This lecture will be recorded





Review of last assignments

Create your own function that in some way modifies the output of COMPAS_SLICER. You can choose any model as a base for the modifications, also your own design.





Advancing computational research

Reproducibility & Upstreaming

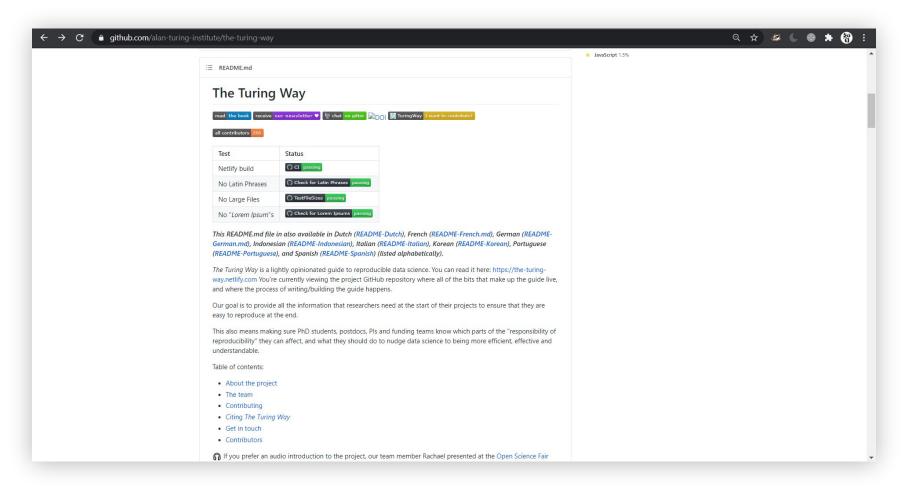


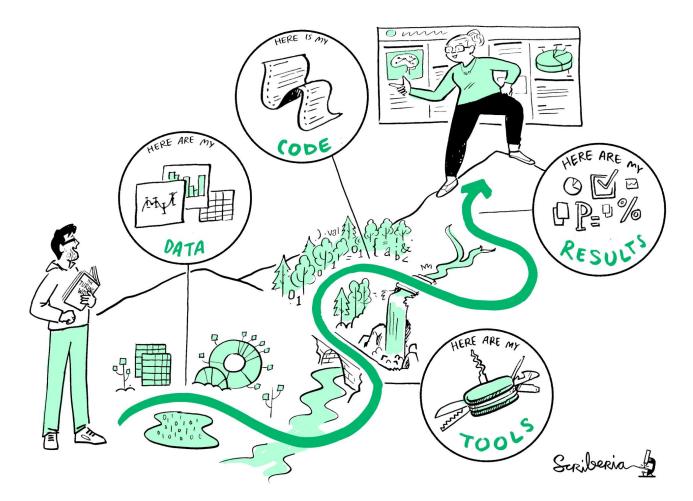
A definition of reproducible research

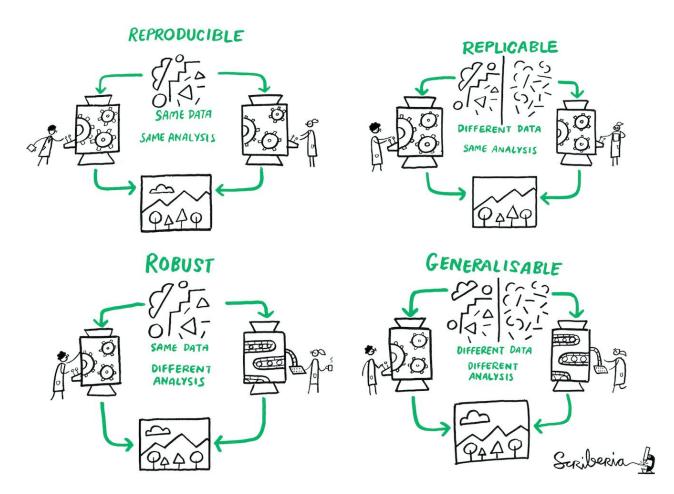
Work that can be **independently recreated** from the **same data** and the **same code** that the original team used.

