

Intro to Reproducibility & Research Data Management

Hermina Ghenu 15 Oct 2024



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- What is reproducibility?



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- Why do I have to annotate my code?
- Why do I have to hand in my code?
- Why shoud I document my file structure?

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Plan for the afternoon: lecture interspersed with activities

Reserach practices:

Reproducibility vs Repeatability vs Generalizability

Reproducibility: Can other scientists (or future you) re-analyze your data & get the exact same result?

Repeatability: Can other scientists replicate your same experiment & achieve a consistent result?

Generalizability: Do other studies exploring the same research question come to the same conclusions?

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Reserach practices:

Reproducibility vs Repeatability vs Generalizability

Reproducibility: Can other scientists (or future you) re-analyze your data & get the exact same result?

- first line of defense in creating repeatable research
- focused on computational or data analysis 🙇

Repeatability: Can other scientists replicate your same experiment & achieve a consistent result?

from initial set-up to final results

Generalizability: Do other studies exploring the same research question come to the same conclusions?

• the \(\frac{1}{2}\) ideal \(\frac{1}{2}\) we strive for in our science

• Why do you think we need reproducibility?

Why we need reproducibility

A reproducible research article is a trusted scientific contribution.

- >85% of ecology & evolution publications are **not** reproducible (e.g., no code).
- Papers that make data & code available are more highly cited.

(Kambouris et al., 2024; Maitner et al., 2024)

Nature is sometimes more complex than we imagined.

 e.g., mouse behavioural responses depend on how they are housed & handled (Nigri et al., 2022)

Mistakes in research can have social / economic impacts.

• e.g., impoverished environment of mice during preclinical studies may explain why most new drug candidates don't work as expected in clinical trials.

(Shemesh & Chen 2023)

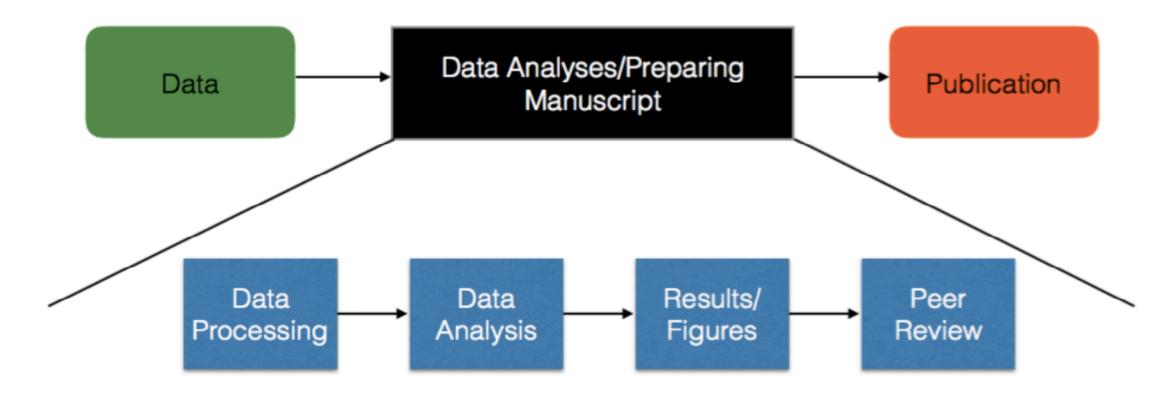
Bad faith actors can diminish our trust in science.

