

REMODEL automated report

A Community Poll on Reproducibility in Computational Geosciences

Robert REINECKE

May 19, 2021

Report last updated: 19th May, 2021

Compilation date: May 19, 2021

This document summerizes a full analysis for detailed results. **It is not a full publication but rather an automated representation of the data present in this repository**

It summarizes the extensive results and builds the foundation for the publication of a journal paper. It will also be distributed along with the data in the course of a journal and data publication.

1 Aim of this survey

Software development has become an integral part of the geosciences¹ as models and data processing get more sophisticated. Paradoxically, it poses a threat to scientific progress as the pillar of science, reproducibility, is seldomly reached². Software code tends to be either poorly written and documented or not shared at all; proper software licenses are rarely attributed. This is especially worrisome as scientific results have potential controversial implications for stakeholders and policymakers and may influence the public opinion for a long time³.

In recent years, progress towards open science has led to more publishers demanding access to data and source code alongside peer-reviewed manuscripts^{4,5}. Still, recent studies find that results can rarely be reproduced^{6,7}.

In this project, we conduct a poll among the geoscience community which is advertised via scientific blogs (AGU, EGU), research networks (researchgate.net and mailing lists), and social media. Therein, we strive to investigate the causes for that lack of reproducibility. We take a peek behind the curtain and unveil how the community develops and maintains complex code and what that entails for reproducibility⁸. Our survey includes background knowledge, community opinion, and behaviour practices regarding reproducible software development. We postulate that this lack of reproducibility⁹ might be rooted in insufficient reward within the scientific community, insecurity regarding proper licencing of

software and other parts of the research compendium as well as scientists' unawareness about how to make software available in a way that allows for proper attribution of their work. We question putative causes such as unclear guidelines of research institutions or that software has been developed over decades¹⁰, by researchers' cohorts without a proper software engineering process¹ and transparent licensing.

To this end, we also summarize solutions like the adaption of modern project management methods from the computer engineering community¹¹ that will eventually reduce costs while increasing the reproducibility of scientific research⁸.

1 A comment to "Most Computational Hydrology is not Reproducible, so is it Really Science?" R.W. Hut, N.C. van de Giesen, N. Drost, Water Resources Research, 2017

2 Hutton, C., Wagener, T., Freer, J., Han, D., Du_y, C., and Arheimer, B., Most computational hydrology is not reproducible, so is it really science? Water Resources Research, 2016

3 Munafo, M., Nosek, B., Bishop, D. et al., A manifesto for reproducible science. Nat Hum Behav, 2017

4 Executive editors, G. Editorial: The publication of geoscientific model developments v1.2. Geoscientific Model Development, 2019

5 Katz, D. S., Niemeyer, K. E., and Smith, A. M., Publish your software: Introducing the journal of open source software (joss), Computing in Science Engineering, 2018

6 Stagge, J. H., Rosenberg, D. E., Abdallah, A. M., Akbar, H., Attallah, N. A., and James, R., Assessing data availability and research reproducibility in hydrology and water resources. Scientific data, 2019

7 Añel, J. A., García-Rodríguez, M., and Rodeiro, J.: Current status on the need for improved accessibility to climate models code, Geosci. Model Dev., 2021

8 Stodden, V., The reproducible research standard: Reducing legal barriers to scientific knowledge and innovation. IEEE Computing in Science & Engineering, 2009

9 <https://www.nature.com/news/1-500-scientists-lift-the-lid-on-reproducibility-1.19970>

10 Muller, C., Schaphoff, S., von Bloh, W., Thonicke, K., and Gerten, D., Going open-source with a model dinosaur and establishing model evaluation standards. EGU, 2018

11 <https://software.rajivprab.com/2019/11/25/the-birth-of-legacy-software-how-change-aversion-feeds-on-itself>

Our larger questions:

- Is reproducibility is an issue in the geosciences? Are bad code and documentation the root cause of that issue?
- Is model software too complex? Does that hinder reproducibility?

- Are researchers missing the tools and know-how (methods, licenses etc.) to build good model code?
- Is missing funding and missing time preventing researchers from making their models more accessible?

We define reproducibility as:

”Reproducibility in the context of modeling in the geosciences means that results obtained by a modeling experiment should be achieved again with a high degree of agreement when the study is replicated with the same model design, inputs, and general methodology by different researchers.

We explicitly exclude the retracing of results by means of using a different modeling environment (including variations in model concept, algorithms, input data or methodology).”

