BASEL JULY 21-25 ISMB ECCB 2019 iSCB

A Practical Introduction to Reproducible Computational Workflows

If you have not installed the required software, please start now!
https://github.com/ISMB-ECCB-2019-Tutorial-AM4/reproducible-computational-workflows

Let us know if you need any help!

BASEL
JULY 21-25
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iSCB
INTERNATIONAL SOCIETY FOR COMPUTATIONAL BIOLOGY

A Practical Introduction to Reproducible Computational Workflows

Introduction

Reproducibility

obtaining consistent results using

the same input data,

computational steps, methods, and code,

and conditions of analysis

Reusability

obtaining new results using

different input data or parameters,

the same computational steps, methods, and code,

and conditions of analysis

Replicability

obtaining consistent results across

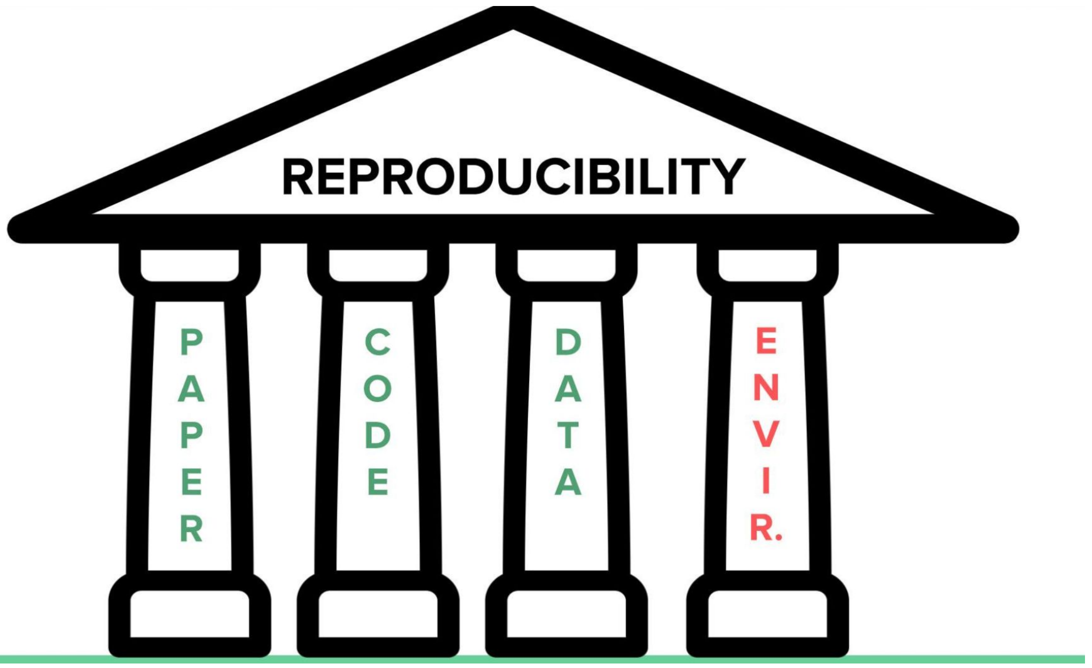
studies aimed at answering the

same scientific question, each of

which has obtained its own data

L. Barba, https://figshare.com/articles/Next_in_Reproducibility_standards_policies_infrastructure_and_human_factors/8194328/1

