Introducing Students to Research and Reproducibility with Open Science Tools

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Open science in research education

Reproducibility, transparency, and openness are all essential factors behind reliable and impactful research. The rapid, global response to understanding the COVID-19 pandemic is attributed to the way researchers openly shared methods and data [1], [2], [3], [4]. Since then, Open Science [5] has been placed at the forefront of an evolving research mission. While the movement is relatively new, it rose to prominence with 2023 delivering the *Year of Open Science* as announced from the White House Office of Science and Technology Policy [6]. Adoption is well in effect, with the National Institutes of Health releasing a new Data Management and Sharing Policy [7] and increasing evidence that open access research articles are a more common route to publication [8]. To meet these growing standards, established researchers likely need to learn Open Science practices on the fly. However, young researchers have an advantage to start practicing Open Science principles as early as their undergraduate education.

Incorporating Open Science into undergraduate education is not new, with researchers aiming to define Open Science broadly and equitably for science education [9]. While it is understandably challenging to learn and apply Open Science principles, a learning-by-doing approach has shown benefits. Open Science modules and activities were introduced in first-year Biology courses [10], a project-based seminar on qualitative research [11], and Psychology courses focused on robust and reproducible research methods [12], [13]. Furthermore, The Collaborative Replications and Education Project [14] and The Hagen Cumulative Science Project [15] implemented projects around replicating existing research in undergraduate education. The increasing effort and awareness around Open Science and reproducible research in undergraduate education inspires a new approach to undergraduate courses that introduce fundamentals of research. This approach introduces broad research practices while simultaneously addressing Open Science practices and tools that enhance reproducibility, transparency and openness.

In this paper, we outline a course opportunity that gave undergraduate students an early exposure to Open Science with hands-on research experience. This course was offered in a set of cohort-focused research and experiential learning courses organized by the Office of the Vice Provost for Education at Carnegie Mellon University (CMU). Titled *Collaborative Research Through Projects*, this set of courses was held in the summer, offering undergraduate students a tuition-free opportunity to undergo a learn-by-doing educational experience.

This paper details a course titled *Enhancing Reproducibility and Collaboration with Open Research Tools.* For eight weeks, classes were held in-person two times a week, led by a STEM Librarian at CMU. This course was designed to help students understand the motivation for the

Open Science movement and be most prepared to navigate these new standards, as they enter a research field. As a team of students and an instructor, we explored high-level concepts of research linked to Open Science, and how modern tools facilitate reproducible research. The observations stated here are not considered comprehensive results from formal research, rather this paper provides reflections from a unique course that may inspire others to incorporate Open Science practices into courses and research.

Reproducibility along the research lifecycle

This course was centered around students understanding and creating reproducible research by developing and assessing open research materials. Reproducibility, which is at the heart of all scientific discoveries and innovation, holds true the most fundamental theories and laws [16]. Without such a crucial step in the scientific process, new findings can only rely on limited trust. Unfortunately, for something so crucial, it has yet to become an established standard. The reproducibility crisis is recognized among researchers, and studies have uncovered plenty of examples where published research cannot be independently reproduced with just information from an article [17], [18], [19], [20].

While the published research article is the standard medium for the evolving research conversation, the metrics of which illustrate a researcher's success, other artifacts and outputs should be considered. These supplemental materials aid the scholarly conversation, promote a researcher's efforts, and invite reuse. These materials may include methods and procedures more detailed than an article's "methods" section, datasets that are openly accessible and well-documented, environmental details of the analysis software, or supplemental project documents managed on open and collaborative platforms.

Creating these artifacts is doable with time, effort, and the proper tools. For detailed methods, there is protocols.io, and for open datasets, there are general repositories like Zenodo or institutional repositories. To preserve and rebuild instances of a computational research environment, there is Code Ocean, and finally, Open Science Framework (OSF) creates a hub for researchers to manage the many moving pieces of a project. In addition, OSF hosts a repository of registered reports and preprints. This collection of tools and platforms is not comprehensive, but was the focus for this course.

