Reproducible Workflows
for Better Science and Efficient Collaboration

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The Reproducibility ~~Crisis~~ Revolution

Reproducibility Project: Cancer Biology

NEWS | 09 December 2021

Half of top cancer studies fail high-profile reproducibility effort

- Goal: Replicate 193 experiments from 53 papers

Errington et al 2021

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Errington et al 2021

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Errington et al 2021

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Errington et al 2021

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Errington et al 2021

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- ~Half **didn't replicate** (much smaller effect sizes)
- **No paper reported** all required data
- **Impossible to repeat** experiments w/o contacting authors
- 1/3 authors **didn't respond or help**

Errington et al 2021

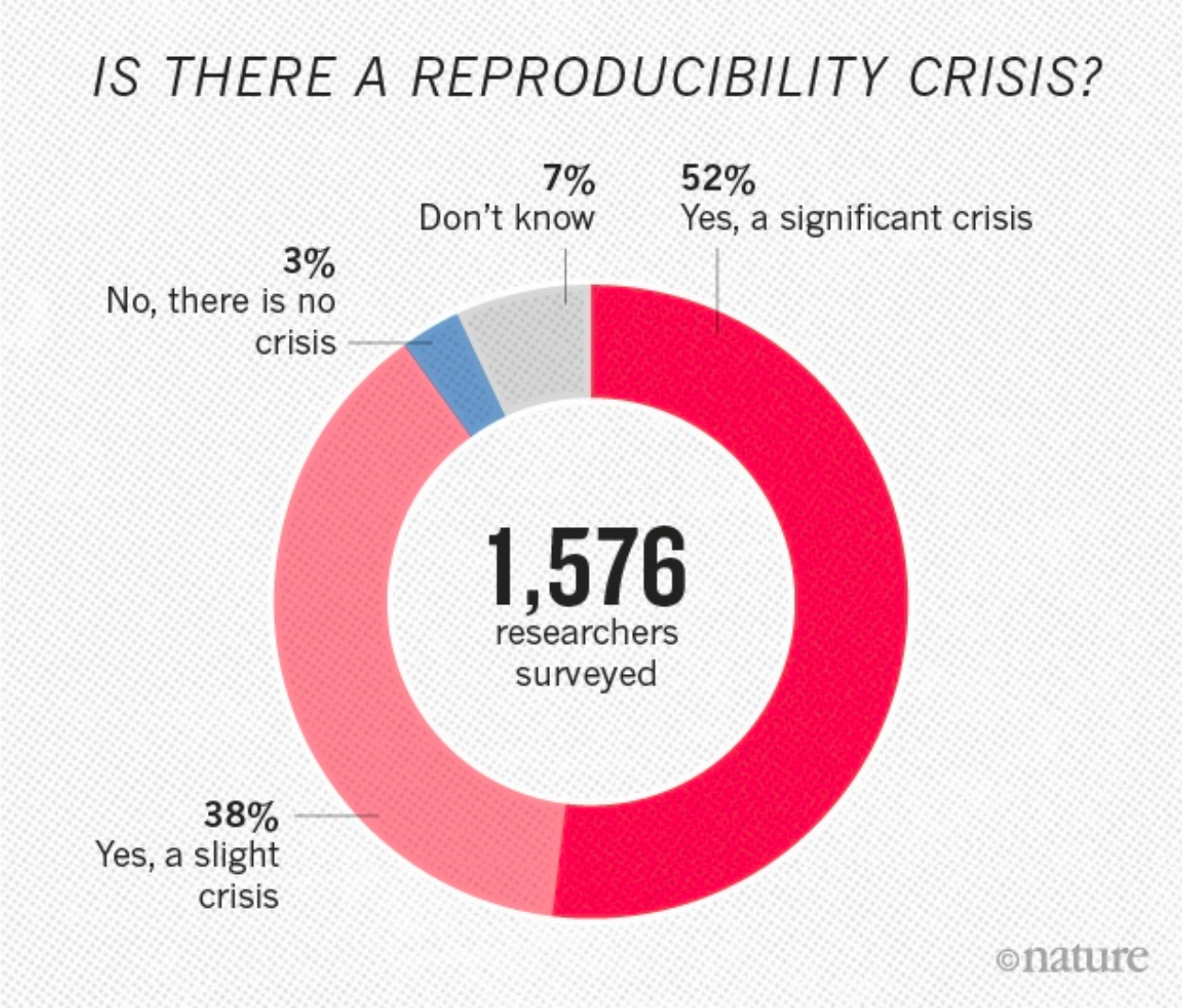
Sylvain Deville ❄️👨‍🎓
@DevilleSy

Trying to reproduce the results of a paper using only what's in the Methods section

