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Practical Tools for Improving Reproducibility (of Bioinformatics)

Johann Dreo

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Practical Tools for Improving Reproducibility (of Bioinformatics)

- Johann Dreo
- 25/11/2021

Abstract

Experimental studies are prevalent in (Bio)informatics, as in many fields involving computer science.

While reproducibility is crucial for science, it is difficult and often overlooked. This presentation introduces a curated list of tools that can help improving reproducibility for experimental computer science.

It may incidentally insist on testing...

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Experimental studies are prevalent in (Bio)informatics, as in many fields involving computer science.

While reproducibility is crucial for science, it is difficult and often overlooked.

This presentation introduces a curated list of tools that can help improving reproducibility for experimental computer science.

It may incidentally insist on testing...

Summary

01

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Why Reproducibility?

02

—

Tools that helps taking
practical actions

03

—

Conclusion

04

—

References



Part 1

Why Reproducibility?

A little bit of Epistemology

The *Reproducibility Crisis*

The scientific method:

- Falsifiability by *experimental* evidence.
- Experimental findings hold under *similar conditions*.
- Making for *predictable* outcomes.
- That can be used to build up *cumulative science*.

A little bit of Epistemology

The problem

Anecdotal evidences:

- More than 70% of researchers have failed in an attempt to reproduce an experiment [Baker 2016].
- Over 50% have even failed to reproduce *THEIR OWN* previous work.

A little bit of Epistemology

Some Terminology

Repeatability: same team, same experiment.

Reproducibility: different team, same experiment.

Replicability: different team, different experiment.

Generalisability: [López-Ibáñez *et al.* 2021]

Possible Actions

Cultural Actions

Researchers in permanent positions, please, think of:

- Incentivize negative results publishing (e.g. reproducibility failure).
- Do not oversell positive results.
- Fight bibliometry optimization.
- Better statistics (avoid p-hacking).
- Refrain from hypothesising after results (HARKing).
- Advertise TESTING.

Possible Actions

Technical Actions YOU can take

In a nutshell: *automate everything.*

- Keep track of Artifacts:
 - Version Control.
 - Lab Notebooks.
 - Archive Code and Data.
 - Save tests.
- Good Engineering:
 - Modular Code.
 - Test, tests, TESTS.
 - Automate Everything.
- Help your future self:
 - Containers.
 - Pipeline Automation.
 - Design of Experiment Automation.
 - Allow Reuse.
 - Publish Code and Data.
 - Automate tests.

Possible Actions

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Part 2

Tools that helps taking practical actions



About This Presentation

Assumptions:

- You know how to read and search documentation.
- Difficulty is to know that a tool exists.
- Everybody likes Python.

This presentation:

- Curated list of tools.
- Insists on TESTING.
- Alternatives and more info in the "see also" section.

Version Control

Git: <https://git-scm.com>

Allows to:

- Keep track of changes you make to your code.
- Go back in time, which helps debugging.
- Work with others on the same codebase.
- Works offline.

Basic idea:

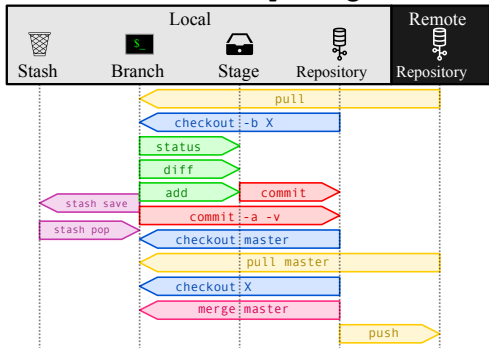
- All the source code is versioned (even tests).
- Note: you only version SOURCES, not generated files or data.
- You *commit* modifications to your code.
- You *merge* commits in the last version.

Version Control

Git: <https://git-scm.com>

See also:

- Shortest tutorial: <https://github.com/nojhan/gitcrux>



- Gitk: <https://www.atlassian.com/git/tutorials/gitk>
- Liquidprompt: <https://github.com/nojhan/liquidprompt>
- Mercurial: <https://www.mercurial-scm.org>

Version Control

Gitlab: <https://about.gitlab.com>

Online service:

- Online backups of Git repositories (see push & pull commands).
- Issue tracker (e.g. test failure report).
- Merge requests from others (e.g. more tests).
- Basic public page hosting.

See also:

- Tutorial:
https://docs.gitlab.com/ee/topics/plan_and_track.html
- Github: <https://github.com>
- DevOps (= automate tests): <https://en.wikipedia.org/wiki/DevOps>

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Notebooks

Jupyter: <https://jupyter.org/>

Interactive page:

- Sequence of paragraphs, executable code, figures.
- Keep track of your ongoing pipeline/experiment.
- Easy to share with others (as a single archive or an online page).
- Perfect for tutorials or demo (tests are good candidates).

