The three R's with R

Research data management

Reproducibility

Reusability

Beautiful data for all the world to see

Dr Jessica Stapley
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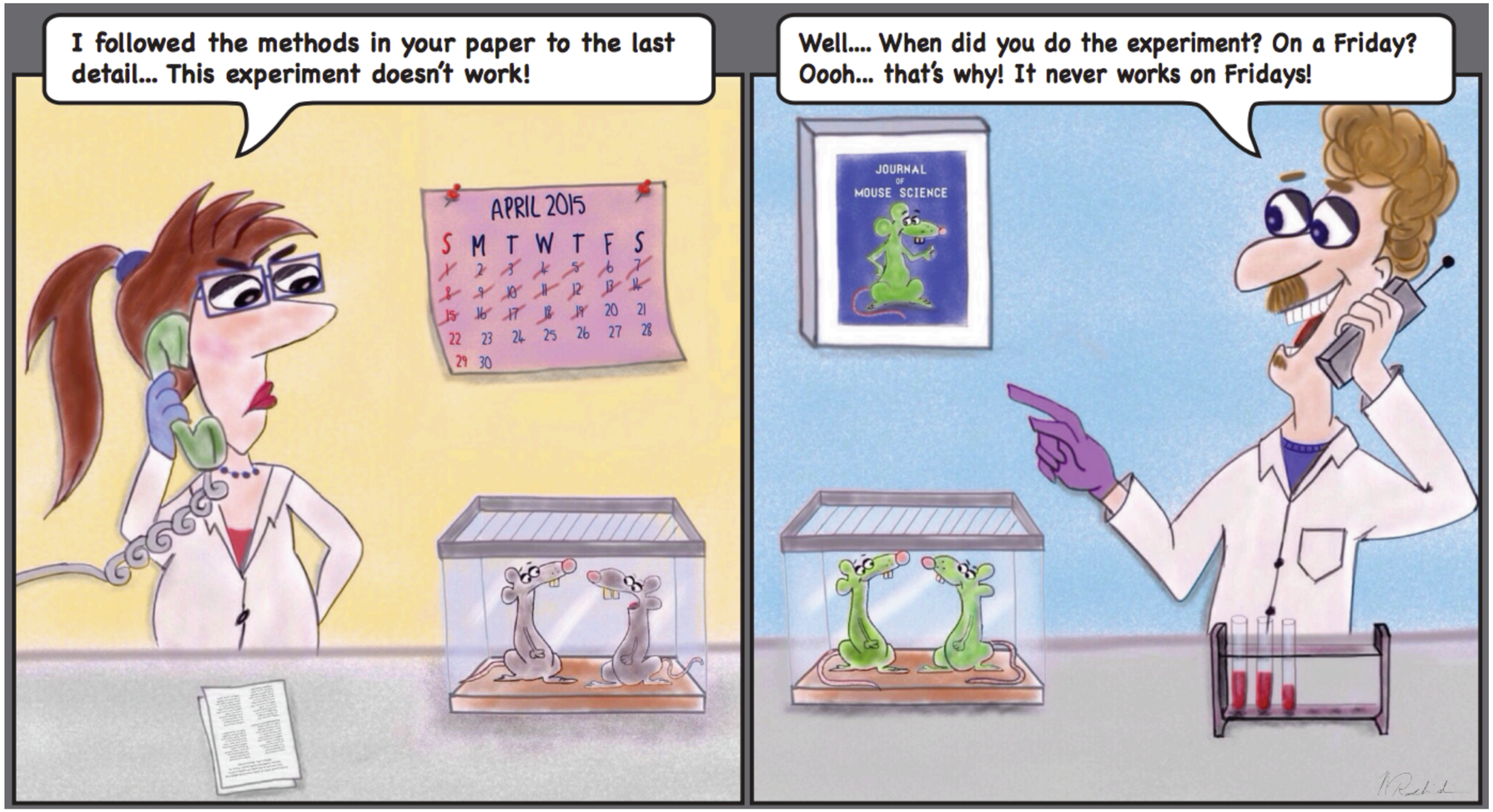
@jessstapley

Reproducibility is a major principle of the scientific method



Reproducibility versus Replication

Reproducibility

An independent researcher can obtain the same results using the original data and original computer code

Replication (Independent verification)

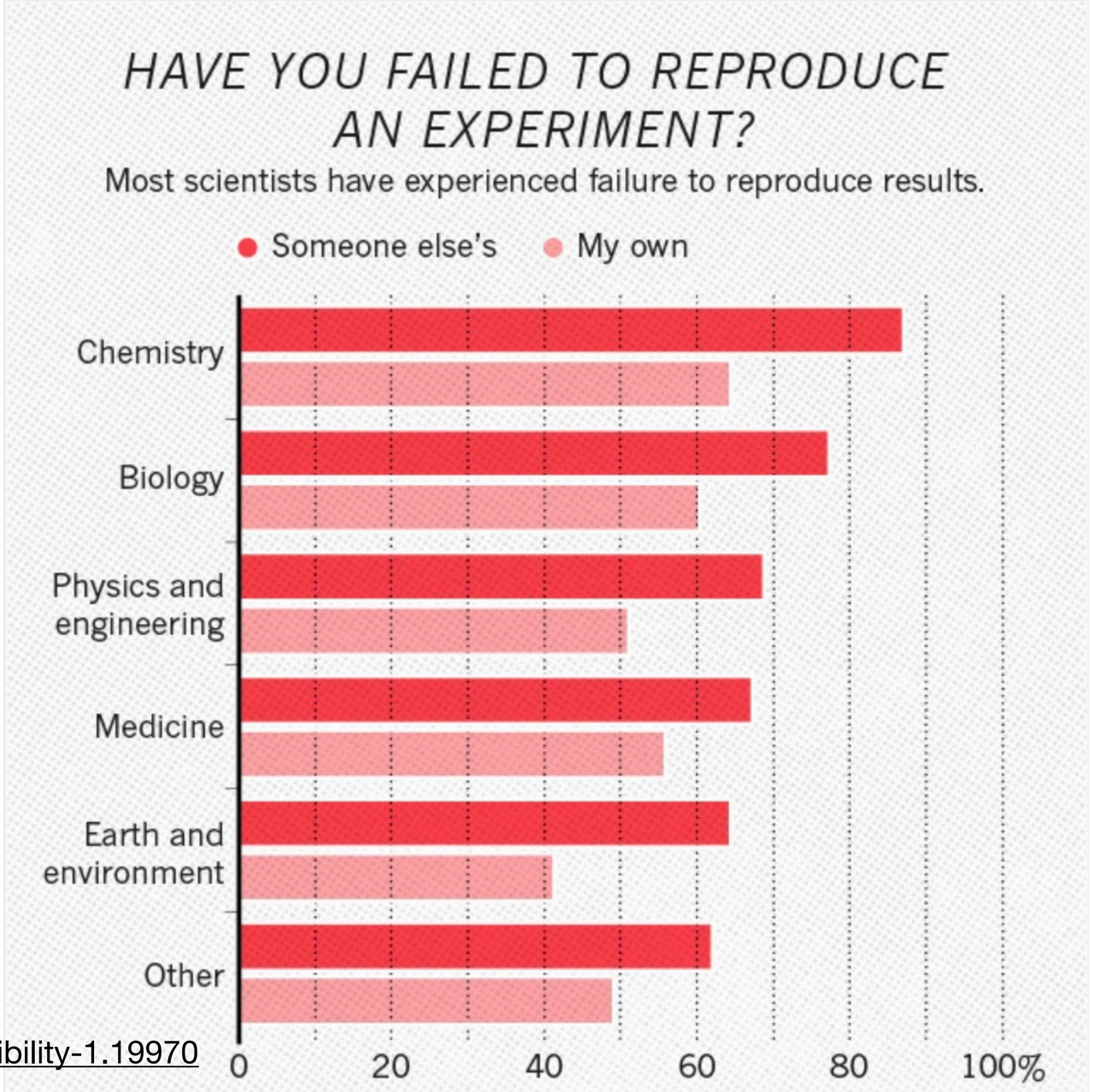
Different researcher/lab conducts an independent study and obtains the same results or comes to the same conclusion as the original study

But how reproducible are most scientific findings?