Most scientific articles

are NOT reproducible

The reproducibility crisis



Baker 2016

Reproducibility

~~CRISIS~~

REVOLUTION

Reproducibility vs Replicability

		Data	
		Same	Different
Analysis	Same	Reproducible	Replicable
	Different	Robust	Generalisable

The Turing Way

We can’t guarantee that

our results are **replicable**.

But at least

they should be **reproducible**.

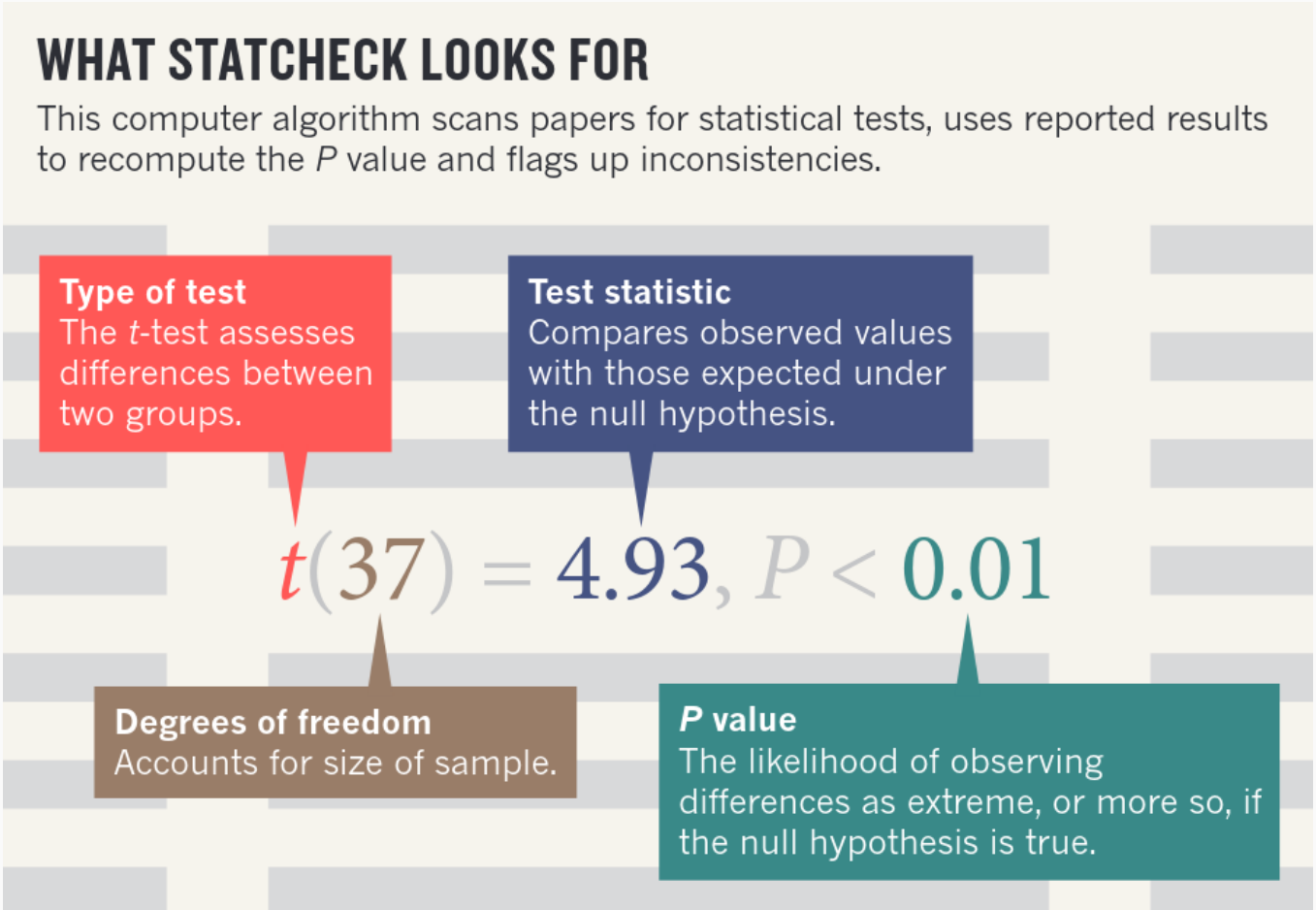
Most scientific articles

are NOT reproducible

Behav Res (2016) 48:1205–1226
DOI 10.3758/s13428-015-0664-2

The prevalence of statistical reporting errors in psychology (1985–2013)