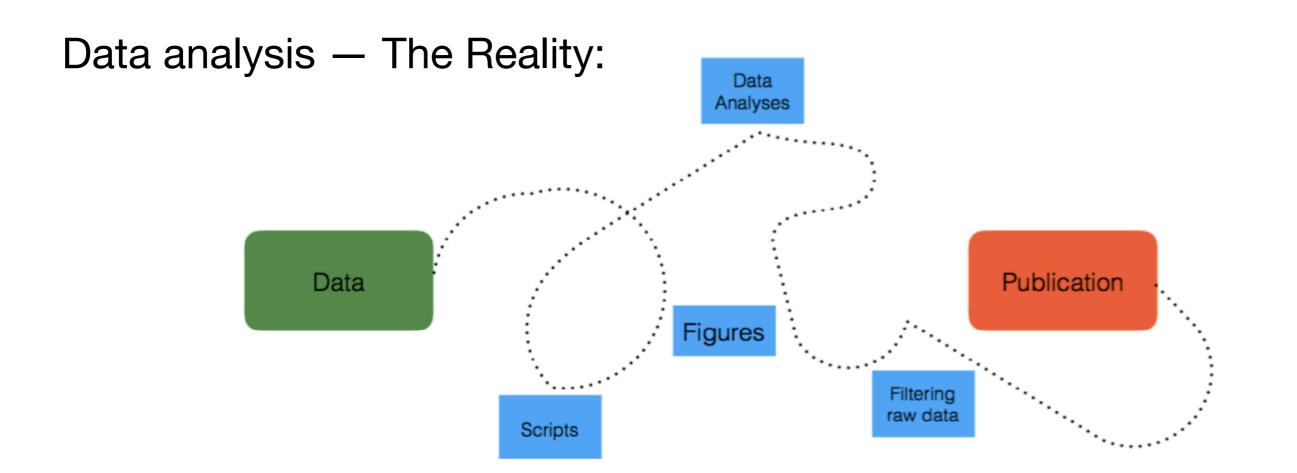
(Kozlov 2022; data forensics details)

Consistent methods for globally coordinated research efforts.

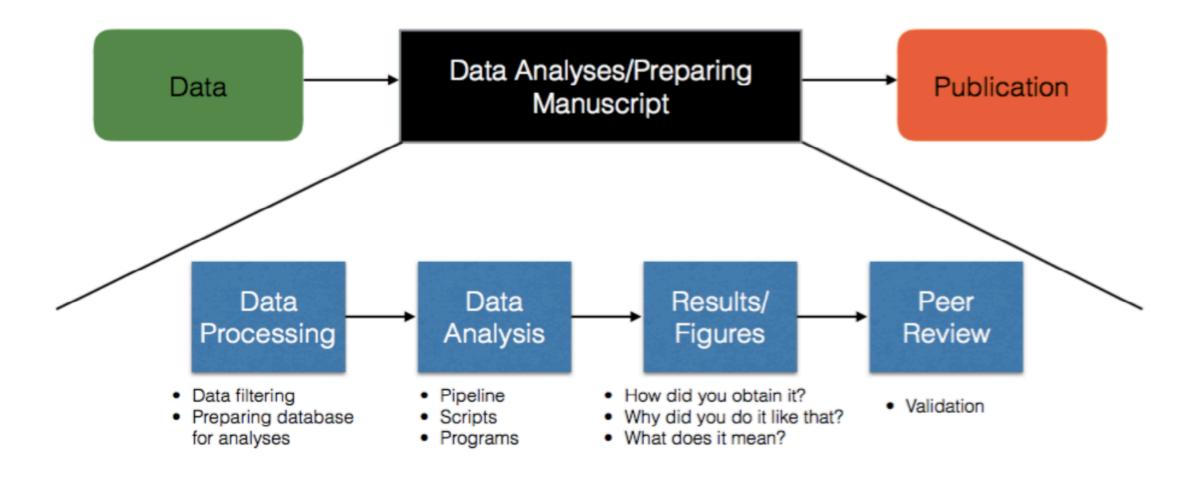
e.g., in combating disease (Park et al., 2021) or climate change (Halbritter et al., 2019)

Data analysis — The Dream:





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A Data Management Plan & Reproducibility Principles help us get closer to this dream

Doing reproducible research

 Goal: able to re-create <u>data and analysis</u> so that you and others can (ideally) arrive at the <u>same</u> interpretations of your results

Doing reproducible research

- Goal: able to re-create <u>data and analysis</u> so that you and others can (ideally) arrive at the <u>same</u> interpretations of your results
- Keep everything!





NOBODY WANTS TO DEAL WITH THIS!!!!!



Doing reproducible research

- Goal: able to re-create <u>data and analysis</u> so that you (ideally) arrive at the <u>same interpretation</u>/ conclusion from your results
- Keep everything!

Doing reproducible research

- Goal: able to re-create <u>data and analysis</u> so that you (ideally) arrive at the <u>same interpretation</u>/ conclusion from your results
- Keep everything!
- Keep everything in such a way that you, or people after you, can (happily?) go back to it

How do you achieve reproducibility in research?