Not very

Survey of >1500 researchers by Nature

- >70% of researchers have tried and failed to reproduce another lab's experiments
- >50% failed to reproduce their own experiments



https://www.nature.com/news/1-500-scientists-lift-the-lid-on-reproducibility-1.19970

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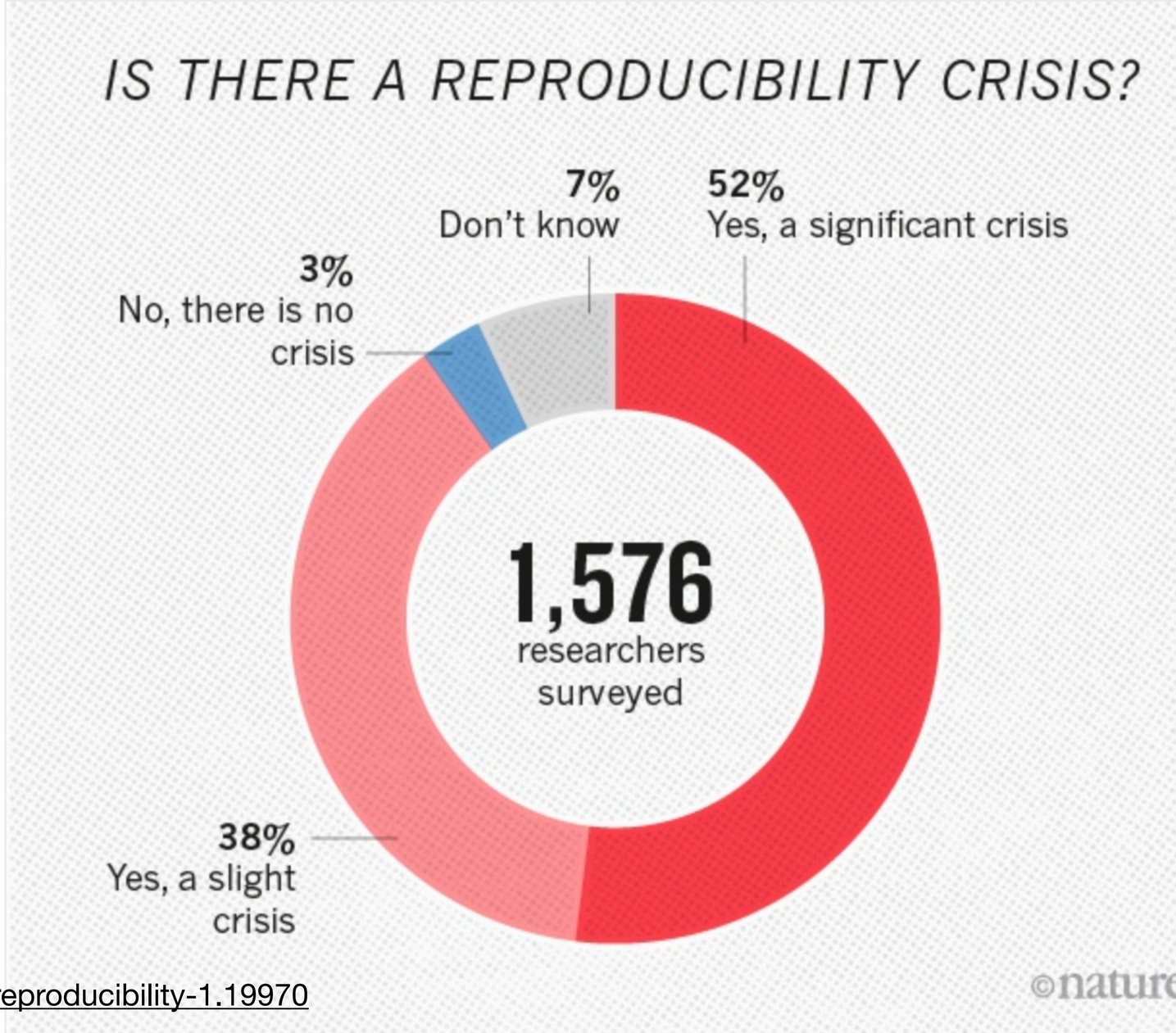
About half the respondents think there is a significant reproducibility crisis



https://www.nature.com/news/1-500-scientists-lift-the-lid-on-reproducibility-1.19970

