

Addressing The Scientific Reproducibility Crisis Through Educational Software
Integration

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Audrey M. Bertin

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Benjamin S. Baumer

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I want to thank a few people.

Preface

This is an example of a thesis setup to use the reed thesis document class (for LaTeX) and the R bookdown package, in general.

Table of Contents

Introduction	1
Chapter 1: An Introduction to Reproducibility	3
1.1 What is reproducibility?	3
1.2 The Reproducibility Crisis	4
1.3 The Components of Reproducible Research	5
1.4 Current Attempts to Address Reproducibility in Scientific Publishing	7
1.4.1 Journal Statements On Reproducibility Across The Sciences	7
1.4.2 Journal Policies In The Statistical And Data Sciences	9
1.4.3 Assessing the Success of Academic Reproducibility Policies	10
1.4.4 Reproducibility Education	11
Chapter 2: Addressing the Challenges of Reproducibility	13
2.1 Review Of Previous Work	13
2.1.1 R Packages and Other Software	13
2.2 Identifying Gaps In Existing Solutions	15
2.3 My Contribution: <code>fertile</code> , An R Package Creating Optimal Conditions For Reproducibility	15
2.3.1 Package Overview	15
2.3.2 Proactive Use	15
2.3.3 Retroactive Use	16
2.3.4 Logging	19
2.3.5 Utility Functions	19
2.3.6 File Path Management	19
2.3.7 File Types	20
2.3.8 Temporary Directories	20
2.3.9 Managing Project Dependencies	21
2.4 How <code>fertile</code> Works	21
2.5 <code>fertile</code> in Practice: Experimental Results From Smith College Student Use	22
Chapter 3: Incorporating Reproducibility Tools Into The Greater Data Science Community	25
3.1 Potential Applications of <code>fertile</code>	25
3.1.1 In Journal Review	25

3.1.2	By Beginning Data Scientists	25
3.1.3	By Advanced Data Scientists	25
3.1.4	For Teaching Reproducibly	25
3.2	Integration Of fertile And Other Reproducibility Tools in Data Science Education	25
	Conclusion	27
	Appendix A: The First Appendix	29
	Appendix B: The Second Appendix, for Fun	31
	References	33

Abstract

The preface pretty much says it all.

Second paragraph of abstract starts here.

Dedication

You can have a dedication here if you wish.

Introduction

Potential sources:

<https://arxiv.org/abs/1401.3269>
<https://academic.oup.com/isp/article-abstract/17/4/392/2528285>
https://dl.acm.org/doi/abs/10.1145/3186266?casa_token=3yv8mooiZXYAAAAA:AUWshgsmm-4ulr7qYK2vm3a6EdJneFLgn3nxplGeaZpT7hgFcIRkRA7edGHdjg_pPvs5p-GoHHFo
https://dl.acm.org/doi/abs/10.1145/3027385.3029445?casa_token=rgNbcFWIA1AAAAAA:cZRPAY1KYewKfheFe74GBDwKzF9Q8X0xMau0AtBVkYSTYrd7apJEnwDY_T8oqh1cZQED1gHjqtq4
<https://berkeleysciencereview.com/2014/06/reproducible-collaborative-data-science/>
<https://guides.lib.uw.edu/research/reproducibility/teaching>
<https://escholarship.org/uc/item/90b2f5xh>
https://www.mitpressjournals.org/doi/full/10.1162/dint_a_00053
<https://www.pnas.org/content/115/11/2584>
<https://www.pnas.org/content/115/11/2561>

Chapter 1

An Introduction to Reproducibility

1.1 What is reproducibility?

In the field of data science, research is considered fully *reproducible* when the requisite code and data files produce identical results when run by another analyst, or more generally, when a researcher can “duplicate the results of a prior study using the same materials as were used by the original investigator”.

Add Source: K. Bollen, J. T. Cacioppo, R. Kaplan, J. Krosnick, J. L. Olds, Social, Behavioral, and Economic Sciences Perspectives on Robust and Reliable Science (National Science Foundation, Arlington, VA, 2015).

This term was first coined in 1992 by computer scientist Jon Claerbout, who associated it with a “software platform and set of procedures that permit the reader of a paper to see the entire processing trail from the raw data and code to figures and tables”.

Add source: J. Claerbout, M. Karrenbach, Electronic documents give reproducible research a new meaning, in Proceedings of the 62nd Annual International Meeting of the Society of Exploration Geophysics, New Orleans, USA, 25 to 29 October 1992.

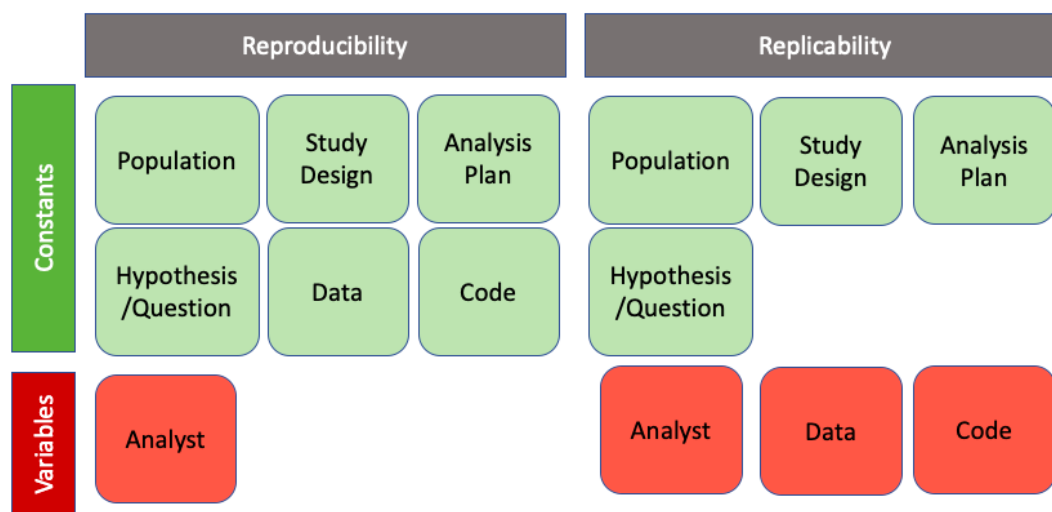
Since its inception, the concept of reproducibility has been applied across many different data-intensive fields, including epidemiology, computational biology, economics, clinical trials, and, now, the more general domain of statistical and data sciences (Goodman, Fanelli, & Ioannidis (2016)).