2 Data processing

We designed the survey according to standards from psychology research. We apply descriptive statistics to analyse demographic background and basic analysis. Further, we apply inferential statistical methods to test the unerlying hypotheses.

The raw data of the survey is stored in the folder **LiveData**. **The raw data has not been modified or cleaned in any way.** To run some basic cleanup run the folloing script:

```
1 import process_data.py as p
2 p.process()
```

3 Results

All data processing and plotting (including building this document) can be executed by running `python run.py`. Plotting details and addtional processing can be found in th script `plot_all.py`.

Our main hypothesis for this analysis where the following:

- **H1** Young scientists develop software more actively than established researchers.
- **H2** Young scientists are more familiar with software licenses than established researchers.
- **H3** Young scientists are more familiar with modern development methods than established researchers.
- **H4** Senior researcher percieve reproducability as a lesser problem than early career researchers.
- **H5** Software complexity is the main reason for a lack of reproducability.

- **H6** Researchers code frequently but without knowledge about proper engineering methods, licences and tools.
- **H7** The most frequently used language is still C/Fortran. Younger scientists tend to use Python and R; this is consistent throughout fields
- **H8** Most researchers are autodidacts when it comes to coding.
- **H9** Most researchers have never reproduced code with the original model. Only with their own model. This differs between fields.
- **H10** Practitioners and researchers perceive the issue of reproducibility differently. Scientists are more aware (?).
- **H11** There are more researchers that apply software than they are ones that develop it. This differs between activities and fields.
- **H12** Most researcher do not know if their software belongs to them.
- **H13** Models that are available are hard to use. Causes?: Bad code, no documentation, no input data
- **H14** Senior researchers are convinced their work is reproducible. (much more at least than young scientists)
- **H15** The smaller the scale the more reproducible and accessible.
- **H16** Researchers think that their software is bug free and always correspond to their intended implementation.
- **H17** Most senior scientists think investment in FOSS doesn't pay off.
- **H18** Senior researchers think that their code/project is easier to understand but that conflicts with reality. And younger researchers have the opposite understanding.
- **H19** We need more funding to enable reproducible computational science.
- **H20** New research software tends to be FOSS, big players are often legacy software grown over decades which is hard to reimplement as FOSS.

3.1 Sample Characteristics (demographics)

Who were our participants? Here we present characteristics of the participants in our poll, i.e. their current career stage, their years of research experience, their geo-scientific field and scale as well as their current focus of work. This is purely descriptive statistics. As we welcomed everyone to our poll, we did not form any assumptions regarding sample characteristics. Also, we tried, but might not have reached a representative sample of the population of geo-scientists.

Here, we report basic sample characteristics. Also, we can check for and report any salient sample properties.

Corresponding survey questions:

- DM01 - What career stage are you in?
- DM02 - For how long have you been working in your research field?
- DM06 - To which field within the geosciences does your research mainly belong?
- DM05 - What geographic scale are you working on?
- DM07 - What is the focus of your work?

