

Addressing The Scientific Reproducibility Crisis Through Educational Software
Integration

Audrey M. Bertin

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Benjamin S. Baumer, Honors Project Advisor

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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.

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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?

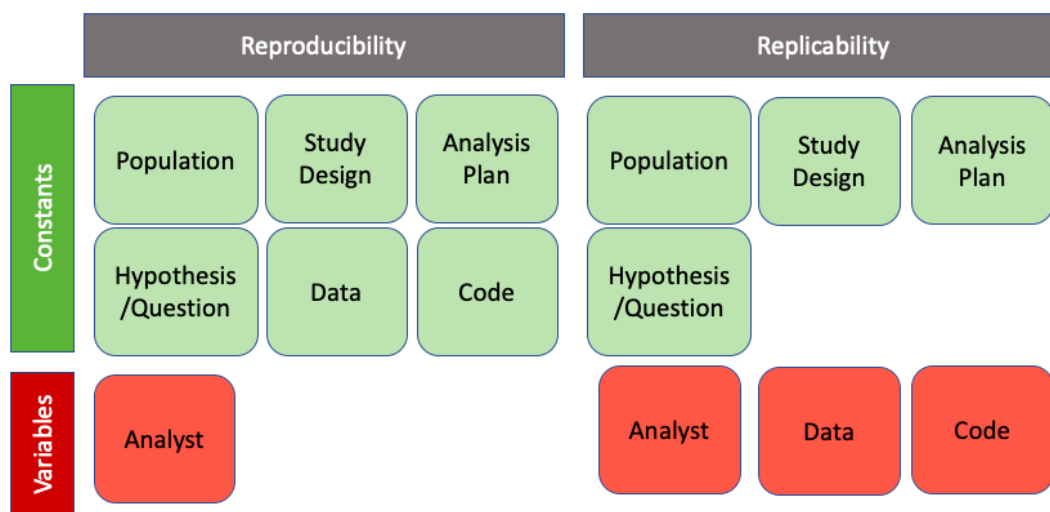
In the field of data science, research is considered fully *reproducible* when the requisite code and data files produce identical results when run by another analyst, or more generally, when a researcher can “duplicate the results of a prior study using the same materials as were used by the original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



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 (Baker (2016)). 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 (Baker (2015), Begley & Ellis (2012)).

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 see why there is an issue with reproducibility and gain a sense of how to solve it, it is important to first understand the components of reproducibility. Essentially, to answer, “What parts does researcher need to include, or what steps do they need to take, to be able to declare their work 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), achieving 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 to the public:
 - 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. Code is readable and consistently styled:
 - 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

In an attempt to increase reproducibility, leaders from academic journals around the world have taken steps to create new standards and requirements for submitted articles. These standards attempt to address the components of reproducibility listed previously, requesting that authors provide certain materials necessary for reproducing their work when they submit an article. However, these standards are highly inconsistent, varying significantly both across and within disciplines, and many only cover one or two of the six primary components, if any at all.

To illustrate this point, we will consider several case studies from journals publishing research on a variety of scientific fields.

1.4.1 Case Studies Across The Sciences

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 (American Journal of Political Science (2016)).

- 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.

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.

For example, 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 (National Institutes of Health (2014)). 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.

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. Additionally, 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 (Cambridge University Press (2020)).

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 (American Economic Association (2020)):

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.

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 Case Studies In The Statistical And Data Sciences



















When considering reproducibility policy, the field of Statistical and Data Sciences performs relatively well. The majority of highly ranked journals in the field 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 (American Statistical Association (2020)).

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 (Journal of Statistical Software (2020)).

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 (Journal of Computational and Graphical Statistics (2020)). 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" (R Journal Editors (2020)).

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 (The American Statistician (2020))s.

Journal Name	Code Sharing Required?	Data Sharing Required?	Other Components Required?
Journal of the American Statistical Association			
Journal of Statistical Software			
Journal of Computational and Graphical Statistics			
The R Journal			
The American Statistician			
The Annals of Statistics			

★ Component recommended, but not required.

◆ Component required, but exceptions granted.

1.4.3 The Bigger Picture

The journals mentioned here are just some of the many academic publishers with reproducibility policies. While they provide a sense of the specific wording and requirements of some policies, they do not necessarily serve as a representative sample of all academic publishing. It is important to also consider the bigger picture, exploring the state of reproducibility policy in academic publishing as a whole.

