

Best practices for teaching reproducibility: motivation, guided instruction and practice

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Introduction

In the graduate and undergraduate data science courses that we teach at the University of British Columbia (UBC), we define data science as the study, development and practice of reproducible and auditable processes to extract insight from data. Using this definition requires that we also define what is meant by a reproducible and auditable analysis. To define reproducible analysis, we embrace the National Academy of Sciences definition, which is reaching the same result given the same input, computational methods, and conditions (2019). For auditable or transparent analysis, we follow how it has been defined by Hilary Parker (2017) and Karthik Ram (2013), which is that there should be a readable record of the steps used to carryout the analysis (i.e., computer code) as well as a record of how the analysis methods evolved (i.e., a version controlled project history). This history is important for recording how and why decisions to use one method or another were made, among other things.

The reason we embrace this definition of data science, is that we believe that data science work should bring insight (e.g., answer an important research question) and employ reproducible and auditable methods so that trustworthy results and data products can be created. Results and data products can be generated without reproducible and auditable methods, however, when they are built this way there is less confidence in how the results or products were created. We believe this stems from non-reproducible and non-auditable analyses:

1. lacking evidence that the results or product could be regenerated given the same input computational methods, and conditions
2. lacking evidence of the steps taken during creation
3. having an incomplete record of how and why analysis decisions were made

In addition to contributing to the trustworthiness of data science work, employing reproducible and auditable methods and workflows bring additional benefits to data scientists, such as in the form of more effective collaboration. Data science is an inherently collaborative science, and the emphasis of reproducible and auditable methods in data science greatly facilitates the act of collaborating in many context, further emphasizing the importance of learning this skill well.

Although the many benefits of reproducible and auditable analyses discussed above may make them seem like an exciting topic for incoming students, the experience when enter a classroom of curious data scientists in training is quite the opposite. Students are usually keen to learn about data science but what they're most excited about is the second part of its definition: extracting insights from the data.

Students are often not even aware of the reproducible and auditable processes of data science, and when they first hear about them, they tend to regard them as an inconvenient means to an end rather than an important skill to master. This outlook is likely at least in part motivated by fact that these processes do not directly lead to novel insights in the same way as a predictive model might, which is what many students have in mind when they envision the work of a data scientist. This negative predisposition creates another barrier to overcome when teaching the reproducible and auditable aspects of data science.

An additional pedagogical challenge is that the tools that we use for reproducibility are not necessarily smooth and easy to learn, but often have a steep learning curve. Over our five years of teaching these topics at UBC we've found three pedagogical strategies that are particularly effective for teaching reproducibility successfully:

1. placing extra emphasis on motivation
2. guided instruction
3. lots of practice

In this paper, we will discuss why we believe each of these are important, provide examples of how to incorporate these in your teaching.

Placing extra emphasis on motivation

Why do we need extra motivation when teaching reproducibility, compared to some other data science topics, such as machine learning? We think this is because students do not have intrinsic excitement or motivation on the topic of reproducibility, they have little prior knowledge on this topic, and reproducibility concepts and in particular tools are challenging to learn.

One example, the version control software that's the most commonly used one for reproducibility, Git, is notorious for being difficult to learn (Figure 1). Furthermore, there are many anecdotes that that most people don not learn it deeply and instead work by trying a variety of commands until they find some things that work. This can lead to learners getting themselves into challenging or perplexing version control situations, with difficult to interpret outputs (e.g., "You are in 'detached HEAD' state. You can look around, make experimental changes and commit them, and you can discard any commits you make in this state without impacting any branches by performing another checkout"). Sometimes these situations are so difficult to get out of, that even professional data scientists and data science educators, for example Jenny Bryan, recommend

the practice of “burning it all down” and starting from scratch - which really defeats many of the purposes of version control.

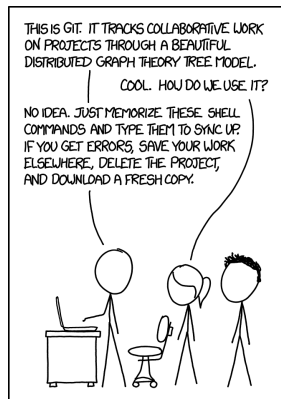


Fig. 1: Infamous xkcd comic that highlights the difficulty of learning and using the version control software Git.