Michèle B. Nuijten[1] · Chris H. J. Hartgerink[1] · Marcel A. L. M. van Assen[1] · Sacha Epskamp[2] · Jelte M. Wicherts[1]



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1/2 articles: **inconsistencies** in p-values

1/8 articles: **grossly inconsistent** p-values

(affecting conclusions -> significance)

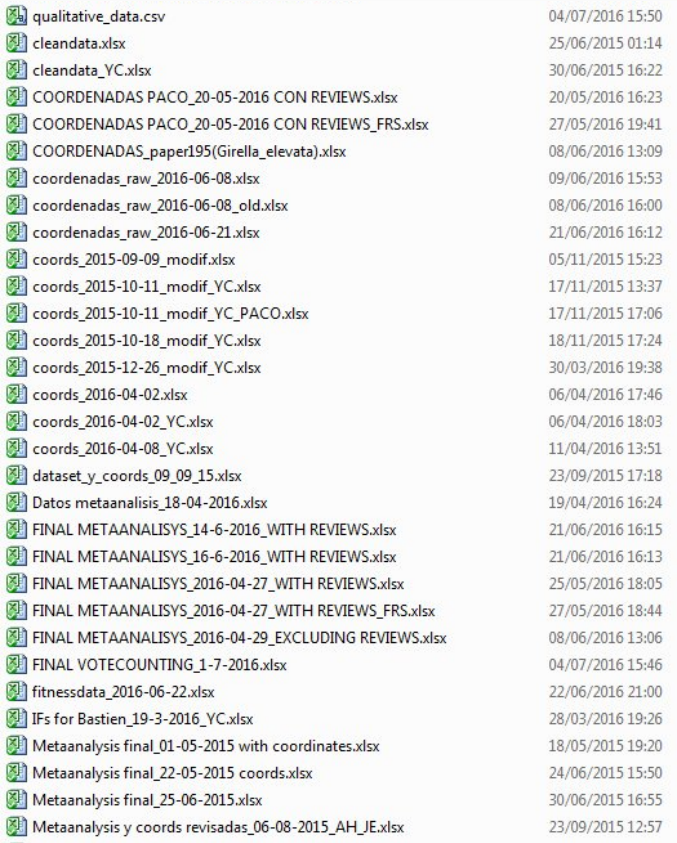
In ecology

< 20% articles are reproducible

Culina et al 2020

We can’t even reproduce our own work

Data/Code lost or unusable



What's a reproducible article?

A scientific article is reproducible if there is **computer code** that can regenerate all results and figures from the **original data**

A scientific article is **advertising**, not scholarship.

The actual scholarship is the **full software environment**,

code and data, that produced the result.

Claerbout & Karrenback 1992

Are we sharing the data?

Are we sharing data?

PERSPECTIVE

Public Data Archiving in Ecology and Evolution: How Well Are We Doing?

Dominique G. Roche[1,2]*, Loeske E. B. Kruuk[1,3], Robert Lanfear[1,4], Sandra A. Binning[1,2]

1 Division of Evolution, Ecology and Genetics, Research School of Biology, The Australian National University, Canberra, Australian Capital Territory, Australia, **2** Éco-Éthologie, Institut de Biologie, Université de Neuchâtel, Neuchâtel, Switzerland, **3** Institute of Evolutionary Biology, School of Biological Sciences, University of Edinburgh, Edinburgh, United Kingdom, **4** Department of Biological Sciences, Macquarie University, Sydney, Australia