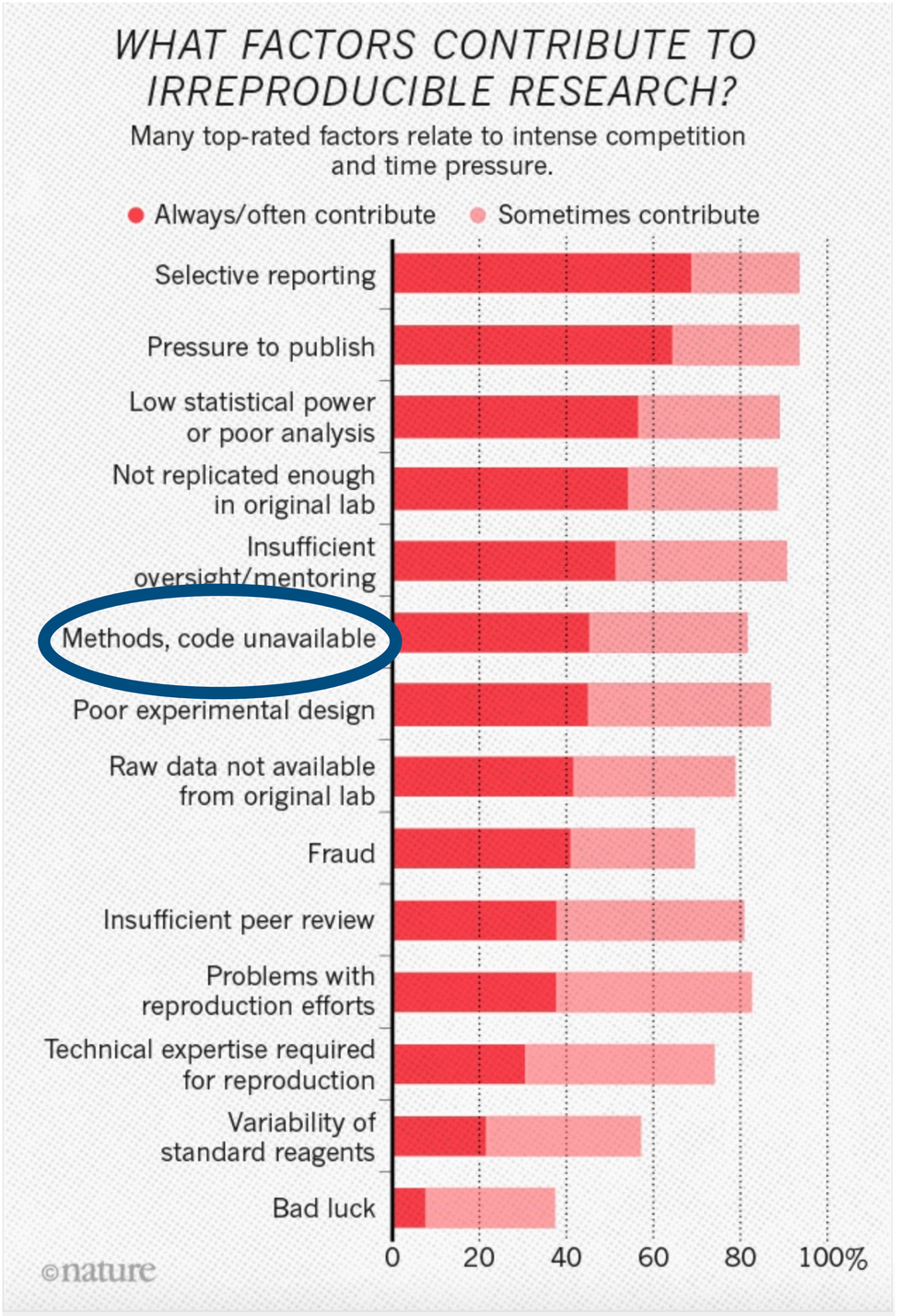
Why can’t we reproduce our work

Major factors relate to some questionable activities

- selective reporting - p-hacking
- pressures to publish

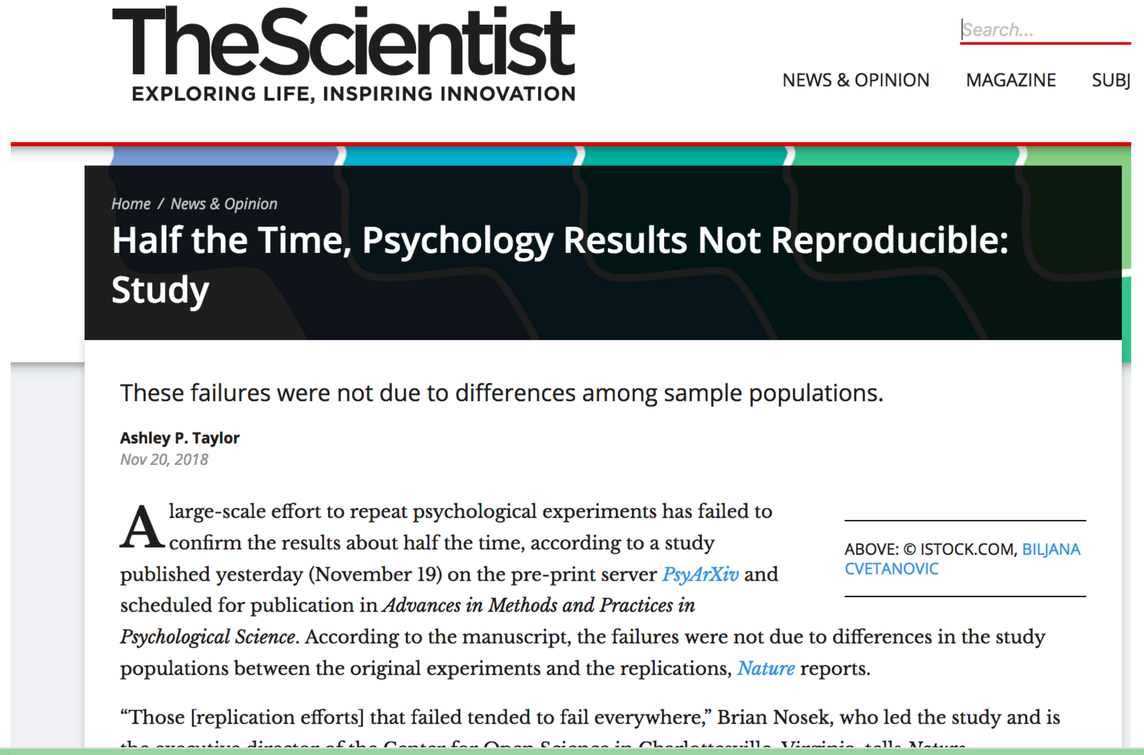
Methods and code not available

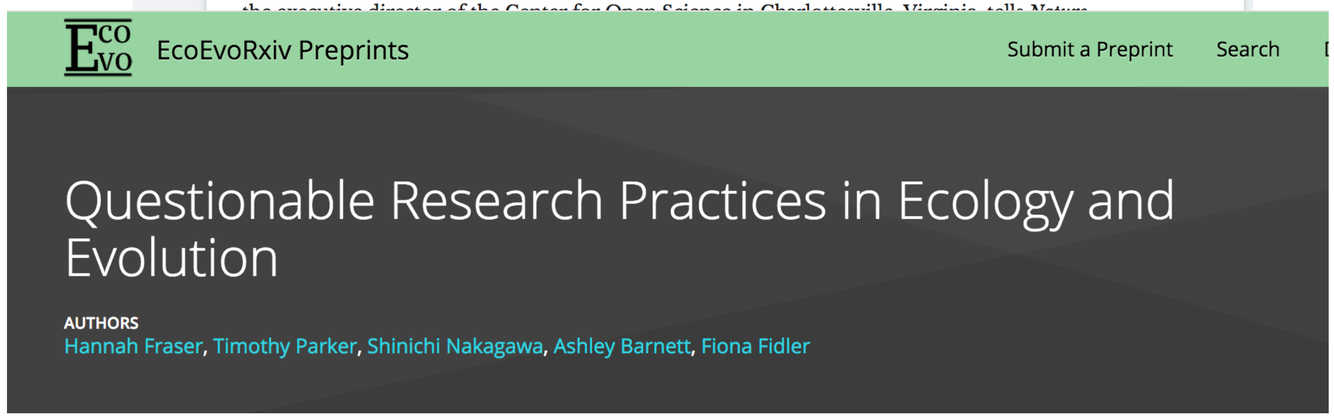
- poorly described exact procedure can not be repeated



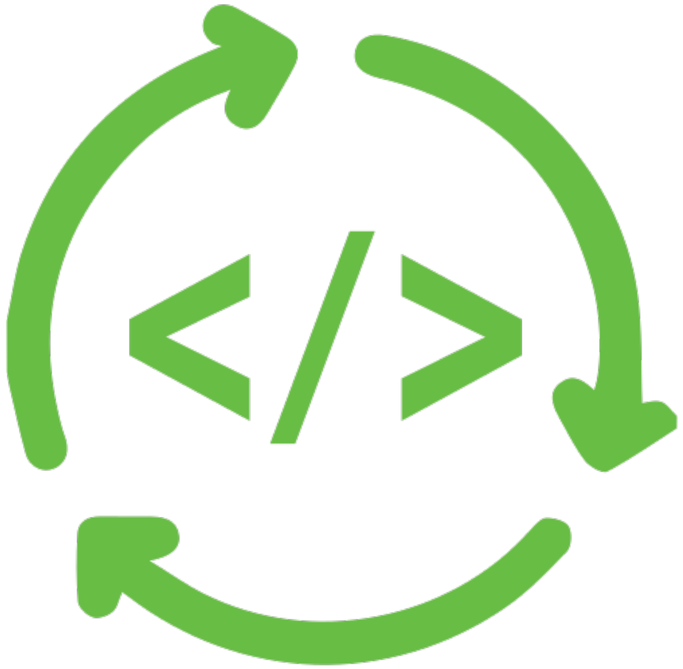
https://www.nature.com/news/1-500-scientists-lift-the-lid-on-reproducibility-1.19970

A similar problem has been found in other surveys and fields - this result has been replicated





To improve the reproducibility and reuse of the data we need to improve computational reproducibility



Dataset and analysis become more complex - accurately describing the analysis is key

Reviewers need access to data and code to be able to reproduce the results if necessary

Funding agencies and publishers require that research data be **FAIR**

Findable

Accessible

Interoperable

Reusable

Open Research Data

FNSNF Swiss National Science Foundation

Research data should be freely accessible to everyone – for scientists as well as for the general public.