Reproducible research has a wide variety of benefits in the scientific community. When researchers provide the code and data used for their work in a well-organized and reproducible format, readers are more easily able to determine the veracity of any findings by following the steps from raw data to conclusions. The creators of reproducible research can also more easily receive more specific feedback (including bug fixes) on their work. Moreover, others interested in the research topic can use the code to apply the methods and ideas used in one project to their own work with minimal effort.

Although often confused, the concept of *reproducibility* is distinct from the similar idea of *replicability*: the ability of a researcher to duplicate the results of a study when

following the original procedure but collecting new data. Replicability has larger-scale implications than reproducibility; the findings of research studies can not be accepted unless a variety of other researchers come to the same conclusions through independent work.

```
knitr::include_graphics("figure/versus.png")
```



Reproducibility and replicability are both necessary to the advancement of scientific research, but they vary significantly in terms of their difficulty to achieve. Reproducibility, in theory, is somewhat simple to attain in data analyses—because code is inherently non-random (excepting applications involving random number generation) and data remain consistent, variability is highly restricted. The achievement of replicability, on the other hand, is a much more complex challenge, involving significantly more variability and requiring high quality data, effective study design, and incredibly robust hypotheses.

1.2 The Reproducibility Crisis

Despite the relative simplicity of achieving reproducibility, a significant proportion of the work produced in the scientific community fails to meet reproducibility standards. 52% of respondents in a 2016 Nature survey believed that science was going through a “crisis” of reproducibility. Additionally, the vast majority of researchers across all fields studied reported having been unable to reproduce another researcher’s results, while approximately half reported having been unable to reproduce their own. <https://www.nature.com/news/1-500-scientists-lift-the-lid-on-reproducibility-1.19970> Other studies paint an even bleaker picture: a 2015 study found that over 50% of studies psychology failed reproducibility tests and research from 2012 found that figure closer to 90% in the field of cancer biology. (<https://www.nature.com/news/over-half-of-psychology-studies-fail-reproducibility-test-1.18248>, <https://www.nature.com/articles/483531a>)

In the past several years, this “crisis” of reproducibility has risen toward the forefront of scientific discussion. Without reproducibility, the scientific community cannot properly verify study results. This makes it difficult to identify which information should be believed and which should not and increases the likelihood that studies sharing misleading information will be dispersed. The rise of data-driven technologies, alongside our newly founded ability to instantly share knowledge worldwide, has made reproducibility increasingly critical to the advancement of scientific understanding, necessitating the development of solutions for addressing the issue.

Academics have recognized this, and publications on the topic appear to have increased significantly in the last several years (Eisner (2018); Fidler & Wilcox (2018); Gosselin (2020); McArthur (2019); Wallach, Boyack, & Ioannidis (2018)).

1.3 The Components of Reproducible Research

In order to address the lack of reproducibility in scientific research, it is important to first consider the question: Which components are necessary to declare research reproducible?

Publications attempting to answer this can be found in all areas of scientific research. However, as Goodman et al. (2016) argue, the language and conceptual framework used to describe research reproducibility varies significantly across the sciences, and there are no clear standards on reproducibility agreed upon by the scientific community as a whole.

At a minimum, according to Goodman et al. (2016), documenting reproducibility requires the sharing of data (raw or processed), relevant metadata, code, and related software. However, according to other authors, the full achievement of reproducibility may require additional components.

Kitzes, Turek, & Deniz (2017) present a collection of case studies on reproducibility practices from across the data-intensive sciences, illustrating a variety of recommendations and techniques for achieving reproducibility. Although their work does not come to a consensus on the exact standards of reproducibility that should be followed, several common trends and principles emerge from their case studies that extend beyond the minimum recommendations of Goodman et al. (2016):

- 1) use clear separation, labeling, and documentation in provided code,
- 2) automate processes when possible, and
- 3) design the data analysis workflow as a sequence of small steps glued together, with outputs from one step serving as inputs into the next. This is a common suggestion within the computing community, originating as part of the Unix philosophy (Gancarz (2003)).

Cooper et al. (2017) focus on data analysis completed in R and identify a similar list of important reproducibility components, reinforcing the need for clearly labeled, well-documented, and well-separated files. In addition, they recommend publishing a list of software dependencies and using version control to track project changes over time.

Broman (2019) reiterates the need for clear naming and file separation while sharing several additional suggestions: keep the project contained in one directory, use relative paths when accessing the file system, and include a `README` file describing the project.

The reproducibility recommendations from R OpenSci, a non-profit initiative founded in 2011 to make scientific data retrieval reproducible, share similar principles to those discussed previously. They focus on a need for a well-developed file system, with no extraneous files and clear labeling. They also reiterate the need to note dependencies and use automation when possible, while making clear a suggestion not present in the previously-discussed literature: the need to use seeds, which allow for the saving and restoring of the random number generator state, when running code involving randomness (Martinez et al. (2018)).

Although these recommendations differ from one another, when considered in combination they provide a well-rounded picture of the components important to research reproducibility across the scientific community:

1. The basic project components are made accessible:
 - Data (raw and/or processed)
 - Metadata
 - Code
 - Related Software
2. The file structure of project is well-organized:
 - Separate folders for different file types.
 - No extraneous files.
 - Minimal clutter.
3. The project is documented well:
 - Files are clearly named, preferably in a way where the order in which they should be run is clear.
 - A `README` is present.
 - Software dependencies are noted.
4. File paths used in code are not system- or user-dependent:
 - No absolute paths.
 - No paths leading to locations outside of a project's directory.
 - Only relative paths, pointing to locations within a project's directory, are permitted.
5. Randomness is accounted for:
 - If randomness is used in code, a seed must also be set.

6. Readable, styled code:

- Though not mentioned in the sources described previously, it is also important that code be written in a coherent style. This is because code that conforms to a style guide or is written in a consistent dialect is easier to read, simplifying the process of following a researcher's work from beginning to end (Hermans & Aldewereld (2017)).

