

Research compendia as R packages

Scientific workflows: Tools and Tips 

2023-07-20

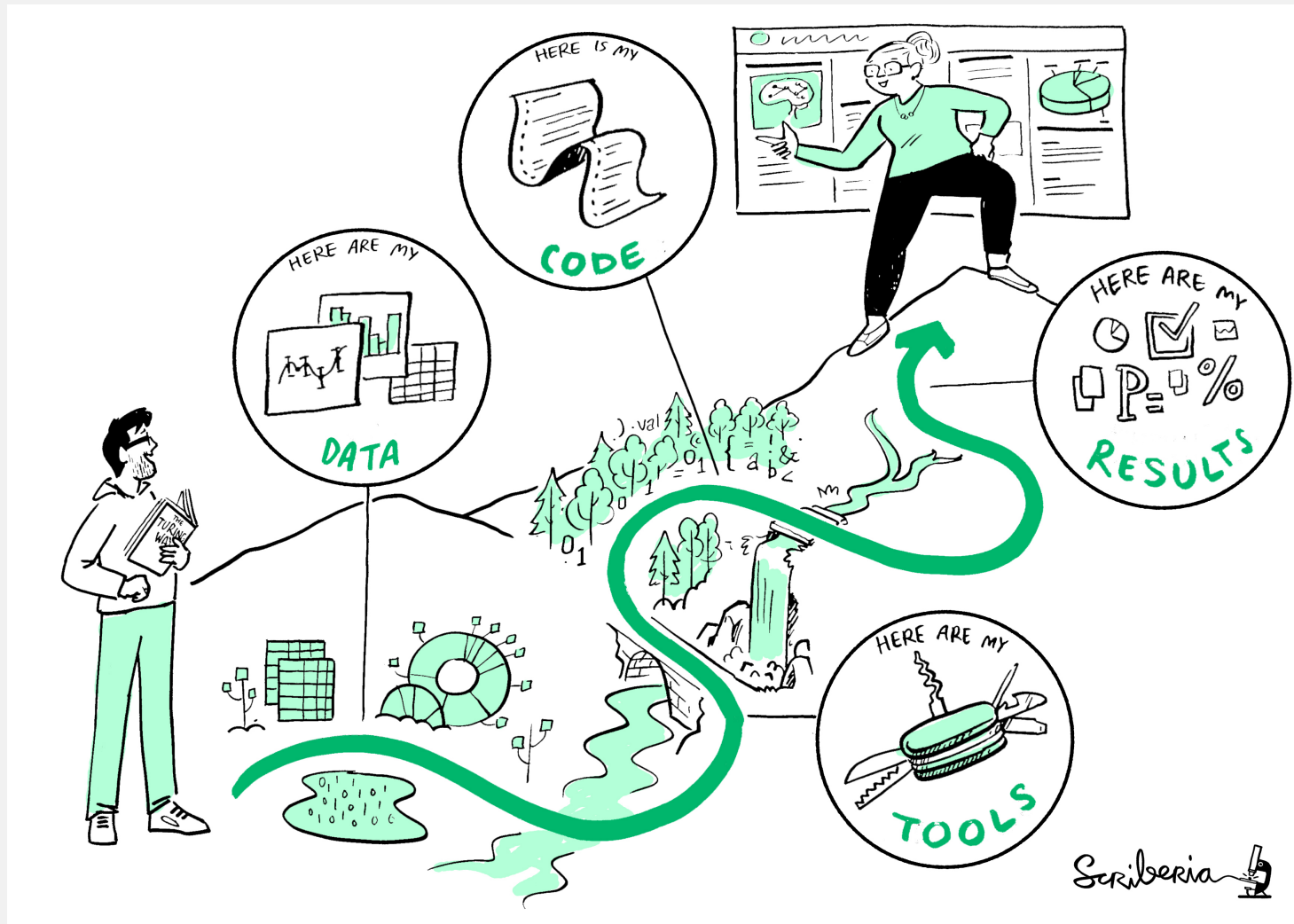
What is this lecture series?

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







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Selina Baldauf // Research compendia as R 

Steps of a scientific project

How to properly structure the project?

I want

-  Reproducibility (for you and others)
-  Reliability (will it work again?)
-  Re-usability (don't re-invent the wheel)
-  Visibility (let others see and use your work)

How? Use a research compendium!



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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.