See also:

- Online demo: <https://jupyter.org/try>
- Tutorial · s: <https://jupyter.readthedocs.io/en/latest/content-quickstart.html>
- Serve notebooks: <https://jupyter.org/hub>

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Modern Engineering

Tests

Golden rule of software engineering:

1. Modular code (= functions).
2. Tests = first lines of defense:
 - 2.1 Asserts on pre and post-conditions.
 - 2.2 Asserts everywhere in the code.
 - 2.3 Unit tests (= stand-alone test of functions, on simple data).
 - 2.4 Integration tests (= with real data).
3. When you finish a feature: RUN TESTS.

Modern Engineering

Test!

```
def f(arg):
    assert(0 < len(arg) <= 100) # Pre-condition.
    assert(all(0 < i <= 10 for i in arg))
    inter = [float(i) for i in arg]
    assert(len(inter) == len(arg)) # Intermediate.
    result = sum(inter)
    assert(0 < result <= len(arg)*10) # Post-condition.
    return result

if __name__ == '__main__':
    assert( f(range(10)) == 45 ) # Basic unit test.
    if __debug__: # Those are declutchable when running python -O
        failed = False
        try:
            res = f([0]*10)
        except AssertionError:
            failed = True
    assert(failed)
```

Modern Engineering

TEST!

Tests helps:

- Avoiding bugs.
- Finding bugs.
- Fixing bugs.
- On the long term.
- Actually coding faster.
- Double-checking intermediate data of your pipeline.

See also:

- R's "stopifnot()" or packages named "assert".
- Python's unittest:
<https://docs.python.org/3/library/unittest.html>
- PyTest Framework: <https://pypi.org/project/pytest>

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Modern Engineering

Continuous Integration

Automate rule #3:

- Every time you push on Gitlab, tests are ran automatically.
- And someone (you) get blamed for pushing bugs.

See also:

- Documentation: <https://docs.gitlab.com/ee/ci/>

Modern Engineering

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Virtualization

Objectives:

- Ease the not-built-here affliction.
- Get rid of the dependencies nightmare.
- Avoid the backward incompatibility plague.

Historically:

- Virtual Machines,
- Package Managers & Virtual Environments,
- Containers.

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Virtualization

VirtualBox: <https://www.virtualbox.org>

Virtual Machine:

- Replace the computer with software.
- Run any OS on any other OS.
- (A bit) slower.
- Takes a lot of space (all the OS is installed).

See also:

- VMware: <https://www.vmware.com/>

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Virtualization

Conda: <https://conda.io>

Package manager + virtual environments:

- Install (several) softwares with (several) specific versions.
- Environment = dependencies that just works.
- Run several environments on your machine.
- Distribute environments configurations.
- Historically for Python, but works for R (and other languages).

See also:

- Bioconda: <https://bioconda.github.io>
- Miniconda: <https://docs.conda.io/en/latest/miniconda.html>

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Virtualization

Singularity: <https://sylabs.io/singularity/>

Containers:

- Virtual OS.
- Run any software on any OS.
- Faster than VM, take less space.
- More stable than virtual environments.
- Install a container on your computer, run it on a cluster.
- (Do not forget to run tests)

See also:

- Docker: <https://www.docker.com>
- Docker hub: <https://hub.docker.com>
- docker2singularity:
<https://github.com/singularityhub/docker2singularity>

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Pipeline Management

SnakeMake <https://snakemake.readthedocs.io>

Pipeline Automation:

- Like a (Python) script calling every steps of your pipeline.
- States which step's input depends on which step's output.
- Automates:
 - parallelization,
 - job submission (e.g. on a cluster),
 - Intermediate step tests.
- Works well with Conda and Singularity.

See also:

- Nextflow: <https://www.nextflow.io>

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Design of Experiment Management

openMOLE: <https://openmole.org>

DoE:

- Explore the parameters space of your model.
- Automates:
 - sampling (understand the response function),
 - calibration (optimize parameters to match reality),
 - sensitivity analysis,
 - job submission.

