

A Framework for Really Reproducible Research

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Chapter 1

Introduction

1.1 Two motivations

This book is about *reproducible research*. A lot of the book is dedicated to fleshing out exactly what that term means, or perhaps what it *should* mean, but moreover, this book is about *really* reproducible research. In order to tell you what *that's* supposed to mean in a relatively concise way, I'm going to talk about the two different kinds of motivations that drive this book.

One type of motivation is the desire to do Good Science. It's my belief that scientific research should be conducted in a way that is maximally replicable, reproducible, transparent, and trustworthy. I think of this as a kind of ethical obligation for scientists, both to the scientific community and to the people that fund our research (usually taxpayers, in my line of work). I also believe that this is inherent to the success of the scientific method, but I am not an expert on the philosophy of science, so I won't go too deeply into that side of things, beyond expressing some of my personal opinions. From this ethical/philosophical point of view, reproducible research is in line with the value system of science, and *really* reproducible research is a set of real-world methods and techniques that do more than lip service to these ideas; they put them into action.

The second type of motivation is the desire to be a Successful Scientist. This is the more practical, pragmatic side of things. In short, being a successful scientist means doing work that gets published frequently in high-quality journals. Obviously for many academics, there are other sides to professional life like teaching, service, etc. Maybe some of the ideas here can apply some to those domains, too, but I'm going to focus on the research side. A successful researcher, from the most concrete point of view, is one with a good publishing record. From this angle, the motivation of reproducible research is to help the researcher be more efficient, effective, and productive, and to produce higher-quality work that is worthy of the most prestigious journals. And similarly, *really* reproducible research is meant to provide a concrete framework that's more than just recapitulating concepts about effective work habits.

Now hopefully, if you're engaged in research, you're interested in one of these

two motivations, maybe both. If you neither care about (a) producing good science worthy of the faith and trust of other scientists and your funding sources, nor (b) being a successful researcher with a great publication record, then maybe you're in the wrong field. The central aim of this book is to talk about how reproducibility — *real* reproducibility — can assist you in both of these goals.

1.2 Three sides of the coin

In order to address these two goals, there are three (count 'em!) sides of the coin we need to explore. One side is the conceptual side, trying to lay out a framework of principles for understanding what it means to be reproducible. The other side is a discussion of how these principles play out in the day-to-day activities of carrying out research. But while this second side is more concrete, it's still framed in terms of general principles that could be implemented in many different ways. The third side is an actual, working implementation. You can see the third side (the edge) of the coin as either the part that connects the two faces of theory and practice, or as I prefer to see it, as the edge of a wheel, where (to mix metaphors) the rubber really meets the road. It's fine to talk about good principles of reproducibility, but without a kind of “manual” for exactly how to put things into practice, there will be a high barrier to entry for most people, which means very little change. If we want *really* reproducible research we have to have an actual working system that enables our good intentions to be realized in a practical way.

This book is aimed at the first two, more conceptual sides. The companion to this book is a repository on GitHub that provides a set of tutorials and guides for using a set of (open source, free) software tools to actually implement the ideas in the book. This “companion” set of materials is ultimately what puts the “really” in the title of the book, but I just couldn't see how to effectively squeeze all those tutorials and things into a useful book format. What I will do is include lots of hyperlinks in this book, in order to make it easier to connect from the idea or motivation for a particular kind of habit, workflow, or tool, to a set of tutorials that will help you get up and running with a tool that actually works as quickly as possible. This brings me to the next section.

1.3 How to use this book

Here's how I imagine (and hope) this book could be used. Read through some of the general chapters in the beginning, to get a sense of the big issues. But then feel free to skip around to particular issues or problems that sound interesting. The material in this book will lay out some of my thoughts on the topic, which will hopefully lead you to arrive at your own thoughts and opinions, and if my ideas intrigue you (either because they sound good, or because they sound terrible), you can follow some links to the GitHub repo to see how I personally attempt to implement my ideas. Those links will teach you how to use some piece of software (or non-software solution, if appropriate) to implement things yourself. All the software and techniques I use are extremely customizable, so if you don't like exactly how I do it and want to tweak it

for your own use, or if you think you can improve on it more generally, my tutorials will hopefully give you a good start towards being able to do that as well.

At some point, I expect this book to become rather static, in the sense that I will revise things as my thinking changes, and as other revisions/corrections need to be made, but if I ever start to change my mind in a big enough way, I may just need to write a different book. But the repository of tutorials and software is going to be a dynamic thing. It is ultimately a selfish endeavor, because I will base the tutorials around my own usage and needs. As those things change, so will the tutorials. However, since I will be using `git` for version control, you will be able to “roll back” any particular tool or tutorial to an earlier phase, if you thought those worked better for you. At least, you’ll be able to do this once you learn how to use `git`, which happens to be the base of what I’m going to recommend for a reproducible workflow! See, this stuff is already sounding useful, and we haven’t even really gotten started yet...

But the point is that the tutorial stuff will change a lot (assuming I can keep up with it), in an ongoing way. I would be very happy to have feedback on any aspect of this whole enterprise, whether you have suggestions or arguments with things in this book, or whether you have suggestions, problems, or alternatives to the implementation stuff on the GitHub site. Please direct all your love/hate mail to shoestringpsycholing1@gmail.com.

1.4 Who this book is for

By trade, I am a cognitive scientist, working in linguistics, psycholinguistics, and second language acquisition. Since this book is inherently a self-centered effort, I will be aiming at those audiences. However, I expect that the basic ideas and concepts should be applicable pretty generally across a lot of different domains of research. In particular, what I’m trying to do in this book is to take a look at some ideas that have been growing in popularity in computational and statistical sciences, and see whether they might apply more generally to research where developing computer code and new statistical/computational algorithms is not inherent to the field. In other words, by talking about how a (non-computational) linguist might be able to employ more reproducible methods, I expect the general principles will be pretty general, beyond the computation-heavy fields.

Thus, the book and the accompanying methods and tutorials are aimed at a pretty broad audience. I do not start out by assuming any particular knowledge of programming, statistics, or anything else. Of course, my implementations are all based around certain kinds of software packages that *do* involve learning at least a little programming, and I’ll argue that this is the most efficient way to implement a reproducible workflow, but the principles and ideas in this book are intended to be aimed at a much more general audience than the set of people who can easily put together a `makefile` (or even know what that is).