The SNSF agrees with this principle. Since October 2017, researchers have to include a data management plan (DMP) in their funding application for most of the funding schemes. At the same time, the SNSF expects that data generated by funded projects are publicly accessible in digital databases provided there are no legal, ethical, copyright or other issues.

Please consult the webpages of the different funding schemes to see whether a DMP is required when submitting an application.

SPRINGER NATURE

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We believe that data should be open, accessible and reusable. Data sharing helps speed up the pace of discovery and its benefits to society.

As a proactive partner to the research community, Springer Nature is pioneering new approaches to data sharing and open data. We're committed to supporting researchers in sharing their data, helping to make data sharing the new normal.

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Open Data

What is open data?

Elsevier supports the principle that "Raw research data should be made freely available to all researchers" and authors should be free to publically post their raw research data (see Author Rights for more details).

We have developed a simple way for authors to do this, by making their research data available on Mendeley Data and linking it to their article on ScienceDirect.

F

F1. (meta)data are assigned a globally unique and eternally persistent identifier.
F2. data are described with rich metadata.
F3. (meta)data are registered or indexed in a searchable resource.
F4. metadata specify the data identifier.

A

A1 (meta)data are retrievable by their identifier using a standardized communications protocol.
A1.1 the protocol is open, free, and universally implementable.
A1.2 the protocol allows for an authentication and authorization procedure, where necessary.
A2 metadata are accessible, even when the data are no longer available.

I

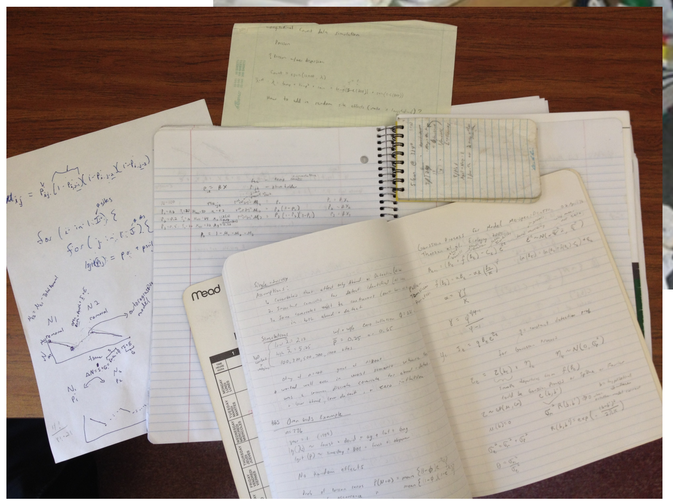
I1. (meta)data use a formal, accessible, shared, and broadly applicable language
I2. (meta)data use vocabularies that follow FAIR principles.
I3. (meta)data include qualified references to other (meta)data.

R

R1. meta(data) have a plurality of accurate and relevant attributes.
R1.1. (meta)data are released with a clear and accessible data usage license.
R1.2. (meta)data are associated with their provenance.
R1.3. (meta)data meet domain-relevant community standards.

SCIENTIFIC DATA | 3:160018 | DOI: 10.1038/sdata.2016.18

Being FAIR - starts with data good management



This is better

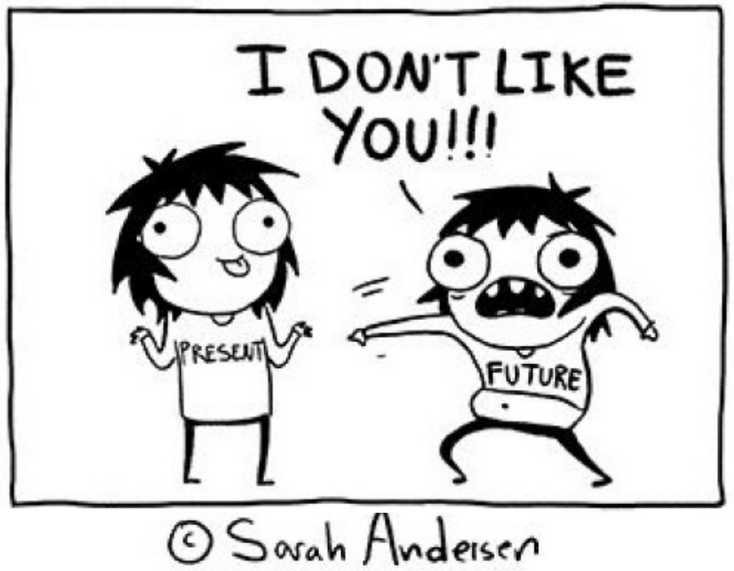
You need to know what you did
Record everything and write meticulous notes
Store your data safely - multiple copies

Data management and Computational reproducibility

- **Reproducible - by you or others**

Reproducible - by you

- The first person who will need to reproduce your results will probably be you
  - New data becomes available
  - Return to the project after some time
  - You give the project to student/collaborator
  - A reviewer suggests a change
  - You find an error and you don know what went wrong



Data management and Computational reproducibility

- **Reproducible - by you or others**

“Someone unfamiliar with your project should be able to look at your computer files and understand in detail what you did and why” - Bill Noble

Data management and Computational reproducibility

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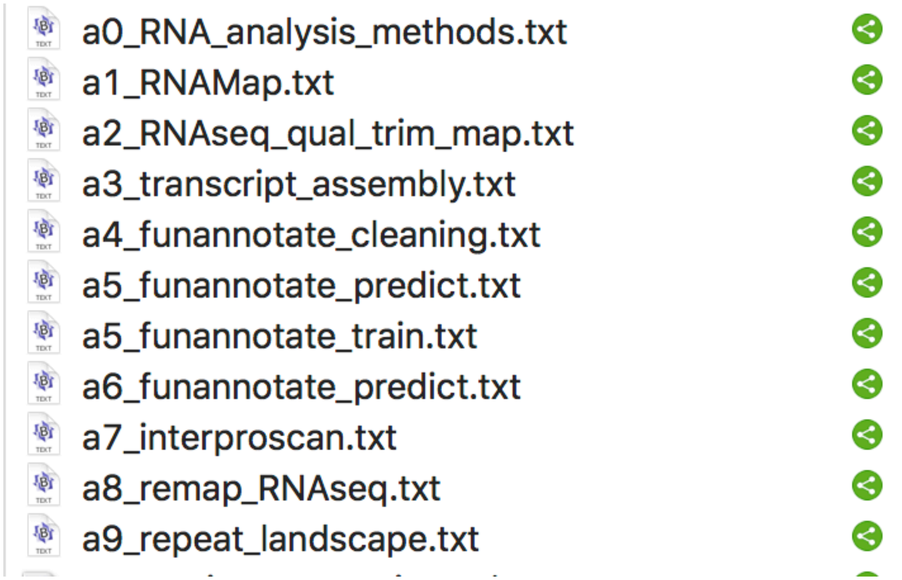
- **Key components**
  - single well structured directory with meaningful subdirectories