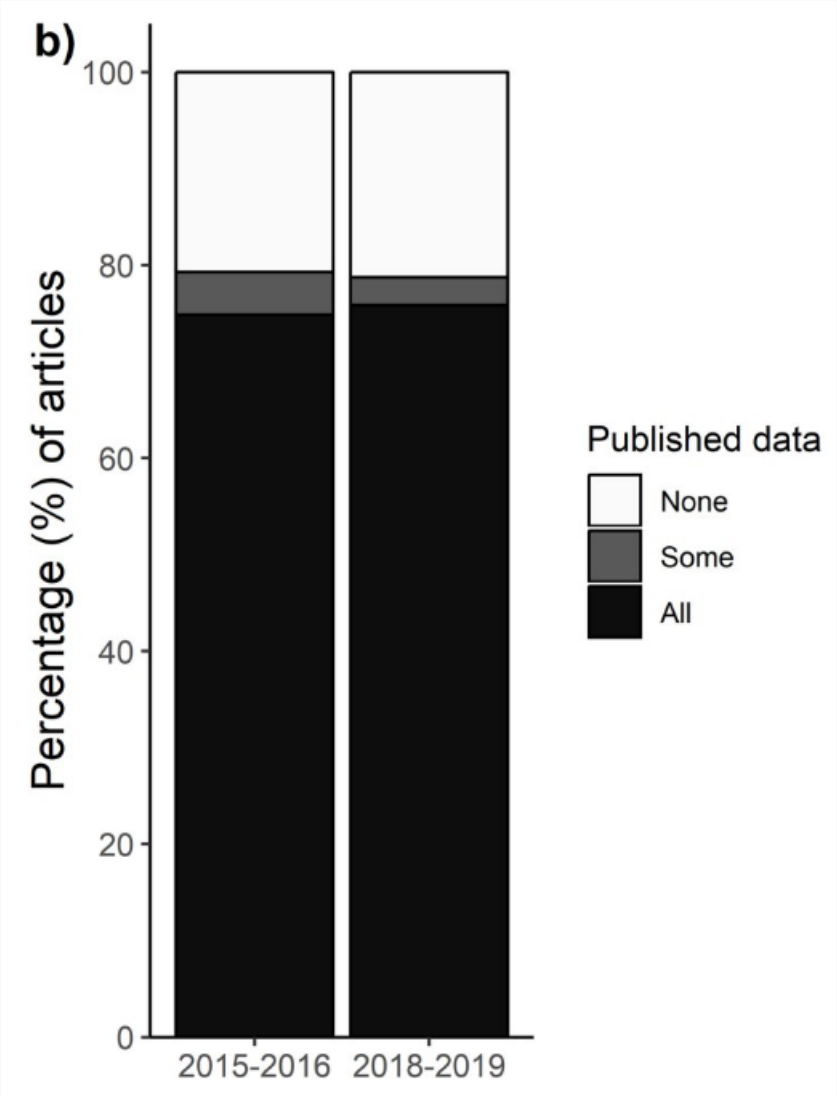
* dominique.roche@mail.mcgill.ca

Abstract

Policies that mandate public data archiving (PDA) successfully increase accessibility to data underlying scientific publications. However, is the data quality sufficient to allow reuse and reanalysis? We surveyed 100 datasets associated with nonmolecular studies in journals that commonly publish ecological and evolutionary research and have a strong PDA policy. Out of these datasets, 56% were incomplete, and 64% were archived in a way that partially or entirely prevented reuse. We suggest that cultural shifts facilitating clearer benefits to authors are necessary to achieve high-quality PDA and highlight key guidelines to help authors increase their data's reuse potential and compliance with journal data policies.

Roche et al. 2015

Are we sharing data?



Culina et al. 2020

Are we sharing data?

Quickly getting better

Campbell et al. 2019

Are we sharing the code?