Another example is R Markdown, which is an implementation of literate code documents (Knuth 1984), that are useful for generating reproducible reports. Many aspects of R Markdown are quite user friendly, however rendering the source R Markdown document to PDF depends on LaTeX. If users make formatting errors that impact LaTeX’s job in the rendering the resulting error messages can be very cryptic and are often not very clear to learners about where the error is coming from and what should be done next to fix the problem. An example of an error from including a `\` character with a reserved LaTeX word outside of a mathematical equation, and the resultant error message is shown in Figure 2. The error message here is interpretable by intermediate and experienced RMarkdown users, but not by novice learners.

Yet another example of a popular reproducibility tool that is challenging to learn is Docker. Docker is a containerization tool that extends beyond just including the package dependencies of your analysis workflow, and instead creates an versioned copy of your entire computational environment including the programming language and any operating system dependencies. This means that you can share an exact copy of your computational environment with your collaborators, even if you work on different operating systems. Docker is an especially challenging one to teach and motivate students to learn because it is so different from writing code to for analysis. This is because software installation is time consuming, which leads to writing and debugging code to automate installation being a slow and painstaking process. This is especially true if certain workflows are not followed. It is also not an exciting part of a data analysis, as things already work on the student’s own computer. This makes it difficult to convince students why they should put effort into learning and using this.

```

2 title: "Untitled"
3 output: pdf_document
4 ---
5
6 ```{r setup, include=FALSE}
7 knitr::opts_chunk$set(echo = TRUE)
8 ```
9
10 Writing reserved LaTeX math words started with a `` outside equations
11 will lead to an error.
12
13 For example, \gamma will prevent this R markdown document from rendering...
14
15 13:68 (Top Level)

```

Console Terminal R Markdown Jobs

```

.../generate_latex_error/generate_latex_error.Rmd
a --self-contained --highlight-style tango --pdf-engine pdflatex --variable graphics --variable 'geometry:margin=1in'
output file: generate_latex_error.knit.md

! Missing $ inserted.
<inserted text>
$
1.75 For example, \gamma
will prevent this R markdown document from

Try to find the following text in generate_latex_error.Rmd:
For example, \gamma

You may need to add $ $ around a certain inline R expression `r` in generate_latex_error.Rmd (see the above hint). See https://github.com/rstudio/rmarkdown/issues/385 for more info.
Error: LaTeX failed to compile generate_latex_error.tex. See https://yihui.org/tinytex/r/#debugging for debugging tips. See generate_latex_error.log for more info.
Execution halted

```

Fig. 2: Latex errors are often cryptic to new learners.

So what do we do to motivate learning reproducibility concepts and tools in our classrooms? We have found the following three strategies helpful:

1. Tell stories from the trenches
2. Study cases of failures with real world consequences
3. Let them fail (in a controlled manner)

Telling stories from the trenches

One successful strategy that we have used is telling stories from the trenches. The instructors who teach these courses at UBC usually have had some experience performing data analyses in their Ph.D.'s or Postdoctoral studies, or are still currently engaged in research where they do this. Through these lived experiences of learning reproducibility tools and applying it to own analyses, we have made mistakes, our collaborators have made mistakes, and thus we can share these experiences with our students. In the Master of Data Science program, many of the students have work experience involving data in the past, and so they also have stories from the trenches. In a classroom with such students, you can carryout think pair share exercises around these stories and get the students to talk about their stories as well as hear yours.

In addition to sharing some consequences of non-reproducible analysis with students (without them having to experience this themselves over a long and drawn out process of self-discovery), these stories come from people the students know (their instructors and peers) and as such, these stories highlight how common and easy it is for such mistakes to happen, to anyone practising data analysis, if care is not taken to follow reproducible workflows and practices. This helps makes the practice of reproducibility seem more applicable and relatable to their own data analysis (which at this stage in their career, may not end up in a published paper).