Four Pillars of Reproducible Research



Open Science

- Open access publications
- Open data
- Open source code
- Open execution environment

http://theoryandpractice.org/2016/05/Reproducibility-Symposium/

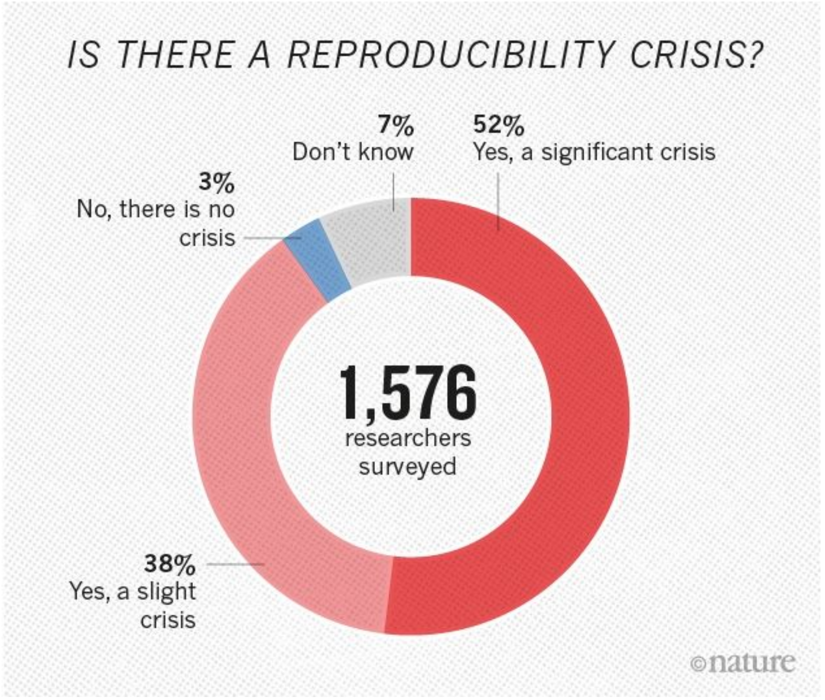
Reproducibility Crisis?

“More than 70% of researchers have tried and failed to reproduce another scientist's experiments, and more than half have failed to reproduce their own experiments.”

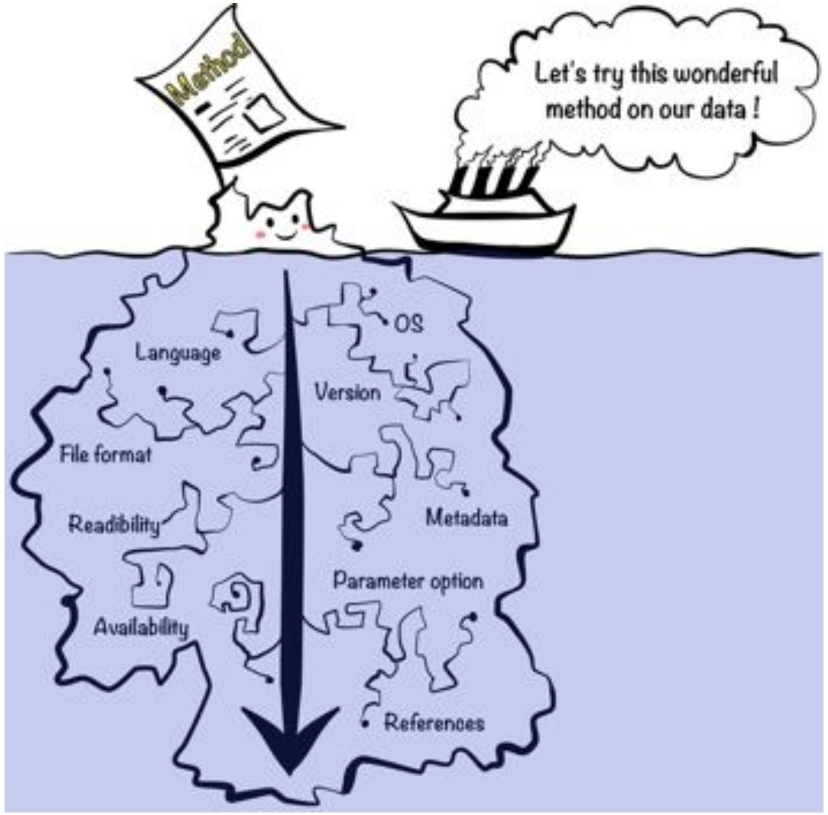
Nature, 2016, M. Baker, 1,500 scientists lift the lid on reproducibility

“Nature journal editors … will, on a case-by-case basis, ask reviewers to check how well the code works.”