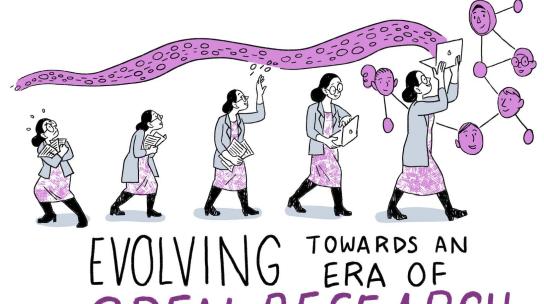
The Turing Way, https://github.com/alan-turing-institute/the-turing-way











OPEN RESEARCH





Elements of open research

Open Data

Documenting and sharing research data openly for re-use.

Open Source Software

Documenting research code and routines, and making them freely accessible and available.



Open Notebooks

An emerging practice, documenting and sharing the experimental process of trial and error.

Open Access

Making all published outputs freely accessible for maximum use and impact.

Open Hardware

Documenting designs, materials, and other relevant information related to hardware, and making them freely accessible and available.



Open Data

- Ensure your data is in a simple, **standard format** or formats which is machine and human-readable.
- Check, reformat or create **metadata to clearly describe what the data is**, how it was collected, and any associated strengths/weaknesses to someone that finds it.
- Identify a relevant, easily discoverable repository or repositories to host your data, and upload it there.
- Assign your data a persistent identifier such as a DOI.



Open Source Software

- Put your code in a freely accessible repository.
- Include a license granting others the right to use, copy and modify your work.
- Include a **README** file containing useful information about a project such as what it is, how
 to use/install it and how to run any tests.
- If you want others to collaborate on the project include contribution guidelines.



Open Hardware

- Make detailed documentation and designs for any hardware you develop openly available.
- Include a **license** granting others the right to use, copy and modify your work.
- Include a **README** file containing useful information about a project (for example, what it is and the materials used).



Open Access

- Publish your research in an **open-access journal**.
- Store a copy or **preprint** of your work in a freely accessible public repository.



Open Notebook

- Keep notes in an **Electronic Lab Notebook**.
- Make your notebooks publicly accessible online.



Licenses



Spectrum of OSS licenses





choosealicense.com

Data







Software



Code management





Reproducible environments

- Tools for reproducible environments:
 - Package managers (conda/pip)
 - Containers (Docker)
- Use and rely on semantic versioning: <u>semver.org</u>
 - MAJOR.MINOR.PATCH
 - o e.g. 1.5.0
- Describe your dependencies meticulously







Code quality

- Always optimize for readability
- Follow naming & style conventions (PEP8)
- Naming is hard, take your time
- Encapsulate complexity: solve it just once
- Don't reinvent the wheel, reuse encapsulated code
- Less code is always more
- Leverage tools to assist your coding (linters, formaters, static analyzers, etc)



Code testing

- There are lots of test types
 - Unit tests
 - Integration tests
 - Performance tests
- But at least, write unit tests. Please, pretty please!
- Test algorithms, not UI
- If you fix a bug, write a test to verify and make sure you don't break it again.
- Run them automatically



Continuous Integration

- Automate all the thingz!
 - Testing
 - o Building/compiling
 - Publishing
 - Style / consistency checks
 - Anything repetitive!
- Makes sure you discover regressions when they occur

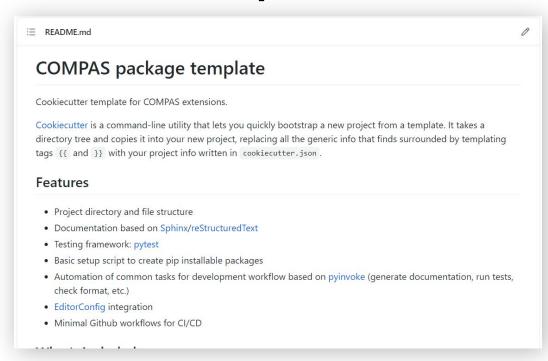




How do I do all that?