1.5 Theses and structure of the book

This is not the first thing that’s ever been written regarding reproducible research. It’s a rather hot topic in some circles, and lots of smart people have been thinking/writing/talking/blogging/tweeting about it. One goal of this book is to push a few new ideas into the discussion. In particular:

1. Whether something is *reproducible* is not an absolute, but is relative to the *range* (i.e., precision, extent) of reproducibility, the *domain* of reproducibility (i.e., what kind of activities are being reproduced?), and the *audience* of reproducibility (i.e., reproducible for whom?).
2. *Reproducible* has to be able to extend beyond just the domain of data analysis; it should apply to all aspects of the cycle of research.

I’ll focus on these two theses more or less in turn. I will start with a broad overview in chapter 2. I’ll review some of the previous work on the general topic, and further flesh out the broad concepts and motivations I’ve alluded to so far. This is more or less re-hashing and re-packaging a lot of things that other people have probably said better, though maybe not all in one place. Then in chapter 3 I’ll talk about the *dimensions* of reproducibility. I will argue that the notion of *reproducibility* is inherently gradient and scalar, and that any definition or standard will have to make some decisions about the target dimensions that qualify something as “in” or “out” with respect to that local definition of what counts as reproducible. In other words, *reproducible* is a relative goal, and while it may be possible to establish standards for a particular field/context, there is no such thing as a useful universal standard. I will then go on to suggest some possible starting points for where to position a reasonably useful definition along these dimensions. That will conclude all of this nosebleed-level discussion.

I’ll then turn to a slightly more concrete discussion of how to make the day-to-day tasks of research more reproducible. In chapter ?? I propose a general schema for the cycle of research, from reading other people’s work to producing your own work. Again, my purpose here is not to go too deep into the philosophy of science, so this is just intended as a way of breaking down the research process into some large chunks. I think this is useful for the present purpose, because these different kinds of activities will involve different issues, problems, and standards regarding what it means to be *reproducible*. But the big point is that this broad view of research goes far beyond the realm of what most people talk about when the term *reproducible research* gets thrown around.

In the chapters that follow (4 through 8), I will focus in one one of these domains of research, and discuss some of the special challenges for reproducibility, and at times grapple with the question of whether (and how) activities in this domain could ever be reproducible. In each of these chapters, I will discuss how the other dimensions (*range* and *audience*) play out for that particular domain. Each chapter will also contain a general description of some practices that could lead to better reproducibility, and I will link heavily to my repository of tutorials that will implement specific software (or non-software) solutions to the implementation problem.

The final chapter will conclude with some parting thoughts.

So let's get started!

Chapter 2

Starting points

2.1 Replication vs. reproduction

Let's start with a terminological clarification. *Replication* and *reproduction* are terms that often get used to talk about similar yet distinct concepts. The basic idea is that *replication* refers to one of the cornerstones of science, which is that someone can perform an experiment, gets some results, and someone *else* can perform a *different* (but possibly similar) experiment, and get a set of results that is consistent with the first. We can say that these results have been *replicated*. *Reproducible* is often used to refer to the ability to get *exactly* the same results starting from the same set of data.

The meaningful distinction here, I propose, is that *replication* is about *results* and *reproduction* is about *methods*. These concepts are somewhat independent, because it may be possible to reproduce a set of methods almost exactly, but if you're collecting data from a different set of participants, you may not end up replicating the initial result. And conversely, it may be difficult or impossible to reproduce someone's methods exactly, or you may be intentionally running an experiment with a variation on the methods, but you still might get a set of results that replicate the earlier findings.

Throughout this book, I will assume that *replication* is a non-negotiable part of the scientific process (though see discussion in section 2.4). If no one can produce results that fit with an earlier set of results, then typically scientists assume there was something wrong with the initial results (all else being equal). I propose that *reproducibility* is a methodological approach (or set of approaches) that should make replication easier if a result is true, and should make aberrant or erroneous results more transparent. In other words, having reproducible methods does not guarantee replication, nor are reproducible methods strictly necessary for replication. But it's my contention (and the opinion of many others) that reproducible methods really facilitate the process in an important way.

With this distinction out of the way, let's talk a little about how the notion of reproducibility has developed recently.

2.2 A sketchy history of reproducibility

I will not go through a detailed, scholarly review of reproducible research, but I will give a brief overview, because to help orient you to how the content of this book fits with other discussions of the general topic.

At its roots, the discussion of reproducible research in the modern context comes from computer science, statistics, and more recently, other disciplines (like genetic biology) that involve increasingly computation-heavy analysis. One of the seminal works is Knuth (1984), which coined the eponymous term “literate programming.” the specific idea was that good programs should be written with the *human* reader in mind, not (just) the computer that runs the programs. This idea has lead to further ideas and developments in methods of documenting code, methods of writing code to be more legible (including developing computer languages themselves to be more legible), and methods of intertwining (or to use the Knuth’s term, “weaving”) human language that explains the code with the code language itself. But the broader idea is the foundation of reproducibility in the computer sciences, which is that in order for a program (and its results) to be shared effectively with the broader community, some care needs to be taken in how it is created. A program that is opaque to people other than its creator will be far less useful than a program that can be understood easily, because the latter can be improved, expanded, adapted, modified, and debugged far more easily.

Jon Claerbout is the next big name on the list, as the coiner of the term “reproducible research” (and, according to Buckheit and Donoho 1995, Claerbout preceded me in using the term “really reproducible” as well), and as an influential early adopter and developer of methods for reproducible computational research. One of Claerbout’s earliest forays was a paper given at the 1992 annual meeting of the Society of Exploration Geophysics,¹ but more recent commentaries are given in Schwab, Karrenbach, and Claerbout (2000) and Fomel and Claerbout (2009), and there are various places (like the Madagascar project, at <http://www.ahay.org/>) where colleagues have implemented complete systems for reproducible research within particular domains.