Study cases of failures with significant real world consequences

A second way to create motivation is through using case studies of irreproducible data analyses that have had significant real world consequences. Such case studies can be used to illustrate the importance and impact of reproducible data analyses. This is something that the authors are currently trying to build into their courses and yet have limited experience with, but think the idea has strong merit and wish to present it here. We believe that this strategy may be particularly important for teaching reproducibility, since the impact and significance of the consequences of not using reproducible practices are not obvious to novices. By presenting case studies where failure to adhering to reproducible practices have led to costly mistakes, we aim to give learners a chance to directly appreciate the connection between the lack of reproducible workflows and the downstream consequences.

While there are many articles outlining recommendations on which reproducible practices to adhere to, case studies of failures are not as frequent in the literature.

We think this partly stems from the fact that such errors are often only discovered internally and never reported, and that there are few incentives for people to spend their time performing proper forensic informatics analysis on others work. Even so, there are several such examples are reported in the literature, one of the most striking leading to putting patients at risk in incorrectly administered clinical trials which we will outline in the next paragraph [ADD REFS TO CLINICAL TRIALS HERE TOO].

These clinical trials took place at Duke in 2006 and involved 110 cancer patients hoping that using personalized gene signatures would identify which treatments were more effective for individuals. The series of scientific papers that formed the basis of these trials were all published in highly regarded “high-impact” journals [CITE THE PAPERS HERE], but they had also raised some concerns among researchers in the field [CITE THIS OR REMOVE THIS CLAIM]. When put under a thorough independent review, these papers were found to contain multiple errors, several related to the use of non-reproducible tools and workflows (Baggerly and Coombes 2009). In the review analysis it was highlighted that most common problems were simple and included mistakes such as “off-by-one” errors where a cell might have been inadvertently deleted in Excel leading to a shift of all remaining values, labelling mix-ups where the treated and not treated groups were assigned labels 0 and 1 instead of meaningful names, which can lead to confusion as to which is the treated and control group, and poor documentation practices leading to lack of transparency which makes it harder and more time-consuming to identify errors (both for the original authors and the reviewers). These clinical trials were eventually terminated over 4 years after they started, around 25 papers papers related to these trials were retracted, and the lead investigators were put under investigation for malpractice. This example highlights the enormous cost associated with not adhering to reproducible practices and having workflows that are opaque and hard to review.

Other examples of case studies that could be used to illustrate the significant real world consequences of reproducibility failures in data analyses are listed in table 1.

Table. 1: Case studies that illustrate the significant real world consequences of reproducibility failures in data analyses.

Reproducibility error	Consequence	Source(s)
Limitations in Excel data formats lead to the loss of 16,000 COVID case records in the Unied Kingdom.	ADD	CITE
Excel’s automatic formatting caused important gene names to be disregarded in scientific studies.	ADD	Zeeberg et al. (2004); Ziemann, Eren, and El-Osta (2016)

Reproducibility error	Consequence	Source(s)
Deletion of a cell caused rows to shift and treatment groups to be mixed up	ADD	Wallensteen et al. (2018)
using binary instead of explanatory labels lead to a mix up of the intervention with the control group	ADD	CITE aboumatar/wise
Mixing up missing data and zero values	Paper retraction	CITE turcing and whitehouse
Incorrectly copying data in a spreadsheet	Delay in the opening a hospital	CITE Picken

Letting them fail (in a controlled manner)

Notably, many instructors (including the authors of this work) have themselves experienced failure in graduate school and during their postdoctoral research in regards to reproducibility, which negatively impacted their work. While these experiences motivate teaching and using reproducibility concepts and tools for instructors, most undergraduates and new graduate students cannot draw on similar professional experiences. Rather than letting new students live through the full perils of irreproducible research, we can set up controlled scenarios to expose them to these downsides in a controlled, accelerated manner while still embodying much of the same motivational benefits.

One way we have done this is providing students an analysis that is not reproducible (i.e., it depends on rare/obscure software packages or specific package versions), and thus will likely fail on someone else's machine. We then ask them to try to run it, and if they cannot run it, we ask them to fix the code or install missing software so they can. Then we provide them the same analysis that has been made reproducible, through the use of shareable compute environments (i.e., `renv`, `conda`, or Docker), instructions on how to use the shared compute environment. The students then experience running the same analysis on their machines without any changing of code or software installation. Under these controlled circumstances failure and frustration can have a positive impact on students overall learning as they experience the many benefits of reproducibility first hand. In a relatively short amount of time, this helps provide motivation to endure the steep learning curves of reproducibility concepts and tools.