Annotate

explain what you're doing and why

Automate

make your decisions explicit by using code

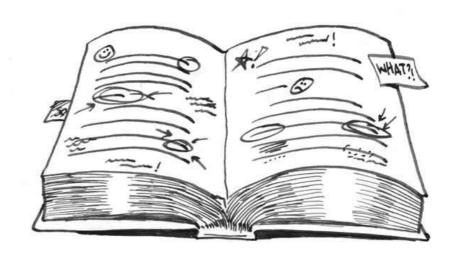
Share

provide access to your work

Hoard

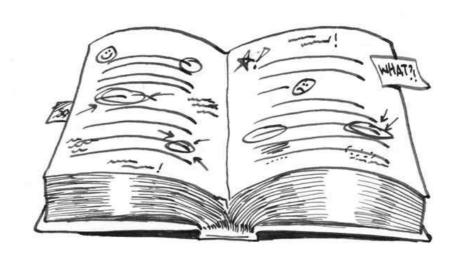
keep (almost) everything

Annotate



Write explanations for your future collaborators
 What? How? Why?!

Annotate



- Write explanations for your future collaborators
 What? How? Why?!
- Habits: use script headers, use meaningful & human-readable names, comment your code
- Tools: notebook documents

Open RStudio and create a new R Notebook document.
 Save then knit the document to pdf. What does this do?

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 - How do you do that?
 - Type "# Annotate!" both inside and outside of the R code block. How are these displayed differently after you knit?

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- Switch the markdown editing mode from Source to Visual.
 What does this do? What objects can you add to the text?

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 What does this do?
- Modify the header to add new fields for "author:" and "date:".
 What other authorship attribution information may be useful?

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Hoard



Keep almost everything

Hoard



- Keep almost everything
- Habits: backup regularly (daily!), exact version of software, store raw data & intermediate steps in data processing, store code & progress on code
- Tools: backup software (e.g. Time Machine), version control (e.g. git), online repositories (e.g. GitHub)

Copy the following code into the code block in your Rnotebook file:

```
# a silly function to multiply the values from 1 to 10
get.multiples1to10 <- function(multiplier){
    numbers <- 1:10
    output <- multiplier*numbers
    return(output)
}

# set the parameter value
current_multiplier <- 3

# run the function
results <- get.multiples1to10(current_multiplier)</pre>
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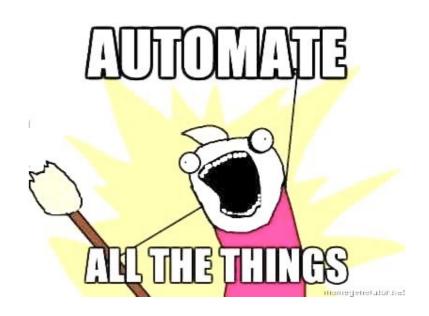
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write.csv(results, filename, row.names = FALSE)
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Are there any annotate habits that we are using here?
 (annotate habits: variable names, annotate code, script headers)

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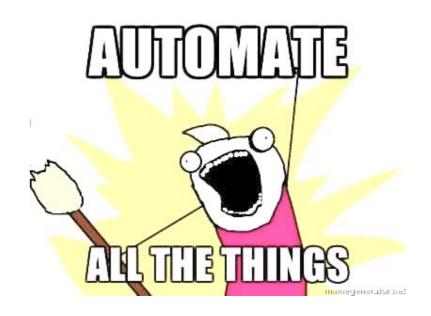
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Automate



- Avoid manual manipulation
 - waste of time, error-prone, decisions are <u>not</u> explicit and can be inconsistent
- Habits: find+replace, use a scripting language for your analyses, automatically save parameters in the filename.
- Tools: notebook documents

Are there any automate habits that we used in this code?
 (automate habits: find+replace, scripting language, filename)

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 Use find+replace to change the name of the function from get_multiples1to10 to a new name that makes sense to you.

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Share



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- Fundamentally, research is about sharing with collaborators, with other scientists
- Habits: think about your <u>audience</u> when analysing (see annotate), share early and often
- Tools: online repositories for data (e.g. Dryad), code (e.g. GitHub), and papers (e.g. bioRxiv)

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Hopefully, by implementing reproducibility principles, our workspace can be more like this:



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