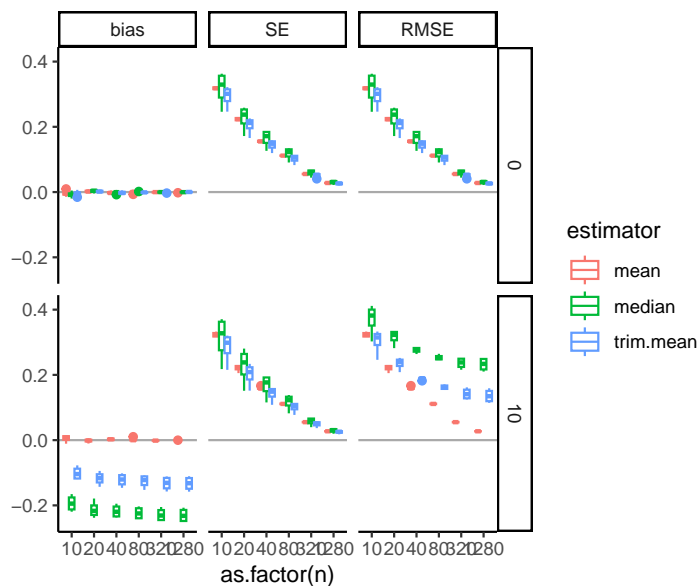
We can also subset to look at how these trade-offs play out when `df0 = 3`, where we are seeing the largest benefits from trimming in our prior analysis. We can then use lines to show the trends, which is a bit clearer:

```
ggplot( filter( res2, df0 == 3 ),
        aes(x=n, y=value, col=estimator ) ) +
    facet_grid( skew ~ Measure ) +
    geom_hline( yintercept=0, col="darkgrey" ) +
    geom_line() + geom_point() +
    scale_x_log10( breaks=ns ) +
    labs( y="" )
```
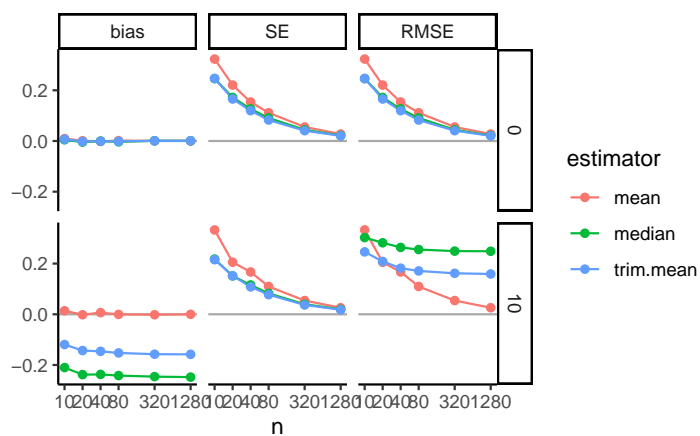

Or maybe we can aggregate without losing too much information:

```r
res2agg <- group_by( res2, n, estimator, skew, Measure ) %>%
  summarise( value = mean(value), .groups = "drop" )

ggplot( filter( res2, df0 == 3 ), aes(x=n, y=value, col=estimator ) ) +
    facet_grid( skew ~ Measure ) +
    geom_hline( yintercept=0, col="darkgrey" ) +
    geom_line() + geom_point() +
    scale_x_log10( breaks=ns ) +
    labs( y="" )
```
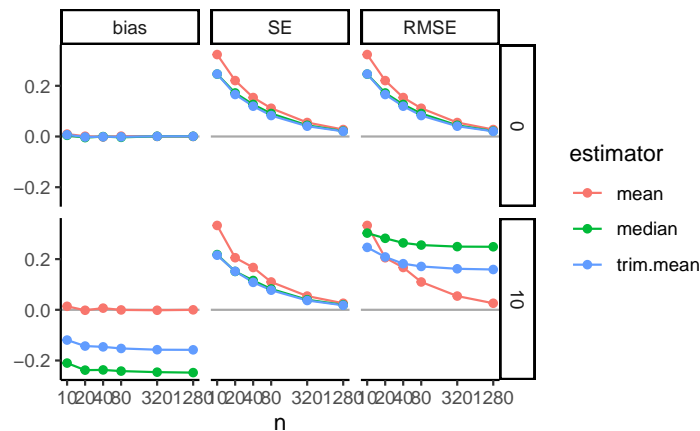

In these *Bias-SE-RMSE* plots, we see how different estimators have different biases and different uncertainties. The bias is negative for our trimmed estimators because we are losing the big outliers above and so getting answers that are too low.

The RMSE captures the trade-off in terms of what estimator gives the lowest overall *error*. For this distribution, the mean wins as the sample size increases because the bias basically stays the same and the SE drops. But for smaller samples the trimming is superior. The median (essentially trimming 50% above and below) is overkill and has too much negative bias.

From a simulation study point of view, notice how we are looking at three different qualities of our estimators. Some people really care about bias, some care about RMSE. By presenting all results we are transparent about how the different estimators operate.

Next steps would be to also examine the associated estimated standard errors for the estimators, seeing if these estimates of estimator uncertainty are good or poor. This leads to investigation of coverage rates and similar.

Chapter 16

Simulations as evidence

We began this book with an acknowledgement that simulation is fraught with the potential for misuse: *simulations are doomed to succeed.* We close by reiterating this point, and then discuss several ways researchers might design their simulations so they more arguably produce real evidence on how well things might work.

When our work is done, ideally we will have generated simulations that provide a sort of "consumer product testing" for the study designs and statistical methods we are exploring. Clearly, it is important to do some consumer product tests that are grounded in how consumers will actually use the product in real life— but before you get to that point, it can be helpful to cover an array of conditions that are probably more extreme than what will be experienced in practice (like dropping things off buildings or driving over them with cars or whatever else). These extreme contexts give us more clear results, and can help us understand the limits of our methods. These extreme contexts are also usually best-case (or at least optimistic) scenarios for when our estimator of interest will excel, giving in effect an upper bound on how well things could go.

Extreme and clear simulations are also usually easier to write, manipulate, and understand. Such simulations can help us learn about the estimators themselves. For example, simulation can help uncover how different aspects of a data generating process affect the performance of an estimator. To discover this, you need a data generation process with clear levers controlling those aspects. Simple simulations can be used to push theory further—we can experiment to gain an inclination of whether a model is a good idea at all, or to verify we are right about an intuition or derivation about how well an estimator can work.

But such simulations cannot be the end of our journey. In general, a researcher should work to ensure their simulation evidence is *relevant.* A set of simulations only using unreaslistic data generating processes may not be that useful. Unless the estimators being tested have truly universally stable properties, we will not

learn much from a simulation that is not relevant to the problem at hand. We have to circle back to providing testing of the sorts of situations an eventual user of our methods might encounter in practice. So how can we make our simulations more relevant?

16.1   Strategies for making relevant simulations

In the following subsections we go through a range of general strategies for making relevant simulations:

1. Use extensive multi-factor simulations
2. Generate simulations based on prior literature.
3. Pick simulation factors based on real data
4. Resample real data directly to get authentic distributions
5. Design a fully calibrated simulation

16.1.1   Make your simulation general with an extensive multi-factor experiment

"If a single simulation is not convincing, use more of them," is one principle a researcher might take. By conducting extensive multifactor simulations, once can explore a large space of possible data generating scenarios. If, across the full range of scenarios, a general story bears out, then perhaps that will be more convincing than a narrower range.

Of course, the critic will claim that some aspect that is not varying is the real culprit. If this aspect is unrealistic, then the findings, across the board, may be less relevant. Thus, pick the factors one varies with care.

16.1.2   Use previously published simulations to beat them at their own game

If a relevant prior paper uses a simulation to make a case, one approach is to replicate that simulation, adding in the new estimator one wants to evaluate. This makes it (more) clear that you are not fishing: you are using something established in the literature as a published benchmark. By constraining oneself to published simulations, one has less wiggle room to cherry pick a data generating process that works the way you want.

16.1.3   Calibrate simulation factors to real data

Use real data to inform choice of factor levels or other data generation features. For example, in James's work on designing methods for meta-analysis, there is often a question of how big sample sizes should be and how many different outcomes per study there should be when simulating effect size estimates from hypothetical studies to be included in a hypothetical meta-analysis. To make

the simulations realistic, James obtained data from a set of past real meta-analyses and fit parametric models to these features, and used the resulting parameter estimates as benchmarks for how large and how varied the simulated meta analyses should be.

In this case, one would probably not use the exact estimated values, but instead use them as a point of reference and possibly explore a range of values around them. For instance, say we find that the distribution of study sizes fits a Poisson(63) pretty well. We might then then simulate study sizes using a Poisson with mean parameters of 40, 60, or 80 (where 40, 60, and 80 would be one factor in our multifactor experiment).

16.1.4 Use real data to obtain directly

You can also use real data directly to avoid a parametric model. For example, say you need a population distribution for a slew of covariates. Rather than using something artificial (like multivariate normal), you can pull population data on a bunch of covariates from some administrative data and then use those data as a (finite) population distribution. You then simple sample (possibly with replacement) rows from your reference population to generate your simulationsample.

The appeal here is that your covariates will then have distributions that are much more authentic than some multivariate normal–they will include both continuous and categorical variables, they will tend to be skewed, and they will be correlated in different ways that are more interesting than anything someone could make up.

As an illustration of this approach, an old paper on heteroscedasticity-robust standard errors (Long and Irvin, 2000) does something similar. It was important in the context that they're studying because the behavior of heteroscedasticity-robust SEs is influenced by leverage, which is a function of the covariate distribution. Getting authentic leverage was hard to do with a parametric model, so getting examples of it from real life made the simulation more relevant.

16.1.5 Fully calibrated simulations

Extending some of the prior ideas even further, one practice in increasing vogue is to generate *calibrated simulations*. These are simulations tailored to a specific applied contexts, where we design our simulation study to more narrowly inform what assumptions and structures are necessary in order to make progress in that specific context.

Often we would do this by building our simulations out of existing data. For an example from above, one might sample, with replacement, from the covariate distribution of an actual dataset so that the distribution of covariates is authentic in how the covariates are distributed and, more importantly, how they co-relate.

But this is not far enough. We also need to generate a realistic relationship between our covariates and outcome to truly assess how well the estimators work in practice. It is very easy to accidentally put a very simple model in place for this final component, thus making a calibrated simulation quite naive in, perhaps, the very way that counts.

We next walk through how you might calibrate further in the context of evaluating estimators for some sort of causal inference context where we are assessing methods of estimating a treatment effect of some binary treatment. If we just resample our covariates, but then layer a constant treatment effect on top, we may be missing critical aspects of how our estimators might fail in practice.

In the area of causal inference, the potential outcomes framework provides a natural path for generating calibrated simulations (Kern et al., 2014). Also see 21 for more discussion of simulations in the potential outcomes framework. Under this framework, we would take an existing randomized experiment or observational study and then impute all the missing potential outcomes under some specific scheme. This fully defines the sample of interest and thus any target parameters, such as a measure of heterogeneity, are then fully known. For our simulation we then synthetically, and repeatedly, randomize and "observe'' outcomes to be analyzed with the methods we are testing. We could also resample from our dataset to generate datasets of different size, or to have a superpopulation target as our estimand.

The key feature here is the imputation step: how do we build our full set of covariates and outcomes? One baseline method one can use is to generate a matched-pairs dataset by, for each unit, finding a close match given all the demographic and other covariate information of the sample. We then use the matched unit as the imputed potential outcome.
By doing this (with replacement) for all units we can generate a fully imputed dataset which we then use as our population, with all outcomes being "real," as they are taken from actual data. Such matching can preserve complex relationships in the data that are not model dependent. In particular, if outcomes tend to be coarsely defined (e.g., on an integer scale) or have specific clumps (such as zero-inflation or rounding), this structure will be preserved.

One concern with this approach is the noise in the matching could in general dilute the structure of the treatment effect as the control- and treatment-side potential outcomes may be very unrelated, creating a lot of so-called idiosyncratic treatment variation (unit-to-unit variation in the treatment effects that is not explained by the covariates). This is akin to measurement error diluting found relationships in linear models. We could reduce such variation by first imputing missing outcomes using some model (e.g., a random forest) fit to the original data, and then matching on all units including the imputed potential outcome as a hidden "covariate." This is not a data analysis strategy, but instead a method of generating synthetic data that both has a given structure of interest and also remains faithful to the idiosyncrasies of an actual dataset.

A second approach that allows for varying the level of a systematic effect is to specify a treatment effect model, predict treatment effects for all units and use those to impute the treatment potential outcome for all control units. This will perfectly preserve the complex structure between the covariates and the $Y_i(0)$s. Unfortunately, this would also give no idiosyncratic treatment variation . To add in idiosyncratic variation we could then need to generate a distribution of perturbations and add these to the imputed outcomes just as an error term in a regression model.

Regardless of how we generate them, once we have a "fully observed" sample with the full set of treatment and control potential outcomes for all of our units, we can calculate any target estimands we like on our population, and then compare our estimators to these ground truths (even if they have no parametric analog) as desired.

Clearly, these calibration games can be fairly complex. They do not lend themselves to a clear factor-based structure that have levers that change targeted aspects of the data generating process (although sometimes you can build in controls to make such levers possible). In exchange, we end up with a simulation that might be more faithfully capturing aspects of a specific context, making our simulations more relevant to answering the narrower question of "how will things work here?"

Part IV

Computational Considerations

Chapter 17

Organizing a simulation project

As we saw earlier, a full multifactor simulation can generate a lot of output that can be hard to navigate. They are complex, multifaceted projects by design. This means that the project itself can be hard to manage. It can be easy to become overwhelmed by a steady accumulation of scripts that generate data, analyze data, run simulations, and so on.

This section is designed to give you the computational skills and ideas that will make it easier to handle complex simulation projects. We start with a discussion of file and project management, then turn to parallel processing, and finally close with some core programming habits that we have found useful for keeping on top of this type of sprawling complexity.

Simulations have two general phases: generate your results and analyze your results. The ending of the first phase should be to save the generated results. The beginning of the second phase should then be to load the results from a file and analyze them. These phases can be in a separate '.R' files. Dividing your simulations in this way allows for easily changing how one *analyzes* an experiment without re-running the entire thing.

This is the simplest version of a general principle of a larger project: put code for different purposes in different files.

For example, at the minimum, for a complex multifactor simulation, you will likely have three general collections of code, not including the code to run the multifactor simulation itself:

- Code for generating data
- Code for analyzing data
- Code for running a single simulation scenario

If each of these pieces is large and complex, you might consider putting them in three different `.R` files. To do this, we need to talk about what kinds of R scripts exist, and also talk about how you can tell one script to load another script.

17.1   Well structured R scripts

In R, there are two critical file types that can hold R code: `.R` files (scripts) and `.Rmd` (or `.qmd`) markdown files. The former just holds R code, while the latter holds a mix of R code and text. The latter is what you would render (or knit) to make a final report–it will run the code, and mix the results in with the text to give a nicely formatted report with code, figures, tables, and other printout nicely embedded. These are what is typically used for smaller projects—all the code and discussion of code would be in a single, convenient place.

For larger projects, you will be more dependant on the first type of file, the `.R` script. Ideally, the principle of modular programming would be applied to these files. Each `.R` file would hold a collection of code that is related to a single task. There are two main types of of `.R` script: those that *just* have functions that can be used for other purposes (meaning that if you run them, the only thing that happens is you end up with some new functions in your current workspace), and those that are traditional scripts such that when you run them, R will do a variety of specified tasks.