The example discussed above was inspired by Jenny Bryan's teaching of STAT 545 at UBC. In her version of this task, she pairs students up and asks them to run each other's code projects that they have been working on in her course. Most usually fail to be able to do this on the first try for the same reasons discussed above. We adapted her teaching method so so that students experience

this in a more limited, controlled manner - which has allowed us to scale this exercise to larger classes with more homogenous experiences.

Guided instruction

We suggest that guided instruction is important in the classroom, specifically when teaching reproducibility. From our experience, reproducibility is not something that most people or students figure out through exploration- and inquiry-based learning, or if they do it is not an efficient process. We hypothesize the reason for this is that reproducibility uses a lot of borrowed tools from software engineering that are being repurposed for science and reproducibility. Thus, a lot of the getting up and getting started with reproducibility has a lot of assumed knowledge behind it, and there are not a lot of like clear and easy on roads for learners who do not have a software engineering background. Part of this may stem from the field being still fairly new and not-yet as widely embraced as we might hope. This means that there is not a lot of culture around using these in data science and statistics, this it is not yet as obvious where the on-ramps are.

Furthermore, similar to why we need extra motivation, the challenge of learning to use the tools due to their steep learning curves suggests that having some guided instruction is beneficial to learners. These points are well stated in a blog post and essay on *The Role of Theory in Data Analysis* by Roger Peng:

There is no need for a new data analyst to learn about reproducibility “from experience.” We don’t need to lead a junior data analysis down a months-long winding path of non-reproducible analysis until they are finally bitten by the non-reproducibility bug (and “therefore learn their lesson”). We can just tell them

“In the past, we’ve found it useful to make our data analysis reproducible Here’s a workflow to guide you in your own analysis.”

Within that one statement, we can “compress” over 20 years of experience.

The authors of this article agree with the statement above and think we owe it to our students to guide them to the best practices that the reproducibility community has arrived on to date and then show them how to use these tools explicitly.

At MDS, we primarily employ guided instructions through three pedagogical strategies:

1. Live demonstration
2. Pre-readings
3. Worksheets

Live demonstration

So how do we use guided instruction in the reproducibility classroom? In data science programming classes it is common to use live demonstration to show how to code in R and Python. A similar pedagogy of live demonstration works well for reproducibility tools, including R Markdown or Jupyter notebooks for reproducible reports, using version control with Git and GitHub, and using Docker to create reproducible and shareable computational environments. We believe that live demonstration makes it more obvious to the students how to use these tools in practice, and facilitates lateral knowledge transfer where learners absorb additional material by observing *how* we work, which would not have been possible from seeing a slide deck. Additionally, when you make mistakes as an instructor in these live demonstrations, it humanizes the reality of working with these tools that are somewhat challenging, even for experts. Intentional mistakes also can provide opportunities to spend more time on that area of the topic and explain the gotchas of a common mistake, and how to fix it.

A word of caution with live demonstration when teaching reproducibility; because we are teaching things that involve graphical user interfaces and/or that come from software engineering, the tech stack moves very fast. This means that each semester we teach these tools, we need to test drive the materials before we share them with the students to see if something has changed.

A relatively recent example of this is from fall 2020, when GitHub decided to change the name of their default branch from master to main (rightfully so). This change broke several of our teaching demos, guided worksheets, and lab homework. It also caused all of our notes to have to be rewritten. Eight months later, this problem is still not completely solved as we have several resources that are still using the master branch that we have not been able to quickly change over. For the reasons argued above, we do believe that it is really important to use guided instruction when teaching reproducibility, however, this should be done with the awareness and the acceptance that these kinds of changes are going to happen relatively frequently. Which means reproducibility instructors are going to have to update or make a new live demos and guided worksheets each year. Without this, the course resources will quickly fall out of usefulness.