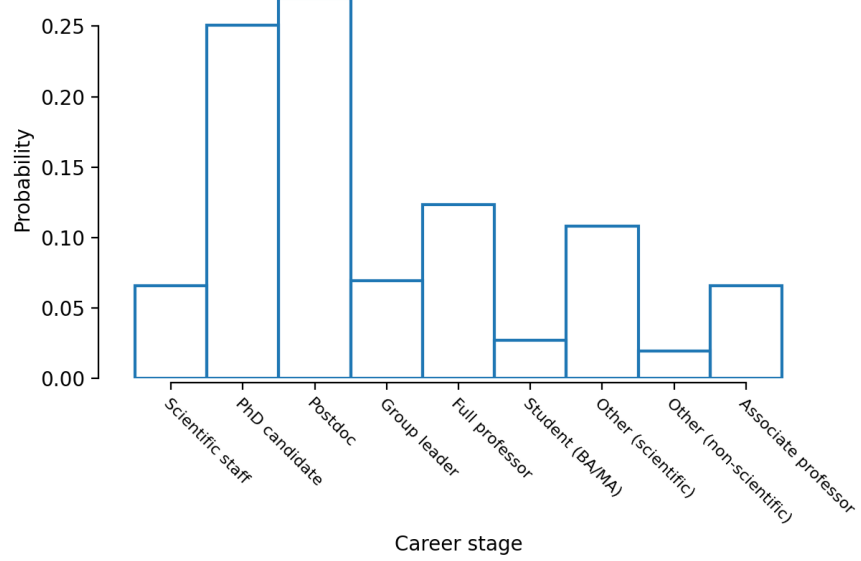


Figure 1: DM01 - Career stage of participants

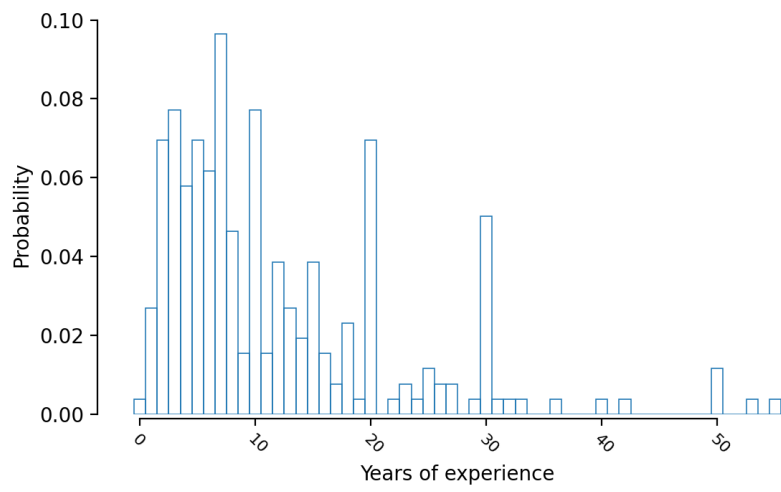


Figure 2: DM02 - For how long have you been working in your field?

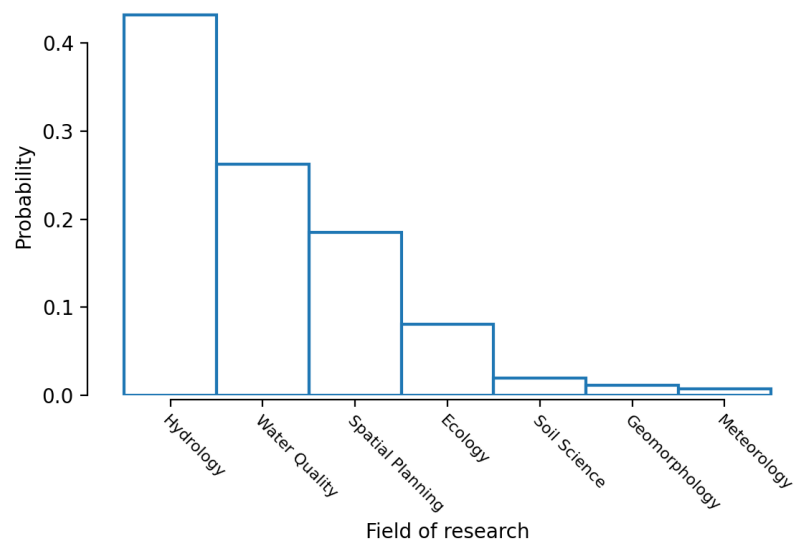


Figure 3: DM06 - Which field do you belong to?

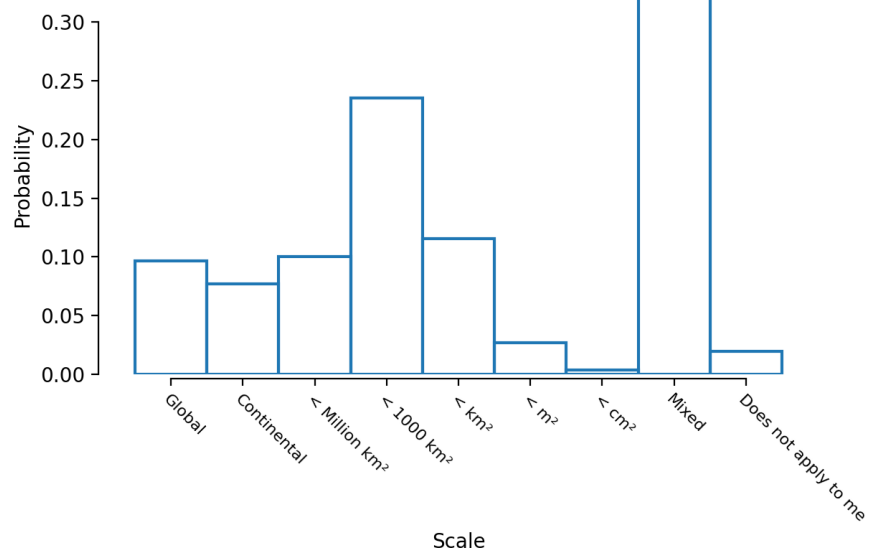


Figure 4: DM05 - What scale are you working on?