Given the scale of the academic publishing network and the sheer number of journals around the world, this is not necessarily an easy task.

In order to simplify this process, academics at the Center for Open Science (COS) attempted to create a metric, called the TOP Factor. The TOP Factor reports the steps that a journal is taking to implement open science practices. It has been calculated for a wide variety of journals, though the COS is still far from scoring all of the publications that are currently available.

The TOP Factor is calculated as follows. Publications are scored on a variety of categories associated with open science and reproducibility. For each category, they receive a score between 0 (poor) and 3 (excellent) based on the degree to which they emphasize each category in their submission/publication policies. A journal's final score, which can range from 0 to 30, is the sum of the individual scores in each of the categories.

	Not Implemented	Level I	Level II	Level III
Citation standards	Journal encourages citation of data, code and materials or says nothing.	Journal describes citation of data in guidelines to authors with clear rules and examples	Article provides appropriate citation for data and materials used consistent with journal's author guidelines	Article is not published until providing appropriate citation for data and materials following journal's author guidelines
Data transparency	Journal encourages data sharing or says nothing	Article states whether data are available and, if so, where to access them	Data must be posted to a trusted repository. Exceptions must be identified at article submission	Data must be posted to a trusted repository, and reported analyses will be reproduced independently prior to publication
Code transparency	Journal encourages code sharing or says nothing	Article states whether code is available and, if so, where to access it	Code must be posted to a trusted repository. Exceptions must be identified at article submission	Code must be posted to a trusted repository, and reported analyses will be reproduced independently prior to publication
Research materials transparency	Journal encourages materials sharing or says nothing	Article states whether materials are available and, if so, where to access them	Materials must be posted to a trusted repository. Exceptions must be identified at article submission	Materials must be posted to a trusted repository, and reported analyses will be reproduced independently prior to publication

Design and analysis transparency	Journal encourages design and analysis transparency or says nothing	Journal articulates design transparency standards	Journal requires adherence to design transparency standards for review and publication	Journal requires and enforces adherence to design transparency standards for review and publication
Study preregistration	Journal says nothing	Article states whether preregistration of study exists and, if so, where to access it	Article states whether preregistration of study exists and, if so, allows journal access during peer review for verification	Journal requires preregistration of studies and provides link and badge in article to meeting requirements
Analysis plan preregistration	Journal says nothing	Article states whether preregistration of study exists and, if so, where to access it	Article states whether preregistration with analysis plan exists and, if so, allows journal access during peer review for verification	Journal requires preregistration of studies with analysis plans and provides link and badge in article to meeting requirements
Replication	Journal discourages submission of replication studies or says nothing	Journal encourages submission of replication studies	Journal encourages submission of replication studies and conducts results blind review	Journal uses registered reports as a submission option for replication studies with peer review prior to observing the study outcomes

When looking at the overall distribution of TOP Factor scores, we see a relatively grim picture: Around 50% of journals score as low as 0-5 overall, while only just over 5% score more than 15, just half of the maximum possible score. Over 40 journals failed to score a single point (Woolston (2020)).

Although it is clear that some journals have relatively strong reproducibility and openness policies, that is clearly not the norm. And many that do appear to have policies lacking in robustness, including exceptions for data privacy and security concerns or phrasing guidelines as recommendations rather than requirements. The field of data science stands out among the rest, with the majority of top journals having relatively robust policies.

1.4.4 Assessing the Success of Academic Reproducibility Policies

We have seen that, although not necessarily the standard, some journals across the sciences have enacted reproducibility policies. 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.

It is important to ask, then, whether academic reproducibility standards *actually* result in a greater number of 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.

Stodden, Seiler, & Ma (2018a) 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.

Hardwicke et al. (2018) conducted a study on the journal *Cognition*, where researchers compared the reproducibility of published work both before and after the journal instituted an open data policy, which required that authors make relevant research data publicly available prior to publication of an article.

The researchers found a considerable increase in the proportion of data available statements (in contrast to ‘data not available’ statements, which could be present due to privacy or security concerns) since the implementation of the policy. Pre-open data policy, only 25% of articles had data available, while that number was a much higher 78% after the policy was put in place.