Code exists but rarely shared

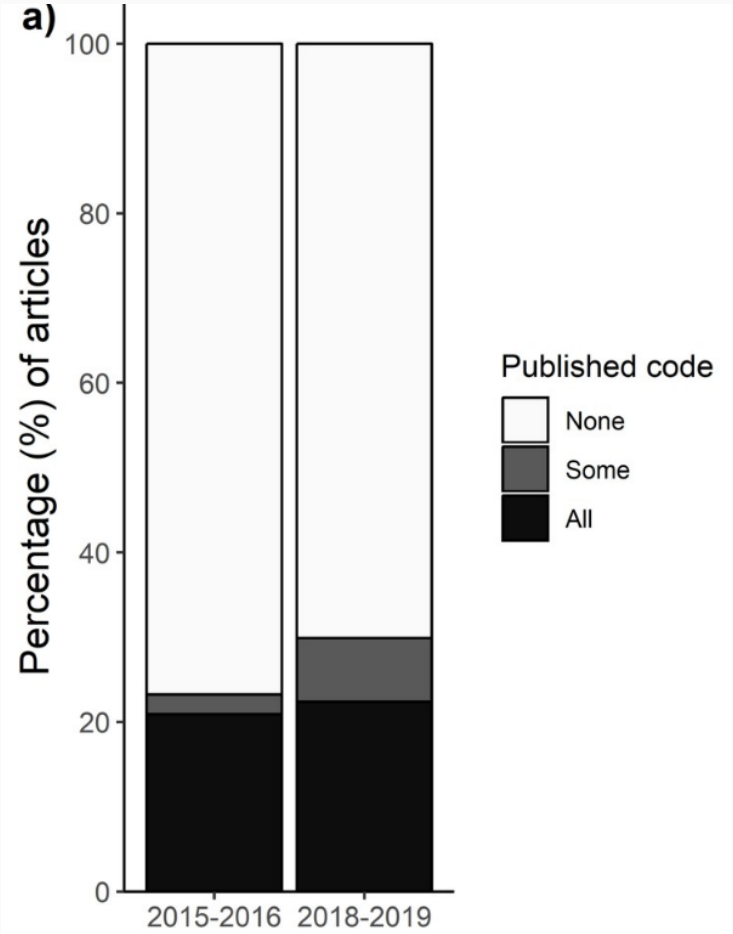
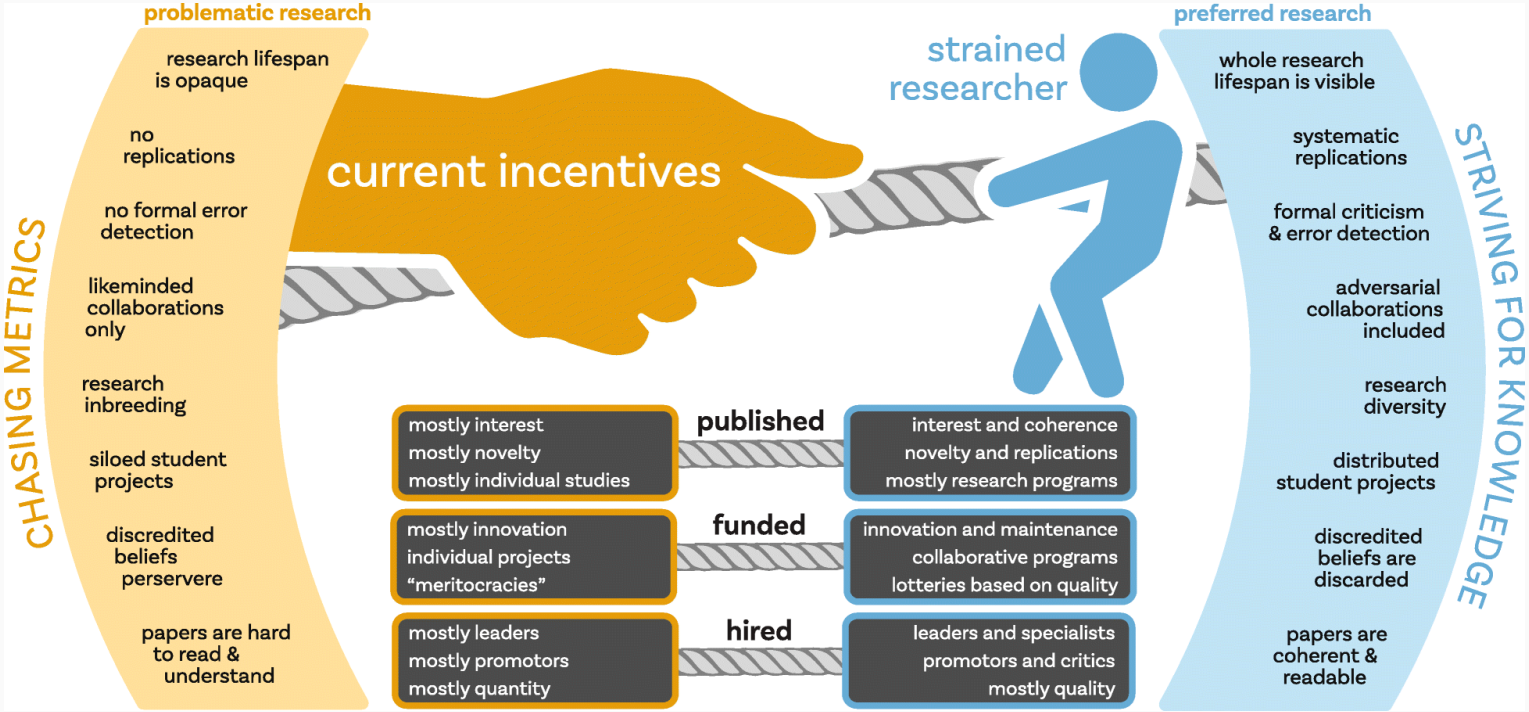