17.1.1   The source command

Inside of an R script you can "source" other `.R` files. The `source()` command essentially "cuts and pastes" the contents of the given file into your R work session. E.g.,

```r
source( here::here( "R/data_generators.R" ) )
source( here::here( "R/estimators.R" ) )
source( here::here( "R/simulation_support.R" ) )
```

If the named file has code to run, it will run it. If the named file has a list of methods, those methods will now be available for use. The `here::here()` command is a convenience function that allows you to specify a file path relative to your R project root directory, so you can easily find your files.

You can even source files inside files that are sourced. For example, `simulation_support.R` could, inside it, source the other two files. You would then only source the single simulation support file in your primary simulation script.

One reason for putting code in individual files is you can then have testing code in each of your files (in False blocks, see below), testing each of your components.

Then, when you are not focused on that component, you don't have to look at that testing code.

Another good reason for this type of modular organizing is you can then allow for a whole simulation universe, writing a variety of data generators that together form a library of options. You can then easily create different simulations that use your different pieces, in your larger project.

For example, in one recent simulation project on estimators for an Instrumental Variable analysis, we had several different data generators for generating different types of compliance patterns (IVs are often used to handle noncompliance in randomized experiments). Our `data_generators.R` code file then had several methods. When we sourced it, we end up wit the following list of methods:

```
> ls()
[1] "describe_sim_data"  "make_dat"          "make.dat_1side"
[4] "make_dat_1side_old" "make_dat_orig"     "make_dat_simple"
[7] "make_dat_tuned"     "rand_exp"          "summarize_sim_data"
```

The `describe()` and `summarize()` methods printed various statistics about a sample dataset; these are used to debug and understand how the generated data looks. We also had a variety of different DGP methods because we had different versions that came up as we were trying to chase down errors in our estimators and understand strange behavior.

Putting the estimators in a different file also had a nice additional purpose: we also had an applied data example in our work, and we could simply source that single file and use those estimators on our actual data. This ensured our simulation and applied analysis were perfectly aligned in terms of the estimators we were using. Also, as we debugged our estimators and tweaked them, we immediately could re-run our applied analysis to update those results with minimal effort.

Modular programming is key.

17.1.2 Putting headers in your .R file

When you write a `.R` script, it is a good idea to put a header at the top of the file, giving a description of the file's purpose. Then, you can also put dividers in your file, e.g.,

```
#-#-#-#-#-#-#-#-#-#-#-#-#-#-#-#-#-#
# Data generating functions ----
#-#-#-#-#-#-#-#-#-#-#-#-#-#-#-#-#-#
```

Note the `----` at the end of the middle line: if you add those trailing dashes, then if you click on the dropdown at the bottom of your RStudio, you will see a pop-up table of contents that allows you to quickly navigate to different parts of your source file.

17.1.3 Storing testing code in your scripts

If you have an extended `.R` file with a list of functions, you might also want to store a lot of code that runs each function in turn, so you can easily remind yourself of what it does, or what the output looks like. One way to keep this code around, but not have it run all the time when you run your script, is to put the code inside a "FALSE block," that might look like so:

```r
# My testing code ----
if ( FALSE ) {
  res <- my_function( 10, 20, 30 )
  res
  # Some notes as to what I want to see.

  sd( res )
  # This should be around 20
}
```

You can then, when you open and look at the script, paste the code inside the block into the console when you want to run it. If you source the script, however, it will not run at all, and thus your code will source faster and not print out any extraneous output. This is a good way to keep your testing code with the code it is testing. When you want to work on just the part of the project captured by your script, you can work inside the single file very easily, ignoring the other parts of your project.

You can also (or instead) write testing code, which we will talk about further below.

17.2 Principled directory structures

We *strongly advocate* keeping a well-organized directory for your simulation. We recommend using RStudio, or a similar IDE, and having a directory structure like the following:

```
my_project/
  proj.Rproj
  README.md
  R/
  data/
  results/
  scripts/
  test/
```

For those who have written R pacakges, this structure will look familiar. The `R/` directory is where you put your core R code. We will have `.R` scripts that just hold our core methods; we can then "load" these scripts into our workspace as needed to gain access to those methods. Saved methods might include the

methods you have developed that you are planning on testing (unless they are in a separate package), and methods to generate data. We *do not* put the scripts that run the actual simulation here. The `R/` folder is to store the building blocks of our simulation only, not the final scripts that use those blocks to run and analyze our simulations themselves.

The `data/` directory is where you put any data files you are using in your simulation. The `results/` directory is where you will save any generated results of your simulation. Sometimes it might be worth having `raw_results` and `results`, where `raw_results` are what you save as soon as you finish running the simulation, and `results` have final results where you may have merged and summarized the raw results.

The `scripts/` directory is where you put your scripts that run the simulation and analyze simulation results. You will likely have one script that runs the simulation, and one or more scripts that analyze the results.

Finally, the `test/` directory is where you put any testing code you have written to test your methods. You can even use the `testthat` package to write unit tests for your methods, and put those in the `test/` directory. This structure is not required, but it is a good idea to have a well-organized project of some type.

17.3 Saving simulation results

Always save your simulation results to a file. Simulations are painful and time consuming to run, and you will invariably want to analyze the results of them in a variety of different ways, once you have looked at your preliminary analysis. We advocate saving your simulation as soon as it is complete. But there are some ways to do better than that, such as saving as you go. This can protect you if your simulation occasionally crashes, or if you want to rerun only parts of your simulation for some reason.

17.3.1 Saving simulations in general

Once your simulation has completed, you can save it like so:

```
dir.create("results", showWarnings = FALSE )
write_csv( res, "results/simulation_CRT.csv" )
```

`write_csv()` is a tidyverse file-writing command; see "R for Data Science" textbook, 11.5.

You can then load it, just before analysis, as so:

```
res = read_csv( "results/simulation_CRT.csv" )
```

There are two general tools for saving. The `read/write_csv` methods save your file in a way where you can open it with a spreadsheet program and look at it.

But your results should be in a vanilla, rectangular format (non-fancy data frame without list columns).

Alternatively, you can use the `saveRDS()` and `readRDS()` methods; these save objects to a file such that when you load them, they are as you left them. The RDS saving keeps your R object as given. The simpler format of a csv file means your factors, if you have them, may not preserve as factors, and so forth.

17.3.2 Saving simulations as you go

If you are not sure you have time to run your entire simulation, or you think your computer might crash half way through, or something similar, you can save each chunk you run as you go, in its own file. You then stack those files at the end to get your final results. With clever design, you can even then selectively delete files to rerun only parts of your larger simulation—but be sure to rerun everything from scratch before you run off and publish your results, to avoid embarrassing errors.

Here, for example, is a script from a research project examining how one might use post-stratification to improve the precision of an IV estimate. This is the script that runs the simulation. Note the sourcing of other scripts that have all the relevant functions; these are not important here. Due to modular programming, we can see what this script does, even without those detail.

```r
source( "R/simulation_functions.R" )

if ( !file.exists("results/frags" ) ) {
    dir.create("results/frags")
}

# Number of simulation replicates per scenario
R = 1000

# Do simulation breaking up R into this many chunks
M_CHUNK = 10

###### Set up the multifactor simulation #######

# chunkNo is a hack to make a bunch of smaller chunks for doing parallel more
# efficiently.
factors = expand_grid( chunkNo = 1:M_CHUNK,
                       N = c( 500, 1000, 2000 ),
                       pi_c = c( 0.05, 0.075, 0.10 ),
                       nt_shift = c( -1, 0, 1 ),
                       pred_comp = c( "yes", "no" ),
                       pred_Y = c( "yes", "no" ),
                       het_tx = c( "yes", "no" ),
```

```r
                        sd0 = 1
                        )
factors <- factors %>% mutate(
    reps = R / M_CHUNK,
    seed = 16200320 + 1:n()
)
```

This generates a data frame of all our factor combinations. This is our list of "tasks" (each row of factors). These tasks have repeats: the "chunks" means we do a portion of each scenario, as specified by our simulation factors, as a process. This would allow for greater parallelization (e.g., if we had more cores), and also lets us save our work without finishing an entire scenario of, in this case, 1000 iterations.

To set up our simulation we make a little helper method to do one row. With each row, once we have run it, we save it to disk. This means if we kill our simulation half-way through, most of the work would be saved. Our function is then going to either do the simulation (and save the result to disk immediately), or, if it can find the file with the results from a previous run, load those results from disk:

```r
safe_run_sim = safely( run_sim )
file_saving_sim = function( chunkNo, seed, ... ) {
    fname = paste0( "results/frags/fragment_", chunkNo, "_", seed, ".rds" )
    res = NA
    if ( !file.exists(fname) ) {
        res = safe_run_sim( chunkNo=chunkNo, seed=seed, ... )
        saveRDS(res, file = fname )
    } else {
        res = readRDS( file=fname )
    }
    return( res )
}
```

Note how we wrap our core `run_sim` method (that takes all our simulation factors and runs a simulation for those factors) in `safely`; `run_sim()` was crashing very occasionally, and so to make the code more robust, we wrapped it so we could see any error messages. Our method cleverly either loads a saved result, or generates it, for a given chunk. This means from whatever is calling the function, it will look exactly the same whether it is loading a saved result or generating a new one.

We next run the simulation by calling `file_saving_sim()` for all of our simulation scenarios.

```r
# Shuffle the rows so we run in random order to load balance.
factors = sample_n(factors, nrow(factors) )
```

```r
if ( TRUE ) {
    # Run in parallel
    parallel::detectCores()

    library(future)
    library(furrr)

    #plan(multiprocess) # choose an appropriate plan from future package
    #plan(multicore)
    plan(multisession, workers = parallel::detectCores() - 2 )

    factors$res <- future_pmap(factors, .f = file_saving_sim,
                            .options = furrr_options(seed = NULL),
                            .progress = TRUE )

} else {
  # Run not in parallel, used for debugging
  factors$res <- pmap(factors, .f = file_saving_sim )
}

tictoc::toc()
```

Note how we shuffle the rows of our task list so that which process gets what task is randomized. If some tasks are much longer (e.g., due to larger sample size) then this will get balanced out across our processes. See 18 for more on parallel processing.

The `if-then` structure allows us to easily switch between parallel and nonparallel code. This makes debugging easier: when running in parallel, stuff printed to the console does not show until the simulation is over. Plus it would be all mixed up since multiple processes are working simultaneously.

The above overall structure allows the researcher to delete one of the "fragment" files from the disk, run the simulation code, and have it just do one tiny piece of the simulation. This means the researcher can insert a `browser()` command somewhere inside the code, and debug the code, in the natural context of how the simulation is being run.

The seed setting ensures reproducibility. Once we are done, we need to clean up our results:

```r
sim_results <-
    factors %>%
    unnest(cols = res)

# Cut apart the results and error messages
sim_results$sr = rep( c("res","err"), nrow(sim_results)/2)
```

```
sim_results = pivot_wider( sim_results, names_from = sr, values_from = res )

saveRDS( sim_results, file="results/simulation_results.rds" )
```

Our final `simulation_results.rds` file will have all the results from our simulation, made by stacking all of the fragments of our simulation together.

17.3.3 Dynamically making directories

If you are generating a lot of files, then you should put them somewhere. But where? It can be nice to dynamically generate a directory for your files on fly. One way to do this is to write a function that will make any needed directory, if it doesn't exist, and then put your file in that spot. For example, you might have your own version of `write_csv` as:

```
my_write_csv <- function( data, path, file ) {

  if ( !dir.exists( here::here( path ) ) ) {
    dir.create( here::here( path ), recursive=TRUE )
  }
  write_csv( data, paste0( path, file ) )
}
```

This will look for a path (starting from your R Project, by taking advantage of the `here` package), and put your data file in that spot. If the spot doesn't exist, it will make it for you.

17.3.4 Loading and combining files of simulation results

Once your simulation files are all generated, the following code will stack them all into a giant set of results, assuming all the files are themselves data frames stored in RDS objects. This function will try and stack all files found in a given directory; for it to work, you should ensure there are no other files stored there.

```
load.all.sims = function( filehead="raw_results/" ) {

  files = list.files( filehead, full.names=TRUE)

  res = map_df( files, function( fname ) {
    cat( "Reading results from ", fname, "\n" )
    rs = readRDS( file = fname )
    rs$filename = fname
    rs
  })
  res
}
```

You would use as so:

```
results <- load.all.sims( filehead="raw_results/" )
results <- bind_rows( results )
```

Chapter 18

Parallel Processing

Especially if you take our advice of "when in doubt, go more general" and if you calculate monte carlo standard errors, you will quickly come up against the limits of your computer. Simultions can be incredibly computationally intensive, and there are a few means for dealing with that. The first, touched on at times throughout the book, is to optimize ones code by looking for ways to remove extraneous calculation (e.g., by writing ones own methods rather than using the safety-checking and thus sometimes slower methods in R, or by saving calculations that are shared across different estimation approaches). The second is to use more computing power. This latter approach is the topic of this chapter.

There are two general ways to do parallel calculation. The first is to take advantage of the fact that most modern computers have multiple cores (i.e., computers) built in. With this approach, we tell R to use more of the processing power of your desktop or laptop. If your computer has eight cores, you can easily get a near eight-fold increase in the speed of your simulation.

The second is to use cloud computing, or compute on a cluster. A computing cluster is a network of hundreds or thousands of computers, coupled with commands where you break apart a simulation into pieces and send the pieces to your army of computers. Conceptually, this is the same as when you do baby parallel on your desktop: more cores equals more simulations per minute and thus faster simulation overall. But the interface to a cluster can be a bit tricky, and very cluster-dependent.

But once you get it up and running, it can be a very powerful tool. First, it takes the computing off your computer entirely, making it easier to set up a job to run for days or weeks without making your day to day life any more difficult. Second, it gives you hundreds of cores, potentially, which means a speed-up of hundreds rather than four or eight.

Simulations are a very natural choice for parallel computation. With a mul-

tifactor experiment it is very easy to break apart the overall into pieces. For example, you might send each factor combination to a single machine. Even without multi factor experiments, due to the cycle of "generate data, then analyze," it is easy to have a bunch of computers doing the same thing, with a final collection step where all the individual iterations are combined into one at the end.

18.1   Parallel on your computer

Most modern computers have multiple cores, so you can run a parallel simulation right in the privacy of your own home!

To assess how many cores you have on your computer, you can use the `detectCores()` method in the **parallel** package:

```
parallel::detectCores()
```

```
## [1] 8
```

Normally, unless you tell it to do otherwise, ***R only uses one core***. This is obviously a bit lazy on R's part. But it is easy to take advantage of multiple cores using the `future` and `furrr` packages.

```
library(future)
library(furrr)
```

In particular, the `furrr` package replicates our `map` functions, but in parallel. We first tell our R session what kind of parallel processing we want using the `future` package. In general, using `plan(multisession)` is the cleanest: it will start one entire R session per core, and have each session do work for you. The alternative, `multicore` does not seem to work well with Windows machines, nor with RStudio in general.

The call is simple:

```
plan(multisession, workers = parallel::detectCores() - 1 )
```

The `workers` parameter specifies how many of your cores you want to use. Using all but one will let your computer still operate mostly normally for checking email and so forth. You are carving out a bit of space for your own adventures.