Other people that have been especially visible in various ways include Robert Gentleman² (e.g., Gentleman and Temple Lang 2004; Gentleman et al. 2005), Roger Peng (e.g., Peng 2009; Peng 2008), and Victoria Stodden (e.g., Stodden 2009; Stodden 2010; Stodden 2011; Stodden 2012).

The common thread with all of these major movers and shakers is that they are primarily in the computational and statistical fields. There is a reason for this. The most common current notion of reproducible research, as forwarded by the people above and others, comes down to sharing the data and code that generate a particular analysis, set of results, figures, etc. This has become a bigger deal in these fields, as the analyses themselves have become more complex and sometimes very computation-intensive. In computer science, it seems obvious that sharing code should be part of the publication process, because in many cases, the code *is* the

¹An “extended abstract” is available here:

<http://sepwww.stanford.edu/doku.php?id=sep:research:reproducible:seg92>

²Yes, [that Robert Gentleman](#).

research! For example, someone writes a piece of software to accomplish X, and then publishes a paper that describes the overall ideas, and maybe some benchmarks or other evidence that it does actually accomplish X. But the primary interest from other people in the field may be in *how* the software actually does what it does. In proprietary contexts, this may be kept secret, so that the owners of the software can sell it and beat their competitors, who are unable to do X. But in scientific contexts, I think secrecy is unacceptable, because it makes it impossible for the scientific community to review, accept, and synthesize the work. Black boxes are not good for science, though they may be good for warfare or profit (*maybe*).

Beyond sharing your code because your code *is* the research, the argument is that sharing your code allows for scientific openness because other people can inspect your code for mistakes, intentional or otherwise. It's a "show your work" kind of argument. In fields where the computations are non-trivial, and *how* you get a results is as much an innovation as *what* the results are, showing your work is an important part of dissemination and communication across the field. So it's no wonder that fields like Peng's (biostatistics) and Stodden's (statistics and computation) are at the forefront of pushing the ideas of reproducible research.

What about fields in the cognitive and social sciences? What about the processes involved in science before you have the data in hand, or after the analyses have been performed? While I think the current movement in reproducible research is great, it doesn't go nearly far enough. That's why I'm writing this book.

2.3 Expanded motivations

If you've gotten this far, I've given you a few teasers in terms of what this is all about, and why you might care. Or maybe you've skipped to this part to decide whether reading this is worth your time. So here I'm going to expand a little on the opening section and enumerate what I think the main "selling points" are for putting in the effort to make your research methods more reproducible.

2.3.1 Being a more successful scientist

I will talk about the "selfish" interests first. I'm talking about producing more and better research, getting more published, and generally being better at your job (if that involves research).

Here are some common issues and questions within research/academia, which can be enormously time-consuming, energy-consuming, and even (if things go poorly) career-threatening:

- You have completed months of data formatting, coding, and analysis, and have spent hours and hours formatting tables of results, creating, formatting, and labeling plots, and inserting statistics into a paper. You (or a colleague, grad student, or especially sharp reviewer) realize that some part of your data was coded wrong, or should be excluded. How long will it take to reproduce everything you've done after fixing your data?

- You are working on a complex data set, and in the process you try several different analyses, some of them very similar, varying only by a single parameter in your statistics software. You decide to report what you think is the best analysis in a paper. Six months later, someone asks you how you did that analysis, because they are trying something similar, and not getting the same results. How do you find the exact sequence of steps and set of options that produced the precise results in your paper? How long will this take?
- Could you pick up one of your own papers of from two years ago (or more) and remember exactly how you analyzed the data? Often the time between doing an analysis and it appearing in print can easily be two years or more. Someone reads your paper “hot off the presses,” (i.e., after a couple of years have passed), and has some good questions. Will you be able to easily remember the details to address those questions?
- You are interested in a particular line of research and want to start your own research by replicating the same pattern of effects someone else has shown. How much effort will this take? If you can’t replicate, how do you compare what you did to what they did? If you ask them to provide details (maybe five or more years after they did the initial work), how likely do you think they will be able to provide sufficient detail to help you? How easy would it be for you to do the same if someone wanted to replicate *your* work?
- How can you be sure that a result/statistic you report in your paper is correct? Detecting typos in prose is relatively easy, since the copyeditor (presumably) knows the language you’re writing in. But how could a copyeditor, or anyone else, catch a typo in your results/stats?
- How quickly can you access a complete bibliography of research that has influenced your thoughts on a particular topic?
- Can you quickly and accurately recall which important theoretical points were developed in which particular papers by a particular author?
- Can you quickly compare notes with someone about papers they’ve read to see if there are any holes in your own reading of the literature?
- Making notes about papers as you’re reading them is often very helpful, and can lead to new insights and new research questions. How easy is it to find those notes when you need them (or even remind yourself that you have notes)? How easy is it to lose those notes, and forget the points you thought about when reading?
- How much time do you spend searching for bibliographic references, even of papers you’ve cited before (or even papers you’ve written)?
- How much time do you spend formatting references, and making sure that the references section of your paper has all and only the references you cite?

- How many times have you made a typo on someone’s name in your references?
- Have you ever wanted to be able to “rewind the tape” on an analysis or draft of a paper, either to revert back to an earlier stage, or recall something that you had removed?
- Have you ever sent dozens of paper drafts back and forth with colleagues via email? How easy is it to find the most updated version, and be confident that it really is the most updated version? Do you have half a dozen different drafts labeled “FINAL”? How easy is it to find a particular draft of the paper, where some critical change was made? How easy is it to attribute certain sections to particular authors?

This is just an initial sampling. I contend that *really* reproducible methods provide you with apparently super-human abilities to address these issues and many more. What if I told you that the answer to the first bullet would be something like “dozens of hours” for non-reproducible methods, and “maybe an hour or two” for really reproducible methods? I also propose that if you have a decent career, you will run into these issues over and over. Therefore, the investment of time and energy into reproducible methods has enormous payback potential.