1.4 Current Attempts to Address Reproducibility in Scientific Publishing

1.4.1 Journal Statements On Reproducibility Across The Sciences

In an attempt to increase reproducibility in the sciences, leaders from academic journals around the world have taken steps to create new standards and requirements for submitted articles. However, these standards are highly inconsistent, varying significantly both across and within disciplines.

The journal whose requirements appear to align most closely with those components defined previously in Section 3 is the *American Journal of Political Science* (AJPS). In 2012, the AJPS became the first political science journal to require authors to make their data openly accessible online, and the publication has instituted stricter requirements since. AJPS now requires that authors submit the following alongside their papers:

- The dataset analyzed in the paper and information about its source. If the dataset has been processed, instructions for manipulating the raw data to achieve the final data must also be shared.
- Detailed, clear code necessary for reproducing all of the tables and figures in the paper.
- Documentation, including a README and codebook.
- Information about the software used to conduct the analysis, including the specific versions and packages used.

ADD SOURCE: https://ajps.org/wp-content/uploads/2018/05/ajps_replication-guidelines-2-1.pdf

These standards are quite thorough and contain mandates for the inclusion of the vast majority of components necessary for complete reproducibility.

Most journals, however, do not come close to meeting such high standards in their reproducibility statements. We will consider examples from several fields:

In the biomedical sciences, a group of editors representing over 30 major journals met in 2014 to address reproducibility in their field, coming to a consensus on a set of principles they wanted to uphold. Listed below are those relating specifically to the use of data and statistical methods:

- 1) Journals in the biomedical sciences should have a mechanism to check the statistical accuracy of submissions.
- 2) Journals should have no (or generous) limit on methods section length.
- 3) Journals should use a checklist to ensure the reporting of key information, including:
 - The article meets nomenclature/reporting standards of the biomedical field.
 - Investigators report how often each experiment was performed and whether results were substantiated by repetition under a range of conditions.
 - Statistics must be fully reported in the paper (including test used, value of N, definition of center, dispersion and precision measures).
 - Authors must state whether samples were randomized and how.
 - Authors must state whether the experiment was blinded.
 - Authors must clearly state the criteria used for exclusion of any data or subjects and must include all results, even those that do not support the main findings.
- 4) All datasets used in analysis must be made available on request and should be hosted on public repositories when possible. If not possible, data values should be presented in the paper or supplementary information.
- 5) Software sharing should be encouraged. At the minimum, authors should provide a statement describing if software is available and how to obtain it.

ADD SOURCE: <https://www.nature.com/news/journals-unite-for-reproducibility-1.16259>

Even though these principles seem well-developed on the surface, they fail to meet even the basic requirements defined by Goodman et al. (2016) previously. Several of the principles are purely recommendations; there is no *requirement* that code be shared, nor metadata, and software requirements are quite loose, requiring no information about dependencies or software version.

We see a similar issue even in journals designed specifically for the purpose of improving scientific reproducibility. *Experimental Results*, a publication created by Cambridge University Press to address some of the reproducibility and open access issues in academia, also falls short of meeting high standards. The journal, which showcases articles from a variety of scientific disciplines, states in their transparency and openness policy:

Whenever possible authors should make evidence and resources that underpin published findings, such as data, code, and other materials, available to readers without undue barriers to access.

The inclusion of code and data are only recommended and no definition of what “other materials” may mean is provided. No components of reproducibility extending beyond those required at a minimum are even considered.

ADD SOURCE: <https://www.cambridge.org/core/journals/experimental-results/information/transparency-and-openness-policy>

The *American Economic Review*, the first of the top economics journals to require the inclusion of data alongside publications, has stronger guidelines than several of those mentioned previously, though not as strong as the *American Journal of Political Science*. Their Data and Code Availability Policy states the following:

It is the policy of the American Economic Association to publish papers only if the data and code used in the analysis are clearly and precisely documented, and access to the data and code is clearly and precisely documented and is non-exclusive to the authors.

SOURCE: <https://www.aeaweb.org/journals/policies/data-code>

These requirements are quite strict, prohibiting exceptions for papers using data or code not available to the public in the way that many other journals claiming to promote reproducibility do.

1.4.2 Journal Policies In The Statistical And Data Sciences

In the field of statistical and data sciences, the majority of highly ranked journals contain statements on reproducibility. Some of these are quite robust, surpassing the requirements of many of the other journals discussed previously, while others are lacking.

The *Journal of the American Statistical Association* stands out as having relatively robust requirements. The publication's guidelines require that data be made publicly available at the time of publication except for reasons of security or confidentiality. It is strongly recommended that code be deposited in open repositories. If data is used in a process form, the provided code should include the necessary cleaning/preparation steps. Data must be in an easily understood form and a data dictionary should be included. Code should also be in a form that can be used and understood by others, including consistent and readable syntax and comments. Workflows involving more than one script should also contain a master script, Makefile, or other mechanism that makes it clear what each component does, in what order to run them, and what the inputs and outputs to each area. **Source here:** <https://jasa-acsgithub.io/repro-guide/pages/author-guidelines>

The *Journal of Statistical Software* also has strong guidelines, though less thorough. Authors must provide *commented* source code for their software; all figures, tables, and output must be exactly reproducible on at least one platform, and random number generation must be controlled; and replication materials (typically in the form of a script) must be provided. **Source here:** <https://www.jstatsoft.org/pages/view/authors#review-process>.

The expectations of the *Journal of Computational and Graphical Statistics* are notably weaker, requiring only that authors “submit code and datasets as online supplements to the manuscript,” with exceptions for security or confidentiality, but providing no further detail. **Source:** <https://www.tandfonline.com/action/authorSubmission?show=instructions&journalCode=ucgs20>. The *R Journal*

has the same requirements, but with no exceptions on the data provision policy, stating that authors should “not use such datasets as examples.” **Source** <https://journal.r-project.org/share/author-guide.pdf>

Perhaps the weakest reproducibility policies come from *The American Statistician* and the *Annals of Statistics*. The former appears to have no requirements, stating only that it “strongly encourages authors to submit datasets, code, other programs, and/or appendices that are directly relevant to their submitted articles,” while the latter appears to have no statement on reproducibility at all. **Sources:** <https://www.tandfonline.com/action/authorSubmission?show=instructions&journalCode=utas20>, <https://imstat.org/journals-and-publications/annals-of-statistics/annals-of-statistics-manuscript-submission/>.