Once you set up your plan, you use `future_pmap()`; it works just like `pmap()` but evaluates across all available workers specified in the plan call. Here we are running a parallel version of the multifactor experiment discussed in Chapter @ref(exp_design) (see chapter @ref(case_Cronback) for the simulation itself).

```
tictoc::tic()
params$res = future_pmap(params,
                         .f = run_alpha_sim,
```

```
                                .options = furrr_options(seed = NULL))
tictoc::tic()
```

Note the `.options = furrr_options(seed = NULL)` part of the argument. This is to silence some warnings. Given how tasks are handed out, R will get upset if you don't do some handholding regarding how it should set seeds for pseudoranom number generation. In particular, if you don't set the seed, the multiple sessions could end up having the same starting seed and thus run the exact same simulations (in principle). We have seen before how to set specific seed for each simulation scenario, but `furrr` doesn't know we have done this. This is why the extra argument about seeds: it is being explicit that we are handling seed setting on our own.

We can compare the running time to running in serial (i.e. using only one worker):

```
tictoc::tic()
params$res2 = dplyr::select(params, n:seed) %>%
  pmap(.f = run_alpha_sim)
tictoc::tic()
```

(The `select` command is to drop the `res` column from the parallel run; it would otherwise be passed as as parameter to `run_alpha_sim` which would in turn cause an error due to the unrecognized parameter.)

18.2 Parallel off your computer

In general, a "cluster" is a system of computers that are connected up to form a large distributed network that many different people can use to do large computational tasks (e.g., simulations!). These clusters will have some overlaying coordinating programs that you, the user, will interact with to set up a "job," or set of jobs, which is a set of tasks you want some number of the computers on the cluster to do for you in tandum.

These coordinating programs will differ, depending on what cluster you are using, but have some similarities that bear mention. For running simulations, you only need the smallest amount of knowledge about how to engage with these systems because you don't need all the individual computers working on your project communicating with each other (which is the hard part of distributed computing, in general).

18.2.1 What is a command-line interface?

In the good ol' days, when things were simpler, yet more difficult, you would interact with your computer via a "command-line interface." The easiest way to think about this is as an R console, but in a different language that the entire computer speaks. A command line interface is designed to do things like

find files with a specific name, or copy entire directories, or, importantly, start
different programs. Another place you may have used a command line inteface
is when working with Git: anything fancy with Git is often done via command-
line. People will talk about a "shell" (a generic term for this computer interface)
or "bash" or "csh." You can get access to a shell from within RStudio by clicking
on the "Terminal" tab. Try it, if you've never done anything like this before,
and type

```
ls
```

It should list some file names. Note this command does *not* have the parenthesis
after the command, like in R or most other programming languages. The syntax
of a shell is usually mystifying and brutal: it is best to just steal scripts from
the internet and try not to think about it too much, unless you want to think
about it a lot.

Importantly for us, from the command line interface you can start an R pro-
gram, telling it to start up and run a script for you. This way of running R
is noninteractive: you say "go do this thing," and R starts up, goes and does
it, and then quits. Any output R generates on the way will be saved in a file,
and any files you save along the way will also be at your disposal once R has
completed.

To see this in action make the following script in a file called "dumb_job.R":

```
library( tidyverse )
cat( "Making numbers\n" )
Sys.sleep(30)
cat( "Now I'm ready\n" )
dat = tibble( A = rnorm( 1000 ), B = runif( 1000 ) * A )
write_csv( dat, file="sim_results.csv" )
Sys.sleep(30)
cat( "Finished\n" )
```

Then open the terminal and type (the ">" is not part of what you type):

```
> ls
```

Do you see your `dumb_job.R` file? If not, your terminal session is in the wrong
directory. In your computer system, files are stored in a directory structure,
and when you open a terminal, you are somewhere in that structure.

To find out where, you can type

```
> pwd
```

for "Print Working Directory". Save your dumb job file to wherever the above
says. You can also change directories using `cd`, e.g., `cd ~/Desktop/temp` means
"change directory to the temp folder inside Desktop inside my home directory"
(the ~ is shorthand for home directory). One more useful commands is `cd ..`
(go up to the parent directory).

Once you are in the directory with your file, type:

```
> R CMD BATCH dumb_job.R R_output.txt --no-save
```

The above command says "Run R" (the first part) in batch mode (the "CMD BATCH" part), meaning source the `dumb_job.R` script as soon as R starts, saving all console output in the file `R_output.txt` (it will be saved in the current directory where you run the program), and where you don't save the workspace when finished.

This command should take about a minute to complete, because our script sleeps a lot (the sleep represents your script doing a lot of work, like a real simulation would do). Once the command completes (you will see your ">" prompt come back), verify that you have the `R_output.txt` and the data file `sim_results.csv` by typing `ls`. If you open up your Finder or Microsoft equivilent, you can actually see the `R_output.txt` file appear half-way through, while your job is running. If you open it, you will see the usual header of R telling you what it loading, the "Making numbers" comment, and so forth. R is saving everything as it works through your script.

Running R in this fashion is the key element to a basic way of setting up a massive job on the cluster: you will have a bunch of R programs all "going and doing something" on different computers in the cluster. They will all save their results to files (they will have files of different names, or you will not be happy with the end result) and then you will gather these files together to get your final set of results.

Small Exercise: Try putting an error in your `dumb_job.R` script. What happens when you run it in batch mode?

18.2.2   Running a job on a cluster

In the above, you can run a command on the command-line, and the command line interface will pause while it runs. As you saw, when you hit return with the above R command, the program just sat there for a minute before you got your command-line prompt back, due to the sleep.

When you properlly run a big job (program) on a cluster, it doesn't quite work that way. You will instead set a program to run, but tell the cluster to run it somewhere else (people might say "run in the background"). This is good because you get your command-line prompt back, and can do other things, while the program runs in the background.

There are various methods for doing this, but they usually boil down to a request from you to some sort of managerial process that takes requests and assigns some computer, somewhere, to do them. (Imagine a dispatcher at a taxi company. You call up, ask for a ride, and it sends you a taxi to do it. The dispatcher is just fielding requests, assinging them to taxis.)

For example, one dispatcher is the slurm (which may or may not be on the cluster you are attempting to use; this is where a lot of this information gets very cluster-specific).

You first set up a script that describes the job to be run. It is like a work request. This would be a plain text file, such as this example (`sbatch_runScript.txt`):

```
#!/bin/bash
#SBATCH -n 32                                              # Number of cores reque
#SBATCH -N 1                                                # Ensure that all co
#SBATCH -t 480                                             # Runtime in minutes
#SBATCH -p stats                                           # Partition to submit
#SBATCH --mem-per-cpu=1000               # Memory per cpu in MB
#SBATCH --open-mode=append                   # Append to output file, don't truncat
#SBATCH -o /output/directory/out/%j.out # Standard out goes to this file
#SBATCH -e /output/directory/out/%j.err # Standard err goes to this file
#SBATCH --mail-type=ALL                      # Type of email notification- BEGIN,EN
#SBATCH --mail-user=email@gmail.com        # Email address

# You might have some special loading of modules in the computing environment
source new-modules.sh
module load gcc/7.1.0-fasrc01
module load R
export R_LIBS_USER=$HOME/apps/R:$R_LIBS_USER

#R file to run, and txt files to produce for output and errors
R CMD BATCH estimator_performance_simulation.R logs/R_output_${INDEX_VAR}.txt --no-sav
```

This file starts with a bunch of variables that describe how sbatch should handle the request. It then has a series of commands that get the computer environment ready. Finally, it has the `R CMD BATCH` command that does the work you want.

These scripts can be quite confusing to understand. There are so many options! What do these things even do? The answer is, for researchers early on their journey to do this kind of work, "Who knows?" The general rule is to find an example file for the system you are working on that works, and then modify it for your own purposes.

Once you have such a file, you could run it on the command line, like this:

```
sbatch -o stdout.txt \
       --job-name=my_script \
       sbatch_runScript.txt
```

You do this, and it will *not* sit there and wait for the job to be done. The `sbatch` command will instead send the job off to some computer which will do the work in parallel.

Interestingly, your R script could, at this point, do the "one computer" parallel type code listed above. Note the script above has 32 cores; your single job could

then have 32 cores all working away on their individual pieces of the simulation, as before (e.g., with `future_pmap`). You would have a 32-fold speedup, in this case.

This is the core element to having your simulation run on a cluster. The next step is to do this *a lot*, sending off a bunch of these jobs to different computers.

Some final tips

- Remember to save a workspace or RDS!! Once you tell Odyssey to run an R file, it, well, runs the R file. But, you probably want information after it's done - like an R object or even an R workspace. For any R file you want to run on Odyssey, remember at the end of the R file to put a command to save something after everything else is done. If you want to save a bunch of R objects, an R workspace might be a good way to go, but those files can be huge. A lot of times I find myself wanting only one or two R objects, and RDS files are a lot smaller.

- Moving files from a cluster to your computer. You will need to first upload your files and code to the cluster, and then, once you've saved your workspace/RDS, you need those back on your computer. Using a scp client such as FileZilla is an easy way to do this file-transfer stuff. You can also use a Git repo for the code, but checking in the simulation results is not generally advisable: they are big, and not really in the spirit of a verson control system. Download your simulation results outside of Git, and keep your code in Git, is a good rule of thumb.

18.2.3 Checking on a job

Once your job is working on the cluster, it will keep at it until it finishes (or crashes, or is terminated for taking up too much memory or time). As it chugs away, there will be different ways to check on it. For example, you can, from the console, list the jobs you have running to see what is happening:

```
sacct -u lmiratrix
```

except, of course, "`lmiratrix`" would be changed to whatever your username is. This will list if your file is running, pending, timed out, etc. If it's pending, that usually means that someone else is hogging up space on the cluster and your job request is in a queue waiting to be assigned.

The `sacct` command is customizable, e.g.,

```
sacct -u lmiratrix --format=JobID,JobName%30,State
```

will not truncate your job names, so you can find them more easily.

You can check on a specific job, if you know the ID:

```
squeue -j JOBID
```

Something that's fun is you can check who's running files on the stats server by typing:

```
showq-slurm -p stats -o
```

You can also look at the log files

```
tail my_log_file.log
```

to see if it is logging information as it is working.

The email arguments, above, cause the system to email you before and after the job is complete. The email notifications you can choose are `BEGIN`, `END`, `FAIL`, and `ALL`; `ALL` is generally good. What is a few more emails?

18.2.4 Running lots of jobs on a cluster

We have seen how to fire off a job (possibly a big job) that can run over days or weeks to give you your results. There is one more piece that can allow you to use even more computing resources to do things even faster, which is to do a whole bunch of job requests like the above, all at once. This multiple dispatching of sbatch commands is the final component for large simulations on a cluster: you are setting in motion a bunch of processes, each set to a specific task.

Asking for multiple, smaller, jobs is also nicer for the cluster than having one giant job that goes on for a long time. By dividing a job into smaller pieces, and asking the scheduler to schedule those pieces, you can let the scheduler share and allocate resources between you and others more fairly. It can make a list of your jobs, and farm them out as it has space. This might go faster for you; with a really big job, the scheduler can't even allocate it until the needed number of workers is available. With smaller jobs, you can take a lot of little spaces to get your work done. Especially since simulation is so independent (just doing the same thing over and over) there is rarely any need for one giant process that has to do everything.

To make multiple, related, requests, we create a for-loop in the Terminal to make a whole series sbatch requests. Then, each sbatch request will do one part of the overall simulation. We can write this program in the shell, just like you can write R scripts in R. A shell scripts does a bunch of shell commands for you, and can even have variables and loops and all of that fun stuff.

For example, the following `run_full_simulation.sh` is a script that fires off a bunch of jobs for a simulation. Note that it makes a variable `INDEX_VAR`, and sets up a loop so it can run 500 tasks indexed 1 through 500.

The first `export` line adds a collection of R libraries to the path stored in `R_LIBS_USER` (a "path" is a list of places where R will look for libraries). The next line sets up a for loop: it will run the indented code once for each number from 1 to 500. The script also specifies where to put log files and names each job with the index so you can know who is generating what file.

```
export R_LIBS_USER=$HOME/apps/R:$R_LIBS_USER

for INDEX_VAR in $(seq 1 500); do

  #print out indexes
  echo "${INDEX_VAR}"

  #give indexes to R so it can find them.
  export INDEX_VAR

  #Run R script, and produce output files
  sbatch -o logs/sbout_p${INDEX_VAR}.stdout.txt \
         --job-name=runScr_p${INDEX_VAR} \
         sbatch_runScript.txt

  sleep 1 # pause to be kind to the scheduler

done
```

One question is then how do the different processes know what part of the simulation they should be working on? E.g., each worker needs to have its own seed so it don't do exactly the same simulation as a different worker! The workers also need their own filenames so they save things in their own files. The key is the `export INDEX_VAR` line: this puts a variable in the environment that will be set to a specific number. Inside your R script, you can get that index like so:

```
index <- as.numeric(as.character(Sys.getenv("INDEX_VAR")))
```

You can then use the index to make unique filenames when you save your results, so each process has its own filename:

```
filename = paste0( "raw_results/simulation_results_", index, _".rds" )
```

You can also modify your seed such as with:

```
factors = mutate( factors,
                  seed = set.seed( 1000 * seed + index ) )
```

Now even if you have a series of seeds within the simulation script (as we have seen before), each script will have unique seeds not shared by any other script (assuming you have fewer than 1000 separate job requests).

This still doesn't exactly answer how to have each worker know what to work on. Conider the case of our multifactor experiment, where we have a large combination of simulation trials we want to run.

There are two approaches one might use here. One simple approach is the following: we first generate all the factors with `expand_grid()` as usual, and

then we take the row of this grid that corresponds to our index.

```
sim_factors = expand_grid( ... )
index <- as.numeric(as.character(Sys.getenv("INDEX_VAR")))
filename = paste0( "raw_results/simulation_results_", index, _".rds" )

stopifnot( index >= 1 && index <= nrow(sim_factors ) )
do.call( my_sim_function, sim_factors[ index, ] )
```

The `do.call()` command runs the simulation function, passing all the arguments listed in the targeted row. You then need to make sure you have your shell call the right number of workers to run your entire simulation.

One problem with this approach is some simulations might be a lot more work than others: consider your simulation with a huge sample size vs. one with a small sample size. Instead, you can have each worker run a small number of simulations of each scenario, and then stack your results later. E.g.,

```
sim_factors = expand_grid( ... )
index <- as.numeric(as.character(Sys.getenv("INDEX_VAR")))
sim_factors$seed = 1000000 * index + 17 * 1:nrow(sim_factors)
```

and then do your usual `pmap` call with `R = 10` (or some other small number of replicates.)

For saving files and then loading and combining them for analysis, see Section 17.3.

18.2.5   Resources for Harvard's Odyssey

The above guidance is tailored for Harvard' computing environment, primarily. For that environment in particular, there are many additional resources such as:

- Odyssey Guide: https://rc.fas.harvard.edu/resources/odyssey-quickstart-guide/
- R on Odyssey: https://rc.fas.harvard.edu/resources/documentation/software/r/

For installing R packages so they are seen by the scripts run by sbatch, see (https://www.rc.fas.harvard.edu/resources/documentation/software-on-odyssey/r/)

Other clusters should have similar documents giving needed guidance for their specific contexts.

18.2.6   Acknowledgements

Some of the above material is based on tutorials built by Kristen Hunter and Zach Branson, past doctoral students of Harvard's statistics department.

Chapter 19

Debugging and Testing

Writing code is not too hard. Writing *correct* code, however, can be quite challenging.

It is often the case that you will write code that does not do what you expect, or that does not work at all. Trying to figure out why can be enormously frustrating and time consuming. There are some tools, however, that can mitigate that to some extent.