Nature, 2018, Does your code stand up to scrutiny?



Barriers to Reproducibility and Reusability



- Missing or incomplete documentation
- Distribution is missing files
- Missing third party package
- Dependencies failed to build
- Runtime error
- Internal compiler error
- My last week:
  - samtools: error while loading shared libraries: libbz2.so.1.0: cannot open shared object file
  - error while loading shared libraries: libz.so.1: failed to map segment from shared object: Operation not permitted
  - /lib64/libc.so.6: version `GLIBC_2.14' not found

https://doi.org/10.1093/gigascience/giy077

S. Turner, bit.ly/madssci-2018-repro

Today you’ll learn techniques and tools to overcome these barriers and publish a reproducible workflow and results!

Tools and Infrastructure

Computational Notebooks:
Jupyter Notebook
Jupyter Lab

Cloud environment to run computational notebooks (including RStudio)

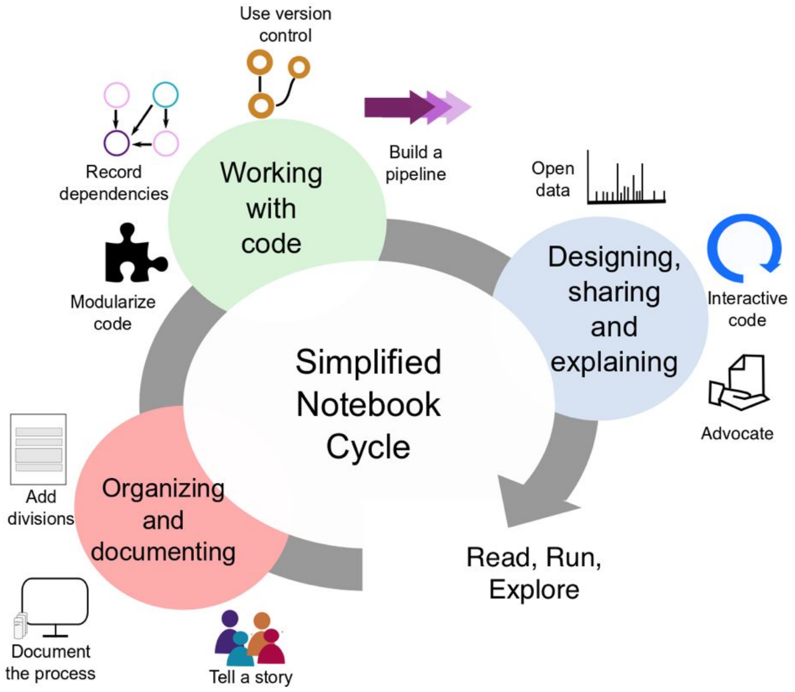
Source package and environment management system

Source code repository

Today’s Sessions

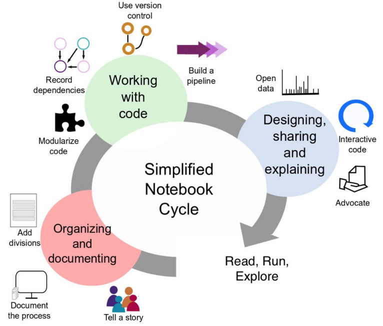
- Set up your environment
  - Introduction to Conda
  - Define your software dependencies
- Create and run Jupyter Notebooks
  - Intro to Jupyter Notebook and Lab
  - Visualize biological data using plugins
- Open-source your code and collaborate using GitHub
- Make your code reproducible by anyone, anywhere
  - Setup Jupyter Notebook [or RStudio] on mybinder.org
  - Share binder links and create badges
  - Other options to share notebooks
- Share you own project
  - Work on own/team project or on provided examples
  - Demo your project