Pre-lecture activities

Although live demonstration is important for the reasons outlined above, it is critical that it does not dominate the time spent in the classroom, so that student have ample time to engage in active learning activities. To ensure that students have sufficient background knowledge to start we complement our live demonstration with assigned pre-lecture activities. These can consist of material that we have created ourselves or external resources and is usually in the form of reading material or videos. Encouraging students to learn the basics before class allows us to have more meaningful live demonstrations and sets students up for a more effective learning experience by spacing out their exposure to the

course material.

Worksheets

After guiding students to foundational knowledge through live demonstration and pre-lecture activities, we challenge them to take a more active learning role by solving worksheet problems on their own in the classroom. This activity occupies most of the in-class time, so that students can engage actively with the material in an environment where they can easily be supported, before working on the homework assignments on their own. Worksheets provide students with many low stakes assessments comprised of short problems that are graded for completion only. In data science, this works well in literate code documents that have automated tests in them to provide feedback. Compared to in-class exercises, worksheets give learners additional change to actively engage with the material while still providing a structured way of providing exercises focused on key learning outcomes. Worksheets are also key for providing students with lots of practice, a topic we discuss in the last section of this article.

Example lesson using guided instruction

Here we provide an example of how we use guided instruction to teach version control in our first year introduction to data science course. In this course, we take a three-pronged approach for directed instruction.

We provide them a textbook reading for them to review before class, then we do a guided instruction in class, where they watch us use the GitHub website, and the Jupyter Git graphical user interface to add, commit, push and pull changes. Then finally they work through a guided worksheet that asks them to do the same thing that we just demonstrated. The guided worksheets also asks them questions along the way to test that they really understand what is adding, what is committing, what is pulling, what is pushing and where is the work going.

The challenge or limitation with this lesson in particular, is that we have chosen to teach using a Git graphical user interface, as opposed to the Git command line tool, due to the very novice level of the learners. Using a graphical user interface, and a newer one, means that we need to more frequently update and fix our lesson as the tool changes. The Git command line tool is more stable, and command line tools have less room to change generally, compared to graphical user interfaces, and thus would be a more stable tool to build a lesson around. However, the trade-off would be that this is a bit less intuitive for new learners, especially those who are also new to the command line in general.

Lots of practice

The third practice we argue for when teaching reproducibility is lots and lots of practice. To build lasting changes in behavior humans need to commit new information to long-term memory, which we can do in two fundamental ways: one

trial learning and repetitive spaced practice. One trial learning usually requires some sort of emotional impact, such as a traumatic event, or a really positive emotional event (a great birthday or a wedding). Forming lasting memories from these emotional experiences, doesn't require repetition. However, that is not how we learn most of the topics taught at school, which tend to be less emotionally salient. Such topics are instead better learned through repetitive spaced practice, where information is committed to long-term memory by revisiting and repeating it multiple times with break in between.

When we teach reproducibility topics, we want students to do more than commit information to long term behavior. We actually want them to act on new information and induce a change in behavior by putting their knowledge into practice, both in the classroom and in their own work. Importantly and in contrast to many other data science topics, students often already have behavioral patterns in place for how they organize and name their files, or how they collaborate with their colleagues. Although these are not reproducible practices, they fill many of the same niches in a learner's workflow, e.g. we want students to replace naming documents `draft-final-version-3.md` with using git and GitHub for version control and substitute collaboration via forks and PR on GitHub for their current habits of using working together on Google docs. Therefore, teaching reproducibility ought to go one step beyond promoting effective retention of information and focus on habitual and behavioral changes, which introduces additional challenges and opportunities.

Habit formation can be defined as the triggering of behavior from contextual cues. In the context of reproducible workflows these cues are the tasks that students desire to execute, such as saving a file after adding new content or wanting to share a document with a colleague. When teaching reproducible workflows we are aiming to replace the behavior with a more reproducible version as a response to the same cue. Although it might sounds like a complex task to not just unlearn an old behavior, but also learn a new one, studies has shown that behavioral change is in fact facilitated when substituting a desirable habit for an undesirable one existing rather than simply trying to unlearn the existing habit (Adriaanse, van Oosten, de Ridder, de Wit, & Evers, 2011).