19.1 Debugging with `print()`

When you follow modular design, you will often have methods you wrote calling other methods you wrote, which call even more methods you wrote. When you get an error, you might not be sure where to look, or what is happening.

A simple method (a method often reviled by professional programmers, but which is still useful for more ordinary folks) for debugging is to use `print()` statements in your code. For example, consider the following code:

```
if ( any( is.na( rs$estimate ) ) ) {
    cat( "There are NAs in the estimates!\n" )
}
```

Here we are printing something out that we suspect might be something we want to check.

There are a few methods for printing to the console: `print()`, which takes any object and prints it out. You can print a dataframe, variable, or a string:

```
print( "My var is ", my_var, "\n" )
print( my_tibble )
```

You can use `cat()`, which is designed to print strings:

```r
cat( "My var is ", my_var, "\n" )
```

You can use the `cli` package, which gives a bit of a nicer printout, and allows for easier formatting:

```r
cli::cli_alert("My var is {my_var}")
```

The problem with printing is it is easy to have a lot of printout statements, and then when you run your code you get a wall of text. For simulations, it is easy to print so much that it will meaningfully slow your simulation down! You can use `print()` statements to help you figure out what is going on, but it is often better to use a more interactive debugging tool, such as the `browser()` function or `stopifnot()` statements, which we will discuss next.

19.2   Debugging with browser

Consider the following code taken from a simulation:

```r
if ( any( is.na( rs$estimate ) ) ) {
    browser()
}
```

The `browser()` command stops your code and puts you in an interactive console where you can look at different objects and see what is happening. Having it triggered when something bad happens (in this case when a set of estimates has an unexpected NA) can help untangle what is driving a rare event.

The interactive console allows you to look at the current state of the code, and you can type in commands to see what is going on. It is just like a normal R workspace, but if you look at the Environment, you will only see what the code has available at the time `browser()` was called. If you are inside a function, for example, you will only see the things passed to the function, and the variables the function has made.

This can be very important to, for example, check what values were passed to your function–many bugs are due to the wrong thing getting passed to some code that would otherwise work.

Once in a browser, you can say `q` to quit out. You can also type `n` to go to the next line of code. This allows you to walk through the code step by step, seeing what happens as you move along. Much of the time, RStudio will even jump to the part of your script where you paused, so you can see the code that will be run with each step.

19.3   Debugging with debug

Another useful debugging tool is the `debug()` function. This function allows you to set a breakpoint in your code, so that when you call the function, it will stop at the beginning of the function and put you in the same browser discussed above. You use it like this:

```
debug( gen_dat )
run_simulation( some_parameters )
```

Now, when `run_simulation()` eventually calls `gen_dat` the script will stop, and you can see exactly what was passed to `gen_dat` and also then walk through `gen_dat` line by line to see what is going on.

19.4   Protecting your functions with "stop"

When writing functions, especially those that take a lot of parameters, it is often wise to include `stopifnot()` statements at the top to verify the function is getting what it expects. These are sometimes called "assert statements" and are a tool for making errors show up as early as possible. For example, look at this (fake) example of generating data with different means and variances

```
make_groups <- function( means, sds ) {
  Y = rnorm( length(means), mean=means, sd = sds )
  round( Y )
}
```

If we call it, but provide different lengths for our means and variances, nothing happens, because R simply recycles the standard deviation parameter:

```
make_groups( c(100,200,300,400),
             c(1,100,10000) )
```

```
## [1]   101   204 17426   400
```

What is nasty about this possible error is nothing is telling you that something is wrong! You could build an entire simulation on this, not realizing that your fourth group has the variance of your first, and get results that make no sense to you. You could even publish something based on a finding that depends on this error, which would eventually be quite embarrasing.

If this function was used in our data generating code, we might eventually see some warning that something is off, but this would still not tell us where things went off the rails. We can instead protect our function by putting in an *assert statement* using `stopifnot()`:

```
make_groups <- function( means, sds ) {
  stopifnot( length(means) == length(sds) )
  Y = rnorm( length(means), mean=means, sd = sds )
```

```
  round( Y )
}
```

Now we get this:

```
make_groups( c(100,200,300,400),
             c(1,100,10000) )
```

```
## Error in make_groups(c(100, 200, 300, 400), c(1, 100, 10000)): length(means) == len
```

The `stopifnot()` command ensures your code is getting called as you intended.

These statements can also serve as a sort of documentation as to what you expect. Consider, for example:

```
make_xy <- function( N, mu_x, mu_y, rho ) {
  stopifnot( -1 <= rho && rho <= 1 )
  X = mu_x + rnorm( N )
  Y = mu_y + rho * X + sqrt(1-rho^2)*rnorm(N)
  tibble(X = X, Y=Y)
}
```

Here we see that rho should be between -1 and 1 quite clearly. A good reminder of what the parameter is for.

This also protects you from inadvetently misremembering the order of your parameters when you call the function (although it is good practice to name your parameters as you pass). Consider:

```
a <- make_xy( 10, 2, 3, 0.75 )
b <- make_xy( 10, 0.75, 2, 3 )
```

```
## Error in make_xy(10, 0.75, 2, 3): -1 <= rho && rho <= 1 is not TRUE
```

```
c <- make_xy( 10, rho = 0.75, mu_x = 2, mu_y = 3 )
```

Part V

Complex Data Structures

Chapter 20

Using simulation as a power calculator

We can use simulation as a power calculator. In particular, to estimate power, we generate data according to our best guess as to what we might find in a planned evaluation, and then analyze these synthetic data and see if we detect the effect we built into our DGP. We then do this repeatedly, and see how often we detect our effect. This is power.

Now, if we are generally right about our guesses about our DGP and the associated parameters we plugged into it, in terms of some planned study, then our power will be right on. This is all a power analysis is, using simulation or otherwise.

Simulation has benefits over using power calculators because we can take into account odd aspects of our modeling, and also do non-standard approaches to evaluation that we might not find in a normal power calculator.

We illustrate this idea with a case study. In this example, we are planning a school-level intervention to reduce rates of discipline via a socio-emotional targeting intervention on both teachers and students, where we have strongly predictive historic data and a time-series component. This is a planned RCT, where we will treat entire schools (so a cluster-randomized study). We are struggling because treating each school is very expensive (we have to run a large training and coaching of the staff), so each unit is a major decision. We want something like 4, 5, or maybe 6 treated schools. Our diving question is: Can we get away with this?

20.1   Getting design parameters from pilot data

We had pilot data from school administrative records (in particular discipline rates for each school and year for a series of five years), and we use those to estimate parameters to plug into our simulation. We assume our experimental sample will be on schools that have chronic issues with discipline, so we filtered our historic data to get schools we imagined to likely be in our study.

We ended up with the following data, with log-transformed discipline rates for each year (we did this to put things on a multiplicative scale, and to make our data more normal given heavy skew in the original). Each row is a potential school in the district.

```
datW = read_csv( "data/discipline_data.csv" )
```

```
## Rows: 27 Columns: 6
## -- Column specification ------
## Delimiter: ","
## chr (1): Code
## dbl (5): 2015, 2016, 2017, 2018, 2019
##
## i Use `spec()` to retrieve the full column specification for this data.
## i Specify the column types or set `show_col_types = FALSE` to quiet this message.
```

```
datW
```

```
## # A tibble: 27 x 6
##     Code  `2015` `2016` `2017` `2018` `2019`
##     <chr>  <dbl>  <dbl>  <dbl>  <dbl>  <dbl>
##  1 S1     -2.87  -2.81  -2.93  -3.52  -4.90
##  2 S2     -3.60  -2.83  -2.56  -2.76  -3.32
##  3 S3     -3.00  -2.88  -2.81  -3.39  -4.91
##  4 S4     -3.90  -3.20  -2.53  -3.67  -4.34
##  5 S5     -2.46  -2.00  -3.34  -3.66  -4.71
##  6 S6     -2.86  -2.74  -2.51  -3.21  -3.80
##  7 S7     -2.47  -2.59  -2.69  -2.15  -2.43
##  8 S8     -2.13  -1.93  -1.82  -2.21  -2.95
##  9 S9     -3.36  -3.16  -3.06  -3.26  -3.10
## 10 S10    -2.89  -2.54  -2.26  -2.89  -3.25
## # i 17 more rows
```

We use these to calculate a mean and covariance structure for generating data:

```
lpd_mns = apply( datW[,-1], 2, mean )
lpd_mns
```

```
##       2015      2016      2017      2018      2019
## -3.076298 -2.868337 -2.931562 -3.337221 -4.011440
```

```
lpd_cov = cov( datW[,-1] )
lpd_cov
```

```
##              2015      2016      2017      2018
## 2015 0.4191843 0.2996073 0.2282627 0.3691894
## 2016 0.2996073 0.3656335 0.2014201 0.2511376
## 2017 0.2282627 0.2014201 0.3084799 0.2927782
## 2018 0.3691894 0.2511376 0.2927782 0.5767486
## 2019 0.1921622 0.1623542 0.2541191 0.2927812
##              2019
## 2015 0.1921622
## 2016 0.1623542
## 2017 0.2541191
## 2018 0.2927812
## 2019 0.5425783
```

20.2   The data generating process

We then write a data generator that, given a desired number of control and treatment schools, and a treatment effect, makes a dataset by sampling vectors of discipline rates, and then imposes a "treatment effect" of scaling the discipline rate by the treatment coefficient for the last two years.

```r
make_dat_param = function( n_c, n_t, tx=1 ) {
    n = n_c + n_t
    lpdisc = MASS::mvrnorm( n, mu = lpd_mns, Sigma = lpd_cov )
    lpdisc = exp( lpdisc )
    colnames( lpdisc ) = paste0( "pdisc_", colnames( lpdisc ) )
    lpdisc = as.data.frame( lpdisc ) %>%
        mutate( ID = 1:n(),
                Z = 0 + ( sample( n ) <= n_t ) )

    # Add in treatment effect
    lpdisc = mutate( lpdisc,
                     pdisc_2018 = pdisc_2018 * ifelse( Z == 1, tx, 1 ),
                     pdisc_2019 = pdisc_2019 * ifelse( Z == 1, tx, 1 ) )

    lpdisc %>%
      relocate( ID, Z )
}
```

Our function generates schools with discipline given by the provided mean and covariance structure; we have calibrated our data generating process to give us data that looks very similar to the data we would see in the field.

For our impact model, the treatment kicks in for the final two years, multiplying

discipline rate by `tx` (so `tx = 1` means no treatment effect).

Testing our function gives this:

```r
set.seed( 59585 )
a = make_dat_param( 100, 100, 0.5 )
head( a, n = 4 )
```

```
##   ID Z pdisc_2015 pdisc_2016 pdisc_2017
## 1  1 1 0.03118036 0.05594299 0.03283595
## 2  2 1 0.04209213 0.01716175 0.02388633
## 3  3 1 0.18736890 0.26266248 0.14379326
## 4  4 0 0.04389430 0.04571297 0.03378810
##   pdisc_2018  pdisc_2019
## 1 0.01051475 0.005732411
## 2 0.01155785 0.009120705
## 3 0.04832345 0.027621311
## 4 0.01101846 0.007154335
```

We can group each treatment arm and look at discipline over the years:

```r
aL = a %>%
    pivot_longer( pdisc_2015:pdisc_2019,
                  names_to = c( ".value", "year" ),
                  names_pattern = "(.*)_(.*)" ) %>%
    mutate( year = as.numeric( year ) )

aLg = aL %>% group_by( year, Z ) %>%
    summarise( pdisc = mean( pdisc ) )
ggplot( aLg, aes( year, pdisc, col=as.factor(Z) ) ) +
    geom_line() +
  labs( color = "Tx?" )
```
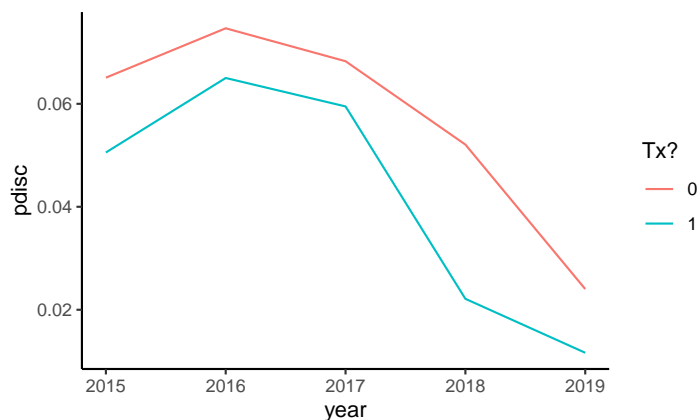

Our treatment group drops faster than the control. We see the nonlinear struc-
ture actually observed in our original data in terms of discipline over time has

been replicated.

We next write some functions to analyze our data. This should feel very familiar:
we are just doing our simulation framework, as usual.

```r
eval_dat = function( sdat ) {

    # No covariate adjustment, average change model (on log outcome)
    M_raw = lm( log( pdisc_2018 ) ~ 1 + Z, data=sdat )

    # Simple average change model using 2018 as outcome.
    M_simple = lm( pdisc_2018 ~ 1 + Z + pdisc_2017 + pdisc_2016 + pdisc_2015,
                   data=sdat )

    # Simple model on logged outcome
    M_log = lm( log( pdisc_2018 ) ~ 1 + Z + log( pdisc_2017) + log( pdisc_2016) + log( pdisc_2015
                data=sdat )

    # Ratio of average disc to average prior disc as outcome
    sdat = mutate( sdat,
                   avg_disc = (pdisc_2018 + pdisc_2019)/2,
                   prior_disc = (pdisc_2017 + pdisc_2016 + pdisc_2015 )/3,
                   disc = pdisc_2018 / prior_disc,
                   disc_two = avg_disc / prior_disc )
    M_ratio = lm( disc ~ 1 + Z, data = sdat )
    M_ratio_twopost = lm( disc_two ~ 1 + Z, data = sdat )

    # Use average of two post-tx time periods, averaged to reduce noise
    M_twopost = lm( log( avg_disc ) ~ 1 + Z + log( pdisc_2017 ) + log( pdisc_2016 ) + log( pdisc_

    # Time and unit fixed effects
    sdatL = pivot_longer( sdat, cols = pdisc_2015:pdisc_2019,
                          names_to = "year",
                          values_to = "pdisc" ) %>%
        mutate( Z = Z * (year %in% c( "pdisc_2018", "pdisc_2019" ) ),
                ID = paste0( "S", ID ) )

    M_2wfe = lm( log( pdisc ) ~ 0 + ID + year + Z,
                 data=sdatL )

    # Bundle all our models by getting the estimated treatment impact
    # from each.
    models <- list( raw=M_raw, simple=M_simple,
                    log=M_log, ratio = M_ratio,
                    ratio_twopost = M_ratio_twopost,
                    log_twopost = M_twopost,
```

```
                        FE = M_2wfe )
    rs <- map_df( models, broom::tidy, .id="model" ) %>%
        filter( term=="Z" ) %>%
        dplyr::select( -term ) %>%
      arrange( model )

    rs
}
```

Our method marches through a host of models; we weren't sure what the gains would be from one model to another, so we decided to conduct power analyses on all of them. Again, we look at what our evaluation function does:

```
dat = make_dat_param( n_c = 4, n_t = 4, tx = 0.5 )
eval_dat( dat )
```

```
## # A tibble: 7 x 5
##   model       estimate std.error statistic p.value
##   <chr>          <dbl>     <dbl>     <dbl>   <dbl>
## 1 FE          -0.644      0.325     -1.98  0.0576
## 2 log         -0.841      0.478     -1.76  0.176
## 3 log_twopost -1.22       0.437     -2.80  0.0680
## 4 ratio       -0.126      0.136     -0.923 0.392
## 5 ratio_twop~ -0.269      0.139     -1.93  0.102
## 6 raw         -0.650      0.300     -2.17  0.0733
## 7 simple      -0.00983    0.0133    -0.742 0.512
```

We have a nice set of estimates, one for each model.