1.4.3 Assessing the Success of Academic Reproducibility Policies

As illustrated by the prior examples, academic publications across many different disciplines have been making an effort to incorporate reproducibility standards into their submission guidelines. The simple implementation of a policy, however, does not ensure that its goals will be achieved. Reproducibility can only be addressed when both authors *and* journal reviewers actively implement publishing standards in practice. Without participation and dedication from all involved, reproducibility guidelines serve more as a theoretical goal than a practical achievement.

So in practice, do academic reproducibility standards actually result in reproducible publications?

Let us consider the case of the journal *Science*. *Science* instituted a reproducibility policy in 2011 and has maintained it ever since. In its original form, their policy stated the following:

All data necessary to understand, assess, and extend the conclusions of the manuscript must be available to any reader of *Science*. All computer codes involved in the creation or analysis of data must also be available to any reader of *Science*. After publication, all reasonable requests for data and materials must be fulfilled. Any restrictions on the availability of data, codes, or materials. . . must be disclosed to the editors upon submission. . .

This policy is similar to many of the others considered previously, requiring the publishing of code and data with exceptions permitted when necessary.

Researchers Victoria Stodden, Jennifer Seiler, and Zhaokun Ma (<https://www.pnas.org/content/115/11/2584>) tested the efficacy of this policy in practice, emailing corresponding authors of 204 articles published in the year after *Science* first implemented its policy to request the data and code associated with their articles. The researchers only received (at least some of) the requested material from 36% of authors. This low rates were due to several factors:

- 26% of authors did not respond to email contact.

- 11% of authors were unwilling to provide the data or code without further information regarding the researchers' intentions.
- 11% asked the researchers to contact someone else and that person did not respond.
- 7% refused to share data and/or code.
- 3% directed the researchers back to their paper's supplemental information section.
- 3% of authors made a promise to follow up and then did not follow through.
- 3% of emails bounced.
- 2% gave reasons why they could not share for ethical reasons, size limitations, or some other reason.

Of the 56 papers they deemed likely reproducible, the authors randomly selected 22 and were able to replicate the results for all but 1, which failed due to its reliance on software that was no longer available.

<https://www.pnas.org/content/115/11/2584>

<https://www.cos.io/about/news/new-measure-rates-quality-research-journals-policies-promote-transparency-and-reproducibility>

<https://www.cos.io/our-services/top-guidelines>

[http://emiguel.econ.berkeley.edu/assets/miguel_research/78/jel.](http://emiguel.econ.berkeley.edu/assets/miguel_research/78/jel.20171350.pdf)

20171350.pdf

https://link.springer.com/chapter/10.1007/164_2019_290#Sec9

<https://royalsocietypublishing.org/doi/full/10.1098/rsos.180448>

Policies can be time consuming to implement in terms of actually reviewing articles for publication. If there's a huge influx, it would be unreasonable to re-run every analysis submitted!

1.4.4 Reproducibility Education

Chapter 2

Addressing the Challenges of Reproducibility

[

The relative simplicity of the reproducibility challenge makes it an ideal candidate for solution-building. Although significant progress on addressing reproducibility on a widespread scale is a long-term challenge, impactful forward progress—if on a smaller scale—can be achieved in the short-term.

My research has focused on doing just this, providing tools to assist with achieving reproducibility in one segment of the scientific community: RStudio users.

] — DO WE NEED THIS?

2.1 Review Of Previous Work

2.1.1 R Packages and Other Software

Much of this work is highly generalized, written to be applicable to users working with a variety of statistical software programs. Because all statistical software programs operate differently, these recommendations are inherently vague and difficult to implement, particularly to new analysts who are relatively unfamiliar with their software. Focused attempts to address reproducibility in specific certain software programs are more likely to be successful. We focus on R, due to its open-source nature, accessibility, and popularity as a tool for statistical analysis.

A small body of R packages focuses on research reproducibility. `rrtools` (Marwick (2019)) addresses some of the issues discussed in Marwick, Boettiger, & Mullen (2018) by creating a basic R package structure for a data analysis project and implementing a basic `testthat::check` functionality. The `orderly` (FitzJohn et al. (2020)) package also focuses on file structure, requiring the user to declare a desired project structure (typically a step-by-step structure, where outputs from one step are inputs into the next) at the beginning and then creating the files necessary to achieve that structure. `workflowr`'s (Blischak, Carbonetto, & Stephens (2019)) functionality is based around version control and making code easily available online. It works to generate a website

containing time-stamped, versioned, and documented results. **checkers** (Ross, DeCicco, & Randhawa (2018)) allows you to create custom checks that examine different aspects of reproducibility. **packrat** (Ushey, McPherson, Cheng, Atkins, & Allaire (2018)) is focused on dependencies, creating a packaged folder containing a project as well as all of its dependencies so that projects dependent on lesser-used packages can be easily shared across computers. **drake** (OpenSci (2020)) analyzes workflows, skips steps where results are up to date, and provides evidence that results match the underlying code and data. Lastly, the **reproducible** (McIntire & Chubaty (2020)) package focuses on the concept of caching: saving information so that projects can be run faster each time they are re-completed from the start.

Many of these packages are narrow, with each effectively addressing a small component of reproducibility: file structure, modularization of code, version control, etc. These packages often succeed in their area of focus, but at the cost of accessibility to a wider audience. Their functions are often quite complex to use, and many steps must be completed to achieve the required reproducibility goal. This cumbersome nature means that most reproducibility packages currently available are not easily accessible to users near the beginning of their R journey, nor particularly useful to those looking for quick and easy reproducibility checks. A more effective way of realizing widespread reproducibility is to make the process for doing so simple enough that it takes little to no conscious effort to implement. You want users to “fall into a hole” (we paraphrase Hadley Wickham) of good practice.

Continuous integration tools provide more general approaches to automated checking, which can enhance reproducibility with minimal code. For example, **wercker**—a command line tool that leverages Docker—enables users to test whether their projects will successfully compile when run on a variety of operating systems without access to the user’s local hard drive (Oracle Corporation (2019)). **GitHub Actions** is integrated into GitHub and can be configured to do similar checks on projects hosted in repositories. **Travis CI** and **Circle CI** are popular continuous integration tools that can also be used to check R code.