The above points are about efficiency. But I also claim that making your work more reproducible will also lead to greater fame (and possibly fortune, depending on your field, I suppose) and higher quality work. By employing more reproducible methods, you will catch mistakes more often, and when you do catch mistakes, it will be easier to correct them. You will be able to explore more lines of thought and experimentation with an analysis or argumentation, and easily “switch back” if the experiment doesn’t work out. The effort you put into making your work reproducible will result in cleaner, more careful work, which should result in a better publication rate, faster publication, quicker resolution of questions by reviewers, and publication in better journals. You will be able to collaborate more effectively, and amplify your output by engaging in more collaborative work. By making your work more reproducible, it will make it easier for other people to build on what you’ve done. This will increase your citations, and lead to a bigger impact on the field than you would have had otherwise.

I’m making some pretty big claims here. Is it snake oil? I don’t think so, but I also don’t have much in the way of empirical results to give you to back it up, either. My personal experience thus far is that when I’ve taken the time to make my work more reproducible, that has *always* paid off. Every time. No exceptions. I have found that I *always* need to recall certain details or update an analysis after some change, or compare an alternative, etc., etc., and more reproducible methods make all of those things much less painful and less time-consuming.

Of course, I have also spent quite a bit of time fiddling around with different software packages, trying out methods that don’t work all that well, and generally sinking a lot of time into learning a bunch of different tools. One of my hopes for this book and the accompanying tutorials is to greatly reduce this cost of entry for you, gentle reader. It’s also a good way for me to iron things out for myself, so this isn’t entirely altruistic. But the other benefit is that the more people use these

methods, the easier collaboration becomes. I'm a huge fan of the \LaTeX system, but it can make collaboration difficult when other people don't use it. The more people use it and other tools that allow more reproducibility, the better, but the cost of entry needs to be sufficiently low.

In the end, though, I'm doing all this myself because I have a firm belief that it will pay off for me personally. I have already seen evidence of this. Whether it works for you is up to you to find out.

2.3.2 Doing better science

As I claimed in the beginning section, reproducible methods should also lead to better science, and reproducibility is partly an ethical responsibility for scientists. We live in an exciting but perilous time for science. The rise of the internet into a mature infrastructure, the continuing advances in personal and large-scale computing, great strides in terms of data collection and analysis of types we could barely contemplate 10 or 20 years ago, and so on, provide an exciting new global realm of scientific discovery and collaboration. On the other hand, because of various domains of economic and social change, science is also under attack. Basic scientific education (for both “hard” and “soft” sciences) is in jeopardy in many spheres of public education. Funding for basic science³ is becoming harder to come by, and more competitive. Several severe cases of academic fraud have received a lot of exposure in the popular press. So while the potential for advances in sciences — including cognitive and social sciences — has never been greater, issues of risk, accountability, and demonstrating value to society loom heavy over the academic landscape.

An absolutely critical piece for both sides of this picture is the issue of trust. On the one hand, as possibilities for new data sources and analyses and collaborations explode, reproducibility is key, in order to maintain trust and order within the scientific community. For example, some advances in statistical methods that have recently become much more accessible (e.g., mixed-effects models, Bayesian analysis) are still not fully integrated or fully understood by researchers in many fields. This means both that some researchers may be employing methods they do not (yet) fully understand, and that some journal reviewers may be resistant to new methods, even if they do not have good reason to be, simply because they are unfamiliar. More transparent, reproducible methods of employing these and other more novel analyses would greatly facilitate the ability to share, evaluate, and critique these methods. In many cases, the publication standards that journals require simply cannot keep up with innovations in analysis, and so a journal article may simply not contain the information that someone would need to know enough about what the authors had

³“Basic” science is typically described as “science for sciences’ sake.” In other words, science for the sake of increasing understanding. This is contrasted with “applied” science, which is science with an aim of addressing some real-world problem with direct social, economic, or military applications. So for example, theoretical particle physics (e.g., the search for the Higgs boson) or theoretical linguistics (e.g., the search for abstract linguistic universals) are basic science, and developing a particular branch of particle physics to explore some new energy weapon, or applying a theory of universal grammar to problems in machine translation, are examples of applied science. In reality, there's a large continuum. The point here is that in all sorts of domains, it's harder and harder to do research without some kind of applied angle to justify funding.

done in order to evaluate the work. Reproducible methods fill that gap, and make it easier for researchers to share findings and confidence in those findings, whether or not journals require certain things.

More broadly, reproducible methods promote transparency and trust. When people outside the academic scientific community can pick up and replicate analyses and results, it can help break down the “ivory tower” metaphor. It increases accountability and decreases the possibilities for fraud and scandal. If anyone with a computer can re-run and inspect for themselves some important analysis of (e.g.) climate change, voter fraud, economic disparity, health issues, etc., then there is far more opportunity to bring discourse of such topics into the realm of facts and better decisions, and out of the realm of hearsay and fact-twisting partisanship. There is a growing practice of people circulating various plots and graphs through social media like Facebook or Twitter, showing things like debt growth under Democrats vs. Republicans, relationships between gun laws and gun violence, etc., etc. But without an ability to replicate the methods (and directly inspect the data) that went into creating such graphs, there is no real reason to trust any of them. A bar graph can lie just as easily as anything else, especially if you can’t see how it was made.

Within academia, there has been a growing recognition of and dissatisfaction with the problem of replication. The standards for publications in most fields reward studies (by publication and dissemination) for showing effects, while “null results” or failed replications of the same studies may have an extremely difficult time getting published, even though the existence of many well-done failed replications should cast significant doubt on the initial published effects. To make matters worse, replication is more difficult and resource-consuming if the original study is not very thoroughly described. By making replication easier, we can save time and money by reducing the amount of resources wasted on failed replication attempts. There are some interesting current projects trying to address the so-called “file drawer” problem of unreported failed replications, but increased reproducibility is a critical piece of making such efforts successful.

Another hot-button issue that relates to reproducibility is the notion of open access. The current fact of the matter is that a great deal of research is funded by taxpayers, but very few taxpayers are able to access the products of the research (i.e., published papers) without having to pay additional fees to a publisher. Universities (also largely funded by taxpayers) pay often exorbitant fees to access the journals that their faculty are publishing in or need access to for their research. While open access and reproducibility are not necessarily related, they would both thrive in world where open, transparent, reproducible methods were the norm. If researchers could easily share their work in formats that other researchers could more easily inspect, reconstruct, and critique, then peer-review should be facilitated, alleviating some of the pressure for journals to be “gatekeepers” of quality.