Before these tools were introduced, the course covered reproducible research ranging from broad fundamentals to specific practices. We first discussed the fundamental process of the scientific method and the tangible steps of the research lifecycle, including the outputs and artifacts produced along the way. Discussions then focused on the limitations of closed research artifacts, or those prepared and shared with minimal effort. From these experiences, tools were introduced to assess reproducibility of open research artifacts.

Table 1: List of Topics Covered Each Week (Two Class Periods)

Week	Topic
1	The Scientific Method
2	The Research Lifecycle
3	Open Science and Research
4	Reproducibility
5	Computational Reproducibility
6	Reproducibility Assessment (Closed Phase)
7	Introduction to Open Science Tools
8	Reproducibility Assessment (Open Phase)

Overview of class sessions and assignments

Lectures occurred mostly as discussions, with simple prompts to facilitate. Outside of lecture, reading passages were distributed with questions to guide student reflections. The main modules of instruction included The Scientific Method, The Research Lifecycle, Open Science and Research, and Reproducibility.

Module 1: The Scientific Method

The first module of the course covered the basics of the scientific method. The first discussion started with a simple question: "How do you do research?" We discussed this process and listed basic steps of research. The following steps were recorded from the in-class discussion between students and instructor:

1. Find a problem
2. Find information about the problem
3. Read literature written from others studying the problem, and reassess if the problem was already solved
4. Develop a hypothesis, identifying variables to measure and study
5. Find or produce data, by conducting an experiment or extracting from other research
6. Analyze the data
7. Check the results against the hypothesis

8. Write up whether the hypothesis was correct or incorrect
9. Reassess and develop a new experiment, identify different variables or biases

We compared our list of steps to the following list, which was prepared before lecture by the instructor based on their own experience and interpretation:

1. Make an observation
2. Ask a question
3. Develop a hypothesis
4. Do background research and identify appropriate variables
5. Conduct an experiment to test the hypothesis and selected variables
6. Analyze results
7. Write conclusions
8. Iterate

Several parallels exist between the two lists, with the major difference being that the list developed in class provides more explicit details. From this exercise, considerations around reproducibility were gradually introduced, starting with a new question: "How will you preserve your progress along each step of the scientific method?" As a class, simple approaches were noted. For research design and planning steps such as initial observations, research questions and hypotheses, here is an overall summary of the concepts noted:

- Write down ideas in digital documents such as Google Docs, where collaborators can share this information through email, social media, or other online locations, with varying permissions for viewing or editing.
- Write down ideas on physical paper to quickly draw visual depictions with distinguishable colors and penmanship, where physical copies are lendable and digital scans are shareable.

For collection and analysis, such as background research, experimental results and analysis, we noted:

- Searching in Google or using resources from a library, creating a list of all found resources in a document, saving copies in folders, or bookmarking pages or sections.
- Writing notes about articles, making annotations, or writing summaries or important facts.
- Saving quantitative data in spreadsheets, recording commentary of qualitative data, or storing physical artifacts or samples in a secure location.
- Creating visualizations from raw data or observations such as graphs, flowcharts, and schematics.

- Uploading code or data to the cloud such as Google Drive, GitHub, or other online sources.

For the final steps in decision/conclusion making and moving forward with iterations, we noted:

- Writing down all conclusions and potentially publishing conclusions despite their nature.
- Refining notes, data, analyses and conclusions by creating new copies of original records.

The first homework assignment focused on *The Practice of Science* and the linearity and non-linearity of the scientific method [21]. Students reflected by considering the ways that the scientific process seems most sensible, describing steps that can be linear, non-linear, or both. Interesting considerations were returned among the reflections, summarized below:

- Single research projects, and research as a whole, is non-linear, as we refer back to the work and knowledge from research in the past.
- The scientific process can be looked at a high level, where there is a linear progression in identifying questions first, then making attempts to solve and assess the problem.
- The scientific process follows a linear path, but the path is always subject to change, with iteration occurring in a single step, circling back to previous steps, or even starting somewhere later in the process.
- Some steps in the process may mix, such as how observations lead to doing background research, while this research leads to further observations.