However, while these tools can be useful, they are generalized so as to be useful to the widest audience. As a result, their checks are not designed to be R-specific, which makes them sub-optimal for users looking to address reproducibility issues involving features specific to the R programming language, such as package installation and seed setting.

2.2 Identifying Gaps In Existing Solutions

2.3 My Contribution: **fertile**, An R Package Creating Optimal Conditions For Reproducibility

2.3.1 Package Overview

fertile attempts to address these gaps in existing software by providing a simple, easy-to-learn reproducibility package that, rather than focusing intensely on a specific area, provides some information about a wide variety of aspects influencing reproducibility. **fertile** is flexible, offering benefits to users at any stage in the data analysis workflow, and provides R-specific features, which address certain aspects of reproducibility that can be missed by external project development software.

fertile is designed to be used on data analyses organized as R Projects (i.e. directories containing an `.Rproj` file). Once an R Project is created, **fertile** provides benefits throughout the data analysis process, both during development as well as after the fact. **fertile** achieves this by operating in two modes: proactively (to prevent reproducibility mistakes from happening in the first place), and retroactively (analyzing code that has already been written for potential problems).

Much of the available literature focuses on file structure, organization, and naming, and **fertile**'s features are consistent with this. Marwick et al. (2018) provide the framework for file structure that **fertile** is based on: a structure similar to that of an R package (R-Core-Team (2020), Wickham (2015)), with an R folder, as well as `data`, `data-raw`, `inst`, and `vignettes`.

2.3.2 Proactive Use

Proactively, the package identifies potential mistakes as they are made by the user and outputs an informative message as well as a recommended solution. For example, **fertile** catches when a user passes a potentially problematic file path—such as an absolute path, or a path that points to a location outside of the project directory—to a variety of common input/output functions operating on many different file types.

```
library(fertile)
file.exists("~/Desktop/my_data.csv")
```

```
[1] TRUE
```

```
read.csv("~/Desktop/my_data.csv")
```

Error: Detected absolute paths

```
read.csv("../.../Desktop/my_data.csv")
```

Error: Detected paths that lead outside the project directory

`fertile` is even more aggressive with functions (like `setwd()`) that are almost certain to break reproducibility, causing them to throw errors that prevent their execution and providing recommendations for better alternatives.

```
setwd("~/Desktop")
```

Error: `setwd()` is likely to break reproducibility. Use `here::here()` instead.

These proactive warning features are activated immediately after attaching the `fertile` package and require no additional effort by the user.

2.3.3 Retroactive Use

Retroactively, `fertile` analyzes potential obstacles to reproducibility in an RStudio Project (i.e., a directory that contains an `.Rproj` file). The package considers several different aspects of the project which may influence reproducibility, including the directory structure, file paths, and whether randomness is used thoughtfully.

The end products of these analyses are reproducibility reports summarizing a project's adherence to reproducibility standards and recommending remedies for where the project falls short. For example, `fertile` might identify the use of randomness in code and recommend setting a seed if one is not present.

Users can access the majority of `fertile`'s retroactive features through two primary functions, `proj_check()` and `proj_analyze()`.

The `proj_check()` function runs fifteen different reproducibility tests, noting which ones passed, which ones failed, the reason for failure, a recommended solution, and a guide to where to look for help. These tests include: looking for a clear build chain, checking to make sure the root level of the project is clear of clutter, confirming that there are no files present that are not being directly used by or created by the code, and looking for uses of randomness that do not have a call to `set.seed()` present. A full list is provided below:

```
list_checks()
```

-- The available checks in 'fertile' are as follows: ----- fertile 0.0.0.9027 --

```
[1] "has_tidy_media"          "has_tidy_images"
[3] "has_tidy_code"           "has_tidy_raw_data"
[5] "has_tidy_data"           "has_tidy_scripts"
[7] "has_readme"              "has_no_lint"
[9] "has_proj_root"           "has_no_nested_proj_root"
[11] "has_only_used_files"     "has_clear_build_chain"
[13] "has_no_absolute_paths"   "has_only_portable_paths"
[15] "has_no_randomness"
```

Subsets of the fifteen tests can be invoked using the `tidyselect` helper functions (Henry & Wickham (2020)) in combination with the more limited `proj_check_some()` function.

```
proj_dir <- "project_miceps"
```

```
proj_check_some(proj_dir, contains("paths"))
```

```
-- Compiling... ----- fertile 0.0.0.9027
-- Rendering R scripts... ----- fertile 0.0.0.9027
-- Running reproducibility checks ----- fertile 0.0.0.9027
v Checking for no absolute paths
v Checking for only portable paths
-- Summary of fertile checks ----- fertile 0.0.0.9027
v Reproducibility checks passed: 2
```

Each test can also be run individually by calling the function matching its check name.

The `proj_analyze()` function creates a report documenting the structure of a data analysis project. This report contains information about all packages referenced in code, the files present in the directory and their types, suggestions for moving files to create a more organized structure, and a list of reproducibility-breaking file paths used in code.

```
proj_analyze(proj_dir)
```

```
-- Analysis of reproducibility for project_miceps ----- fertile 0.0.0.9027
-- Packages referenced in source code ----- fertile 0.0.0.9027

# A tibble: 9 x 3
  package      N used_in
  <chr>      <int> <chr>
1 broom         1 project_miceps/analysis.Rmd
2 dplyr         1 project_miceps/analysis.Rmd
3 ggplot2       1 project_miceps/analysis.Rmd
4 purrr         1 project_miceps/analysis.Rmd
5 readr         1 project_miceps/analysis.Rmd
6 rmarkdown     1 project_miceps/analysis.Rmd
7 skimr         1 project_miceps/analysis.Rmd
8 stargazer     1 project_miceps/analysis.Rmd
9 tidyr         1 project_miceps/analysis.Rmd
```

```
-- Files present in directory ----- fertile 0.0.0.9027 --
```