20.3   Running the simulation

Now we put it all together in our classic simulator:

```
sim_run = function( n_c, n_t, tx, R, seed = NULL ) {
    if ( !is.null( seed ) ) {
        set.seed(seed)
    }
    cat( "Running n_c, n_t =", n_c, n_t, "tx =", tx, "\n" )
    rps = rerun( R, {
        sdat = make_dat_param(n_c = n_c, n_t = n_t, tx = tx)
        eval_dat( sdat )
    })
    bind_rows( rps )
}
```

We then do the usual to run across a set of scenarios, running `sim_run` on each row of the following:

```r
res = expand_grid( tx = c( 1, 0.75, 0.5 ),
                   n_c = c( 4, 5, 6, 8, 12, 20 ),
                   n_t = c( 4, 5, 6 ) )
res$R = 1000
res$seed = 1010203 + 1:nrow(res)
```

For evaluation, we load our saved results and calculate rejection rates (we use an alpha of 0.10 since we are doing one-sided testing):

```r
res = readRDS( file="data/discipline_simulation.rds" )

sres <- res %>% group_by( n_c, n_t, tx, model ) %>%
    summarise( E_est = mean( estimate ),
               SE = sd( estimate ),
               E_SE_hat = mean( std.error ),
               pow = mean( p.value <= 0.10 ) ) # one-sided testing
sres
```

```
## # A tibble: 378 x 8
## # Groups:   n_c, n_t, tx [54]
##      n_c   n_t    tx model    E_est      SE E_SE_hat
##    <dbl> <dbl> <dbl> <chr>    <dbl>   <dbl>    <dbl>
## 1      4     4   0.5 FE      -0.693  0.313    0.277
## 2      4     4   0.5 log     -0.694  0.476    0.430
## 3      4     4   0.5 log_~   -0.692  0.431    0.383
## 4      4     4   0.5 ratio   -0.374  0.219    0.203
## 5      4     4   0.5 rati~   -0.291  0.151    0.139
## 6      4     4   0.5 raw     -0.719  0.535    0.515
## 7      4     4   0.5 simp~   -0.0195 0.0194   0.0157
## 8      4     4  0.75 FE      -0.292  0.310    0.274
## 9      4     4  0.75 log     -0.295  0.488    0.435
## 10     4     4  0.75 log_~   -0.305  0.424    0.373
## # i 368 more rows
## # i 1 more variable: pow <dbl>
```

20.4   Evaluating power

Once our simulation is run, we can explore power as a function of the design characteristics. In particular, we eventually want to calculate the chance of noticing effects of different sizes, given various sample sizes we might employ. Our driving question is how few schools on the treated side can we get away with? Also, we want to know how much having more schools on the control side allows us to get away with fewer schools on the treated side.

20.4.1   Checking validity of our models

Before we look at power, we need to check on whether our different models are valid. This is especiallt important as we are in a small n context, so we know asymptotics may not hold as they should. To check our models for validity we subset our trials to where `tx = 1`, and look at the rejection rates.

We first run a regression to see if rejection is a function of sample size (are smaller samples more invalid) and treatment-control imbalance. We center both variables so our intercepts are overall average rejection rates for each model considered:

```r
sres = mutate( sres,
               n = n_c + n_t,
               imbalance = pmax( n_t / n_c, n_c / n_t ) - 1 )
sres$n = (sres$n - mean(sres$n)) / sd(sres$n)
mod = lm( pow ~ 0 + (n + imbalance) * model - n - imbalance,
          data = filter( sres, tx == 1 ) )
broom::tidy(mod) %>%
  knitr::kable( digits = 3)
```

term	estimate	std.error	statistic	p.value
modelFE	0.143	0.006	24.593	0.000
modellog	0.099	0.006	16.999	0.000
modellog_twopost	0.093	0.006	15.939	0.000
modelratio	0.090	0.006	15.437	0.000
modelratio_twopost	0.093	0.006	15.967	0.000
modelraw	0.092	0.006	15.751	0.000
modelsimple	0.091	0.006	15.571	0.000
n:modelFE	-0.003	0.006	-0.459	0.647
n:modellog	0.001	0.006	0.141	0.888
n:modellog_twopost	-0.005	0.006	-0.919	0.360
n:modelratio	0.000	0.006	0.071	0.944
n:modelratio_twopost	0.002	0.006	0.414	0.680
n:modelraw	-0.006	0.006	-1.008	0.316
n:modelsimple	0.001	0.006	0.191	0.849
imbalance:modelFE	0.005	0.005	0.857	0.394
imbalance:modellog	-0.003	0.005	-0.587	0.558
imbalance:modellog_twopost	0.004	0.005	0.708	0.480
imbalance:modelratio	0.000	0.005	-0.001	0.999
imbalance:modelratio_twopost	0.001	0.005	0.249	0.804
imbalance:modelraw	0.006	0.005	1.154	0.251
imbalance:modelsimple	0.001	0.005	0.180	0.858

We can also plot the nominal rejection rates under the null:

```r
sres %>% filter( tx == 1 ) %>%
ggplot( aes( n_c, pow, col=model ) ) +
```

```r
facet_wrap( ~ n_t, nrow=1 ) +
geom_line() +
geom_hline( yintercept = 0.10 ) +
scale_x_log10(breaks=unique(sres$n_c) )
```
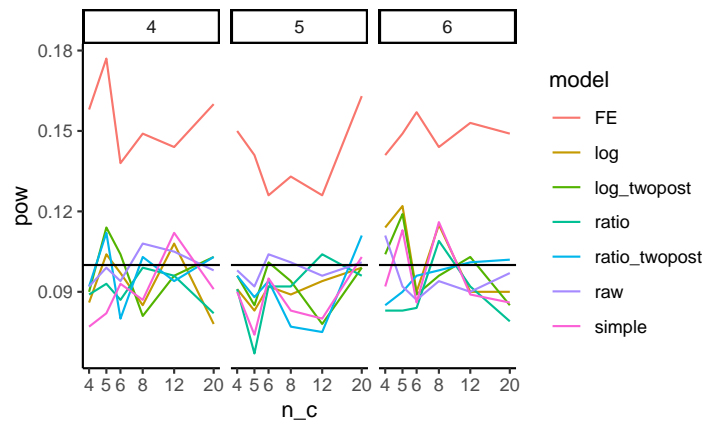

We see the fixed effect models have elevated rates of rejection. Interestingly, these rates do not seem particularly dependent on sample size or treatment-control imbalance (note lack of significant coefficeints on our regression model). The other models all appear valid.

We can also check for bias of our methods:

```r
sres %>% group_by( model, tx ) %>%
  summarise( E_est = mean( E_est ) ) %>%
  pivot_wider( names_from="tx", values_from="E_est" )
```

```
## # A tibble: 7 x 4
## # Groups:   model [7]
##   model           `0.5`   `0.75`        `1`
##   <chr>           <dbl>    <dbl>      <dbl>
## 1 FE             -0.692  -0.290  -0.000703
## 2 log            -0.692  -0.288   0.00120
## 3 log_twopost    -0.692  -0.291   0.00241
## 4 ratio          -0.372  -0.187  -0.000937
## 5 ratio_twopost  -0.289  -0.145  -0.00108
## 6 raw            -0.694  -0.290   0.00327
## 7 simple         -0.0206 -0.0104  0.0000998
```

We see our models are estimating different things, none of which are the treatment effect as we parameterized it. In particular, "FE," "log," "raw," and "log_twopost" are all estimating the impact on the log scale. Note that $log(0.5) \approx -0.69$ and $log(0.75) \approx -0.29$. Our "simple" estimator is estimating the impact on the absolute scale; reducing discipline rates by 50% corresponds

to about a 2% reduction in actual cases. Finally, "ratio" and "ratio_twopost" are estimating the change in the average ratio of post-policy discipline to pre; they are akin to a gain score as compared to the log regressions.

20.4.2 Assessing Precision (SE)

Now, which methods are the most precise? We look at the true standard errors across our methods (we drop "simple" and the "ratio" estimators since they are not on the ratio scale):

```r
sres %>%
  group_by( model, n_c, n_t ) %>%
  summarise( SE = mean(SE ) ) %>%
  filter( !(model %in% c( "simple", "ratio", "ratio_twopost" ) ) ) %>%
  ggplot( aes( n_c, SE, col=model )) +
    facet_grid( . ~ n_t ) +
    geom_line() + geom_point() +
    geom_hline( yintercept = 0 ) +
  labs( colour = "Model" )
```
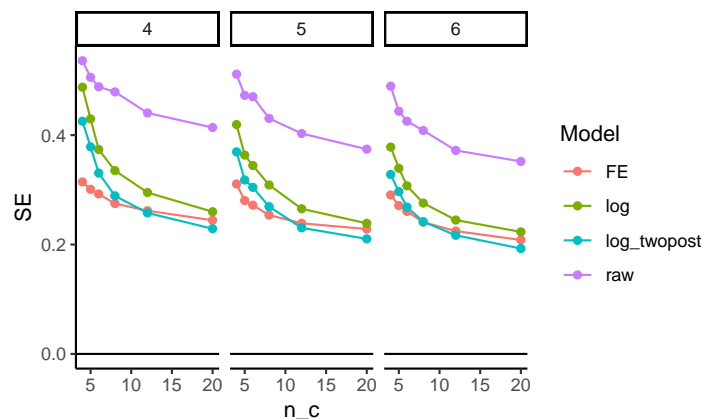

It looks like averaging two years for the outcome is helpful, and bumps up precision. The two way fixed effects model seems to react to the number of control units differently than the other estimators; it is way more precise when the number of controls is few, but the other estimators catch up. The "raw" estimator gives a baseline of no covariate adjustment; everything is substantially more precise than it. The covariates matter a lot.

20.4.3 Assessing power

We next look at power over our explored contexts, for the models that we find to be valid (i.e., not FE).

```r
sres %>%
  filter( model != "FE",tx != 1 ) %>%
```

```
ggplot( aes( n_c, pow, col=model )) +
  facet_grid(  . ~ tx + n_t, labeller = label_both ) +
  geom_line() + geom_point() +
  geom_hline( yintercept = 0, col="grey" ) +
  geom_hline( yintercept = c( 0.10, 0.80 ), lty=2 ) +
theme_minimal()+ theme( legend.position="bottom",
                        legend.direction="horizontal",
                        legend.key.width=unit(1,"cm"),
                        panel.border = element_blank() ) +
labs( title="Power for various methods vs number of controls.",
    y = "Power" )
```


Power for various methods vs number of controls.
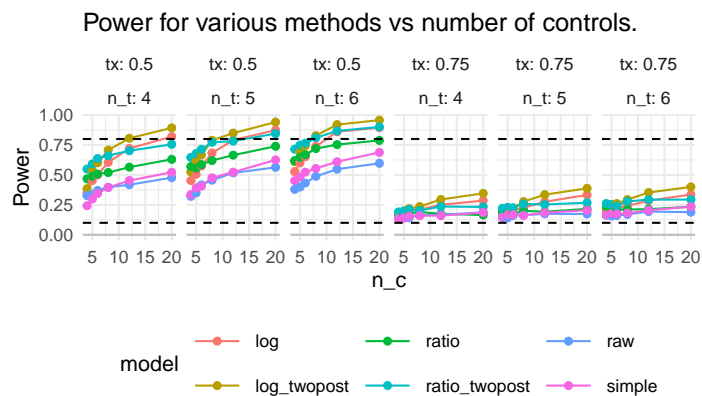
We mark 80% power with a dashed line. For a 25% reduction in discipline, nothing reaches desired levels of power. For 50% reduction, some designs do, but we need substantial numbers of control schools. Averaging two years of outcomes post-treatment seems important: the "twopost" methods have a distinct power bump. For a single year of outcome data, the log model seems our best bet.

20.4.4 Assessing Minimum Detectable Effects

Sometimes we want to know, given a design, what size effect we might be able to detect. The usual measure for this is the Minimum Detectable Effect (MDE), which is usually the size of the smallest effect we could detect with power 80%.

To calculate Minimal Detectable Effects (MDEs) for the log-scale estimators, we first average our SEs over our different designs, grouped by sample size, and then convert the SEs to MDEs by multiplying by 2.8. We then have to convert to our treatment scale by flipping the sign and exponentiating, to get out of the log scale.

```
sres2 = sres %>%
  group_by( model, n_c, n_t ) %>%
  summarise( SE = mean( SE ),
             E_SE_hat = mean( E_SE_hat ) ) %>%
```

```r
  mutate( MDE = exp( - (1.64 + 0.8) * SE ) )

sres2 %>%
  filter( !(model %in% c( "simple", "ratio", "ratio_twopost" ) ) ) %>%
  ggplot( aes( n_c, MDE, col=model ) ) +
  facet_wrap( ~ n_t, labeller = label_both ) +
  geom_point() + geom_line()  +
  geom_hline( yintercept = 0.5 ) +
  theme_minimal() +
  scale_x_log10( breaks = unique( sres$n_c ) ) +
  theme( legend.position="bottom",
         legend.direction="horizontal", legend.key.width=unit(1,"cm"),
         panel.border = element_blank() ) +
  labs( x = "Number of control units", y = "MDE (proportion reduction of rate)",
        caption = "A MDE of 0.6 means a 60% reduction (more than half) in discipline r
        title = "MDE vs number of control units for various methods" )
```


A MDE of 0.6 means a 60% reduction (more than half) in discipline rates
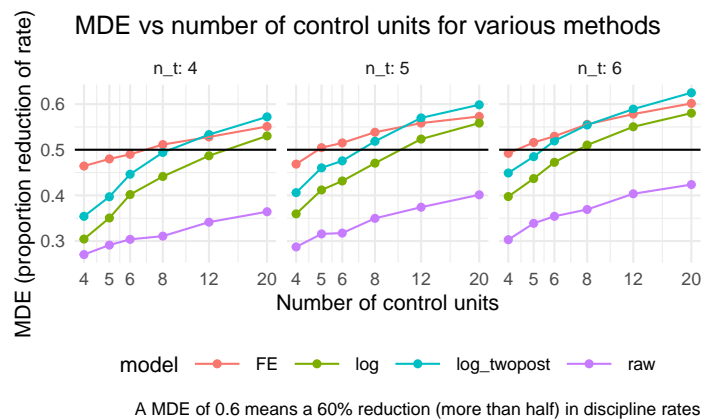
Corresponding with our findings regarding precision, above, the twopost estimator is the most sensitive, finding the smallest effects.

Chapter 21

Simulation under the Potential Outcomes Framework

If we are in the business of evaluating how various methods such as matching or propensity score weighting work in practice, we would probably turn to the potential outcomes framework for our simulations. The potential outcomes framework is a framework typically used in the causal inference literature to make very explicit statements regarding the mechanics of causality and the associated estimands one might target when estimating causal effects. While we recommend reading, for a more thourough overview, either [CITE Raudenbush or Field Experiments textbook], we briefly outline this framework here to set out our notation.