The argument, therefore, is two-fold. First, science is facilitated by openness. If your methods provide a barrier to openness, that is an impediment to science. In some sense, this impediment is inherent to the task of communicating our thoughts in a way that other people can interpret them and expand upon them, but the more reproducible your methods are, the more this natural impediment is removed. Second, science exists not in a vacuum but as part of a social contract between the

people that enable scientists (taxpayers, employers, etc.) and the scientists themselves. Reproducible methods should help promote trust and accountability. On efficiency grounds alone, if reproducible methods help researchers do more research and waste less time, then such methods are part of a responsible use of the resources (time and money) given to researchers.

While I do not personally believe that intentional waste and fraud is widespread in academia, there are certain areas that are more vulnerable than others, like research on pharmaceuticals or other big medical issues, and those are inevitably the areas where there is the most to gain or lose by fraud. Would reproducible methods have prevented the terrible debacle of the [Duke cancer trials](#)? Maybe not, but one of the major people involved in uncovering the faults of the study ([Keith Baggerly](#)) believes pretty strongly that reproducible methods would have made it much easier (thus much less time-intensive and much less expensive) to catch the mistakes.⁴ And if you think this kind of thing is an isolated case, spend some time reading or listening to Ben Goldacre.⁵ Goldacre focuses on the deception and bad science behind many medical studies. He doesn't focus explicitly on reproducible methods, but one of his big themes is the selective withholding of data. If a pharmaceutical company withholds the data from 75% of the trials done on their drug, how confident can we be that the effects reported are real? A fully open, reproducible set of methods is a key piece in making all kinds of findings open to other academics, to policymakers and decision-makers, and to the public.

But what about low-stakes (i.e., most) research in cognitive science, or other disciplines? Do I really think that linguists are insidiously withholding data in order for them to defend their pet theory within Minimalist syntax? Not exactly, but the effects of publication bias are well-known and discussed in many places. In essence, since there is a bias to publish positive findings (i.e., “statistically significant” results), many of the studies that have attempted a replication but found no results will not be published, meaning that the literature will present a skewed, and perhaps completely false picture of the actual pattern of findings. Worse, Uri Simonsohn and colleagues (Simmons, Nelson, and Simonsohn 2011) have shown that many of the typical practices of researchers in psychology and other cognitive sciences result in the ability to find nearly any effect to be “statistically significant,” but *only when these practices go unreported*.

There are two points here. First, flaws and inaccuracies in the ways that research findings are presented are not limited to high-stakes, big-money areas. Even very well-meaning and experienced researchers can inadvertently fall into some of the traps. Research is *difficult*, after all! Second, while reproducible methods are not a panacea, they go a long way towards improving the situation. Back to the issue of ethics, what if your “slightly fudged” results end up sparking a lot of interest, and several people get grants to pursue issues based on those findings? That could be millions of dollars and years of work wasted. Transparent, reproducible methods don't ensure that this could never happen, but they discourage it.

⁴See here for a video and slides of a talk he's given:

http://videlectures.net/cancerbioinformatics2010_baggerly_irrh/

⁵Who is actually very entertaining! See this talk for example:

http://www.ted.com/talks/ben_goldacre_battling_bad_science.html

2.3.3 Summary of motivations

I've argued for two different kinds of reasons to at least consider reproducible research methods. One is that it will help you *personally* to be more productive, to publish better papers, and to have a bigger impact in your field, the more reproducible your methods are. The other is that reproducible methods help promote and enforce the trust inherent in the social contract of research.

2.4 A dissenting opinion and a rejoinder

I would be remiss if I didn't recognize that not everyone is convinced. In a recent unpublished manuscript, Drummond (2012) offers a "dissenting opinion." He outlines four points that he interprets to be the main points of the reproducible research "movement" that he sees growing, and he offers responses to each. The following are lifted verbatim from Drummond (2012, p.2–3):

1. **Claim for reproducible research** It is, and always has been, an essential part of science; not doing so is simply bad science.

Drummond's rebuttal Reproducibility, at least in the form proposed, is not now, nor has it ever been, an essential part of science.

2. **Claim for reproducible research** It is an important step in the "Scientific Method" allowing science to progress by building on previous work; without it progress slows.

Drummond's rebuttal The idea of a single well defined scientific method resulting in an incremental, and cumulative, scientific process is highly debatable.

3. **Claim for reproducible research** It requires the submission of the data and computational tools used to generate the results; without it results cannot be verified and built upon.

Drummond's rebuttal Requiring the submission of data and code will encourage a level of distrust among researchers and promote the acceptance of papers based on narrow technical criteria.

4. **Claim for reproducible research** It is necessary to prevent scientific misconduct; the increasing number of cases is causing a crisis of confidence in science.

Drummond's rebuttal Misconduct has always been part of science with surprisingly little consequence. The public's distrust is likely more to with [sic] the apparent variability of scientific conclusions.

I'll address these points in turn. First, Drummond starts by articulating a position pretty similar to the distinction I draw in section 2.1. What I call "replication" — finding results that are consistent with a pattern of results found in a different study — he calls "Scientific Replication," and he seems to admit that this is pretty

important. His point is that the *exact* reproduction of an analysis from the same data set is a pretty novel development in the history of science, and not at all a cornerstone of scientific progress. I don't disagree with his point, but I think it's missing the bigger issue. That is, I agree that strictly speaking, reproducible methods are not *necessary* for the kind of replication that advances scientific knowledge. As Drummond points out, getting the same pattern of results with a near-identical experiment is less impressive (for the purposes of generalization) than getting the same results under a different set of circumstances. But I think this strict reading is missing the benefit that reproducible methods can have. Are they *necessary* or even *sufficient* for scientific progress. No, of course not. Will they *facilitate* scientific progress? I believe so. Drummond's third point argues "no," but I'll get to that shortly.