	file	ext	size	
1	Estrogen_Receptors.docx	docx	10.97K	
2	citrate_v_time.png	png	188.38K	
3	proteins_v_time.png	png	377.76K	
4	Blot_data_updated.csv	csv	14.43K	
5	CS_data_redone.csv	csv	7.39K	
6	mice.csv	csv	14.33K	
7	README.md	md	39	
8	miceps.Rproj	Rproj	204	
9	analysis.Rmd	Rmd	4.94K	
				mime
1	application/vnd.openxmlformats-officedocument.wordprocessingml.document			
2				image/png
3				image/png
4				text/csv
5				text/csv
6				text/csv
7				text/markdown
8				text/rstudio
9				text/x-markdown

```
-- Suggestions for moving files ----- fertile 0.0.0.9027 --
```

	path_rel	dir_rel
1	Blot_data_updated.csv	data-raw
2	CS_data_redone.csv	data-raw
3	Estrogen_Receptors.docx	inst/other
4	analysis.Rmd	vignettes
5	citrate_v_time.png	inst/image
6	mice.csv	data-raw
7	proteins_v_time.png	inst/image

```
1 file_move('project_miceps/Blot_data_updated.csv', fs::dir_create('project_miceps/dat
2 file_move('project_miceps/CS_data_redone.csv', fs::dir_create('project_miceps/dat
3 file_move('project_miceps/Estrogen_Receptors.docx', fs::dir_create('project_miceps/inst/
4 file_move('project_miceps/analysis.Rmd', fs::dir_create('project_miceps/vign
5 file_move('project_miceps/citrate_v_time.png', fs::dir_create('project_miceps/inst/
6 file_move('project_miceps/mice.csv', fs::dir_create('project_miceps/dat
7 file_move('project_miceps/proteins_v_time.png', fs::dir_create('project_miceps/inst/
```

```
-- Problematic paths logged ----- fertile 0.0.0.9027 --
```

```
NULL
```


2.3.4 Logging

fertile also contains logging functionality, which records commands run in the console that have the potential to affect reproducibility, enabling users to look at their past history at any time. The package focuses mostly on package loading and file opening, noting which function was used, the path or package it referenced, and the timestamp at which that event happened. Users can access the log recording their commands at any time via the `log_report()` function:

```
log_report()
```

```
# A tibble: 6 x 4
  path      path_abs      func      timestamp
  <chr>      <chr>      <chr>      <dtm>
1 package:re~ <NA>      base::r~ 2020-09-06 17:30:44
2 package:th~ <NA>      base::r~ 2020-09-06 17:30:44
3 package:th~ <NA>      base::l~ 2020-09-06 17:30:44
4 package:pu~ <NA>      base::l~ 2020-09-07 13:47:42
5 package:fo~ <NA>      base::l~ 2020-09-07 13:47:42
6 project_mi~ /Users/audreybertin/Docume~ readr::~ 2020-09-07 13:47:42
```

The log, if not managed, can grow very long over time. For users who do not desire such functionality, `log_clear()` provides a way to erase the log and start over.

2.3.5 Utility Functions

fertile also provides several useful utility functions that may assist with the process of data analysis.

2.3.6 File Path Management

The `check_path()` function analyzes a vector of paths (or a single path) to determine whether there are any absolute paths or paths that lead outside the project directory.

```
# Path inside the directory
check_path("project_miceps")
```

```
# A tibble: 0 x 3
# ... with 3 variables: path <chr>, problem <chr>, solution <chr>
```

```
# Absolute path (current working directory)
check_path(getwd())
```

```
Error: Detected absolute paths
```

```
# Path outside the directory  
check_path("../fertile.Rmd")
```

Error: Detected paths that lead outside the project directory

2.3.7 File Types

There are several functions that can be used to check the type of a file:

```
is_data_file(fs::path(proj_dir, "mice.csv"))
```

```
[1] TRUE
```

```
is_image_file(fs::path(proj_dir, "proteins_v_time.png"))
```

```
[1] TRUE
```

```
is_text_file(fs::path(proj_dir, "README.md"))
```

```
[1] TRUE
```

```
is_r_file(fs::path(proj_dir, "analysis.Rmd"))
```

```
[1] TRUE
```

2.3.8 Temporary Directories

The `sandbox()` function allows the user to make a copy of their project in a temporary directory. This can be useful for ensuring that projects run properly when access to the local file system is removed.

```
proj_dir
```

```
[1] "project_miceps"
```

```
fs::dir_ls(proj_dir) %>% head(3)
```

```
project_miceps/Blot_data_updated.csv  
project_miceps/CS_data_redone.csv  
project_miceps/Estrogen_Receptors.docx
```

```
temp_dir <- sandbox(proj_dir)
temp_dir
```

```
/var/folders/v6/f62qz88s0sd5n3yqw9d8sb300000gn/T/RtmpRIZRSt/project_miceps
```

```
fs::dir_ls(temp_dir) %>% head(3)
```

```
/var/folders/v6/f62qz88s0sd5n3yqw9d8sb300000gn/T/RtmpRIZRSt/project_miceps/Blot_data
/var/folders/v6/f62qz88s0sd5n3yqw9d8sb300000gn/T/RtmpRIZRSt/project_miceps/CS_data_r
/var/folders/v6/f62qz88s0sd5n3yqw9d8sb300000gn/T/RtmpRIZRSt/project_miceps/Estrogen_
```

2.3.9 Managing Project Dependencies

One of the challenges with ensuring that work is reproducible is the issue of dependencies. Many data analysis projects reference a variety of R packages in their code. When such projects are shared with other users who may not have the required packages downloaded, it can cause errors that prevent the project from running properly.

The `proj_pkg_script()` function assists with this issue by making it simple and fast to download dependencies. When run on an R project directory, the function creates a .R script file that contains the code needed to install all of the packages referenced in the project, differentiating between packages located on CRAN and those located on GitHub.

```
install_script <- proj_pkg_script(proj_dir)
cat(readChar(install_script, 1e5))
```

```
# Run this script to install the required packages for this R project.
# Packages hosted on CRAN...
install.packages(c( 'broom', 'dplyr', 'ggplot2', 'purrr', 'readr', 'rmarkdown', 'ski
# Packages hosted on GitHub...
```

2.4 How fertile Works

Much of the functionality in `fertile` is achieved by writing **shims link to wikipedia page here**. `fertile`'s shimmed functions intercept the user's commands and perform various logging and checking tasks before executing the desired function. Our process is:

1. Identify an R function that is likely to be involved in operations that may break reproducibility. Popular functions associated with only one package (e.g., `read_csv()` from `readr`) are ideal candidates.
2. Create a function in `fertile` with the same name that takes the same arguments (and always the dots ...).