Take a sample of experimental units, indexed by i. For each unit, we can treat it or not. Denote treatment as $Z_i = 1$ for treated or $Z_i = 0$ for not treated. Now we imagine each unit has two potential outcomes being the outcome we would see if we treated it ($Y_i(1)$) or if we did not ($Y_i(0)$). Finally, our observed outcome is then

$$Y_i^{obs} = Z_i Y_i(1) + (1 - Z_i) Y_i(0).$$

For a unit, the treatment effect is $\tau_i = Y_i(1) - Y_i(0)$; it is how much our outcome changes if we treat vs. not treat. Frustratingly, for each unit we can only see one of its two potential outcomes, so we can never get an estimate of these individual τ_i. Under this view, causality is a missing data problem: if we only were able to impute the missing potential outcomes, we could have a dataset where we could calculate any estimands we wanted. E.g., the true average treatment effect *for the sample $\mathcal{S}$* would be:

$$ATE_{\mathcal{S}} = \frac{1}{N} \sum_i Y_i(1) - Y_i(0).$$

The average proportion increase, by contrast, would be

$$API_{\mathcal{S}} = \frac{1}{N} \sum_i \frac{Y_i(1)}{Y_i(0)}$$

21.1 Finite vs. Superpopulation inference

Consider a sample of n units, $\mathcal{S}$, along with their set of potential outcomes. We can talk about the true ATE of the sample, or, if we thought of the sample as being drawn from some larger population, we could talk about the true ATE of that larger population.

This is a tension that often arises in potential outcomes based simulations: if we are focused on $ATE_{\mathcal{S}}$ then for each sample we generate, our estimand could be (maybe only slightly) different, depending on whether our sample has more or fewer units with high τ_i. If, on the other hand, we are focused on where the units came from (which is our data generating model), our estimand is a property of the DGP, and would be the same for each sample generated.

The catch is when we calculate our performance metrics, we now have two possible targets to pick from. Furthermore, if we are targeting the superpopulation ATE, then our error in estimation may be due in part to the representativeness of the sample, *not* the estimation or uncertainty due to the random assignment.

We will follow this theme throughout this chapter.

21.2 Data generation processes for potential outcomes

If we want to write a simulation using the potential outcomes framework, it is clear and transparent to first generate a complete set of potential outcomes, then generate a random assignment based on some assignment mechanism, and finally generate the observed outcomes as a function of assignment and original potential outcomes.

For example, we might say that our data generation process is as follows: First generate each unit $i = 1, \ldots, n$, as

$$
\begin{aligned}
X_i &\sim exp(1) - 1 \\
Y_i(0) &= \beta_0 + \beta_1 X_i + \epsilon_i \text{ with } \epsilon_i \sim N(0, \sigma^2) \\
\tau_i &= \tau_0 + \tau_1 X_i + \alpha u_i \text{ with } u_i \sim t_{df} \\
Y_i(1) &= Y_i(0) + \tau_i
\end{aligned}
$$

with $exp(1)$ being the standard exponential distribution and t_{df} being a t distribution with df degrees of freedom. We subtract 1 from X_i to zero-center it (it is often convenient to have zero-centered covariates so we can then, e.g., interpret τ_0 as the true superpopulation ATE of our experiment).

The above model is saying that we first, for each unit, generate a covariate. We then generate our two potential outcomes. I.e., we are generating what the outcome would be for each unit if it were treated and if it were not treated. We are driving both the level and the treatment effect with X_i, assuming β_1 and τ_1 are non-zero.

One advantage of generating all the potential outcomes is we can then calculate the finite-sample estimands such as the true average treatment effect for the generated sample: we just take the average of $Y_i(1) - Y_i(0)$ for our sample.

Here is some code to illustrate the first part of the data generating process (we leave treatment assignment to later):

```r
gen_data <- function( n = 100,
                      R2 = 0.5,
                      beta_0 = 0, beta_1 = 1,
                      tau_0 = 1, tau_1 = 1,
                      alpha = 1, df = 3 ) {
  stopifnot( R2 >= 0 && R2 < 1 )
  X_i = rexp( n, rate = 1 ) - 1
  beta_1 = sqrt( 1 - R2 )
  sigma_e = sqrt( R2 )
  Y0_i = beta_0 + beta_1 * X_i + rnorm( n, sd=sigma_e )
  tau_i = tau_0 + tau_1 * X_i + alpha * rt( n, df = df )
  Y1_i = Y0_i + tau_i

  tibble( X = X_i, Y0 = Y0_i, Y1 = Y1_i )
}
```

And now we see our estimand can change:

```r
set.seed( 40454 )
d1 <- gen_data( 50 )
mean( d1$Y1 - d1$Y0 )
```

```
## [1] 0.6374925
```

```r
d2 <- gen_data( 50 )
mean( d2$Y1 - d2$Y0 )
```

```
## [1] 0.5479788
```

In reviewing our code, we know our superpopulation ATE should be `tau`, or 1 exactly. If our estimate for `d1` is 0.6 do we say that is close or far from the target? From a finite sample performance approach, we nailed it. From

superpopulation, less so.

Also in looking at the above, there are a few details to call out:

- We can store the latent, intermediate quantities (both potential outcomes, in particular) so we can calculate the estimands of interest or learn about our data generating process. When we hand the data to an estimator, we would not provide this "secret" information.
- We are using a trick to index our DGP by an R2 value rather than co-efficients on X so we can have a standardized control-side outcome (the expected variation of $Y_i(0)$ will be 1). The treatment outcomes will have more variation due to the heterogeniety of the treatment impacts.
- If we were generating data with a constant treatment impact, then $ATE_{\mathcal{S}} = ATE$ always; this is typical for many similations in the literature. That being said, treatment variation is what causes a lot of methods to fail and so having simulations that have this variation is usually important.

Once we have our *schedule of potential outcomes*, we would then generate the *observed outcomes* by assigning our (synthetic, randomly generated) n units to treatment or control. For example, say we wanted to simulate an observational context where treatment was a function of our covariate. We could model each unit as flipping a weighted coin with some probability that was a function of X_i as so:

$$
\begin{aligned}
p_i &= logit^{-1}(\xi_0 + \xi_1 X_i) \\
Z_i &= Bern(p_i) \\
Y_i &= Z_i Y_i(1) + (1 - Z_i) Y_i(0)
\end{aligned}
$$

Here is code for assigning our data to treatment and control:

```r
assign_data <- function( dat,
                         xi_0 = -1, xi_1 = 1 ) {
  n = nrow(dat)
  dat = mutate( dat,
                p = arm::invlogit( xi_0 + xi_1 * X ),
                Z = rbinom( n, 1, prob=p ),
                Yobs = ifelse( Z == 1, Y1, Y0 ) )
  dat
}
```

We can then add our assignment variable to our given data as so:

```r
assign_data( d2 )
```

```
## # A tibble: 50 x 6
##           X     Y0     Y1      p     Z    Yobs
##       <dbl>  <dbl>  <dbl>  <dbl> <int>   <dbl>
```

```
## 1  0.670     0.667   2.58  0.418     1    2.58
## 2  0.371     0.314   4.57  0.348     1    4.57
## 3  1.94      1.29    3.03  0.719     0    1.29
## 4 -0.244     0.119 -10.0   0.224     1 -10.0
## 5  0.00850   1.44    2.88  0.271     0    1.44
## 6  1.41      1.14    5.02  0.600     1    5.02
## 7 -0.864     0.461   0.802 0.134     1    0.802
## 8 -0.00533 -0.914   -1.17  0.268     0   -0.914
## 9 -0.907    -0.202   0.555 0.129     1    0.555
## 10 -0.363   -0.141   1.16  0.204     1    1.16
## # i 40 more rows
```

Note how `Yobs` is, depending on `Z`, either `Y0` or `Y1`. Separating our our DGP and our random assignment underscores the potential outcomes framework adage of the data are what they are, and we the experimenters (or nature) is randomly assigning these whole units to various conditions and observing the consequences.

In general, we might instead put the `p_i` part of the model in our code generating the outcomes, if we wanted to view the chance of treatment assignment as inherent to the unit (which is what we usually expect in an observational context).

21.3   Finite sample performance measures

Let's generate a single dataset with our DGP from above, and run a small experiment where we actually randomize units to treatment and control:

```
n = 100
set.seed(442423)
dat = gen_data(n, tau_1 = -1)
dat = mutate( dat,
              Z = 0 + (sample( n ) <= n/2),
              Yobs = ifelse( Z == 1, Y1, Y0 ) )
mod = lm( Yobs ~ Z, data=dat )
coef(mod)[["Z"]]
```

```
## [1] 0.8914992
```

We can compare this to the true finite-sample ATE:

```
mean( dat$Y1 - dat$Y0 )
```

```
## [1] 1.154018
```

Our finite-population simulation would be:

```
rps <- rerun( 1000, {
  dat = mutate( dat,
               Z = 0 + (sample( n ) <= n/2),
```

```
              Yobs = ifelse( Z == 1, Y1, Y0 ) )
  mod = lm( Yobs ~ Z, data=dat )
  tibble( ATE_hat = coef(mod)[["Z"]],
          SE_hat = arm::se.coef(mod)[["Z"]] )
}) %>%
bind_rows()
```

```
## Warning: `rerun()` was deprecated in purrr 1.0.0.
## i Please use `map()` instead.
##    # Previously
## rerun(1000, {
## dat = mutate(dat, Z = 0 + (sample(n) <= n / 2),
## Yobs = ifelse(Z == 1, Y1, Y0))
## mod = lm(Yobs ~ Z, data = dat)
## tibble(ATE_hat = coef(mod)[["Z"]], SE_hat =
## arm::se.coef(
## mod)[["Z"]])
## })
##
##    # Now
## map(1:1000, ~ {
## dat = mutate(dat, Z = 0 + (sample(n) <= n / 2),
## Yobs = ifelse(Z == 1, Y1, Y0))
## mod = lm(Yobs ~ Z, data = dat)
## tibble(ATE_hat = coef(mod)[["Z"]], SE_hat =
## arm::se.coef(
## mod)[["Z"]])
## })
## This warning is displayed once every 8 hours.
## Call `lifecycle::last_lifecycle_warnings()` to
## see where this warning was generated.
```

```
rps %>% summarise( EATE_hat = mean( ATE_hat ),
                   SE = sd( ATE_hat ),
                   ESE_hat = mean( SE_hat ) )
```

```
## # A tibble: 1 x 3
##   EATE_hat     SE ESE_hat
##      <dbl> <dbl>   <dbl>
## 1     1.16 0.248   0.307
```

We are simulating on a single dataset. In particular, our set of potential outcomes is entirely fixed; the only source of randomness (and thus the randomness behind our SE) is the random assignment. Now this opens up some room for critique: what if our single dataset is non-standard?

Our super-population simulation would be, by contrast:

```r
rps_sup <- rerun( 1000, {
  dat = gen_data(n)
  dat = mutate( dat,
             Z = 0 + (sample( n ) <= n/2),
             Yobs = ifelse( Z == 1, Y1, Y0 ) )
  mod = lm( Yobs ~ Z, data=dat )
  tibble( ATE_hat = coef(mod)[["Z"]],
          SE_hat = arm::se.coef(mod)[["Z"]] )
}) %>%
  bind_rows()
```

```
## Warning: `rerun()` was deprecated in purrr 1.0.0.
## i Please use `map()` instead.
##   # Previously
## rerun(1000, {
## dat = gen_data(n)
## dat = mutate(dat, Z = 0 + (sample(n) <= n / 2),
## Yobs = ifelse(Z == 1, Y1, Y0))
## mod = lm(Yobs ~ Z, data = dat)
## tibble(ATE_hat = coef(mod)[["Z"]], SE_hat =
## arm::se.coef(
## mod)[["Z"]])
## })
##
##   # Now
## map(1:1000, ~ {
## dat = gen_data(n)
## dat = mutate(dat, Z = 0 + (sample(n) <= n / 2),
## Yobs = ifelse(Z == 1, Y1, Y0))
## mod = lm(Yobs ~ Z, data = dat)
## tibble(ATE_hat = coef(mod)[["Z"]], SE_hat =
## arm::se.coef(
## mod)[["Z"]])
## })
## This warning is displayed once every 8 hours.
## Call `lifecycle::last_lifecycle_warnings()` to
## see where this warning was generated.
```

```r
rps_sup %>% summarise( EATE_hat = mean( ATE_hat ),
                    SE = sd( ATE_hat ),
                    ESE_hat = mean( SE_hat ))
```

```
## # A tibble: 1 x 3
##   EATE_hat    SE ESE_hat
##      <dbl> <dbl>   <dbl>
## 1     1.00 0.381   0.378
```

First, note our superpopulation simulation is not biased for the superpopulation ATE. Also note the true SE is larger than our finite-sample simulation; this is because part of the uncertainty in our estimator is the uncertainty of whether our sample is representative of the superpopulation.

Finally, this clarifies that our linear regression estimator is estimating standard errors assuming a superpopulation model. The true finite sample standard error is less than the expected estimated error: from a finite sample perspective, our estimator is giving overly conservative uncertainty estimates. (This discrepancy is often called the correlation of potential outcomes problem.)

21.4   Nested finite simulation procedure

We just saw a difference between a specific, single, finite-sample dataset and a superpopulation. What if we wanted to know if this phenomenon was more general across a set of datasets? This question can be levied more broadly: if we run a simulation on a single dataset, this is even more narrow than running on a single scenario: if we compare methods and find one is superior to another for our single dataset, how do we know this is not an artifact of some specific characteristic of *that data* and not a general phenomenon at all?

One way forward is to run a nested simulation, where we generate a series of finite sample datasets, and then for each dataset run a small simulation. We then calculate the expected finite sample performance across the datasets. One could almost think of the datasets themselves as a "factor" in our multifactor experiment. This is what we did in [CITE estimands paper]

Borrowing from the simulation appendix of [CITE estimands paper], repeat R times:

1. Generate a dataset using a particular DGP. This data generation is the "sampling step" for a superpopulation (SP) framework. The DGP represents an infinite superpopulation. Each dataset includes, for each observation, the potential outcome under treatment or control.

2. Record the true finite-sample ATE, both person and site weighted.

3. Then, three times, do a finite simulation as follows:

a. Randomize units to treatment and control.
b. Calculate the corresponding observed outcomes.
c. Analyze the results using the methods of interest, recording both the point estimate and estimated standard error for each.

Having only three trials will give a poor estimate of within-dataset variability for each dataset, but the average across the R datasets in a given scenario gives a reasonable estimate of expected variability across datasets of the type we would see given the scenario parameters.