Module 2: The Research Lifecycle

The second module focused on the research lifecycle, where more concrete tasks and artifacts of research exist. We framed the discussion around a simple list of stages aligned with services at CMU Libraries [22]:

1. Design
2. Plan
3. Collect
4. Analyze
5. Publish and Archive
6. Reuse

We aimed to connect the previous module by placing each step of the scientific method under corresponding stages to the research lifecycle. We observed interestingly that most or all of the scientific method applies in the early half of the research lifecycle, while the later half that includes publishing, archiving, and reuse, only fit with the “conclusions” and “iteration” in the scientific method. This helped us see that the pieces of research related to testing hypotheses, running experiments, and collecting and analyzing data are easy to associate with the scientific method, while stages more prominent in academic research, like publishing, sharing, impact, and reuse, are not so easily associated. Once again we brainstormed ways we can preserve our ideas and discoveries along this lifecycle. We arrived at a more diverse list of artifacts that follows more closely to modern research outputs like research proposals, bibliographies, notes on methods and procedures, manuscripts, and repositories.

The reading reflection included passages from *Navigating the Research Lifecycle for the Modern Researcher* [23]. Students were prompted to reflect on how their own skills and familiarity with tools aligned with practices in research. Students brought up some of the following skills, summarized below:

- Communication skills that help researchers collaborate and share ideas and feedback.
- Having a curiosity and fascination with exploring the unknown.
- Using mathematical knowledge to process and manipulate data.
- Organization and willingness to expand curiosity to varying topics, which helps a researcher explore.
- Using tools for programming and data analysis, which help in collecting and analyzing.

Module 3: Open Science and Research

In the third module, we shifted to Open Science and research, particularly, the movement, practices, and the FAIR principles [24]. This course fortuitously occurred during 2023, so the Year of Open Science from the White House OSTP memo [6] was the first talking point in introducing and emphasizing the Open Science movement. Following this, we reviewed a list of components and practices of Open Science that are regularly referenced [5], [22], [25], [26]:

- Pre-Registration
- Open Access Publications
- Open Data
- Open-Source Software
- Open Educational Resources
- Open Peer Review
- Open Notebooks
- Open Protocols
- Open Collaboration
- Open Research Metrics

In an exercise similar to previous sessions, we mapped the components of Open Science to the stages in the research lifecycle. We did not discuss each component in great detail, but students chose those that were interesting. We found that some fit in single stages, spanned multiple in succession, or fit in multiple stages in segments. A few examples are summarized below:

- Pre-registration fits in research design and planning.
- Open peer review fits in publishing and archive.
- Open data and open-source software fit in collecting, analyzing, publishing, archiving, and reuse.
- Open access fits first in design and planning, then later in the lifecycle with publishing and archiving.
- Open notebooks span the entire lifecycle.

For homework, students read about the Open Science challenge to adopt individual practices that align with widely shared values [25]. In the written reflections, students connected an Open Science practice discussed in class to widely shared core values of science (Objectivity, Honesty, Openness, Accountability, Fairness, and Stewardship) [25], [27].

Module 4: Reproducibility

The last of the main modules connected everything by covering reproducibility in the context of the practices and products along the research lifecycle, while following the scientific method. We first discussed reproducibility through problems in modern research, such as the recognition of the reproducibility crisis and examples of failed replication studies [17], [18]. We then narrowed our focus towards computational research and what defines reproducibility in this area. For instance, we discussed different definitions as illustrated in the Turing Way Handbook, [28] where reproducibility and replicability of a computational analysis depends on whether the same data is used. We also discussed best practices in data management and computational research, such as version control, storing and organizing files with naming conventions, using relative paths over absolute paths, recording software versions and dependencies, and adopting software licenses.

In the reading reflection assignment, the students dove further into the evidence of the reproducibility crisis [17] and also reflected about barriers that researchers face around reproducibility [28]. Students highlighted the following barriers summarized below:

- Reproducibility is not normally considered for promotion and there is a challenging balance of selfless needs, like sharing for the research community, and self-centered needs, like considering progress of your own research for further funding, promotion, and achievement.