Directory structure

```
project
|   README.md
└──data/
|       └──raw_data/
|           |   data_orig.csv
|       └──processed_data/
|           |   data_clean.csv
|       └──results/
|           |   model_results.csv
└──documents/
|       meeting_notes.md
|       data_dictionary.md
└──code/
|       └──exploration/
|           |   01_data_exploration.Rmd
|           |   02_model_results.Rmd
|       └──scripts/
|           |   01_do_clean_data.R
|           |   02_do_model_data.R
|           └──functions/
|               |   01_funs_clean_data.R
|               |   02_funs_model_data.R
```

Example of my own analysis scripts



http://www.rebeccabarter.com/blog/2019-03-07_reproducible_pipeline/

Directory naming

Keep path names short (< 256 characters)

Recommendation for file names:
Unique, reflect content (if possible)

Use only ASCII (American Standard Code for Information Interchange) characters
- NO SPACES
- Be aware of case sensitivity

Bad examples

data%20management%20plan.docx
sup figure 2.png
lab meeting 19.10.2019.pptx

Good examples

Data_management_plan_SNF.docx
sup_figure_02_summary_stats.png
lab_meeting_2019-10-19.pptx

Data management and Computational reproducibility

- **Reproducible - by you or others**

“Someone unfamiliar with your project should be able to look at your computer files and understand in detail what you did and why” - Bill Noble

- **Key components**
  - single well structured directory with meaningful subdirectories
  - data processing and analysis should carefully documented in interactive notebooks based on open access software (e.g. Jupyter notebook, R markdown)

Data processing and analysis

- Interactive Notebooks - combine documentation, code, input and output generated by the code, e.g. graphs)
- Open access software - accessible
- Avoid WORD and EXCEL - versions, hidden characters, auto-filling, auto-formatting, scaleability

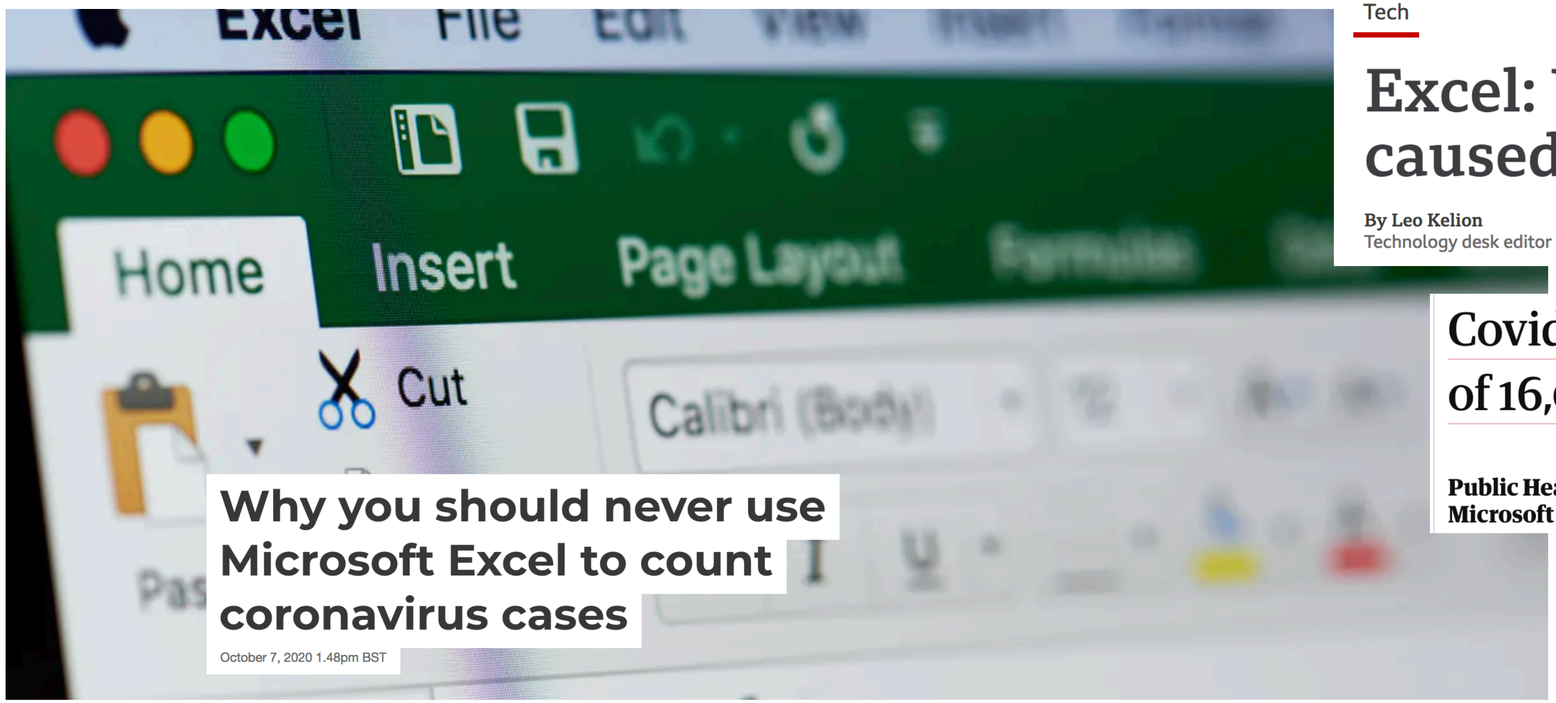
R Markdown

from RStudio

https://rmarkdown.rstudio.com/

https://jupyter.org/

It is OK, I have an excel spreadsheet with all my data



PixieMe/Shutterstock

Tech

Excel: Why using Microsoft's tool caused Covid-19 results to be lost

By Leo Kelion
Technology desk editor

Covid: how Excel may have caused loss of 16,000 test results in England

Public Health England data error blamed on limitations of Microsoft spreadsheet

- 16000 coronavirus cases were missing from daily reports between 25.09-02.10.2020
- Underestimate the scale of infections
- Delayed Track and Trace - possibly increasing community transmission and risk of infection

Data processing and analysis

- Interactive Notebooks - combine documentation, code, input and output generated by the code, e.g. graphs)
- Open access software - accessible
- Avoid WORD and EXCEL - versions, hidden characters, auto-filling, auto-formatting, scaleability
  - if you use excel - convert xls. files to files that are ‘open format’ not proprietary (e.g. csv, txt). Check the conversion of data, e.g. conversion to dates

R Markdown

from RStudio

https://rmarkdown.rstudio.com/

https://jupyter.org/

Data management and Computational reproducibility

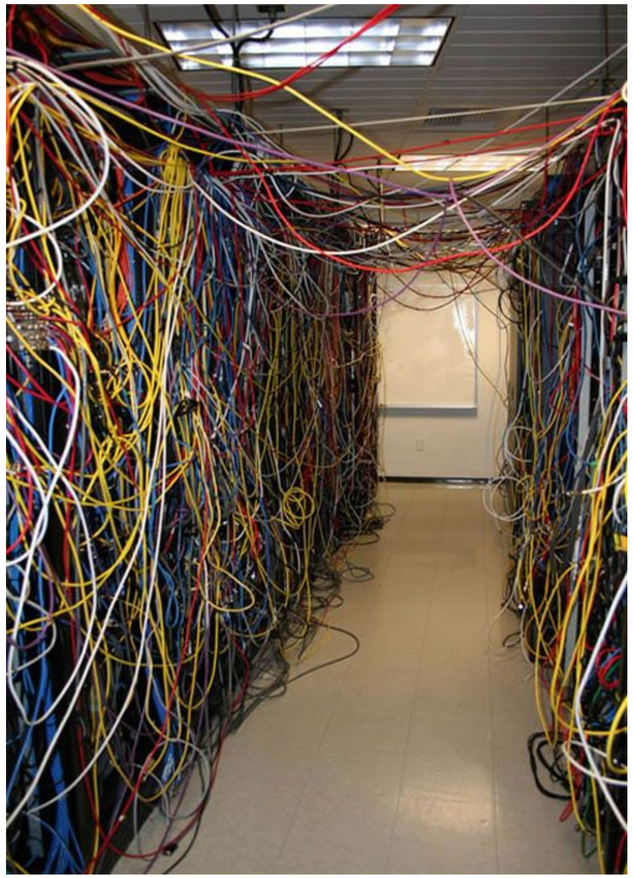
- **Reproducible - by you or others**

“Someone unfamiliar with your project should be able to look at your computer files and understand in detail what you did and why” - Bill Noble