To demonstrate we first make a mini-finite sample driver:

```r
one_finite_run <- function( R0 = 3, n = 100, ... ) {
  dat = gen_data( n = n, ... )
  rps <- rerun( R0, {
        dat = mutate( dat,
                    Z = 0 + (sample( n ) <= n/2),
                    Yobs = ifelse( Z == 1, Y1, Y0 ) )
        mod = lm( Yobs ~ Z, data=dat )
        tibble( ATE_hat = coef(mod)[["Z"]],
                SE_hat = arm::se.coef(mod)[["Z"]] )
    }) %>%
    bind_rows()
  rps$ATE = mean( dat$Y1 - dat$Y0 )
  rps
}
```

This driver also stores the finite sample ATE for future reference:

```r
one_finite_run()
```

```
## Warning: `rerun()` was deprecated in
## purrr 1.0.0.
## i Please use `map()` instead.
##    # Previously
## rerun(3, {
## dat = mutate(dat, Z = 0 +
## (sample(n) <= n / 2),
## Yobs = ifelse(Z == 1, Y1,
## Y0))
## mod = lm(Yobs ~ Z, data =
## dat)
## tibble(ATE_hat =
## coef(mod)[["Z"]], SE_hat =
## arm::se.coef(
## mod)[["Z"]])
## })
##
##    # Now
## map(1:3, ~ {
## dat = mutate(dat, Z = 0 +
## (sample(n) <= n / 2),
## Yobs = ifelse(Z == 1, Y1,
## Y0))
## mod = lm(Yobs ~ Z, data =
## dat)
## tibble(ATE_hat =
```

```
## coef(mod)[["Z"]], SE_hat =
## arm::se.coef(
## mod)[["Z"]])
## })
## This warning is displayed
## once every 8 hours.
## Call
## `lifecycle::last_lifecycle_warnings()`
## to see where this warning was
## generated.

## # A tibble: 3 x 3
##   ATE_hat SE_hat   ATE
##     <dbl>  <dbl> <dbl>
## 1   0.348  0.421 0.768
## 2   1.32   0.472 0.768
## 3   1.17   0.549 0.768
```

We then run a bunch of finite runs.

```
runs <- rerun( 500, one_finite_run() ) %>%
  bind_rows( .id = "runID" )
```

```
## Warning: `rerun()` was deprecated in
## purrr 1.0.0.
## i Please use `map()` instead.
##   # Previously
##   rerun(500,
##   one_finite_run())
##
##   # Now
##   map(1:500, ~
##   one_finite_run())
## This warning is displayed
## once every 8 hours.
## Call
## `lifecycle::last_lifecycle_warnings()`
## to see where this warning was
## generated.
```

We use `.id` because we will need to separate out each finite run and analyze separately, and then aggregate.

Each finite run is a very noisy simulation for a fixed dataset. This means when we calculate performance measures we have to be careful to avoid bias in the calculations; in particular, we need to focus on estimating SE^2 across the finite runs, not SE, to avoid the bias caused by having a few observations with every estimate.

```r
fruns <- runs %>% group_by( runID ) %>%
  summarise( EATE_hat = mean( ATE_hat ),
             SE2 = var( ATE_hat ),
             ESE_hat = mean( SE_hat ),
             .groups = "drop" )
```

And then we aggregate our finite sample runs:

```r
res <- fruns %>%
  summarise( EEATE_hat = mean( EATE_hat ),
             EESE_hat = sqrt( mean( ESE_hat^2 ) ),
             ESE = sqrt( mean( SE2 ) ) ) %>%
  mutate( calib = 100 * EESE_hat / ESE )

res
```

```
## # A tibble: 1 x 4
##   EEATE_hat EESE_hat   ESE calib
##       <dbl>    <dbl> <dbl> <dbl>
## 1     0.996    0.380 0.331  115.
```

We see our expected standard error estimate is, across the collection of finite sample scenarios all sharing a similar parent superpopulation DGP, 15% too large for the true expected finite-sample standard error.

We need to keep the squaring. If we look at the SEs themselves, we have further apparent bias due to our *estimated* `ESE_hat` being so unstable due to too few observations:

```r
mean( sqrt( fruns$SE2 ) )
```

```
## [1] 0.2944556
```

We can use our collection of mini-finite-sample runs to estimate superpopulation quantities as well. Given that the simulation datasets are i.i.d. draws, we can simply take expectations across all our simulations. The only concern is our estimates of MCSE will be off due to the clustering in our simulation runs.

Here we calculate superpopulation performance measures (both with the squared SE and without; we prefer the squared version):

```r
runs %>%
  summarise( EATE_hat = mean( ATE_hat ),
             SE_true = sd( ATE_hat ),
             SE_hat = mean( SE_hat ),
             SE2_true = var( ATE_hat ),
             SE2_hat = mean( SE_hat^2 ) ) %>%
  pivot_longer( cols = c(SE_true:SE2_hat ),
                names_to = c( "estimand", ".value" ),
```

```
                names_sep ="_" ) %>%
  mutate( inflate = 100 * hat / true )
```

```
## # A tibble: 2 x 5
##   EATE_hat estimand  true    hat inflate
##      <dbl> <chr>    <dbl> <dbl>   <dbl>
## 1    0.996 SE       0.389 0.377    96.9
## 2    0.996 SE2      0.151 0.142    93.9
```

Chapter 22

The Parametric bootstrap

An inference procedure very much connected to simulation studies is the parametric bootstrap. The parametric bootstrap is a bootstrap technique designed to obtain standard error estimates for an estimated parametric model. It can do better than the case-wise bootstrap in some circumstances, usually when there is need to avoid the discrete, chunky nature of a casewise bootstrap (which will only give values that exist in the original dataset).

For a parametric bootstrap, the core idea is to fit a given model to actual data, and then take the parameters we estimate from that model as the DGP parameters in a simulation study. The parametric bootstrap is a simulation study for a specific scenario, and our goal is to assess how variable (and, possibly, biased) our estimator is for this specific scenario. If the behavior of our estimator in our simulated scenario is similar to what it would be under repeated trials in the real world, then our bootstrap answers will be informative as to how well our original estimator performs in practice. This is the bootstrap principle, or analogy with an additional assumption that the real-world is effectively well specified as the parameteric model we are fitting.

In particular we do the following:

1. generate data from a model with coefficients as estimated on the original data.
2. repeatedly estimate our target quantity on a series of synthetic data sets, all generated from this model.
3. examine this collection of estimates to assess the character of the estimates themselves, i.e. how much they vary, whether we are systematically estimating too high or too low, and so forth.
4. The variance and bias of our estimates in our simulation is probably like the actual variance and bias of our original estimate (this is precisely the bootstrap analogy).

A key feature of the parametric bootstrap is it is not, generally, a multifactor simulation experiment. We fit our model to the data, and use our best estimate of the world, as given by the fit model, to generate our data. This means we generally want to simulate in contexts that are (mostly) *pivotal*, meaning the distribution of our test statistic or point estimate is relatively stable across different scenarios. In other words, we want the uncertainty of our estimator to not heavily depend on the exact parameter values we use in our simulation, so that if we are simulating with incorrect parameters our bootstrap analogy will still hold.

Often, to achieve a reasonable claim of being pivotal, we will focus on standardized statistics, such as the *t*-statistic of

$$t = \frac{est}{\widehat{SE}}$$

It is more common for the distribution of a standardized test statistic to have a canonical distribution across scenarios than an absolute estimate.

22.1   Air conditioners: a stolen case study

Following the case study presented in [CITE bootstrap book], consider some failure times of air conditioning units:

```
dat = c( 3, 5, 7, 18, 43, 85, 91, 98, 100, 130, 230, 487 )
```

We are interested in the log of the average failure time:

```
n = length(dat)
y.bar = mean(dat)
theta.hat = log( y.bar )

c( n = n, y.bar = y.bar, theta.hat = theta.hat )
```

```
##           n       y.bar   theta.hat
##   12.000000 108.083333    4.682903
```

We are interested in this because we are modeling the failure time of the air conditioners with an exponential distribution. This means we will generate new failure times with an exponential distribution:

```
reps = replicate( 10000, {
    smp = rexp(n, 1/y.bar)
    log( mean( smp ) )
})

res_par = tibble(
  bias.hat = mean( reps ) - theta.hat,
```

```
  var.hat = var( reps ),
  CIlog_low = theta.hat + bias.hat - sqrt(var.hat) * qnorm(0.975),
  CIlog_high = theta.hat + bias.hat - sqrt(var.hat) * qnorm(0.025),
  CI_low = exp( CIlog_low ),
  CI_high = exp( CIlog_high ) )
res_par
```

```
## # A tibble: 1 x 6
##   bias.hat var.hat CIlog_low CIlog_high CI_low
##      <dbl>   <dbl>     <dbl>      <dbl>  <dbl>
## 1  -0.0420  0.0856      4.07       5.21   58.4
## # i 1 more variable: CI_high <dbl>
```

Note how we are, as usual, in our standard simulation framework of repeatidly (1) generating data and (2) analyzing the simulated data. Nothing is changed.

The nonparametric, or case-wise, bootstrap (this is what people normally mean when they say bootstrap) would look like this:

```
reps = replicate( 10000, {
    smp = sample( dat, replace=TRUE )
    log( mean( smp ) )
})

res_np = tibble(
  bias.hat = mean( reps ) - theta.hat,
  var.hat = var( reps ),
  CIlog_low = theta.hat + bias.hat - sqrt(var.hat) * qnorm(0.975),
  CIlog_high = theta.hat + bias.hat - sqrt(var.hat) * qnorm(0.025),
  CI_low = exp( CIlog_low ),
  CI_high = exp( CIlog_high ) )


bind_rows( parametric = res_par,
           casewise = res_np, .id = "method") %>%
  mutate( length = CI_high - CI_low )
```

```
## # A tibble: 2 x 8
##   method      bias.hat var.hat CIlog_low CIlog_high
##   <chr>          <dbl>   <dbl>     <dbl>      <dbl>
## 1 parametric   -0.0420  0.0856      4.07       5.21
## 2 casewise     -0.0651  0.132       3.90       5.33
## # i 3 more variables: CI_low <dbl>,
## #   CI_high <dbl>, length <dbl>
```

This is *also* a simulation: our data generating process is a bit more vague, however, as we are just resampling the data. This means our estimands are

not as clearly specified. For example, in our parameteric approach, our target parameter is known to be true. In the case-wise, the connection between our DGP and the parameter `theta.hat` is less explicit.

Overall, in this case, our parametric bootstrap can model the tail behavior of an exponential better than case-wise. Especially considering the small number of observations, it is going to be a more faithful representation of what we are doing–provided our model is well specified for the real world distribution.

Appendix A

Coding Reference

In this appendix chapter we give a bit more detail on some core programming skills that we use throughout the book.

A.1 How to repeat yourself

At the heart of simulation is replication: we want to do the same task over and over. In this book we have showcased a variety of tools to replicate a random process. In this section we give a formal presentation of these tools.

A.1.1 Using `replicate()`

The `replicate( n, expr, simplify )` method is a base-R function, which takes two arguments: a number `n` and an expression `expr` to run repeatedly. You can set `simplify = FALSE` to get the output of the function as a list, and if you set `simplify = TRUE` then R will try to simplify your results into an array.

For simple tasks where your expression gives you a single number, replicate will produce a vector of numbers:

```
replicate( 5, mean( rpois( 3, lambda = 1 ) ) )
```

```
## [1] 0.6666667 1.0000000 0.6666667 1.0000000
## [5] 0.6666667
```

If you do not simplify, you then will need to massage your results:

```
one_run <- function() {
  dd = rpois( 3, lambda = 1 )
  tibble( mean = mean( dd ), sd = sd( dd ) )
}
```

```
rps <- replicate( 2, one_run(), simplify = FALSE )
rps
```

```
## [[1]]
## # A tibble: 1 x 2
##    mean    sd
##   <dbl> <dbl>
## 1  1.67  1.53
##
## [[2]]
## # A tibble: 1 x 2
##    mean    sd
##   <dbl> <dbl>
## 1  1.33  1.15
```

In particular, you will probably stack all your tibbles to make one large dataset:

```
rps <- bind_rows( rps )
rps
```

```
## # A tibble: 2 x 2
##    mean    sd
##   <dbl> <dbl>
## 1  1.67  1.53
## 2  1.33  1.15
```

Note that you give replicate a full piece of code that would run on its own. You can even give a whole block of code in curly braces. This is exactly the same code as before:

```
rps <- replicate( 2, {
  dd = rpois( 3, lambda = 1 )
  tibble( mean = mean( dd ), sd = sd( dd ) )
}, simplify = FALSE ) %>%
  bind_rows()
```

The `replicate()` method is good for simple tasks, but for more general use, you will probably want to use `map()`.

A.1.2   Using `map()`

The tidyverse way of repeating oneself is the `map()` method. The nice thing about `map()` is you map over a list of values, and thus can call a function repeatedly, but with a shifting set of inputs.

```
one_run_v2 <- function( N ) {
  dd = rpois( N, lambda = 1 )
  tibble( mean = mean( dd ), sd = sd( dd ) )
```

```
}
n_list = c(2, 5)
rps <- map( n_list, one_run_v2 )
rps
```

```
## [[1]]
## # A tibble: 1 x 2
##     mean    sd
##    <dbl> <dbl>
## 1   0.5 0.707
##
## [[2]]
## # A tibble: 1 x 2
##     mean    sd
##    <dbl> <dbl>
## 1   0.8 0.837
```

You again would want to stack your results:

```
bind_rows(rps)
```

```
## # A tibble: 2 x 2
##     mean    sd
##    <dbl> <dbl>
## 1   0.5 0.707
## 2   0.8 0.837
```

We have a small issue here, however, which is we lost what we *gave* `map()` for each call. If we know we only get one row back from each call, we can add the column directly:

```
rps$n = n_list
```

A better approach is to *name* your list of input parameters, and then your `map` function can add those names for you as a new column when you stack:

```
n_list %>%
  set_names() %>%
  map( one_run_v2 ) %>%
  bind_rows( .id = "n" )
```

```
## # A tibble: 2 x 3
##    n     mean    sd
##    <chr> <dbl> <dbl>
## 1 2        2    0
## 2 5      1.4  1.14
```

An advantage here is if you are returning multiple rows (e.g., one row for each estimator tested in a more complex simulation), all the rows will get named

correctly and automatically.

In older tidyverse worlds, you will see methods such as `map_dbl()` or `map_dfr()`. These will automatically massage your output into the target type. `map_dfr()` will automatically bind rows, and `map_dbl()` will try to simplify the output into a list of doubles. Modern tidyverse no longer likes this, which we find somewhat sad.

To read more about `map()`, check out out Section 21.5 of R for Data Science (1st edition), which provides a more thorough introduction to mapping.

A.1.3   map with no inputs

If you do not have parameters, but still want to use `map()`, you can. E.g.,

```
map_dfr( 1:3, \(.) one_run() )
```

```
## # A tibble: 3 x 2
##     mean     sd
##    <dbl> <dbl>
## 1 1       1
## 2 0.667 0.577
## 3 0       0
```

The weird "(.)" is a shorthand for a function that takes one argument and then calls `one_run()` with no arguments. We are using the 1:3 notation to just make a list of the right length (3 replicates, in this case) to map over. A lot of fuss! Just use `replicate()`

To make all of this more clear, consider passing arguments that you manipulate on the fly:

```
map_dfr( n_list, \(x) one_run_v2( x*x ) )
```

```
## # A tibble: 2 x 2
##     mean     sd
##    <dbl> <dbl>
## 1  1      1.41
## 2  1.16  1.11
```

Anonymous functions, as these are called, can be useful to connect your pieces of simulation together.

A.1.4   Other approaches for repetition

In the past, there was a tidyverse method called `rerun()`, but it is currently out of favor. Originally, `rerun()` did exactly that: you gave it a number and a block of code, and it would rerun the block of code that many times, giving you the results as a list. `rerun()` and `replicate()` are near equivalents. As we saw, `replicate()` does what its name suggests—it replicates the result of

an expression a specified number of times. Setting `simplify = FALSE` returns the output as a list (just like `rerun()` did).

A.2 Default arguments for functions

To write functions that are both easy to use and configurable, set default arguments. For example,

```
my_function = function( a = 10, b = 20 ) {
    100 * a + b
}

my_function()
```

```
## [1] 1020
```
```
my_function( 5 )
```

```
## [1] 520
```
```
my_function( b = 5 )
```

```
## [1] 1005
```
```
my_function( b = 5, a = 1 )
```

```
## [1] 105
```

We can still call `my_function()` when we don't know what the arguments are, but then when we know more about the function, we can specify things of interest. Lots of R commands work exactly this way, and for good reason.

Especially for code to generate random datasets, default arguments can be a life-saver as you can then call the method before you know exactly what everything means.

