Research compendia as R packages

Scientific workflows: Tools and Tips :hammer_and_wrench:

2023-07-20

What is this lecture series?

Scientific workflows: Tools and Tips 🎇





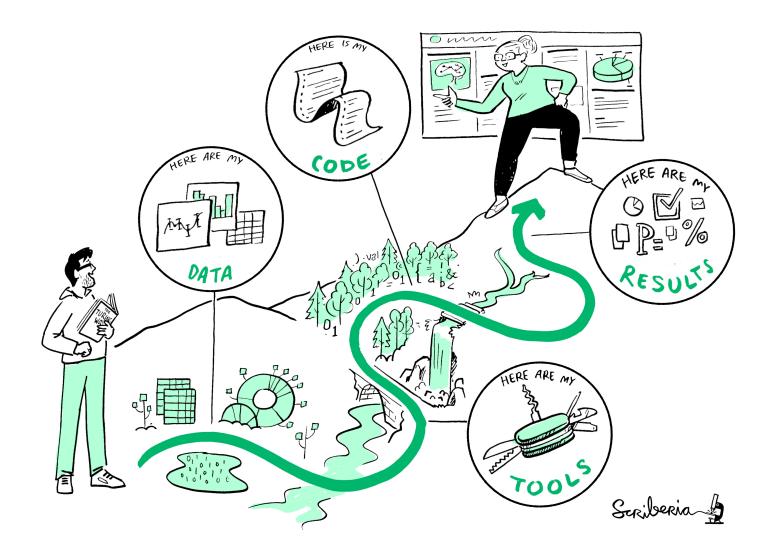
Every 3rd Thursday 🕓 4-5 p.m. 🕯 Webex





- One topic from the world of scientific workflows
- For topic suggestions send me an email
- If you don't want to miss a lecture
 - Check out the lecture website
 - Subscribe to the mailing list
- Slides provided on Github

Steps of a scientific project



Steps of a scientific project

How to properly structure the project?

I want

- Reproduciblity (for you and others)
- Property Reliablity (will it work again?)
- Re-usablity (don't re-invent the wheel)
- Visiblity (let others see and use your work)



How? Use a research compendium!



This image was created by Scriberia for The Turing Way community and is used under a CC-BY licence (DOI 10.5281/zenodo.3332807).

What is a research compendium?

 Collection of all digital parts of a research project (data + code + text)

The goal of a research compendium is to provide a **standard and easily recognizable** way for organizing the digital materials of a project to enable others to **inspect**, **reproduce**, **and extend** the research.

From Marwick et al. 2018

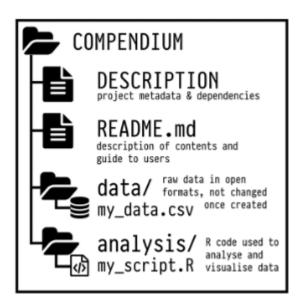


Principles for building research compendia

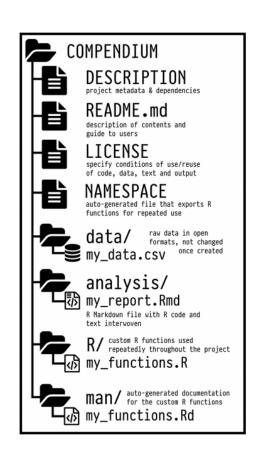
- Stick with the conventions in your field
- Keep data, methods and output separate
- Specify the computational environment
- Key components for sharing the compendium include
 - Licence
 - Version control
 - Metadata
 - Persistent identifier (e.g DOI)

Examples of different complexities

Small compendium



Medium size compendium



They are R packages!

R packages as research compendia



NOT PEER-REVIEWED

Packaging data analytical work reproducibly using R (and friends)

Ben Marwick
University of Washington, University of Wollongong
and
Carl Boettiger
University of California, Berkeley
and
Lincoln Mullen
George Mason University

March 20, 2018

Basic idea: Hijack the R package development ecosystem to build a research compendium

Different use cases, e.g.

- Publish code, data and analysis scripts alongside your paper
- Publish a dataset in a way that other people can work with it in R



Some benefits of R packages

- Benefit from quality control mechanisms built around R packages
- Additional packages around this ecosystem to make your life easier
- Easy documentation
- Easy sharing of data

Hands-on: Create a research compendium with the R package structure

Find a detailed step-by-step guide on the website

Summary and Conclusions

It's convenient to have standards you can follow

- R packages provide an helpful development ecosystem that we can hijack for our research compendia
- You can develop your compendium in different ways
 - A package that is meant to be installed with install.packages()
 - A compendium that won't be installed but uses quality checks from package ecosystem
- usethis is a great workflow package (not only for package development)

Outlook

- Include large datasets with piggyback
- Automated tests with Github actions
- Unit tests to test your functions using testthat
- Easily connect Github repo to Zenodo to get a DOI
- holepunch package to build a Docker image

The nice thing:

- Also this easy to set up with usethis and friends
- They are also documented on the lecture series website

Next lecture

Summer/Conference break in August and September!

Time for some feedback from you!

Please fill out the questionnaire if you have time (5 mins)

Topic of next lecture t.b.a.

- 19th October (3) 4-5 p.m. P Webex
- Subscribe to the mailing list
- For topic suggestions and/or feedback send me an email

Thank you for your attention:)

Questions?

References

- Marwick, Ben, Carl Boettiger, and Lincoln Mullen. 2018. "Packaging Data Analytical Work Reproducibly Using R (and Friends)." American Statistician 72 (1): 80–88.
 - https://doi.org/10.1080/00031305.2017.1375986.
- The Turing Way website is a very useful guide to reproducible data science
- Slides and list of resources for research compendia by Karthik