3. Write this new function so that it:

- a) captures any arguments,
- b) logs the name of the function called,
- c) performs any checks on these arguments, and
- d) calls the original function with the original arguments. Except where warranted, the execution looks the same to the user as if they were calling the original function.

Most shims are quite simple and look something like what is shown below for `read_csv()`.

```
fertile::read_csv
```

```
function(file, ...) {
  if (interactive_log_on()) {
    log_push(file, "readr::read_csv")
    check_path_safe(file)
    readr::read_csv(file, ...)
  }
}
<bytecode: 0x7f92d06179b0>
<environment: namespace:fertile>
```

fertile shims many common functions, including those that read in a variety of data types, write data, and load packages. This works both proactively and retroactively, as the shimmed functions written in **fertile** are activated both when the user is coding interactively and when a file containing code is rendered.

In order to ensure that the **fertile** versions of functions (“shims”) always supersede (“mask”) their original namesakes when called, **fertile** uses its own shims of the **library** and **require** functions to manipulate the R search path so that it is always located in the first position. In the **fertile** version of **library()**, we detach **fertile** from the search path, load the requested package, and then re-attach **fertile**. This ensures that when a user executes a command, R will check **fertile** for a matching function before considering other packages. While it is possible that this shifty behavior could lead to unintended consequences, our goal is to catch a good deal of problems before they become problematic. Users can easily disable **fertile** by detaching it, or not loading it in the first place.

2.5 **fertile** in Practice: Experimental Results From Smith College Student Use

fertile is designed to: 1) be simple enough that users with minimal R experience can use the package without issue, 2) increase the reproducibility of work produced

by its users, and 3) educate its users on why their work is or is not reproducible and provide guidance on how to address any problems.

To test *fertile*'s effectiveness, we began an initial randomized control trial of the package on an introductory undergraduate data science course at Smith College in Spring 2020 **ADD FOOTNOTE** (This study was approved by Smith College IRB, Protocol #19-032).

The experiment was structured as follows:

1. Students are given a form at the start of the semester asking whether they consent to participate in a study on data science education. In order to successfully consent, they must provide their system username, collected through the command `Sys.getenv("LOGNAME")`. To maintain privacy the results are then transformed into a hexadecimal string via the `md5()` hashing function.
2. These hexadecimal strings are then randomly assigned into equally sized groups, one experimental group that receives the features of *fertile* and one group that receives a control.
3. The students are then asked to download a package called *sds192* (the course number and prefix), which was created for the purpose of this trial. It leverages an `.onAttach()` function to scan the R environment and collect the username of the user who is loading the package and run it through the same hashing algorithm as used previously. It then identifies whether that user belongs to the experimental or the control group. Depending on the group they are in, they receive a different version of the package.
4. The experimental group receives the basic *sds192* package, which consists of some data sets and R Markdown templates necessary for completing homework assignments and projects in the class, but also has *fertile* installed and loaded silently in the background. The package's proactive features are enabled, and therefore users will receive warning messages when they use absolute or non-portable paths or attempt to change their working directory. The control group receives only the basic *sds192* package, including its data sets and R Markdown templates. All students from both groups then use their version of the package throughout the semester on a variety of projects.
5. Both groups are given a short quiz on different components of reproducibility that are intended to be taught by *fertile* at both the beginning and end of the semester. Their scores are then compared to see whether one group learned more than the other group or whether their scores were essentially equivalent. Additionally, for every homework assignment submitted, the professor takes note of whether or not the project compiles successfully.

Based on the results, we hope to determine whether *fertile* was successful at achieving its intended goals. A lack of notable difference between the *experimental* and *control* groups in terms of the number of code-related questions asked throughout the semester would indicate that *fertile* achieved its goal of simplicity. A higher average for the *experimental* group in terms of the number of homework assignments

that compiled successfully would indicate that **fertile** was successful in increasing reproducibility. A greater increase over the semester in the reproducibility quiz scores for students in the *experimental* group compared with the *control* group would indicate that **fertile** achieved its goal of educating users on reproducibility. Success according to these metrics would provide evidence showing **fertile**'s benefit as tool to help educators introduce reproducibility concepts in the classroom.

Chapter 3

Incorporating Reproducibility Tools Into The Greater Data Science Community

3.1 Potential Applications of `fertile`

3.1.1 In Journal Review

3.1.2 By Beginning Data Scientists

3.1.3 By Advanced Data Scientists

3.1.4 For Teaching Reproducibility

3.2 Integration Of `fertile` And Other Reproducibility Tools in Data Science Education

Conclusion

fertile is an R package that lowers barriers to reproducible data analysis projects in R, providing a wide array of checks and suggestions addressing many different aspects of project reproducibility, including file organization, file path usage, documentation, and dependencies. **fertile** is meant to be educational, providing informative error messages that indicate why users' mistakes are problematic and sharing recommendations on how to fix them. The package is designed in this way so as to promote a greater understanding of reproducibility concepts in its users, with the goal of increasing the overall awareness and understanding of reproducibility in the R community.

The package has very low barriers to entry, making it accessible to users with various levels of background knowledge. Unlike many other R packages focused on reproducibility that are currently available, the features of **fertile** can be accessed almost effortlessly. Many of the retroactive features can be accessed in only two lines of code requiring minimal arguments and some of the proactive features can be accessed with no additional effort beyond loading the package. This, in combination with the fact that **fertile** does not focus on one specific area of reproducibility, instead covering (albeit in less detail) a wide variety of topics, means that **fertile** makes it easy for data analysts of all skill levels to quickly gain a better understanding of the reproducibility of the work.

In the moment, it often feels easiest to take a shortcut—to use an absolute path or change a working directory. However, when considering the long term path of a project, spending the extra time to improve reproducibility is worthwhile. **fertile**'s user-friendly features can help data analysts avoid these harmful shortcuts with minimal effort.