For example, consider the `blkvar` package that has some code to generate blocked randomized datasets. We might locate a promising method, and type it in:

```
library( blkvar )
generate_blocked_data()
```

```
## Error in generate_blocked_data(): argument "n_k" is missing, with no default
```

That didn't work, but let's provide some block sizes and see what happens:

```
generate_blocked_data( n_k = c( 3, 2 ) )
```

```
##   B        Y0       Y1
## 1 B1  0.1651598 6.371708
```

```
## 2 B1 -0.7767558 5.613676
## 3 B1 -1.4736741 4.856552
## 4 B2 -1.0636928 4.448634
## 5 B2  0.1533518 4.334540
```

Nice! We see that we have a block ID and the control and treatment potential outcomes. We also don't see a random assignment variable, so that tells us we probably need some other methods as well. But we can play with this as it stands right away.

Next we can see that there are many things we might tune:

```
args( generate_blocked_data )
```

```
## function (n_k, sigma_alpha = 1, sigma_beta = 0, beta = 5, sigma_0 = 1,
##     sigma_1 = 1, corr = 0.5, exact = FALSE)
## NULL
```

The documentation will tell us more, but if we just need some sample data, we can quickly assess our method before having to do much reading and understanding. Only once we have identified what we need do we have to turn to the documentation itself.

A.3   Optimizing code (and why you often shouldn't)

Optimizing code is when you spend a bit more human effort to write code that will run faster on your computer. In some cases, this can be a critical boost to running a simulation, where you inherently will be doing things a lot of times. Cutting runtime down will always be tempting, as it allows you to run more replicates and get more precisely estimated performance measures for your simulation.

That being said, generally optimize code only after discovering you need to. Optimizing as you go usually means you will spend a lot of time wrestling with code far more complicated than it needs to be. For example, often it is the estimation method that will take a lot of computational time, so having very fast data generation code will not help shorten the overall run time of a simulation much, as you are tweaking something that is only a small part of the overall pie, in terms of time. Keep things simple; in general your time is more important than the computer's time.

In the next sections we will look at a few optimization efforts applied to the ANOVA example in the prior chapters.

A.3.1 Hand-building functions

In the Welch example above, we used the system-implemented ANOVA. An alternative approach would be to "hand roll" the ANOVA F statistic and test directly. Doing so by hand can set you up to implement modified versions of these tests later on. Also, although hand-building a method does take more work to program, it can result in a faster piece of code (this actually is the case here) which in turn can make the overall simulation faster.

Following the formulas on p. 129 of Brown and Forsythe (1974) we have (using data as generated in Chapter 6:

```r
ANOVA_F <- function(sim_data) {

  x_bar <- with(sim_data, tapply(x, group, mean))
  s_sq <- with(sim_data, tapply(x, group, var))
  n <- table(sim_data$group)
  g <- length(x_bar)

  df1 <- g - 1
  df2 <- sum(n) - g

  msbtw <- sum(n * (x_bar - mean(sim_data$x))^2) / df1
  mswn <- sum((n - 1) * s_sq) / df2
  fstat <- msbtw / mswn
  pval <- pf(fstat, df1, df2, lower.tail = FALSE)

  return(pval)
}


ANOVA_F(sim_data)
```

```
## [1] 0.002497797
```

To see the difference between our version and R's version, we can use an R package called `microbenchmark` to test how long the computations take for each version of the function. The `microbenchmark` function runs each expression 100 times (by default) and tracks how long the computations take. It then summarizes the distribution of timings:

```r
library(microbenchmark)
timings <- microbenchmark(Rfunction = ANOVA_F_aov(sim_data),
                          direct    = ANOVA_F(sim_data))
```

```
## Warning in microbenchmark(Rfunction =
## ANOVA_F_aov(sim_data), direct =
## ANOVA_F(sim_data)): less accurate nanosecond
## times to avoid potential integer overflows
```

```
timings
```

```
## Unit: microseconds
##       expr     min       lq     mean   median
##  Rfunction 195.160 203.2575 240.4105 213.8765
##     direct  83.886  91.6760 102.7107  96.1245
##       uq      max neval
##  234.725 1727.535    100
##  103.443  349.115    100
```

The direct function is 2.3 times faster than the built-in R function.

This result is not unusual. Built-in R functions usually include lots of checks and error-handling, which take time to compute. These checks are crucial for messy, real-world data analysis but unnecessary with our pristine, simulated data. Here we can skip them by doing the calculations directly. In general, however, this is a trade-off: writing something yourself gives you a lot of chance to do something wrong, throwing off all your simulations. It might be faster, but you may pay dearly for it in terms of extra hours coding and debugging. Optimize only if you need to!

A.3.2   Computational efficiency versus simplicity

An alternative approach to having a function that, for each call, generates a single set of data, would be to write a function that generates *multiple* sets of simulated data all at once.

For example, for our ANOVA example we could specify that we want `R` replications of the study and have the function spit out a matrix with `R` columns, one for each simulated dataset:

```r
generate_data_matrix <- function(mu, sigma_sq, sample_size, R) {

  N <- sum(sample_size)
  g <- length(sample_size)

  group <- rep(1:g, times = sample_size)
  mu_long <- rep(mu, times = sample_size)
  sigma_long <- rep(sqrt(sigma_sq), times = sample_size)

  x_mat <- matrix(rnorm(N * R, mean = mu_long, sd = sigma_long),
                  nrow = N, ncol = R)
  sim_data <- list(group = group, x_mat = x_mat)

  return(sim_data)
}
```

```
generate_data_matrix(mu = mu, sigma_sq = sigma_sq,
                     sample_size = sample_size, R = 4)
```

```
## $group
##  [1] 1 1 1 2 2 2 2 2 2 3 3 4 4 4 4
##
## $x_mat
##               [,1]       [,2]        [,3]       [,4]
##  [1,] -1.1790632 0.7805722   0.7711074 1.2753672
##  [2,]  2.4160302 3.1073488  -1.6081629 0.4196167
##  [3,]  0.4950409 4.1031245   2.7664053 1.7352006
##  [4,]  2.4804740 1.6636922   3.9830638 4.1231762
##  [5,]  0.7434552 1.2039138   0.2647096 1.6756596
##  [6,]  3.2185066 0.3496457   2.3249747 2.1554411
##  [7,]  4.0411462 2.4233487   2.5393216 1.4254521
##  [8,]  3.7780351 0.7254293   4.0446210 0.5131817
##  [9,]  2.6685690 1.6684263   2.1747235 3.0994807
## [10,]  6.4508882 5.1857268   4.8141904 8.4568769
## [11,]  1.8542667 3.8682330   2.4237823 5.4617181
## [12,]  5.7922912 6.2489447   5.6722027 6.3249945
## [13,]  5.5627116 6.2221245   5.9849752 4.6089806
## [14,]  6.0355414 7.1686699   5.7994605 4.8935517
## [15,]  6.1857938 7.2068300   7.1912594 5.4974888
```

This approach is a bit more computationally efficient because the setup calculations (getting `N`, `g`, `group`, `mu_full`, and `sigma_full`) only have to be done once instead of once per replication. It also makes clever use of vector recycling in the call to `rnorm()`. However, the structure of the resulting data is more complicated, which will make it more difficult to do the later estimation steps. Furthermore, if the number of replicates `R` is large and each replication produces a large dataset, this "all-at-once" approach will entail generating and holding very large amounts of data in memory, which can create other performance issues. On balance, we recommend the simpler approach of writing a function that generates a single simulated dataset per call (unless and until you have a principled reason to do otherwise).

A.3.3 Reusing code to speed up computation

Computational and programming efficiency should usually be a secondary consideration when you are starting to design a simulation study. It is better to produce accurate code, even if it is a bit slow, than to write code that is speedy but hard to follow (or even worse, that produces incorrect results). All that said, there is some glaring redundancy in the two functions used for the ANOVA simulation. Both `ANOVA_F` and `Welch_F` start by taking the simulated data and calculating summary statistics for each group, using the following code:

```r
x_bar <- with(sim_data, tapply(x, group, mean))
s_sq <- with(sim_data, tapply(x, group, var))
n <- table(sim_data$group)
g <- length(x_bar)
```

In the interest of not repeating ourselves, it would better to pull this code out as a separate function and then re-write the `ANOVA_F` and `Welch_F` functions to take the summary statistics as input. Here is a function that takes simulated data and returns a list of summary statistics:

```r
summarize_data <- function(sim_data) {

  res <- sim_data %>%
    group_by( group ) %>%
    summarise( x_bar = mean( x ),
               s_sq = var( x ),
               n = n() )
  res
}
```

We just packaged the code from above, and puts our results in a nice table (and thus pivoted to using tidyverse to calculate these things):

```r
sim_data = generate_data(mu=mu, sigma_sq=sigma_sq, sample_size=sample_size)
summarize_data(sim_data)
```

```
## # A tibble: 4 x 4
##    group x_bar  s_sq     n
##    <int> <dbl> <dbl> <int>
## # 1      1 0.817 6.28      3
## # 2      2 2.18  3.33      6
## # 3      3 3.62  0.165     2
## # 4      4 5.96  0.102     4
```

Now we can re-write both F-test functions to use the output of this function:

```r
ANOVA_F_agg <- function(x_bar, s_sq, n) {
  g = length(x_bar)
  df1 <- g - 1
  df2 <- sum(n) - g

  msbtw <- sum(n * (x_bar - weighted.mean(x_bar, w = n))^2) / df1
  mswn <- sum((n - 1) * s_sq) / df2
  fstat <- msbtw / mswn
  pval <- pf(fstat, df1, df2, lower.tail = FALSE)

  return(pval)
}
```

```r
summary_stats <- summarize_data(sim_data)
with(summary_stats, ANOVA_F_agg(x_bar = x_bar, s_sq = s_sq, n = n))
```

```
## [1] 0.007878319
```

```r
Welch_F_agg <- function(x_bar, s_sq, n) {
  g = length(x_bar)
  w <- n / s_sq
  u <- sum(w)
  x_tilde <- sum(w * x_bar) / u
  msbtw <- sum(w * (x_bar - x_tilde)^2) / (g - 1)

  G <- sum((1 - w / u)^2 / (n - 1))
  denom <- 1 +  G * 2 * (g - 2) / (g^2 - 1)
  W <- msbtw / denom
  f <- (g^2 - 1) / (3 * G)

  pval <- pf(W, df1 = g - 1, df2 = f, lower.tail = FALSE)

  return(pval)
}

with(summary_stats, ANOVA_F_agg(x_bar = x_bar, s_sq = s_sq, n = n))
```

```
## [1] 0.007878319
```

The results are the same as before.

We should always test any optimized code against something we know is stable, since optimization is an easy way to get bad bugs. Here we check against R's implementation:

```r
summary_stats <- summarize_data(sim_data)
F_results <- with(summary_stats,
                ANOVA_F_agg(x_bar = x_bar, s_sq = s_sq, n = n))
aov_results <- oneway.test(x ~ factor(group), data = sim_data,
                        var.equal = TRUE)
all.equal(aov_results$p.value, F_results)
```

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

```r
W_results <- with(summary_stats,
                Welch_F_agg( x_bar = x_bar,
                            s_sq = s_sq, n = n))
aov_results <- oneway.test(x ~ factor(group),
                          data = sim_data,
                          var.equal = FALSE)
all.equal(aov_results$p.value, W_results)
```

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

Here we are able to check against a known baseline. Checking estimation functions can be a bit more difficult for procedures that are not already implemented in R. For example, the two other procedures examined by Brown and Forsythe, the James' test and Brown and Forsythe's $F*$ test, are not available in base R. They are, however, available in the user-contributed package `onewaytests`, found by searching for "Brown-Forsythe" at http://rseek.org/. We could benchmark our calculations against this package, but of course there is some risk that the package might not be correct. Another route is to verify your results on numerical examples reported in authoritative papers, on the assumption that there's less risk of an error there. In the original paper that proposed the test, Welch (1951) provides a worked numerical example of the procedure. He reports the following summary statistics:

```r
g <- 3
x_bar <- c(27.8, 24.1, 22.2)
s_sq <- c(60.1, 6.3, 15.4)
n <- c(20, 20, 10)
```

He also reports $W = 3.35$ and $f = 22.6$. Replicating the calculations with our `Welch_F_agg` function:

```r
Welch_F_agg(x_bar = x_bar, s_sq = s_sq, n = n)
```

```
## [1] 0.05479049
```

We get slightly different results! But we know that our function is correct—or at least consistent with `oneway.test`—so what's going on? It turns out that there was an error in some of Welch's intermediate calculations, which can only be spotted because he reported all of his work in the paper.

We then put all these pieces in our revised `one_run()` method as so:

```r
one_run_fast <- function( mu, sigma_sq, sample_size ) {
  sim_data <- generate_data(mu = mu, sigma_sq = sigma_sq,
                            sample_size = sample_size)
  summary_stats <- summarize_data(sim_data)
  anova_p <- with(summary_stats,
                  ANOVA_F_agg(x_bar = x_bar,s_sq = s_sq, n = n))
  Welch_p <- with(summary_stats,
                  Welch_F_agg(x_bar = x_bar, s_sq = s_sq, n = n))
  tibble(ANOVA = anova_p, Welch = Welch_p)
}

one_run_fast( mu = mu, sigma_sq = sigma_sq,
              sample_size = sample_size )
```

```
## # A tibble: 1 x 2
```

```
##      ANOVA   Welch
##      <dbl>   <dbl>
## 1 0.0000835 0.00116
```

The reason this is important is we are now doing our group aggregation only once, rather than once per method. We can use our microbenchmark to see our speedup:

```
library(microbenchmark)
timings <- microbenchmark(noagg = one_run(mu = mu, sigma_sq = sigma_sq,
                                          sample_size = sample_size),
                          agg = one_run_fast(mu = mu, sigma_sq = sigma_sq,
                                          sample_size = sample_size) )
timings
```

```
## Unit: microseconds
##   expr      min       lq      mean    median
##  noagg  563.545  622.216  855.8635  658.4805
##    agg 1366.489 1504.351 1714.5036 1588.7705
##       uq      max neval
##  721.436 14493.13   100
## 1745.001  5950.33   100
```

And our relative speedup is:

```
with(summary(timings), round(mean[1] / mean[2], 1))
```

```
## [1] 0.5
```

To recap, there are two advantages of this kind of coding:

1. Code reuse is generally good because when you have the same code in multiple places it can make it harder to read and understand your code. If you see two blocks of code you might worry they are only mostly similar, not exactly similar, and waste time trying to differentiate. If you have a single, well-named function, you immediately know what a block of code is doing.

2. Saving the results of calculations can speed up your computation since you are saving your partial work. This can be useful to reduce calculations that are particularly time intensive.

Appendix B

Further readings and resources

We close with a list of things of interest we have discovered while writing this text.

- Morris, White, & Crowther (2019). Using simulation studies to evaluate statistical methods.
- High-level simulation design considerations.
- Details about performance criteria calculations.
- Stata-centric.
- SimDesign R package (Chalmers, 2019)
- Tools for building generic simulation workflows.
- Chalmers & Adkin (2019). Writing effective and reliable Monte Carlo simulations with the SimDesign package.
- DeclareDesign (Blair, Cooper, Coppock, & Humphreys)
- Specialized suite of R packages for simulating research designs.
- Design philosophy is very similar to "tidy" simulation approach.
- SimHelpers R package (Joshi & Pustejovsky, 2020)
- Helper functions for calculating performance criteria.
- Includes Monte Carlo standard errors.

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