- Reproducibility is challenging when using big data and complex computational infrastructures, such as sharing large datasets across the world, and creating compatibility with different formats and structure of data.
- Producing open and reproducible research offers limited incentives when these practices require more effort but give evidence against yourself, further opening up yourself to critique, and being held at a higher standard than less open researchers.

In the remaining weeks of the course, we transitioned to a hands-on reproducibility assessment. This phase provided the best opportunity for students to practice research and gain first-hand experience with open and closed research artifacts. The subjects of the study were computational research samples in data science and numerical simulation. To ensure that students were prepared to interact with the research samples, the course included several parallel sessions covering basic Python programming for data science. In addition, we covered best practices in reproducible research code with additional parallel sessions on version control with Git and GitHub. The Python curriculum was adapted from the Carpentries lessons [29], and version control was adapted from passages in the Turing Way Handbook [28].

Reproducibility assessment

In the final portion of the class, the students practiced research methods and best practices in a reproducibility assessment. Overall, the assessment involved samples of computational experiments that students would attempt to reproduce as well as modify to attempt to produce new results. The assessment underwent two phases: a closed phase, where students received limited materials that followed minimal open and reproducible practices in preparation, and an open phase, where students received a greater collection of materials that were prepared using tools and platforms that followed open and reproducible principles. In both phases, students uploaded their work to Open Science Framework [30]. These deliverables would include figures and data that could only be produced by properly re-executing the experiment and written reflections about their experience.

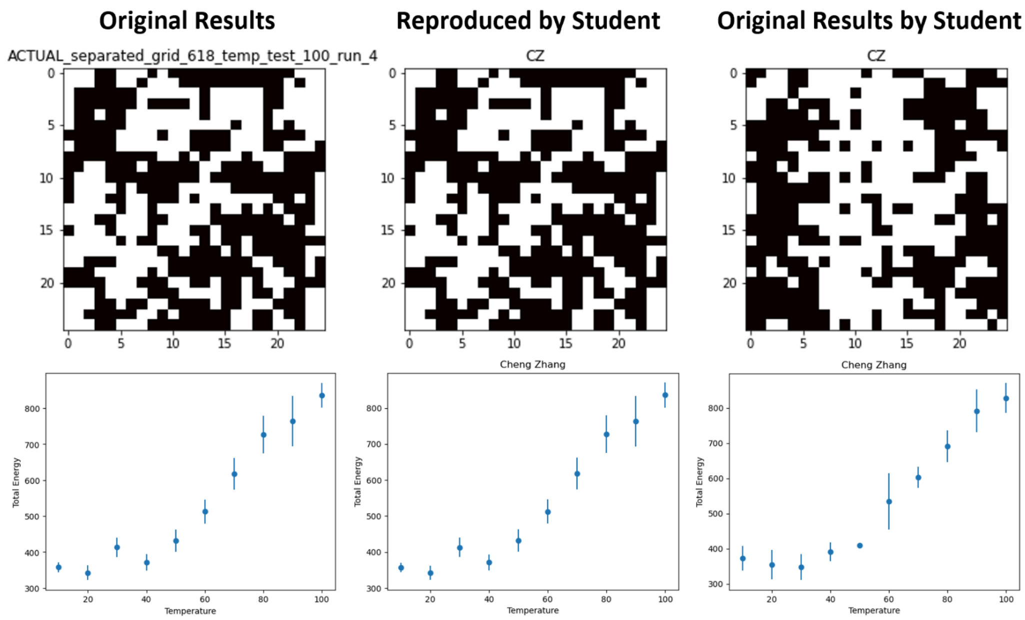

Figure 1: Example of results from a research sample (left), results reproduced by a student (middle), and original results produced by a student (right).

