Creating targets-based scientific workflows

Reproducible Scientific Workflows in R - Part 2

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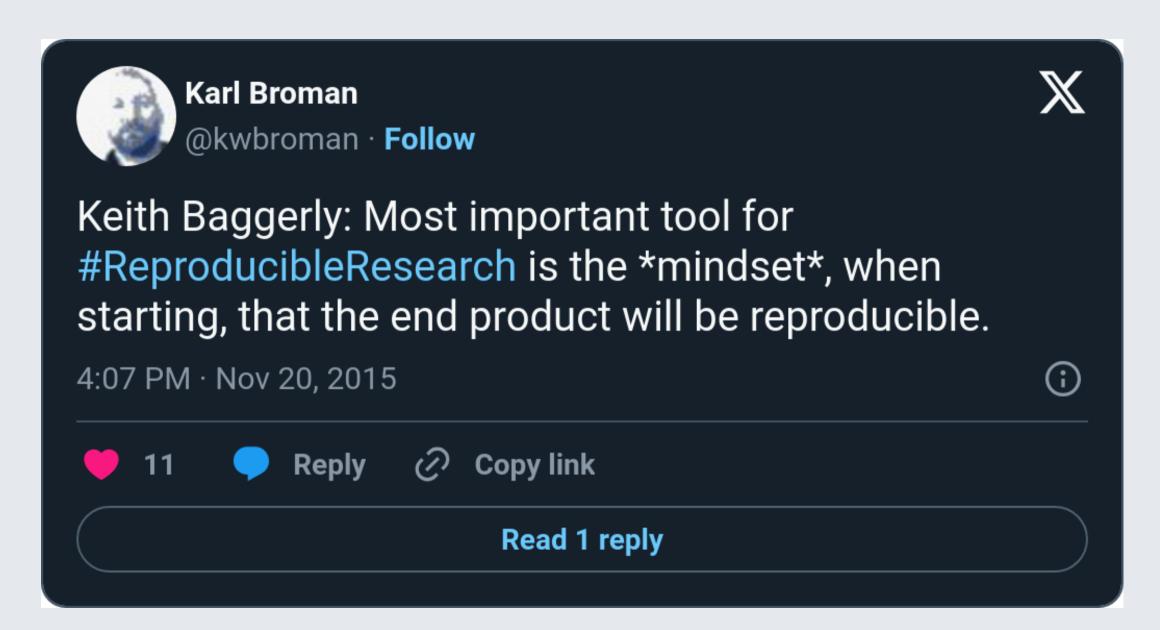
2024-02-12

Outline

- Concepts on scientific workflows
- The {targets} package
- Practical session

Concepts on scientific workflows

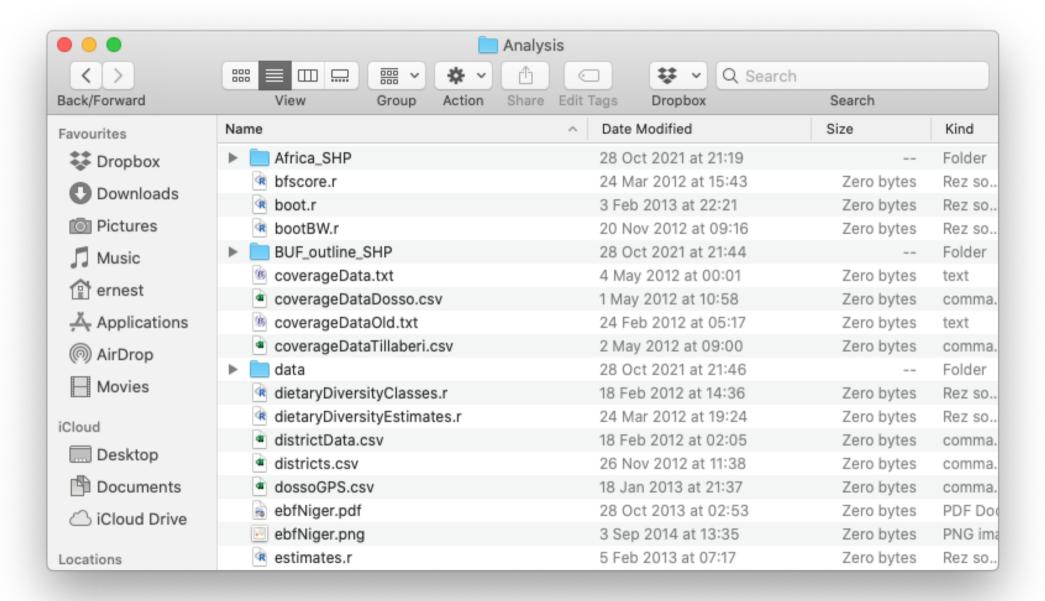
Concept #1: Reproducibility, reproducibility, reproducibility!