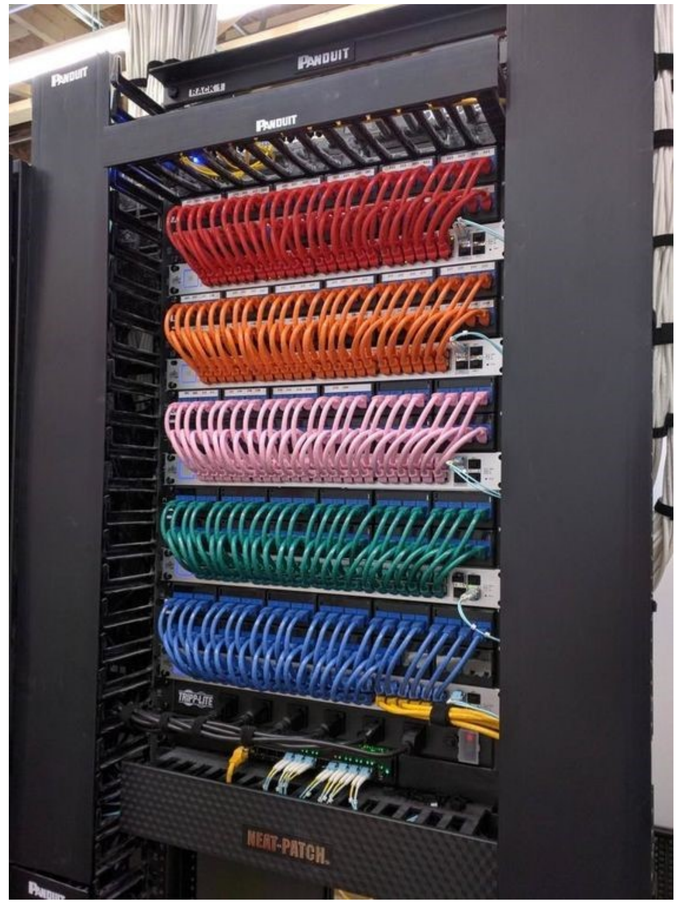
- **Key components**
  - single well structured directory with meaningful subdirectories
  - data processing and analysis should carefully documented in interactive notebooks based on open access software (e.g. Jupyter notebook, R markdown)
  - accessible and hosted on a repository (e.g. github)

Computational reproducibility

This is fine



This is better



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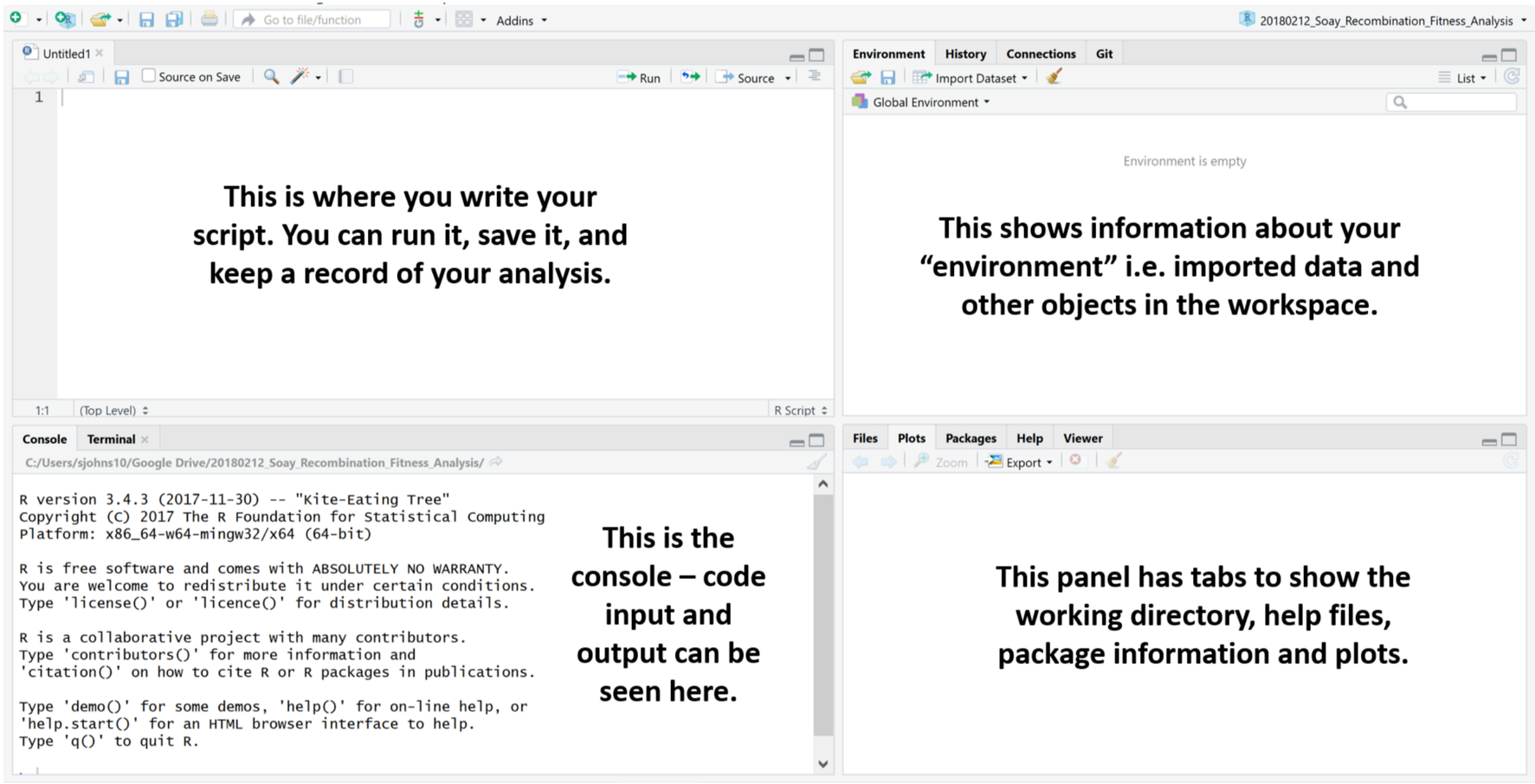
RStudio®