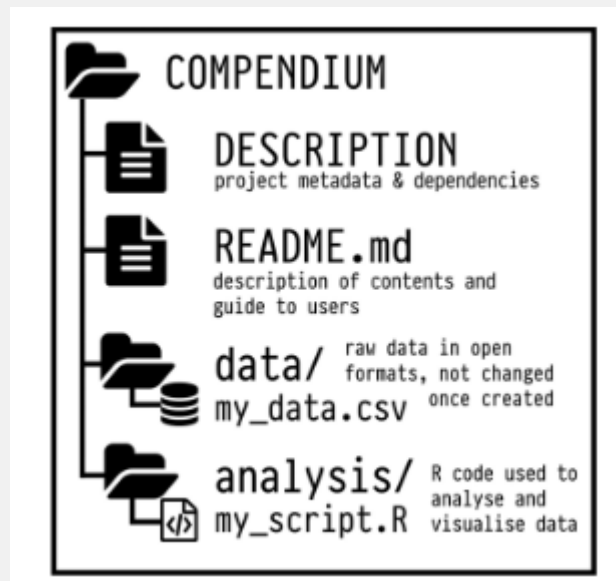
From [Marwick et al. 2018](#)

Principles for building research compendia

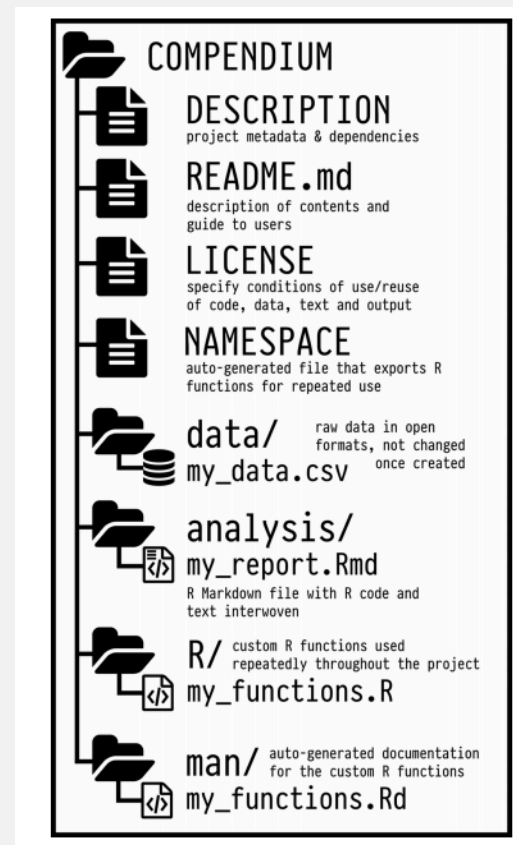
- Stick with the conventions in your field
- Keep **data**, **methods** and **output** separate
- Specify the computational environment
- Key components for sharing the compendium include
 - Licence
 - Version control
 - Metadata
 - Persistent identifier (e.g DOI)

Examples of different complexities

Small compendium

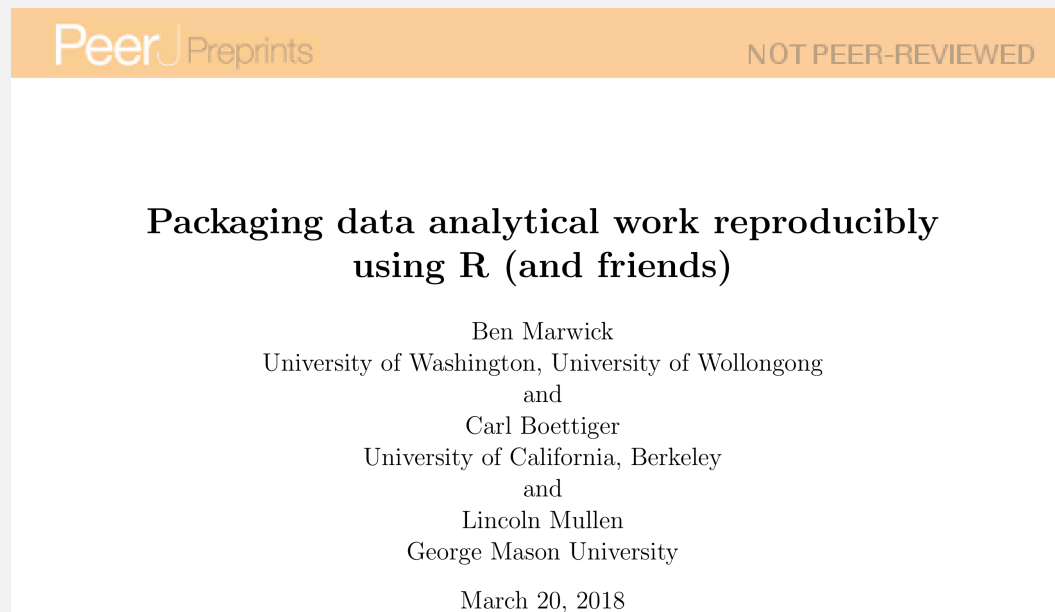


Medium size compendium



They are R packages!

R packages as research compendia



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  4-5 p.m.  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](#)