Concept #2: Organisation

File organization and naming are powerful weapons against chaos.

@JennyBryan



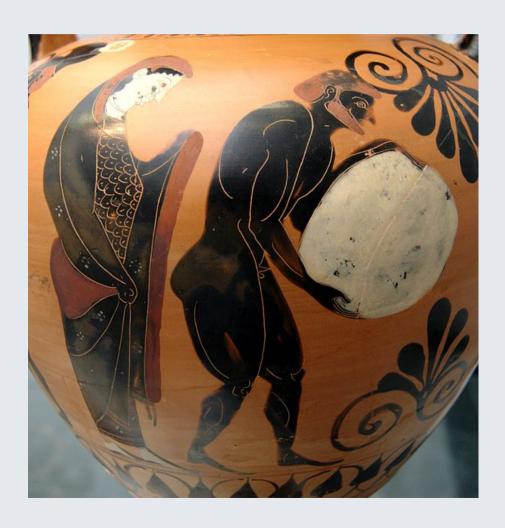
Concept #3: DRY - Don't repeat yourself

Don't repeat yourself. It's not only repetitive, it's redundant, and people have heard it before.

Lemony Snicket

```
# Overlay maps of Niger and Nigeria to clean-up the map
par(new=TRUE)
plot(nigeria, axes = FALSE, xlim = mapXLimits, vlim = mapYLimits, border = "white", col = "white")
par(new = TRUE)
plot(boundaries, axes = FALSE, xlim = mapXLimits, ylim=mapYLimits, lwd = 0.5, border = "black")
par(new = TRUE)
plot(n1, axes = FALSE, xlim = mapXLimits, vlim=mapYLimits, lwd = 0.25, col = "blue")
par(new = TRUE)
plot(n4, axes = FALSE, xlim = mapXLimits, ylim=mapYLimits, lwd = 0.25, col = "blue")
par(new = TRUE)
plot(n5, axes = FALSE, xlim = mapXLimits, ylim=mapYLimits, lwd = 0.25, col = "blue")
par(new = TRUE)
plot(n6, axes = FALSE, xlim = mapXLimits, ylim=mapYLimits, lwd = 0.25, col = "blue")
par(new = TRUE)
plot(n6.27, axes = FALSE, xlim = mapXLimits, ylim=mapYLimits, lwd = 0.25, col = "blue")
par(new = TRUE)
plot(n7, axes = FALSE, xlim = mapXLimits, ylim=mapYLimits, lwd = 0.25, col = "blue")
par(new = TRUE)
plot(n14, axes = FALSE, xlim = mapXLimits, ylim=mapYLimits, lwd = 0.25, col = "blue")
```

Sisyphean loop



- 1. Launch the code.
- 2. Wait while it runs.
- 3. Discover an issue.
- 4. Restart from scratch.

Concept #3: Frequency reduces difficulty



Jenny Bryan · Follow

X

If it hurts, do it more often. – @martinfowler

We shared this idea in a recent workshop and it resonated with many.

Applies to all sorts of things: git tasks (pushing & pulling), keeping your s/w stack current, sharing your work with others, etc.