Habitual behavior has been proposed to protect individuals from motivational lapses, where a desired good behavior is not expressed due to a momentary lack of willpower (TODO ref Review paper habit formation). By promoting the formation of habits in students, they opt for the reproducible workflow "by default," shielding them from relying on willpower to not "take the easy way out" and employ in a familiar, but irreproducible fashion workflow strategy.

Habits are best learned through frequent, regular, and sustained cue exposure. To support the formation of reproducible workflow habits, we therefore complement guided instruction with plenty of embed practice in the classroom, where we intentionally pause during the demos and say "okay students your turn, do what i just did." This is a more controlled form of practice, which sets students up for practicing these habits on their own. As mentioned above, we also provide

students with worksheets that can be used both in the class room and at home, as students receive feedback through autograding.

Importantly, habit formation is not a linear process. Instead, each successful action following a cue, adds to the formation of a new habit in an asymptotic fashion, where the initial events are the most important and the learning rate eventually plateaus as the habitual pattern solidifies. While popular literature often refers to ~30 days as the “all it takes,” to develop new habits, studies have reported anything from and average of 60 to 100 days before reaching the plateau phase of habit development. We therefore believe it is paramount that learners have sustained frequent practice in reproducible workflows, which is interleaved with other topics where they would employ and benefit from these skills in real life.

To give students adequate time and practice to cement their reproducible workflow habits, we have taken intentional choices of which learning technologies and platforms are used throughout the program. This ensures that students are practicing using reproducible tools for the full 10 months as part of the course learning technology mechanics (homework submission, grading, etc) and interleaved with learning other topics, just as they will do later in their careers (a detailed example follows in the next section). We also intentionally choose to use authentic data science reproducibility tools to provide opportunities for practicing and gaining confidence with these tools in “sharp” authentic scenarios rather than just in constructed exercises. This sustained practice not only enforces students’ habits, but also increases their proficiency with these tools and they can run into problems in an environment where they can easily reach out for help without feeling intimidated to ask.

Example lesson(s) of lots of practice

A specific example of how we use lots of practice is used in almost all of the UBC Master of Data Science courses (20 one-credit courses taken over an eight-month period). In these courses we use version control, particularly Git and GitHub as our course management system. In these courses, the homework instructions and assignments are distributed to the students as GitHub repositories and the only way that they can submit their homework is by putting their homework in that GitHub repository. So they have to go through the cloning procedure, or at least be able to somehow download their assignments from the GitHub website, as well as be able to (hopefully through using Git) upload their work back to that GitHub repository.

To incentivize doing this using Git (as opposed to the GitHub web user interface) we also assign some marks of each assignment to a mechanics grade. For this we assess whether they have at least three commits associated with every single assignment and have written meaningful commit messages. We do this because we’re trying to build these good habits and practices. There are good reasons why you use version control, not just to submit your homework but to active as

a backup, for collaboration, or in case you want to go back in time and change things. By the end of this program the students have version controlled their work in over 80 different GitHub repositories. We hope this results in using version control becoming a habit, to the point that if they're going to work on a project it's going to go under version control by default - even when they leave the program and are no longer receiving grades for doing this.

One exciting technology that we have recently started incorporating in our teaching of reproducible workflows is GitHub actions. This tool has allowed us to automate the building of individual “playgrounds” of complex Git scenarios that would take much effort and typically fail to stage in a large classroom. One of the GitHub repositories that we created for these activities (<https://github.com/ttimbers/review-my-pull-request>) serves the purpose of providing a playground where students can explore and practice to learn how to use GitHub's code review feature for pull requests. To use it, students create their own copy of the repository on GitHub, create a branch named pr and then a pull request is automatically created for them by a bot. After this simple setup, the students can spend the rest of the exercise exploring how to perform code reviews on GitHub.

Conclusions

We think over the past five years from teaching in the Master of Data Science and our Introduction to Data Science course that key things for teaching reproducibility in the data science classroom are providing extra emphasis on motivation, providing guided instruction so it's not a mystery of how you get started and what you need to do, as well as lots and lots of practice so that we can not only teach them the material and the concepts but so that this actually changes their practices and their workflows and they will use it after leaving your classroom.

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