Closed phase

At the start of the closed phase, we discussed the computational research subjects that would be used for the assessment, an introductory machine learning tutorial with the Iris dataset [31], and a simple example of simulated annealing to separate randomly mixed numbers in a matrix [32]. To embark on the first tasks of this assessment, students were provided links to basic GitHub repositories that contained Jupyter Notebooks and datafiles. Students were asked to download every file, look through the Jupyter Notebooks, and simply attempt to run all of the code from top to bottom. From these attempts, we could assess each other's experience by checking if the code could all run successfully, and if not, discuss what happened and what errors came up. It was strongly emphasized that there were no penalties if code could not run, as reflections from each student's experience was most valuable for the learning in this course. If all of the code did run, students were asked to upload specific figures or copies of data, which verifies that the code could produce outputs. (See Closed Reproducibility Study on OSF [30]) Students could verify that their outputs match the original by referring back to the original outputs in the GitHub repository.

The students found that the experience was overall simple and educational, with these projects seeming overall reproducible. They did run into several technical errors, with a summary of errors listed below:

- Some file paths needed to be changed to properly read and write files.
- Some file paths referred to folders that needed to be created manually.
- Original data was overwritten and the resulting figures from the analysis looked different, but similar trends were observable.
- Some code ran for considerable time, suggesting that a warning could help future users.
- Statistical scores used for parameter optimization in machine learning models would differ upon each run of the code.
- Formatting and appearance in figures had differences from the original.

In addition, students had the opportunity to expand on each experiment in the second assignment. With properly running code, students were asked to make a change such as a different value for a parameter or variable. Such changes were expected to make a noticeable difference to some of the outputs requested in the previous assignment. Again, students uploaded these outputs and a written reflection about their experience. The students' discoveries are summarized below:

- Part of the code required a seed for a random number generator, so this parameter was selected to alter. However, seed declaration occurred multiple times, so multiple lines of code had to be altered. Similar trends in figures were observed after random number seeds were changed.
- Altering parameters beyond random number seeds was also possible, such as sizes of matrices in the simulated annealing example. Increasing the sizes of matrices created different trends than the original study, but also required some sections of code to run significantly longer.
- Outputs needed to be redirected to a new folder so that original outputs were not replaced.
- It was possible to complete the task without running all of the code in a notebook, however, this lowered confidence in the results.

Introducing Open Science tools

Once the students finished working with closed research outputs by troubleshooting any technical errors, we transitioned towards the idea of tools that aim to avoid such errors and confusion. The tools in the focus of this lesson were an institutional repository, LabArchives, protocols.io, and Code Ocean. We briefly discussed each and contemplated how these tools may have helped reproducibility in the closed phase. Following this lesson, students completed an exercise to practice with some of these tools. This included finding a research deposit in the institutional repository, creating a protocol that outlines a task, and creating a capsule on Code Ocean with data and code (example).

Open phase

With newfound knowledge of Open Science tools, we transitioned into the open phase. Students worked again with just one of the research samples (simulated annealing), now using code, data, and protocols all prepared with Open Science tools. Students were instructed to complete the same tasks as the closed phase, but students were also given links to a protocol [33] and a Code Ocean capsule [34]. Students followed the protocol and edited a fork of the capsule to rerun code in Jupyter notebooks and produce and upload copies of data and figures. Again, the following task involved expanding on the experiment, where students made changes to variables or parameters in the code and uploaded new outputs. (See Open Reproducibility Study on OSF [30]) Students wrote new reflections on this process, and specifically, they recalled any challenges faced during the closed phase, commenting on whether or not they thought that tools like Code Ocean and protocols.io would have helped alleviate those challenges. Many of the students reflected on the following:

- There were no longer any challenges associated with file paths.
- In Code Ocean, some code requires more time to complete, which may be due to the code no longer running locally. While running the code takes relatively longer, and results aren't viewable until the run is finished, it was assuring to see the ongoing steps displayed in Code Ocean. However, It was sometimes preferred to run code in a JupyterLab environment, either locally or as a cloud workstation in Code Ocean. This way, it was possible to see intermediate results as the code ran.
- Tracking changes through version control in Code Ocean was simpler to manage and visualize compared to GitHub.
- When running new analyses, all new versions of data and code files were not saved in the folders designated for data and code in the capsule. One workaround involved creating new folders and rewriting the code to save new outputs to these folders. However, these directories were found to sometimes disappear.
- Some confusion arose due to inconsistencies with the steps written in the protocol and the instructions for the assignment. Despite this, steps in the protocol listed as "Computational Step" or steps that included warnings increased confidence when reproducing the analysis.