Writing and Sharing Computational Analyses in Jupyter Notebooks



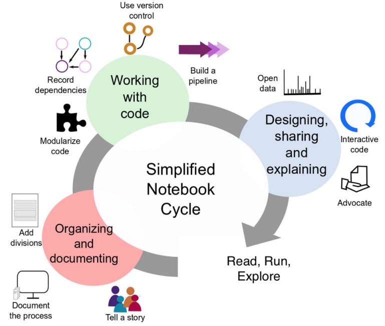
Ten Simple Rules for Writing and Sharing Computational Analyses in Jupyter Notebooks, PLOS Comp. Biol. in press, preprint: https://arxiv.org/abs/1810.08055

Organizing and Documenting



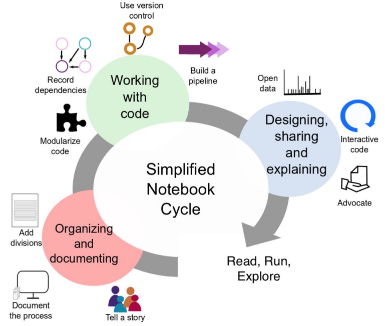
- Rule 1: Tell a Story for an Audience
  - Beginning - introduce topic
  - Middle - describe steps
  - End - interprets results
  - Describe not just what you did, by why you did it, how the steps are connected, and what it all means.
  - Adjust your description depending on the intended audience
- Rule 2: Document the process, not just the results
  - Add descriptive notes, e.g., why a particular parameter was chosen
- Rule 3: Use cell divisions to make steps clear
  - Avoid long cells
  - Limit each cell to one meaningful step
  - Split long notebooks into a series of notebooks
  - Keep a top-level index notebook with links to the individual notebooks

Working with Code



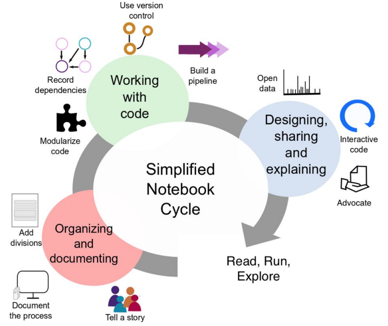
- Rule 4: Modularize Code
  - Use functions instead of duplicating code cells
- Rule 5: Record Dependencies
  - Manage your dependencies explicitly from the start using a tool such as
    - Conda’s environment.yml
    - pip’s requirements.txt
- Rule 6: Use Version Control
  - Consider using a public repository from the beginning of a project
  - Tie research results to specific software versions
- Rule 7: Build a Pipeline
  - Design notebooks with reuse in mind (different input data and parameters)
  - Define key input data and parameters at the top of each notebook
  - Break long notebooks into smaller notebooks that focus on one or a few analysis steps.

Sharing, explaining



- Rule 8: Share and Explain Your Data
  - Share your data in a repository with a persistent identifier, e.g., DOI or ARK
    - Bio repositories, e.g., NCBI, Ensemble, PDB
    - General repositories, e.g., Zenodo https://zenodo.org/
  - Small datasets can be stored in GitHub with our source code
    - E.g., in a /data folder
  - Very large datasets
    - Consider using a sample of the data and a link to the original data
  - Save intermediate data after data processing
    - E.g., in /intermediate_data folder
    - Can be used to verify each step in a workflow