While the institution of an open data policy appears to have been associated with a significant increase in the percentage of studies with data available, further research indicates that the policy was perhaps not as effective as intended. Many of the datasets were usable in theory, but not in practice. Only 62% of the articles with data available statements had truly reusable datasets—in this case, meaning that the data were accessible, complete, and understandable. Though this is an increase from the pre-policy period, which saw 49% of articles with data availability statements as reusable in practice, it is still far from ideal.

Combining these two data points indicates that *less than half* of articles published after the open data policy was instituted actually contained truly usable data.

In this small sample of cases, we see that purely having a reproducibility statement does not necessarily mean that all, or even a majority, of published work will truly be reproducible.

1.5 Limitations on Achieving Reproducibility in Scientific Publishing

There are several reasons for this apparent divide between journal reproducibility standards and the true proportion of submitted articles that are truly reproducible. Some of these are challenges faced by the article authors, while others are faced by the journal editors.

1.5.1 Challenges for Authors

Stodden, Seiler, & Ma (2018b) conducted a survey asking over 7,700 researchers about one of the key characteristics of reproducibility – open data – and gathered information about the reasons why authors found difficulties in making their data available to the public

The main challenges listed by respondents were as follows:

- 46% identified “Organizing data in a presentable and useful way” to be difficult.
- 37% had been “Unsure about copyright and licensing.”
- 33% had problems with “Not knowing which repository to use.”
- 26% cited a “Lack of time to deposit data.”
- 19% found the “Costs of sharing data” to be high.

The relative frequency of these issues varied across several characteristics, including author seniority, subject area, and geographical location, though authors in all categories faced some issues.

Given the relatively high frequency of concern over achieving reproducibility, it follows that researchers will not make the necessary effort to do so if journal guidelines provide a way out. Policies that *recommend* the inclusion of data or that allow exceptions to open data for certain reasons are likely to be associated with a lower proportion of reproducible articles than those that make open data mandatory.

1.5.2 Challenges for Journals

In addition to the challenges faced on the part of the authors, journal reviewers face their own difficulties in ensuring reproducibility.

In order to make sure that all submitted articles comply with reproducibility guidelines, reviewers must go through them one by one and reproduce all of the results by hand using the provided materials.

This is an incredibly intensive process, as we will see in the example of the *American Journal for Political Science* (AJPS), whose reproducibility policy was discussed previously in Chapter 1.4.1.

Jacoby, Lafferty-Hess, & Christian (2017) describe the AJPS process in detail:

Acceptance of an article for publication in the AJPS is contingent on successful reproducibility of any empirical analyses reported in the article.

After an article is submitted, staff from a third party vendor hired by AJPS go through the provided materials to ensure that they can be preserved, understood, and used by others. They then run all of the analyses in the article using the code, instructions, and data provided by the authors and compare their results to the submitted articles. Authors are then given an opportunity to resolve any issues that come up. This process is repeated until reproducibility is ensured.

Although providing a significant benefit to the scientific community, this thorough process is associated with high costs.

The verification process slows down the journal review process significantly, adding a median 53 days to the publication workflow, as many submitted articles require one or more rounds of resubmission (the average number of resubmissions is 1.7). It is also quite labor intensive, taking an average of 8 person-hours per manuscript to reproduce the analyses and prepare the materials for public release and adding significant monetary cost to AJPS.

Journals are often reluctant to take on such an intensive task due to the drastically increased burden it places on reviewers and on the publication's financial resources. This is particularly true given that the number of submitted articles per year has been increasing over time (Leopold (2015)). Every additional submission increases the burden of achieving reproducibility, and with a large enough volume, the challenge can quickly become seemingly impossible to manage reasonably.

As a result, journals often encourage reviewers to consider authors' compliance with data sharing policies, but do not formally require that they ensure it as a criterion for acceptance (Hrynaszkiewicz (2020)).

1.6 Attempts to Address These Limitations

The previous discussion makes clear that, although reproducibility is critically important to scientific progress and academic journals are taking steps to encourage it, the scientific community is far from achieving the desired level of widespread reproducibility. In large part, this appears due to the challenge and complexity of actually achieving reproducibility. Those attempting to improve the reproducibility of work can face issues with concerns over legality of sharing data, large commitments of time or money, challenges finding a good repository, and organizing all of the many components of their work in an understandable way, among other things.

Additionally, science faces the additional challenge that many publishers do not emphasize reproducibility at all, providing many opportunities for all authors except those personally dedicated to producing reproducible work to leave reproducibility by the wayside. Many journals have no reproducibility requirements, and those that do often do not take the necessary steps to ensure that they are actually met.