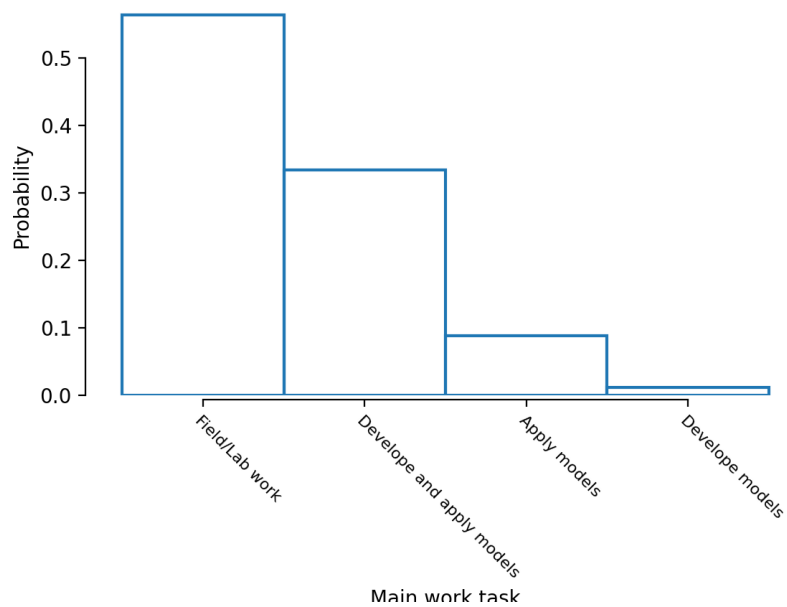


Figure 5: DM07 What is the focus of your work?

3.2 Community Opinion on Reproducibility

This part covers people's view and opinion. We assume that our definition of reproducibility was used (annotated at several points in the poll).

Analysis Steps:

- plot corresponding questions (across full sample)
- perform statistical testing of our above stated hypotheses (across sub-groups, e.g. early career vs senior researcher)
- perform further data exploration (NOT hypothesis testing) - this might inspire future research, e.g. correlation analysis

Corresponding survey questions:

- O101 - How strongly do you agree with the following statements?
- O103 - What are the reasons for a lack of reproducibility?
- S113 - How long do you think does it take for an average PhD student to efficiently work with your research software?

Corresponding hypotheses

- H4 Senior researcher perceive reproducibility as a lesser problem than early career researchers.
- H5 Software complexity is the main reason for a lack of reproducibility.
- H10 Practitioners and researchers perceive the issue of reproducibility differently. Scientists are more aware (?).
- H13 Models that are available are hard to use. Causes?: Bad code, no documentation, no input data.
- H14 Senior researchers are convinced their work is reproducible. (much more at least than young scientists).
- H16 Researchers think that their software is bug free and always correspond to their intended implementation.

O101: Opinion on Reproducibility in Geo-Sciences: How strongly did participants generally agree with statements? Do they consider it a problem at all? Do they think that their work is reproducible?

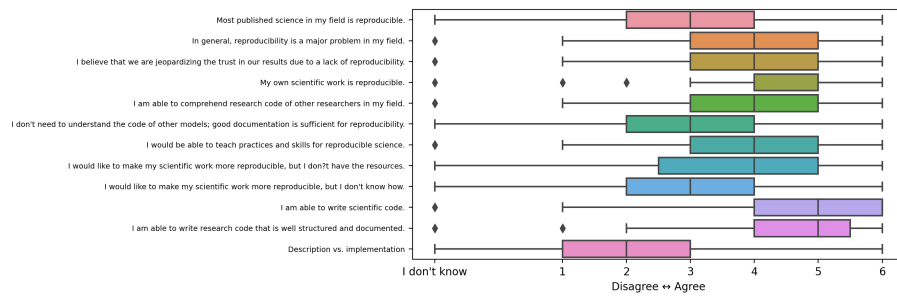


Figure 6: O101 How strongly do you agree with the following questions?