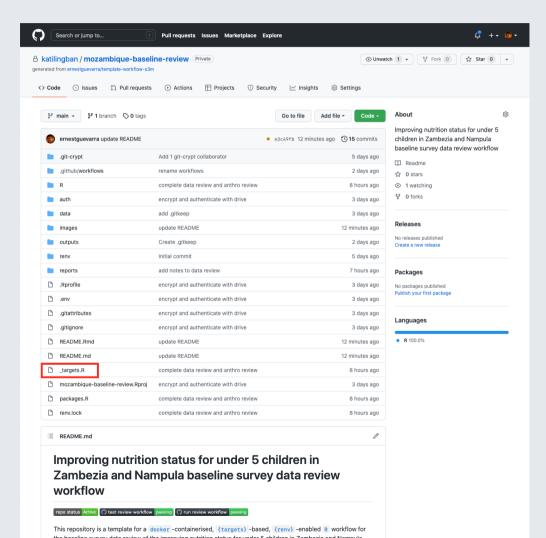
martinfowler.com/bliki/Frequenc...

The {targets} package



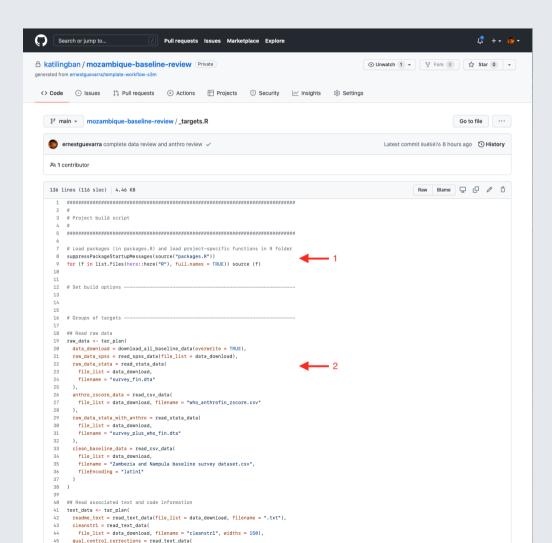
- a pipeline toolkit for Statistics and data science in R
- maintain a reproducible workflow without repeating yourself
- learns how your workflow fits together
- skips costly runtime for tasks that are already up-to-date
- runs only the necessary computation
- supports implicit parallel computing
- abstracts files as R objects
- shows tangible evidence that the results match the underlying code and data

{targets} file organisation



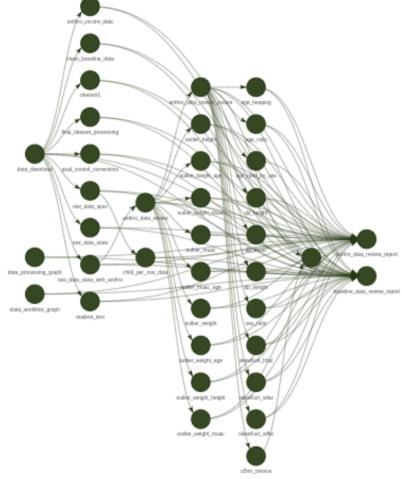
- this is a typical file structure with user-defined components of any project-oriented workflow
- the _targets.R file, however, is special and specific to a {targets} workflow - it is the target script file
- the target script file should be in the project's root directory

{targets} script file



- Load the packages required (1)
- Load custom functions (1)
- Define individual targets intermediate step of the workflow (2)
- End with a list of targets objects

{targets} workflow





Up to date



Stem

Questions?

Practical session

We will all continue to go through Exercise #1 in the Practical R for Epidemiologists book

Questions?

Thank you!

Slides can be viewed at https://oxford-ihtm.io/open-reproducible-science/session9.html

PDF version of slides can be downloaded at https://oxford-ihtm.io/open-reproducible-science/pdf/session9reproducible-scientific-workflows.pdf

R scripts for slides available here