See also:

- modeFrontier: <https://engineering.esteco.com/modefrontier>
- ModelCenter:
<https://www.phoenix-int.com/product/modelcenter-integrate/>

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Metadata

CookieCutter: <https://cookiecutter.readthedocs.io>

Projects Templates:

- Create project directories and base files.
- Allows to follow best practices.
- Avoids forgetting important features.
- Example: cookiecutter

`gh:snakemake-workflows/cookiecutter-snakemake-workflow`

See also:

- Search for templates:

`https://github.com/search?q=cookiecutter&type=Repositories`

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License · s

Authors Rights Belongs to:

- Writings = you.
- Diagrams = you.
- Code = your employer(s).
- (But information disclosure authorizations may be limited)

License = what Authors Rights are given to Users, covers:

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- Modification of the work,
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Free (Software) Licenses

Guarantee Freedom of:

- Use (run) the work,
- Study the source code,
- Redistribute the work,
- Improve the work.

These freedoms are necessary to reproducibility, even more for replicability.

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Suggested Licenses

For source code:

- Affero GPL v3: <https://www.gnu.org/licenses/agpl-3.0.en.html>
- LGPL v3: <https://www.gnu.org/licenses/lgpl-3.0.html>
- Apache license: <https://www.apache.org/licenses/LICENSE-2.0>

For generic work:

- Creative Commons Attribution Share-Alike (CC-BY-SA):
<https://creativecommons.org/licenses/by-sa/4.0/>

See also:

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Publication

Open-Access

Reproducibility needs open-access.

Preprints repositories:

- arXiv: <https://arxiv.org>
- bioRxiv: <https://www.biorxiv.org>
- HAL: <https://hal.archives-ouvertes.fr>

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Publication

Zenodo: <https://zenodo.org>

Long term archiving of code and data associated with a publication:

- Archive Code (with tests),
- Link to a Git tag on Github,
- Archive Data,
- Link to/from publications (via DOI or preprint ID),
- Get a DOI (easier to cite),
- Allows versions.

See also:

- Software Heritage: <https://www.softwareheritage.org>

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Part 3

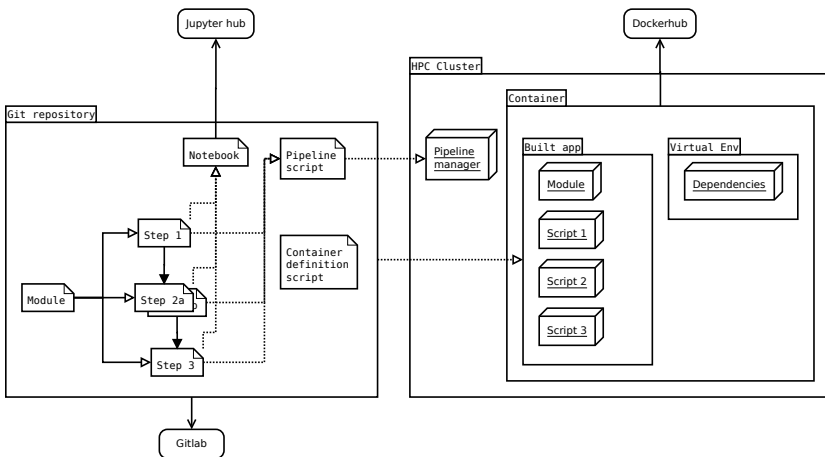
Conclusion

Minimal Workflow

- You start with a notebook, coding a simple proof of concept,
- Once it works, you modularize out some functions,
- You code a module, in a local Git repository.
- You add asserts as you type.
- When a function works, you write the related test.
- The notebook becomes a tutorial on a how to use your code.
- When a feature works, you test it in a container.
- The container installs dependencies *via* Conda.
- To run experiments, you write a pipeline script, calling the container.
- You push your repository on Gitlab.
- You archive the code & data on Zenodo.
- You write the publication, citing the archives.
- You put the publication on a preprint archive.

Summary

App management



Summary

Essential tools

- Git — <https://git-scm.com>
- Gitlab — <https://about.gitlab.com>
- Jupyter — <https://jupyter.org>
- Conda — <https://conda.io>
- Singularity — <https://syslabs.io/singularity>
- SnakeMake — <https://snakemake.readthedocs.io>
- openMOLE — <https://openmole.org>
- CookieCutter — <https://cookiecutter.readthedocs.io>
- AGPLv3 — <https://www.gnu.org/licenses/agpl-3.0.en.html>
- bioRxiv — <https://www.biorxiv.org>
- Zenodo — <https://zenodo.org>

Happy reproducing.

Read more about reproducible pipelines: [Wratten *et al.* 2021]

—




Do not hesitate to test your code & to ask questions:

`johann.dreo@pasteur.fr`

Part 4

References



-
-  Baker, M., Is there a reproducibility crisis? *Nature* 533, 2016, 452–454.
 -  Wratten, L., Wilm, A. & Göke, J., Reproducible, scalable, and shareable analysis pipelines with bioinformatics workflow managers. *Nat Methods* 18, 2021, 1161–1168.
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