The second point is a case of pedantic nitpicking, in my opinion. He points out that not everyone is convinced that science proceeds by incremental steps. This is exactly why I also admitted early on that I am not an expert in the philosophy of science. Because I do not think the usefulness of reproducible methods hinges on some acceptance of what the philosophically "correct" view of science is. I don't think there necessarily needs to be a single "correct" view. All I claim is that transparency of methods and increased ability for people to understand and reproduce each other's work will only grease the skids, whatever the actual trajectory of scientific progress is. I don't think any of the benefits of reproducible research depend on a notion of science as incremental and cumulative. Maybe some proponents believe otherwise, but at least I propose that one can find value in reproducible methods without adhering to this (or any other) narrow view of what "science" is.

The third point is what I think is really at the heart of Drummond's complaint, and I think the most legitimate concern. In short, he seems worried that if journals start to impose arbitrary constraints on what the authors need to provide, then the system of peer-review will get clogged with data and software, and there will be a much greater burden on authors, reviewers, and editors. It just sounds like a big hassle to him, and not worth it. He also thinks it will foster distrust, because it would treat everyone as if they had something to hide, by forcing them to put data and code out into the open.

There are several issues here. One of the more disturbing comments Drummond makes is that submitting code will "simply result in an accumulation of questionable software (p. 5)." This is disturbing to me, because if one really believes that the software that generated the results of a paper is questionable, why would you ever trust the results reported in the paper? I think what he means is that most pieces of code that researchers throw together to do their analyses are not the cleanest, most efficient, most generally useful pieces of software. I think this is probably fair, given that I would think that most researchers are not also expert software developers, and are thus putting together scripts that are designed to get the answers they need, not produce general-purpose software that could be used in a "production-level" context. However, I think if researchers took the reproducible research goals seriously, they would be producing code that more cleanly replicates and produces the results of the paper. If you still have doubts about the code, at least you are able to actually inspect the code and confirm or disconfirm your doubts. If you think most people's

code is crap, and you don't ask them to provide their code, then you really have no reason to read any of the papers in the first place.

This segues into Drummond's point about reviewers. I think he imagines a situation where reviewers are called upon not only to review the paper, but to review the (messy, "questionable") code. I think this is only one way it could play out. If we imagine a really reproducible paper like the kind I will discuss in this book, the paper *cannot exist* without the code. If you take the code away, then there will be no tables of results, no figures, no reporting statistics at all. In this kind of set-up, as long as the reviewers believe the results, then there's no reason to question the code, because by definition, the authors have produced code that results in the paper. Only in the case where a reviewer is familiar with the type of analysis and wishes to know about a detail not reported in the main body of the paper (which happens *very* frequently, in my limited experience), those details can be obtained by inspecting the code. Maybe the authors would be asked to point out where in the code such-and-such can be found, or why they chose to implement something in a particular way, but if the research is *really* reproducible, the reviewer should be able to verify or falsify any particular concern they have. But if the reviewer doesn't care about the code, I don't see how it would be any different from the current situation if they merely trust that the authors' code does what they say it does, and trust the results as reported in the paper. All it would change is provide a much more thorough and expedient way for reviewers' questions and concerns to be addressed. But I think Drummond's point is well-taken that journals may not always come up with the best policies regarding reproducible research, so some effort should be taken to get things right, if a journal decides to enforce some degree of reproducibility.

Another technical downside is that if code and data are shared in addition to papers, this could represent an exponential increase in the burden on journals to host such material. This is a legitimate concern, since it starts to put a very real price tag on reproducible methods. But since publishers currently charge for access to an article *in perpetuity*, it doesn't seem unfair to me that they would therefore have the responsibility of hosting the materials in perpetuity. Maybe some more obscure articles' materials get "retired" to archives that don't need to be kept in on-demand storage on a disk somewhere. But I think if this became the norm, there would be some effort in figuring out how to host things in a cost-effective way. And again, this is only a downside towards the mandatory *publishing* of reproducible methods. All of my arguments above are based on the idea that people would use reproducible methods first for their own private benefit (regardless of journal requirements), and second in order to facilitate sharing their work (again, regardless of whether that sharing is done through a journal publisher or not). So this concern about clogging publisher's servers is not a general problem.

The bigger issue, from my perspective, is the burden that reproducible methods put on *researchers*. If it were automatic and easy to implement reproducible methods, then everyone would be doing it already. It's my belief that implementing reproducible methods, and learning the techniques/software that enable the implementation are all worth the time and energy expended. But it's hard to say if it's really worth it to everyone, if some people would benefit more than others, or what. And it's hard to put a precise price tag on it. Most people were not initially trained

on the tools that I will recommend for an implementation of reproducible measures. That means that virtually any research in the fields I work it will have some learning curve in order to start doing more and more reproducible research. And changing work habits is difficult!

To this objection, I can only say that my personal experience has been that it's more than worth it. Some people have naturally gravitated towards these kinds of techniques, and they will naturally appeal more to some people than to others. This book and the accompanying tutorials are a big experiment. Maybe they will help enable people to implement reproducible research, where they never would have otherwise. Or maybe it will just help a subset of people, who may have eventually stumbled on some similar ideas anyway, to find these techniques faster. Or maybe it will only help me! This is still an empirical question, so I'm writing the book to find out the answer.

Drummond's final point seems to be that misconduct in science is not a new phenomenon, and in fact scientific progress is remarkably robust against the bad effects of misconduct. Somewhat paradoxically, he seems to suggest (referring to the Duke cancer trials) that perhaps the solution is that we should be "more skeptical about the results of scientific experiments (p. 7)." This is really perplexing to me, because he seems to be suggesting that requiring reproducible research would increase distrust in the scientific community, but then suggests that instead of reproducible methods, we should simply distrust more science? The biggest point about the Duke trials is not that reproducible methods would have prevented the problem (which was apparently largely due to some very basic problems in data formatting: having one column displaced by a row with respect to the values in the other columns), but if we are to believe Baggerly, *thousands* of man-hours could have been saved if they had not had to go through the excruciating work of reconstructing methods that were not provided. Skepticism is natural (or acquired) tendency of all good scientists; reproducible methods merely make it easier to satisfy one's skepticism.