Discussion

Overall, the combination of procedural documentation on protocols.io and a Code Ocean capsule gave students an improved experience in reproducing and altering an original analysis. Code Ocean capsules are designed to let an outside researcher reproduce results from research code with a press of a button. In the scenario presented to the class, students were able to easily do this, but ambiguity rose when students attempted to alter and rerun variations of the original code. The technical errors associated with this issue are likely tied to the strict optimization for reproducibility when completing a “Reproducible Run” in Code Ocean [35]. This feature is not built to run modified versions of the code and data. Therefore, it is best to run new analyses from a cloud workstation in Code Ocean or download the capsule and run in a different environment. It was not clear how to best share or publish a modified version of a published capsule. This produced challenges for us to review and collaborate on our work.

An outlined procedure on protocols.io [33] provided further guidance for reproducibility and modification of the original research, but there were associated challenges as well. The tasks outlined in this phase of the reproducibility assessment were inconsistent with instructions in the protocol. The simulated annealing research sample involved two separate notebooks: one for generating the data, and one for analyzing the data. The protocol was written so that users knew how to run and edit each notebook in Code Ocean separately, however the protocol listed these steps in an order that conflicted with the order of instructions for the assignment. Despite this confusion, the protocol offered further guidance and instructions.

There were also details in the research outputs that affected reproducibility. In the notebook that was written for data generation, the simulated annealing algorithm executed many iterations that involved randomly generated numbers. For the original experiment, executing this code was obviously the first step for the original analysis, but for reproducibility, rerunning this code overwrites the original data. While similar trends should arise from subsequent analysis, it is not possible to perfectly reproduce all numerical results. There are a few solutions for further iterations of this type of research example, such as creating a record of seeds that will be set in each iteration, and writing intermediate results after each iteration. This will increase computational demand, but all recorded seeds and data will ensure a proper snapshot of the simulation. Though it is not the recommended practice, it may be best to separate data production and analysis steps when preparing Code Ocean capsules. This will allow users to reproduce and modify steps independently.

The reproducibility assessment gave students a real-world experience of the complexities that any researcher may find when using the outputs from another. In the closed phase of this assessment, students learned how to identify challenges linked to research shared without best practices. Students identified file paths that were not consistent with the organization of files downloaded from a repository, exact results were not reproduced due to random numbers, and parts of code ran for a surprisingly large amount of time. Transitioning to the open phase, which incorporated protocols.io and Code Ocean, the students interacted with novel research artifacts that guide researchers to properly reproduce steps and obtain the exact results despite the organizational and environmental requirements necessary for computational research. Students were able to identify how these tools helped them avoid the errors and subsequent troubleshooting required to work with raw outputs from the closed phase. Although the research samples were fictitious, the students worked with research outputs that are identical to the kinds that actual researchers encounter.

Conclusion

By integrating Open Science practices and tools into an undergraduate research course, students learned first-hand reproducible research practices. This course equipped students with foundational knowledge of the scientific method and research lifecycle and provided hands-on experience in utilizing digital tools for transparent and open dissemination of research outputs. While simultaneously learning about the steps to create and share research outputs, students learned how opening these outputs help outside researchers, collaborators, and themselves. Through research samples in Jupyter Notebooks in a reproducibility assessment, students uncovered insights into the practical application and impact of Open Science tools and practices on the reproducibility of computational research. Comparing and contrasting the steps and processes in reproducing exact results between open and closed research outputs, students gained real-world insights into the experiences faced by actual researchers. The observations shared here aim to inspire current and future researchers and educators to adopt transparent and reproducible research methodologies, so that we all can collectively enhance the quality of future scientific education and research.

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