COMPAS Templates

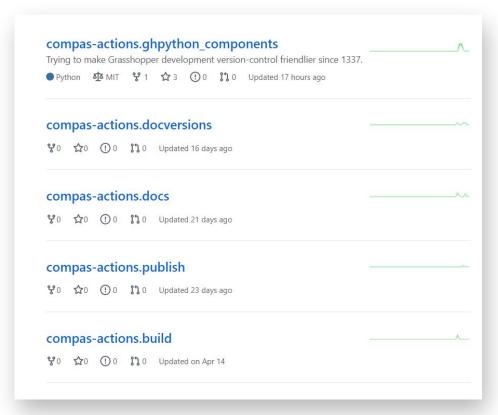




New extension/package: https://github.com/compas-dev/tpl-extension



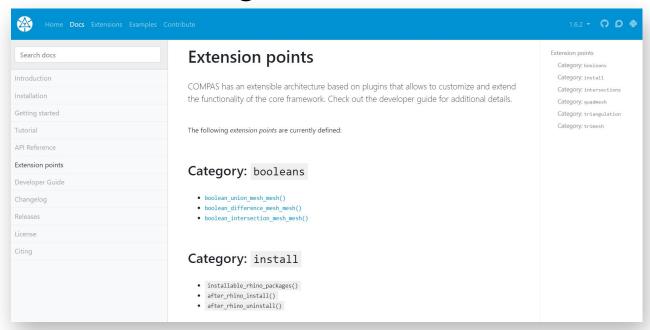
COMPAS Actions







COMPAS Plugins



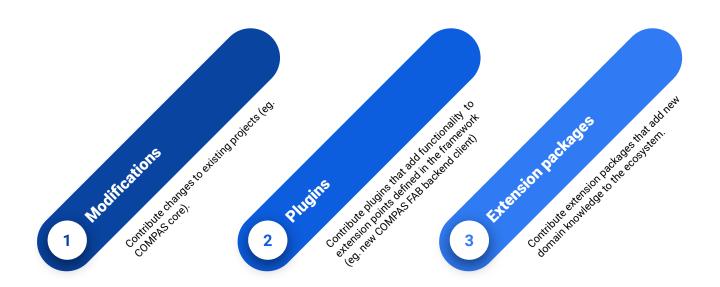


Upstreaming research

...is the process of **contributing** private research source code **back to the open source sphere**.

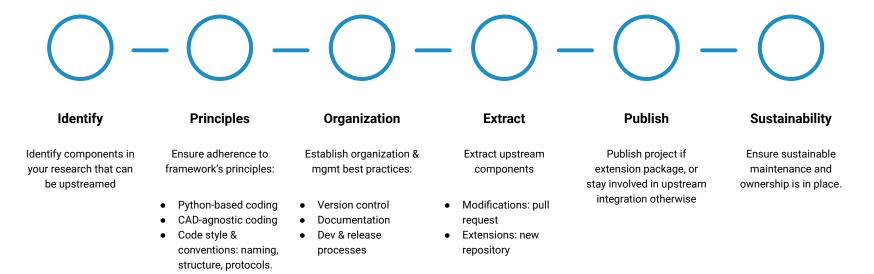


Upstream contribution types





Upstream process





More resources

The Turing Way

https://the-turing-way.netlify.app

Awesome Reproducible Research (and other awesome-* lists)

https://github.com/leipzig/awesome-reproducible-research

COMPAS Exchange (Tomorrow, 10-12am, registration required):

https://ethz.zoom.us/meeting/register/u5Eocu2oqjkqGdVZ0m7FzQdX_FaZIKLjvHaC



Next week



Thanks!