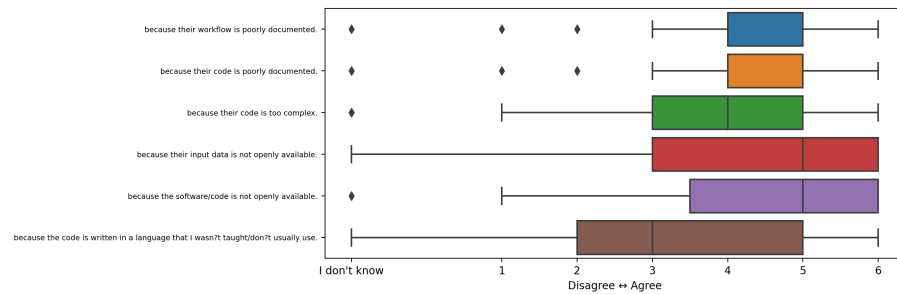


Figure 7: O103 What are the reasons for poor reproducibility?

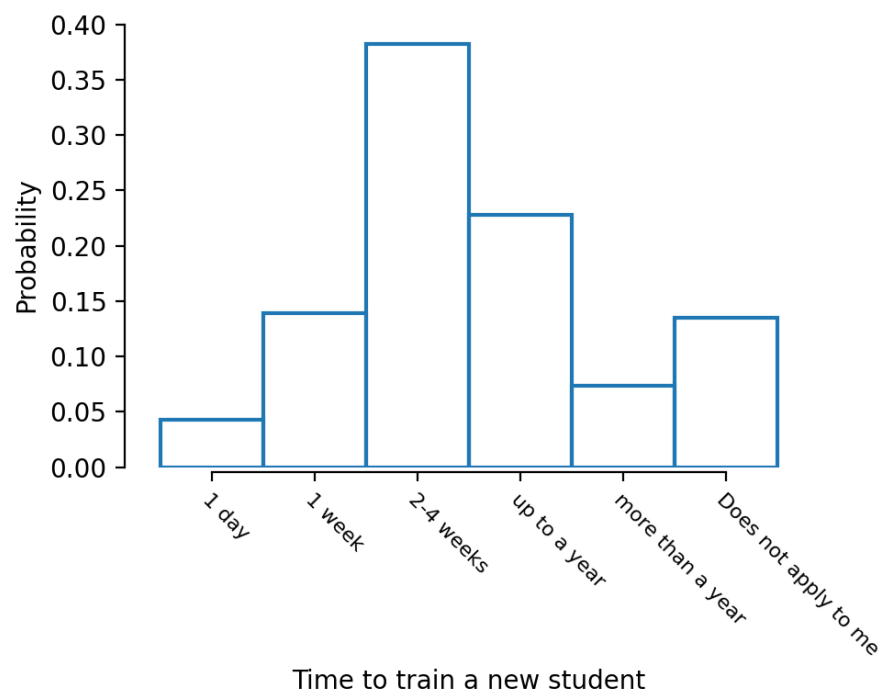


Figure 8: S113 How long does it take to train a new student in your software?

3.2.1 H4 Differences in Opinion on Reproducibility

Established researchers 32 Young researchers 177 Mean agreement to reproducibility without don't know 3.1185770750988144
Mean agreement among Y 3.023121387283237
Mean agreement among O 3.6129032258064515
Median agreement to reproducibility 3.0
Median agreement among Y 3.0
Median agreement among O 4.0 Career has no normal distribution
No statistical test possible, samples of Prof. too low to do a proper Wilcoxon or even t-test

3.2.2 H5 Reasons for lack of reproducibility

!Include don't know Mean workflow: 4.223938223938224, code documentation : 4.146718146718147, code complexity: 3.583011583011583, input data not available: 4.374517374517374, code availability: 4.351351351351352, written language: 3.1621621621621623
Main reason: Input data. 2: code availability, 3: workflow, 4: documentation, 5: complexity
Mean agreement code complexity without don't know 3.8847736625514404
Mean agreement among Y 3.784431137724551
Mean agreement among O 4.033333333333333
Median agreement 4.0
Median agreement among Y 4.0
Median agreement among O 4.0

3.2.3 H10 Practitioners are less aware of the issue

No Data to investigate this question. Only scientists answered the poll.

3.2.4 H13 Reasons for reproducibility

See H5. No additional data to explore this further.