To put this another way, it *might* be the case that the scientific process is robust against the "base rate" of misconduct (though one has to wonder when you hear Ben Goldacre talk about the pervasiveness of it in some medical sciences). But even in the examples that Drummond gives, reproducible methods would have helped enormously. He brings up the claim of "cold fusion" by Pons and Fleischmann in 1989. And he mentions that the impact of this study were "short lived." But in doing so, he mentions that "many scientists did attempt to reproduce the result and failed (p. 7)." Is the implication that the time and money spent in all those failed replications was negligible? Those scientists had nothing better to do? That's hard for me to believe. Of course, even with reproducible methods, some time and expense would be lost in trying to replicate false finding like this, but the point is that (almost by definition) the more reproducible the methods are, the less time and money would be wasted in the process.

In the end, I think Drummond's points mostly stack in *favor* of reproducible research. While reproducibility is not a *necessity* of science, it facilitates what he calls "Scientific Replication" (and what I call just "replication" in section 2.1) by providing more transparency and facilitating the process of replication. The fact that not everyone has the same view of what the "scientific method" is also comes

out favoring reproducible research, because perhaps an author is making some set of judgment calls as to which of his results are “important” or not. If this is not transparent in a way that allows others to examine the impact of alternatives, then the work would be of little use, or even misleading to someone with different views. In other words, greater transparency and reproducibility benefits more viewpoints, not fewer. Finally, the consistent presence of misconduct is not likely to disappear from science, no more than from any other sphere of human endeavor. However, reproducible measures should both discourage “accidental” misconduct, and make all kinds of misconduct and Bad Science (to use [Goldacre’s term](#)) easier to catch and less onerous to correct.

2.5 Some core values

We’ve already discussed replication, but what else is at stake here? Why should we care about reproducibility?

Chapter 3

Dimensions of reproducibility

So we're a few chapters in, and I have managed to only hint vaguely at what *reproducible* really means. The reason for this is that ultimate, I think reproducibility is most useful when thought of as a *relative* concept. I'll present a conceptual framework in this chapter for what I think the most important dimensions of reproducibility are. But moreover, I think reproducibility is relative in a very practical sense. That is, I believe that we should be less caught up in defining some ideal for reproducibility, and more invested in finding out how to make our work more reproducible than it is currently, and reaping the benefits.

That said, the thesis I present in this chapter is as follows. Evaluating whether research is reproducible (or how reproducible it is) depends on three dimensions: the *domain*, the *range*, and the *audience*. In brief, these refer to *what* is being reproduced, *how precise* the reproduction is, and *who* is expected to be able to do the reproduction.

I'll talk about each of these dimensions in turn.

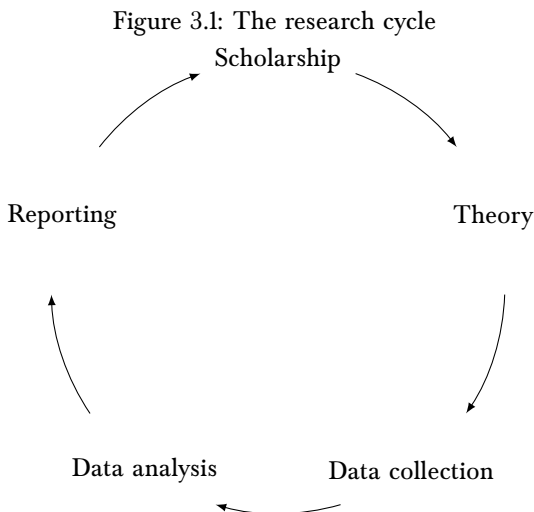
3.1 Domain: what is being reproduced?

In order to talk about reproducibility, we have to consider what aspects of the research process — or more concretely, what research *tasks* — are intended to be reproduced. The current “state of the art,” as forwarded by the most visible proponents of reproducible research, boils down to a reproduction of data analysis. Sharing data and code that reproduces the analysis, figures, etc. in a paper is a great start, but only focuses on one slice of the research process.

But even this slice can be broken down, and we can talk about some aspects of the data analysis process being more reproducible than others, for any given case. For example, someone might publish all the code that went into their analysis, but for some reason were not able to (or not willing to) provide the raw data. This is a step in the right direction, and it makes the analysis more reproducible than if they hadn't provided their code, but it's more limited in the *domain* of reproducibility.

However, to really push the idea of reproducible research to its limits, we need

to expand the domain to consider *all* aspects of the research process, not just the data analysis part. Again, I'm not a philosopher of science, but from my point of view, the research process breaks down into five big chunks, which are inter-related in various ways, but which basically form a cycle. This is schematized in figure 3.1.



Here's how I see the basic cycle happening:

1. **Scholarship:** Reading and synthesizing previous work on a topic. Very few ideas in science come from nowhere. Science is a long, protracted dialogue. So the processes involved in scholarship are the processes of listening to that dialogue and coming to some understanding of it and where you might be able to add to it.
2. **Theory:** This is basically the “ideas” bucket. In the process of doing research and reading the literature, you eventually come up with your own ideas, or pick some aspect of existing ideas to test. That is, there is a process of narrowing in on some aspect of a theory that you are wanting to falsify, clarify, develop, or support.
3. **Data collection:** At the heart of all kinds of science is the idea that you need to make some kind of observations about the world, that is, collect data. I'm simplifying a great deal to place this step after theory, because in many cases, observations precede theory, but I think one could defend the idea that all observation is made in the context of some theory, even if that theory is a rough “pre-theoretical” conceptualization of a problem or domain. Either way, if the reader would prefer to add more lines and circles to the diagram, they are welcome to. The point here is that the process of data collection frequently interacts with theoretical understanding, and includes both designing experiments and all manner of collection processes, such as

running a psycholinguistic experiment with undergraduates, collecting data from a corpus or scraping it from the web, running lab experiments, collecting naturalistic observations, etc., etc.