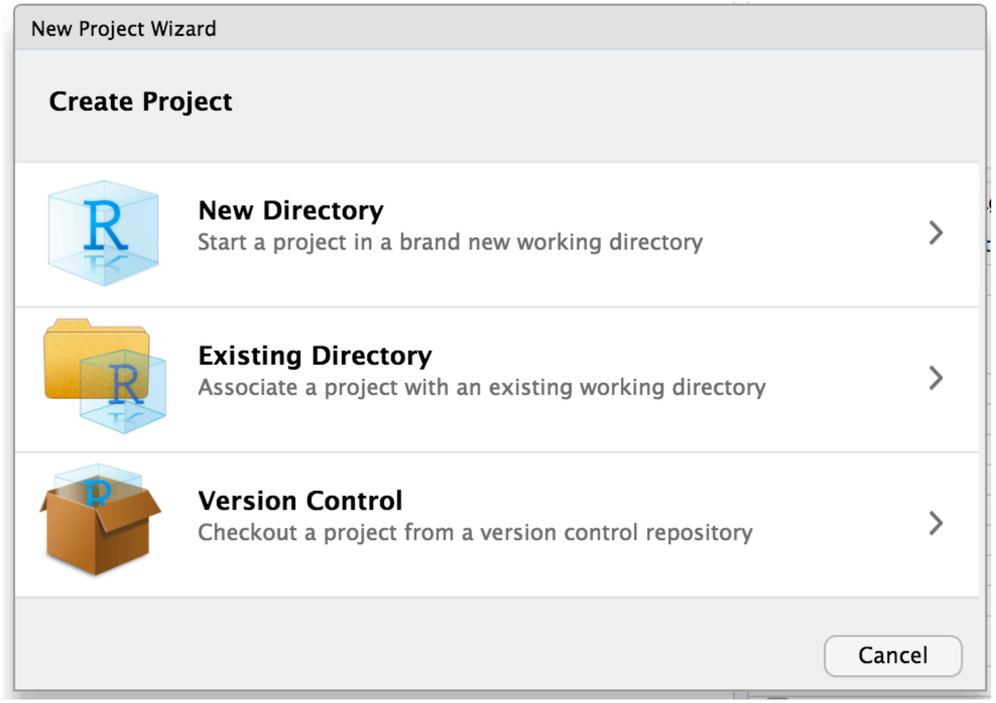
R projects and R markdown

Jessica Stapley

- RStudio is an integrated development environment (IDE) for R
- makes working with R easier - includes
  - drop down menus
  - syntax highlighting
  - code completion
  - smart indentation
  - workspace browser
  - data viewer
  - plot history
  - … and much more



R studio - R projects and R Markdown

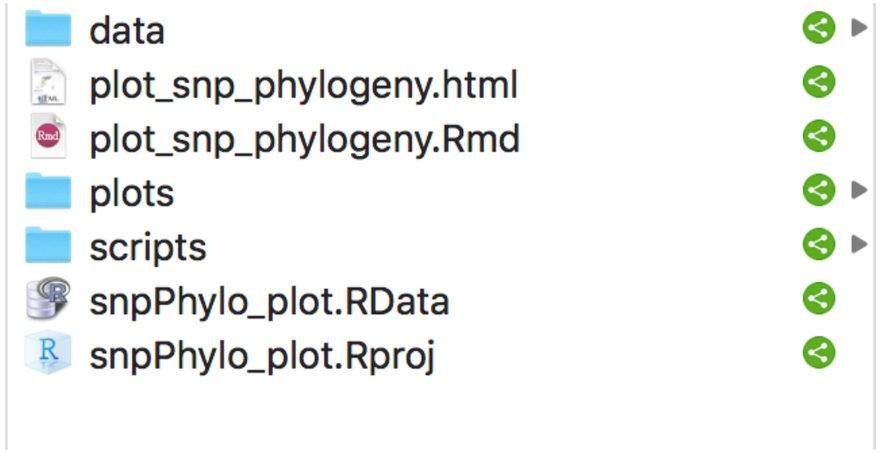


Jessica Stapley

R projects

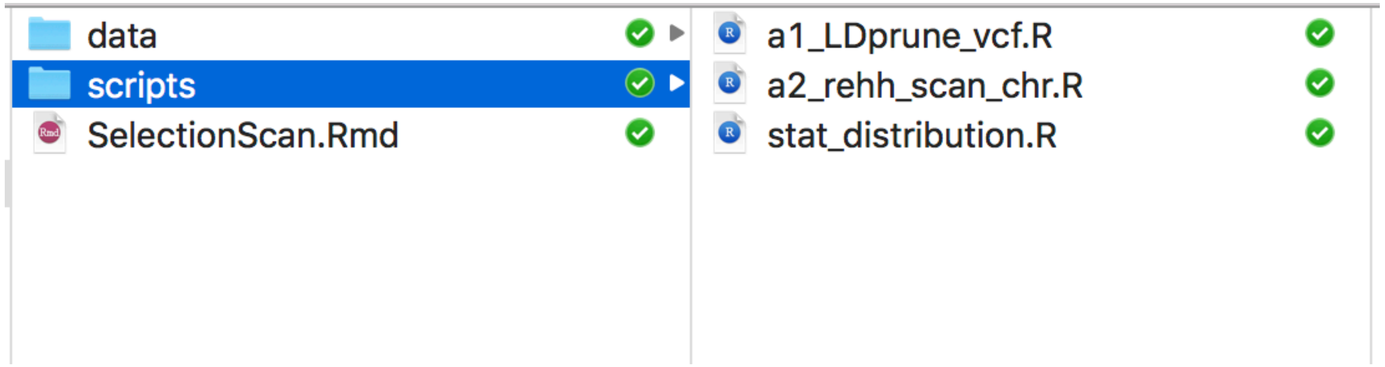
R projects

- creates a directory where all files and relevant metadata are kept
- keeps data reliable, portable, shareable and reproducible
- sets the environment (e.g.working directory) so the code will run on any machine



No single way to structure the project

- (raw)data: contains data for project (read only protected)
- R scripts - sequentially named so order can be easily seen
- plots: plots of the data



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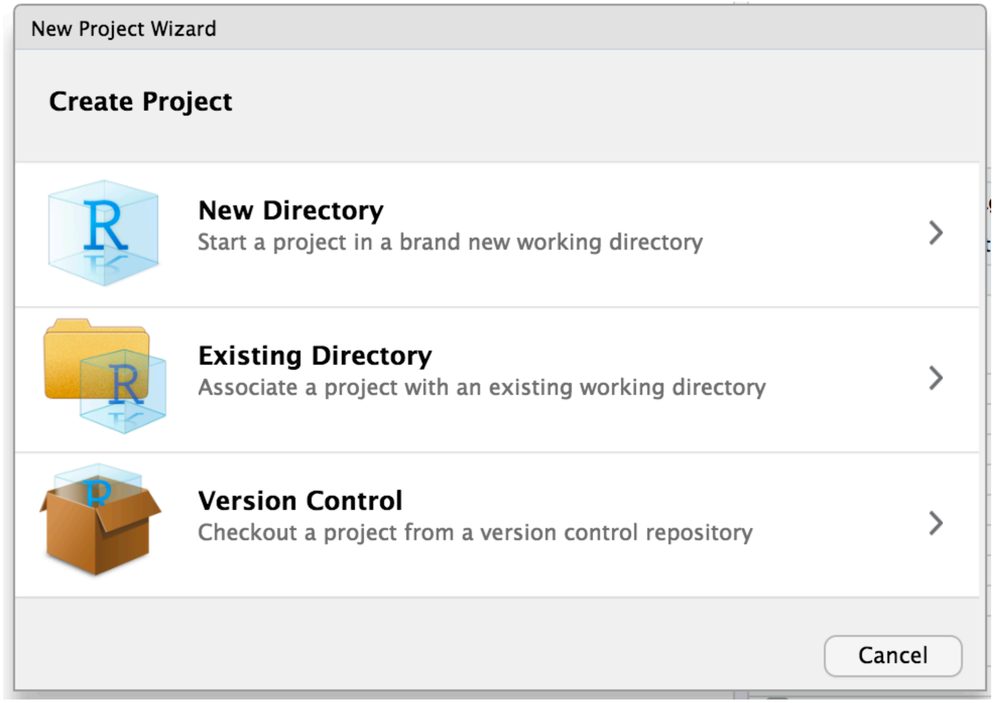