3.2.5 H14 Senior researchers are convinced their work is reproducible. (much more at least than young scientists).

Mean agreement my own research is reproducible 4.431372549019608
Mean agreement among Y 4.417142857142857
Mean agreement among O 4.5625
Median agreement 5.0
Median agreement among Y 5.0
Median agreement among O 5.0

3.2.6 H16 Researchers think that their software is bug free and always correspond to their intended implementation.

We did not ask a question that perfectly relates. Parts are answered in Fig. 6. Main relation to question: Implementing an algorithm based on a description from a publication yourself is the same as using the exact software package/original code that was used in that very publication.

Mean agreement description is same as implementation (including don't know)
2.1969111969111967

3.3 Reproducibility Practices and Skills

This part covers "actual" behaviour. (still only self-report assessment, but we can't change that)

Start here with summary of our hypotheses

We expected to see that... (formulate in a neutral tone)

Analysis Steps: plot corresponding questions (across full sample) perform statistical testing of our above stated hypotheses (across subgroups, e.g. early career vs senior researcher) perform further data exploration (NOT hypothesis testing) - this might inspire future research, e.g. correlation analysis

Corresponding hypotheses

- H6 Researchers code frequently but without knowledge about engineering methods licences and tools.
- H9 Most researchers have never reproduced code with the original model. Only with their own model. This differs between fields.
- H12 Most researchers don't know if their software belongs to them.
- H2 Young scientists are more familiar with licencing issues.

Corresponding survey questions:

- O102 -
- S103
- S110
- S202
- S112
- S101
- S111
- S104
- S105
- S106

3.3.1 H9 Activity of reproduction

XX

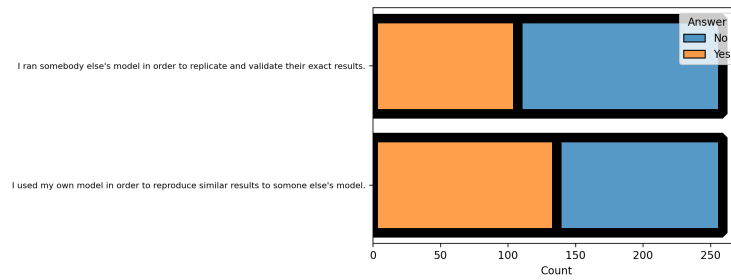
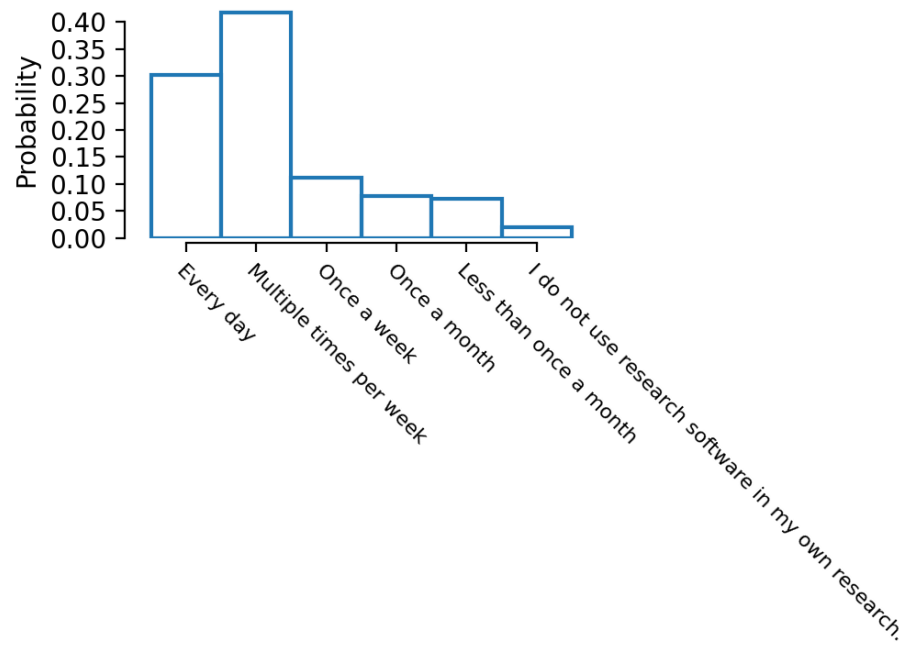
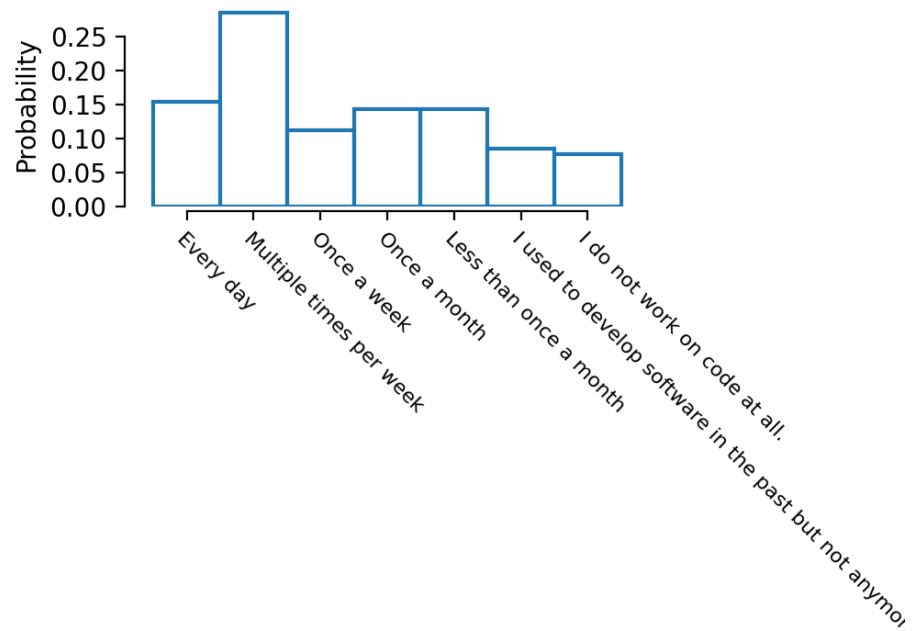