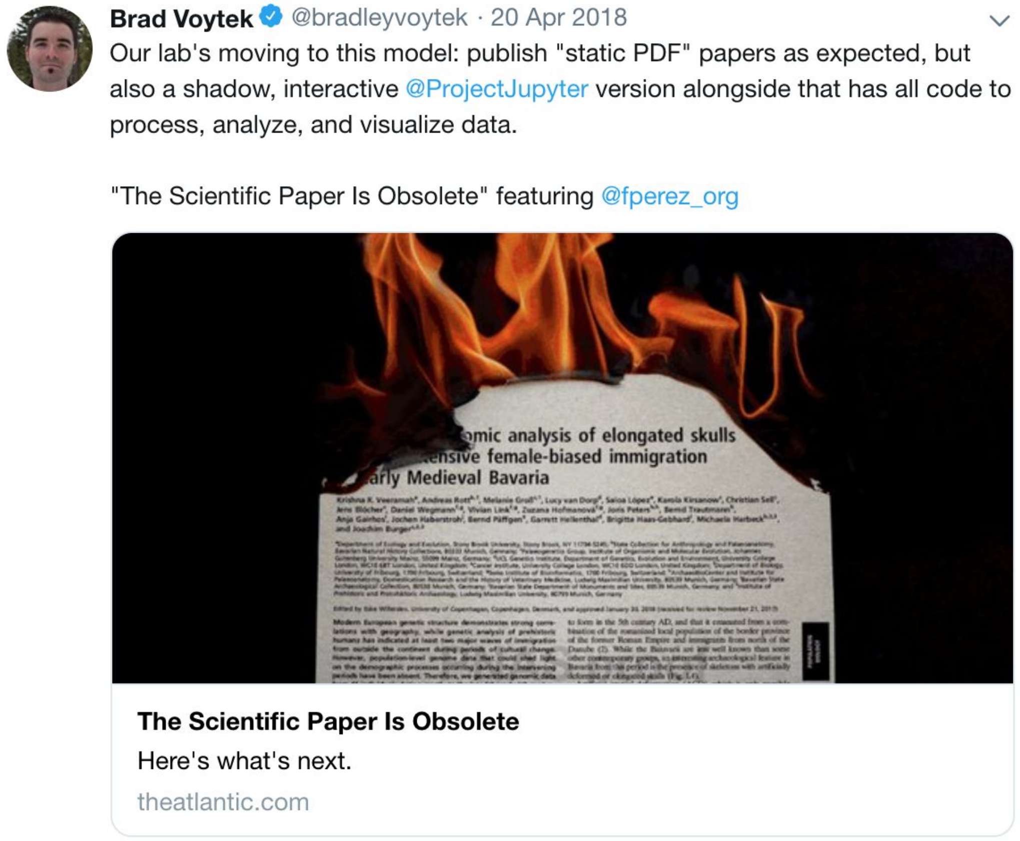
Sharing, explaining cont.



- Rule 9: Design your notebooks to be read, run, and explored
  - Git repository
    - Add a descriptive README file
    - Add a LICENCE file (liberal licence, e.g., MIT, Apache 2)
    - Add a static HTML/PDF file of your notebooks for long-term preservation
    - Add Binder badge/link to launch notebooks in the cloud (https://mybinder.org/)
  - Consider using ipywidgets to add menus or sliders to enable interactive exploration of parameters

Sharing, explaining cont.

- Rule 10: Advocate for open research
  - Apply what you learned in this tutorial in your own research and be an advocate for open and reproducible research in your lab or workplace
  - Publish a fully reproducible paper! Create all figures, data tables, and all other computational results using Jupyter Notebook and deposit in Github.


omic analysis of elongated skulls
ensive female-biased immigration
arly Medieval Bavaria

Brad Voytek @bradleyvoytek · 20 Apr 2018

Our lab's moving to this model: publish "static PDF" papers as expected, but also a shadow, interactive @ProjectJupyter version alongside that has all code to process, analyze, and visualize data.

"The Scientific Paper Is Obsolete" featuring @fperez_org

The Scientific Paper Is Obsolete

Here's what's next.

theatlantic.com

Demo of the Ten Simple Rules using Jupyter Notebook run on mybinder.org

https://github.com/jupyter-guide/ten-rules-jupyter