These issues, however, are not impossible to overcome. Proponents of reproducibility have taken action to help address them, both through education on reproducibility and through software that helps simplify the process of achieving it.

1.6.1 Through Education

1.6.2 Through Software

Several researchers and members of the Statistical and Data Sciences community have taken action to develop software focused on reproducibility which removes some of the load on data analysts by automating reproducibility processes and checking whether certain components are achieved.

Much of this software has been written for users of the coding and data analysis language **R**. **R** is very popular in the data science community due to its open-source nature, accessibility, extensive developer and user base, and statistical analysis-specific features.

Some of the existing software solutions are listed below:

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 de-

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.

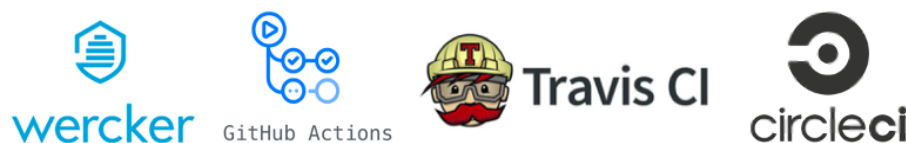


There have also been several **Continuous integration** tools developed outside of R which can be used by those coding in almost any language. These provide more general approaches to automated checking, which can enhance reproducibility with minimal code.

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.



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 Identifying Gaps In Existing Solutions

on r packages 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.

**** on continuous integration **** 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 My Contribution: **fertile**, An R Package Creating Optimal Conditions For Reproducibility

2.2.1 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`.

2.2.2 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.

2.2.3 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 --

# A tibble: 9 x 4
  file                ext      size mime
  <fs::path>          <chr> <fs::byt> <chr>
1 Estrogen_Recepto~ docx    10.97K application/vnd.openxmlformats-of~
2 citrate_v_time.p~ png     184.83K image/png
3 proteins_v_time.~ png     377.15K image/png
4 Blot_data_update~ csv      14.43K text/csv
5 CS_data_redone.c~ csv       7.39K text/csv
6 mice.csv           csv     14.33K text/csv
7 README.md          md         39 text/markdown
8 miceps.Rproj       Rproj      204 text/rstudio
9 analysis.Rmd       Rmd      4.94K text/x-markdown

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

# A tibble: 7 x 3
  path_rel      dir_rel  cmd
  <fs::path>    <fs::path> <chr>
1 Blot_data_updated~ data-raw  file_move('project_miceps/Blot_data_u~
2 CS_data_redone.csv data-raw  file_move('project_miceps/CS_data_red~
3 Estrogen_Receptor~ inst/other file_move('project_miceps/Estrogen_Re~
4 analysis.Rmd      vignettes file_move('project_miceps/analysis.Rm~
5 citrate_v_time.png inst/image file_move('project_miceps/citrate_v_t~
6 mice.csv          data-raw  file_move('project_miceps/mice.csv', ~
7 proteins_v_time.p~ inst/image file_move('project_miceps/proteins_v_~

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

NULL
```

2.2.4 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~	2020-09-12 18:43:44
2	package:th~	<NA>	base::r~	2020-09-12 18:43:44
3	package:th~	<NA>	base::l~	2020-09-12 18:43:44
4	package:pu~	<NA>	base::l~	2020-09-12 18:45:27
5	package:fo~	<NA>	base::l~	2020-09-12 18:45:27
6	project_mi~	/Users/audreybertin/Docume~	readr::~	2020-09-12 18:45:28

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.

2.2.5 Utility Functions

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

2.2.6 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

2.2.7 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
```

2.2.8 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/RtmpqEI2kb/project_miceps
```

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

```
/var/folders/v6/f62qz88s0sd5n3yqw9d8sb300000gn/T/RtmpqEI2kb/project_miceps/Blot_data  
/var/folders/v6/f62qz88s0sd5n3yqw9d8sb300000gn/T/RtmpqEI2kb/project_miceps/CS_data_r  
/var/folders/v6/f62qz88s0sd5n3yqw9d8sb300000gn/T/RtmpqEI2kb/project_miceps/Estrogen_
```

2.2.9 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', 'skimr', '
```

```
# Packages hosted on GitHub...
```

2.3 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: 0x7f862e922cb0>
<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.

2.4 *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)
```

Appendix B

The Second Appendix, for Fun

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