4. **Data analysis:** Whatever kind of data you end up collecting, there has to be some kind of analysis involved. In the context of reproducible research, the assumption is normally that this involves quantitative (statistical) analysis, but this doesn't necessarily have to be the case. However, the data is analyzed, that process is integral to understanding how the data actually bear on the theory being tested/developed, and so the process should be as reproducible and transparent as possible. I'd go so far as to say that things like formal mathematical proofs are a type of analysis, and show how one gets from A to B, from premises (theory and scholarship; preceding work) to conclusions. More on all this, but the point is that there's a lot that could qualify as "data analysis" in the broader view I'm setting up here.
5. **Reporting:** A critical piece following an analysis is to report the results, conclusions, etc. in some kind of formal, written fashion. There's a cute picture on the web of Adam Savage from the *Mythbusters* show with the caption: "**Remember kids, the only difference between screwing around and science is writing it down.**" In a slightly more serious venue, Andrew Gelman says more or less the same thing in his blog: "**science *is* science communication.**" Regardless of the philosophy, writing papers and getting published is one of the primary things researchers are expected to do in the course of their careers. This involves a lot of things, but it represents a pulling together of some part of the analysis (often not all of it!) of some of the data (often not all of it!) and discussion of some of the literature (often not all of it!). . . you get the picture. Reporting is a lot more than just putting down the previous four steps to paper; it involves a lot of choices that could be made more transparent or reproducible. And finally, a published paper becomes part of the dialogue of science, feeding back into the cycle.

Again, the idea I'd like to push is that reproducibility is not necessarily limited to just the data analysis part of the cycle, though that's been the primary focus of people that have been waving the banner of Reproducible Research. In the next several chapters, I will work through each of these parts of the cycle, discussing how the activities in that domain could be made more reproducible, and how this could be a good idea. But before diving into that, I still need to talk about *precision* and *audience*.

3.2 Range: the precision of reproducibility

Once you narrow in on *what* you're trying to reproduce, you can talk about how *precise* the reproduction is, or should be. If your goal is to reproduce an analysis, the assumption is that usually it should be pretty precise. That is, if you want to show how you got from a set of data to a particular statistic or figure, and someone runs

your code with your data, the expectation is that the reproduction should be *exact*. But even “exact” may have some tolerance for variation. You’ll only get an exact figure if the code also specifies things like aspect ratio, or precise colors. But maybe variation in some of these details is tolerable for one’s purposes. That’s the broader point here, that “reproducible” can represent a wide range of values for how precise the reproduction needs to be in order to be acceptable, depending on the context.

To take another example, data collection methods should be fairly reproducible, so that other people can see exactly how you collected your data, and so that they could collect similar data on their own. But if it involves collecting data from a sample (like collecting data from human participants), it will be impossible to collect precisely the same set of data. Even automated methods like scraping websites or processing Google search results may be impossible to reproduce exactly, because of the constantly changing nature of the internet. But even if the collected data won’t be exactly the same, providing the code and stimuli for running your experiment is a much more reproducible case than simply describing generally how the experiment was designed.

Reproducibility is not an all-or-nothing proposal. Simply moving your methods down the scale towards “higher precision of reproducibility” has a great deal of value, however far you’re able to push them. But if institutions (like journals) wish to set thresholds for minimum standards, then the precision of reproducibility needs to be carefully considered.

3.3 Audience: who is going to do the reproduction?

The dimension of *audience* may be one of the most important dimensions, but I have seen little if any direct discussion of it. It can be a deal-breaker in many cases, especially if you are interested in *really* reproducible research, not just *theoretically* reproducible research. For example, you could provide a complete set of code to generate all of your results and figures, but if you provide it in FORTRAN, or something esoteric like `brainf***`, the number of people who could actually reproduce your work would be pretty small. To take a more realistic example, while the statistical software R continues to grow in popularity, proprietary statistical packages like SPSS are still much more prevalent. I will argue later that using R has many advantages for creating reproducible research, but it may be that for a particular audience, it is *harder* for them to reproduce an analysis in R than it is in SPSS. Similarly, while I will argue that \LaTeX is a superior system for writing reproducible papers, Microsoft Word is still dominant for many researchers, and reproducible collaboration with \LaTeX can run into real problems.

Even more broadly, an analysis might be reproducible for some other academic working in the same field, but might be totally opaque to a non-academic. This is a real issue, and can undercut some of the lofty ideals put forward by the reproducible research community. For example, how can reproducible methods provide transparency and accountability to taxpayers, if 99% of taxpayers do not know enough about the software to be able to run the analysis?

Finally, there is also a very special case of audience to consider: yourself. For

many of the benefits I outline in section 2.3.1, the goal is to make it so that you can easily reproduce your own work. If you've never tried it, this turns out to be more difficult than you might expect.

3.4 Interactions

These dimensions are theoretically independent, but in reality, they are often correlated in important ways. For example, if you want to be able to reproduce your own work, it is usually implied that the target precision is pretty high. That is, it's more typical that you want to be able to know or reproduce *exactly* (or as exactly as possible) how you did something. But in typical papers, where you must report your methods in a way so that other researchers could at least attempt a replication of your results, the standard for precision are much lower. To take the example of data collection for an experiment, if you have a successful round in recruiting participants, you will probably be interested in using more or less exactly the same tactics (same flyers, same places where you posted your flyers, same rate of pay, etc.), but this level of detail is virtually never shared in a published paper. Conversely, if you want your analysis to be *really* reproducible by a wide audience, you may have to provide a lot more detail than you would to a graduate student in your lab, since they may already have a great deal of familiarity with your typical practices.

The point is that reproducible methods are not a one-size-fits-all project. Therefore, I will work through a wide range of applications and situations, and discuss what it might mean to have more reproducible methods in that domain, for certain values of precision and audience, but I will not be able to cover all possible combinations in a detailed way. In keeping with a pragmatic focus, I will take self-reproduction (i.e., reproducing your own work) as a starting point, and discuss what I consider to be useful levels of precision, and then expand from there.

Chapter 4

Scholarship

Chapter 5

Theory

Chapter 6

Data collection

Chapter 7

Data analysis

Chapter 8

Reporting

Chapter 9

Conclusions

Chapter 10

Implementation

10.1 Guiding principles

10.1.1 Free and open source

10.1.2 Cross-platform

10.1.3 Stable

10.1.4 Well-documented

10.1.5 Customizable

10.2 Summary of tools

10.2.1 Emacs

10.2.2 Org-mode

10.2.3 Git

10.2.4 L^AT_EX

10.2.5 Python

10.2.6 R

10.2.7 (Emacs) Lisp

10.3 Scholarship

10.4 Data collection

10.5 Data analysis

10.6 Sharing

10.7 Collaboration

10.8 Putting it all together

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