Appendix A

The First Appendix

This first appendix includes all of the R chunks of code that were hidden throughout the document (using the `include = FALSE` chunk tag) to help with readability and/or setup.

In the main Rmd file

```
# This chunk ensures that the thesisdown package is  
# installed and loaded. This thesisdown package includes  
# the template files for the thesis.  
if (!require(remotes)) {  
  if (params$'Install needed packages for {thesisdown}') {  
    install.packages("remotes", repos = "https://cran.rstudio.com")  
  } else {  
    stop(  
      paste('You need to run install.packages("remotes")',  
            "first in the Console.")  
    )  
  }  
}  
  
if (!require(thesisdown)) {  
  if (params$'Install needed packages for {thesisdown}') {  
    remotes::install_github("ismayc/thesisdown")  
  } else {  
    stop(  
      paste(  
        "You need to run",  
        'remotes::install_github("ismayc/thesisdown")',  
        "first in the Console."  
      )  
    )  
  }  
}  
  
library(thesisdown)
```

```
# Set how wide the R output will go  
options(width = 70)
```

In Chapter ??:

Appendix B

The Second Appendix, for Fun

References

- Blischak, J., Carbonetto, P., & Stephens, M. (2019). Workflowr: A framework for reproducible and collaborative data science. Retrieved from <https://CRAN.R-project.org/package=workflowr>
- Broman, K. (2019). Initial steps toward reproducible research: Organize your data and code. *Sitewide ATOM*. Retrieved from <https://kbroman.org/steps2rr/pages/organize.html>
- Cooper, N., Hsing, P.-Y., Croucher, M., Graham, L., James, T., Krystalli, A., & Michonneau, F. (2017). A guide to reproducible code in ecology and evolution. *British Ecological Society*. Retrieved from <https://www.britishecologicalsociety.org/wp-content/uploads/2017/12/guide-to-reproducible-code.pdf>
- Eisner, D. A. (2018). Reproducibility of science: Fraud, impact factors and carelessness. *Journal of Molecular and Cellular Cardiology*, 114, 364–368. <http://doi.org/https://doi.org/10.1016/j.yjmcc.2017.10.009>
- Fidler, F., & Wilcox, J. (2018). Reproducibility of scientific results. In E. N. Zalta (Ed.), *The stanford encyclopedia of philosophy* (Winter 2018). <https://plato.stanford.edu/archives/win2018/entries/scientific-reproducibility/>; Metaphysics Research Lab, Stanford University.
- FitzJohn, R., Ashton, R., Hill, A., Eden, M., Hinsley, W., Russell, E., & Thompson, J. (2020). Orderly: Lightweight reproducible reporting. Retrieved from <https://CRAN.R-project.org/package=orderly>
- Gancarz, M. (2003). *Linux and the unix philosophy* (2nd ed.). Woburn, MA: Digital Press.
- Goodman, S. N., Fanelli, D., & Ioannidis, J. P. A. (2016). What does research reproducibility mean? *Science Translational Medicine*, 8(341), 1–6. <http://doi.org/10.1126/scitranslmed.aaf5027>
- Gosselin, R.-D. (2020). Statistical analysis must improve to address the reproducibility crisis: The access to transparent statistics (acts) call to action. *BioEssays*, 42(1), 1900189. <http://doi.org/10.1002/bies.201900189>
- Henry, L., & Wickham, H. (2020). Tidysselect: Select from a set of strings. Retrieved

- from <https://CRAN.R-project.org/package=tidyselect>
- Hermans, F., & Aldewereld, M. (2017). Programming is writing is programming. In *Companion to the first international conference on the art, science and engineering of programming* (pp. 1–8).
- Kitzes, J., Turek, D., & Deniz, F. (2017). *The practice of reproducible research: Case studies and lessons from the data-intensive sciences*. Berkeley, CA: University of California Press. Retrieved from <https://www.practicereproducibleresearch.org>
- Martinez, C., Hollister, J., Marwick, B., Szöcs, E., Zeitlin, S., Kinoshita, B. P., ... Meinke, B. (2018). Reproducibility in Science: A Guide to enhancing reproducibility in scientific results and writing. Retrieved from <http://ropensci.github.io/reproducibility-guide/>
- Marwick, B. (2019). Rrtools: Creates a reproducible research compendium. Retrieved from <https://github.com/benmarwick/rrtools>
- Marwick, B., Boettiger, C., & Mullen, L. (2018). Packaging data analytical work reproducibly using R (and friends). *The American Statistician*, 72(1), 80–88. <http://doi.org/doi.org/10.1080/00031305.2017.1375986>
- McArthur, S. L. (2019). Repeatability, reproducibility, and replicability: Tackling the 3R challenge in biointerface science and engineering. *Biointerphases*, 14(2), 1–2. <http://doi.org/10.1116/1.5093621>
- McIntire, E. J. B., & Chubaty, A. M. (2020). Reproducible: A set of tools that enhance reproducibility beyond package management. Retrieved from <https://CRAN.R-project.org/package=reproducible>
- OpenSci, R. (2020). Drake: A pipeline toolkit for reproducible computation at scale. Retrieved from <https://cran.r-project.org/package=drake>
- Oracle Corporation. (2019). Wercker. Retrieved from <https://github.com/wercker/wercker>
- R-Core-Team. (2020). Writing r extensions. *R Foundation for Statistical Computing*. Retrieved from <http://cran.stat.unipd.it/doc/manuals/r-release/R-exts.pdf>
- Ross, N., DeCicco, L., & Randhawa, N. (2018). Checkers: Automated checking of best practices for research compendia. Retrieved from <https://github.com/ropenscilabs/checkers/blob/master/DESCRIPTIONr>
- Ushey, K., McPherson, J., Cheng, J., Atkins, A., & Allaire, J. (2018). Packrat: A dependency management system for projects and their r package dependencies. Retrieved from <https://CRAN.R-project.org/package=packrat>
- Wallach, J. D., Boyack, K. W., & Ioannidis, J. P. A. (2018). Reproducible research

practices, transparency, and open access data in the biomedical literature, 2015-2017. *PLOS Biology*, 16(11), 1–20. <http://doi.org/10.1371/journal.pbio.2006930>

Wickham, H. (2015). *R packages* (1st ed.). Sebastopol, CA: O'Reilly Media, Inc.