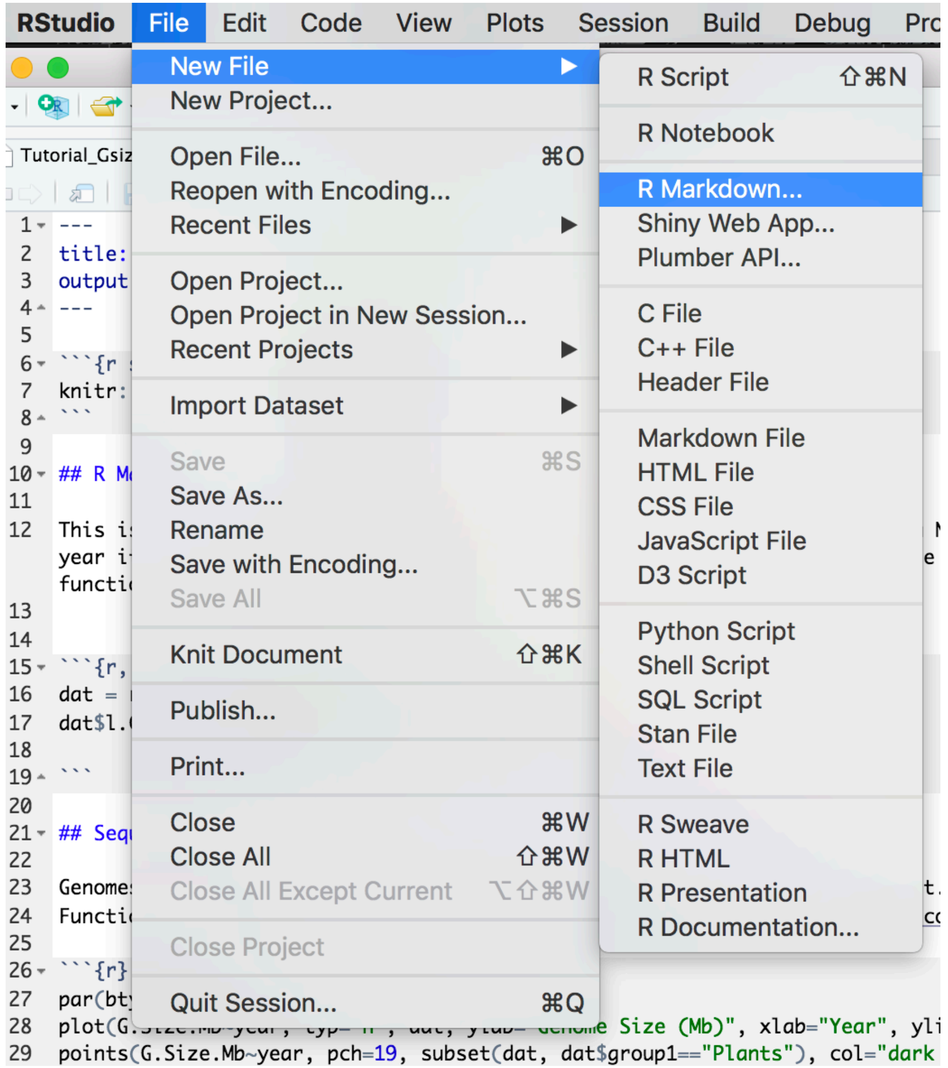

Markup and markdown

Markup - system for annotating text documents, e.g. html

```
<h1>Heading</h1>
<h2>Sub-heading</h2>
<a href="www.webpage.com">Link</a>
<ul>
  <li>List-item1</li>
  <li>List-item2</li>
  <li>List-item3</li>
</ul>
```

Markdown - lightweight markup language which uses plain-text syntax in order to be as unobtrusive as possible, so that a human can easily read it

Jessica Stapley

R studio Markdown

```
---
title: "Genome size of sequenced genomes available on NCBI"
output: html_document
---

```{r setup, include=FALSE}
knitr::opts_chunk$set(echo = TRUE)
```

R Markdown

This is an R Markdown document to create plots of data on genome size from NCBI (as of 20.06.19). Here I plot genome size against the year it was released for all the genomes available on NCBI. I also plot the distribution of log genome size using a kernel denisty function.


```{r, echo=FALSE}
dat = read.table("data/NCBI_eukaryotes.txt", header = TRUE)
dat$l.Gsize = log(dat$G.Size.Mb)

```

Sequenced genome size over time for different taxonomic groups

Genomes on NCBI have been getting bigger. The Axolotl genome is the largest.
Function to position and size the image from https://scrogster.wordpress.com/2014/06/02/adding-phylopic-org-silhouettes-to-r-plots/

```{r}
par(bty="l")
plot(G.Size.Mb~year, typ="n", dat, ylab="Genome Size (Mb)", xlab="Year", ylim=c(0,37000))
points(G.Size.Mb~year, pch=19, subset(dat, dat$group1=="Plants"), col="dark green")
points(G.Size.Mb~I(year+0.25), pch=19, subset(dat, dat$group1=="Animals"), col="blue")
points(G.Size.Mb~I(year+0.5), pch=19, subset(dat, dat$group1=="Fungi"), col="orange")
points(G.Size.Mb~I(year+0.75), pch=19, subset(dat, dat$group1=="Protists"), col="red")


```
```

Genome size of sequenced genomes available on NCBI

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points(G.Size.Mb~I(year+0.25), pch=19, subset(dat, dat$group1=="Animals"), col="blue")
points(G.Size.Mb~I(year+0.5), pch=19, subset(dat, dat$group1=="Fungi"), col="orange")
points(G.Size.Mb~I(year+0.75), pch=19, subset(dat, dat$group1=="Protists"), col="red")
```

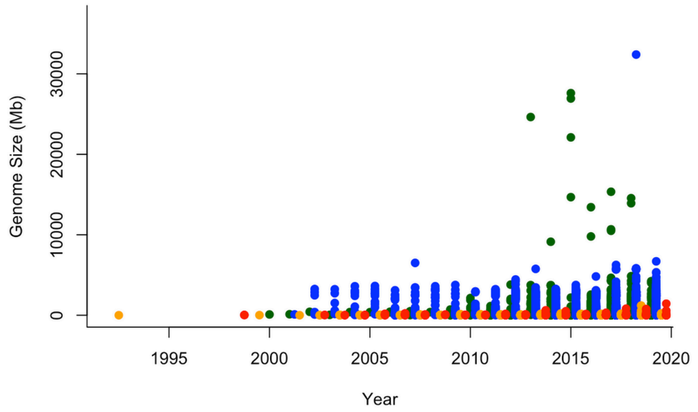

Jessica Stapley

Integration of GitHub and R

- Advanced users
- Happy git with R (https://happygitwithr.com/)
- Git is a version control system developed to help groups of people work together collaboratively on software projects
- Github is a web-based hosting service

Summary

- We need to ensure our research is reproducible
- FAIR - guide to enhance the reusability of their data
- Recommended (required) by publishers and funding bodies
- Assess the FAIRness of your data (https://ardc.edu.au/resources/working-with-data/fair-data/fair-self-assessment-tool/)
- It all starts with good research data management and clear description of what you did and what versions of software you used.
- R studio, R projects, R markdown and integration with Github can help you make your data more open, shareable and reproducible