Figure 9: O102



Usage of research software

Figure 10: S103



Frequency of research code development

Figure 11: S110

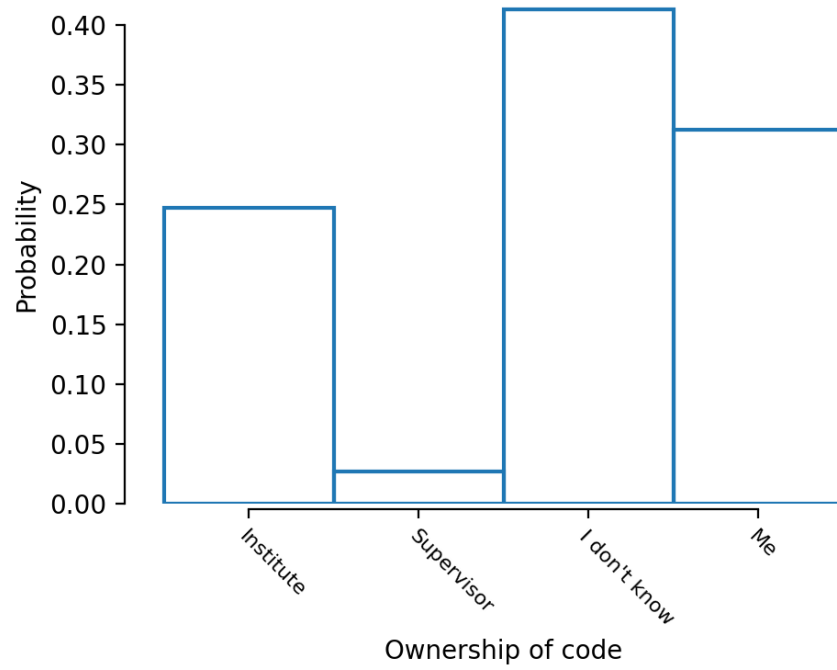


Figure 12: S202

3.4 Hurdles against and Solutions towards Reproducibility

This part covers "actual" behaviour. (still only self-report assessment, but we can't change that)

Start here with summary of our hypotheses

We stated that... (formulate in a neutral tone)

Analysis Steps: plot corresponding questions (across full sample) perform statistical testing of our above stated hypotheses (across subgroups, e.g. early career vs senior researcher) perform further data exploration (NOT hypothesis testing) - this might inspire future research, e.g. correlation analysis

corresponding hypotheses (see Robert's evaluation plan): H7 H13 H3

Corresponding survey questions: S203 S201 S204 (open text)