Fig 1. Code-sharing is at its infancy in ecology, wher

Culina et al. 2020

WHY?

Poor incentives



O'Dea et al 2021

Doing reproducible research can be costly

The Costs of Reproducibility

Russell A. Poldrack[1,*]
[1]Department of Psychology, Stanford University, Stanford, CA, USA
*Correspondence: poldrack@stanford.edu
https://doi.org/10.1016/j.neuron.2018.11.030

PERSPECTIVE

Open science challenges, benefits and tips in early career and beyond

Christopher Allen[1]*, **David M. A. Mehler**[1,2]*

Must value diverse contributions to reproducible research

Credit data generators for data reuse

To promote effective sharing, we must create an enduring link between the people who generate data and its future uses, urge **Heather H. Pierce** and colleagues.

Pierce et al 2019

Let’s knock down psychological barriers

Publish your computer code: it is good enough

Freely provided working code — whatever its quality — improves programming and enables others to engage with your research, says **Nick Barnes**.

Barnes 2010

- Improve training
- Avoid shaming -> constructive critique
- Ugly code better than no code

Why doing reproducible research?

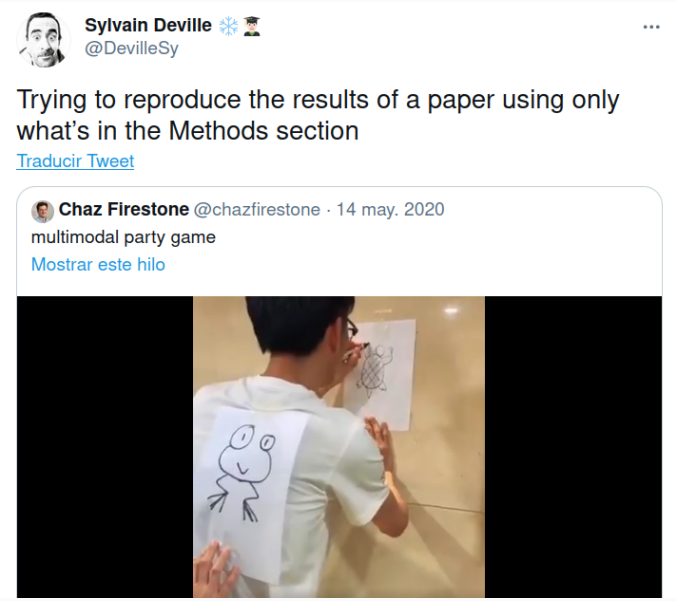
Reproducibility: good for you, good for everyone

Automation (good code) saves time

Trevor Branch
@TrevorABranch

My rule of thumb: every analysis you do on a dataset will have to be redone 10–15 times before publication. Plan accordingly. #Rstats

Code = fully traceable, reproducible analysis



Code advantages:

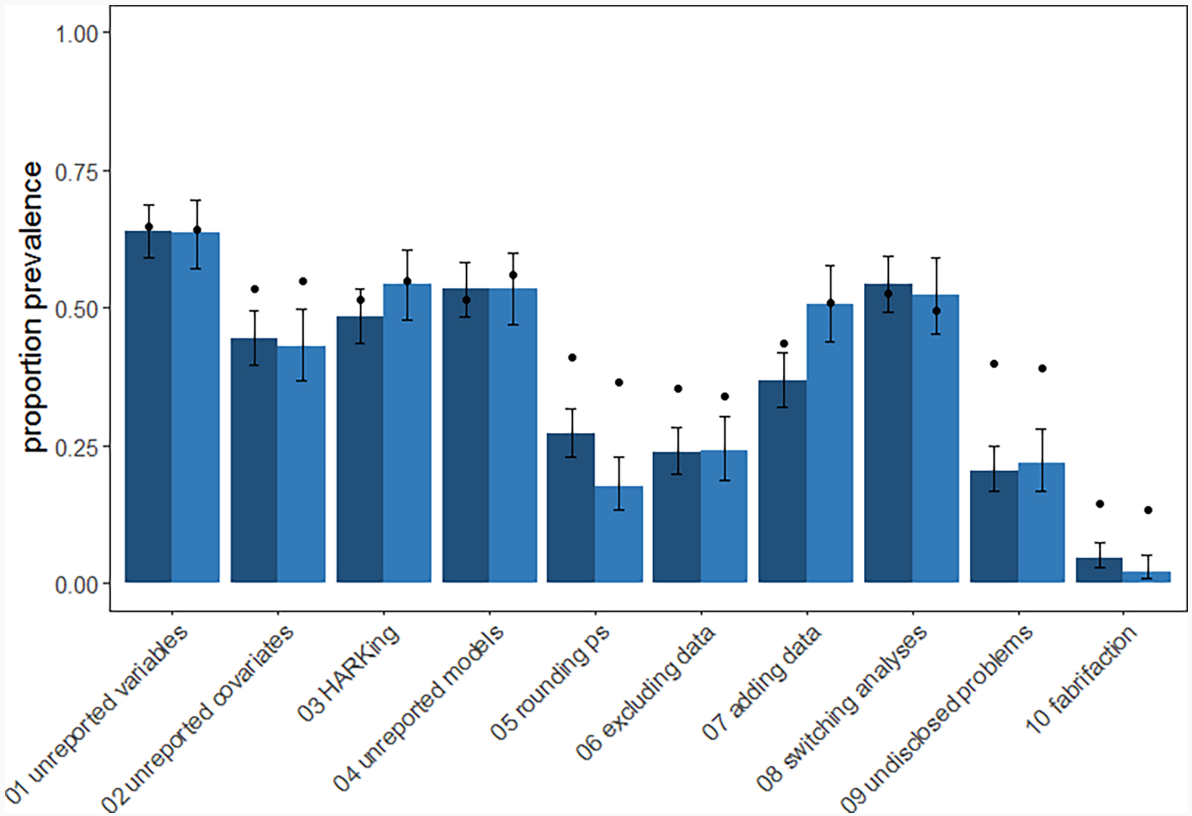
- Easier writing
- Easier, deeper review
- Reusable

Transparency prevents bad practices

RESEARCH ARTICLE

Questionable research practices in ecology and evolution

Hannah Fraser[1]*, Tim Parker[2], Shinichi Nakagawa[3], Ashley Barnett[1], Fiona Fidler[1,4]



p-hacking, HARKing, data fabrication...

Fraser et al 2018

Transparency avoids unnecessary disputes

DOI:10.1063/PT.6.1.20180822a

22 Aug 2018 in Research & Technology

The war over supercooled water

How a hidden coding error fueled a seven-year dispute between two of condensed matter's top theorists.

Ashley G. Smart

Over the next seven years, the perplexing discrepancy would ignite a bitter conflict, with junior scientists caught in the crossfire. At stake were not only the reputations of the two groups but also a peculiar theory that sought to explain some of water's deepest and most enduring mysteries. Earlier this year, the dispute was finally settled. And as it turns out, the entire ordeal was the result of botched code.

Transparency brings better science

Alexey Shiklomanov
@ashiklom711

I'm co-author on a study currently published only as a publicly available discussion paper. My code was on GitHub.

A colleague read the paper, thought the results looked weird, checked my code, found a bug and emailed me about it.

This is how science should work. #openscience

Many journals (and funders) value/require reproducibility

As a condition for publication in ESA journals, all underlying data and statistical code pertinent to the results presented in the publication must be made available in a permanent, publicly accessible data archive or repository, with rare exceptions (see

Many journals value reproducibility

'Papers with exemplary **data and code archiving**

are **more valuable** for future research and [...]

will be given **higher priority** for publication'

(*Molecular Ecology*)

Higher impact: cites, reuse, reputation

RESEARCH ARTICLE

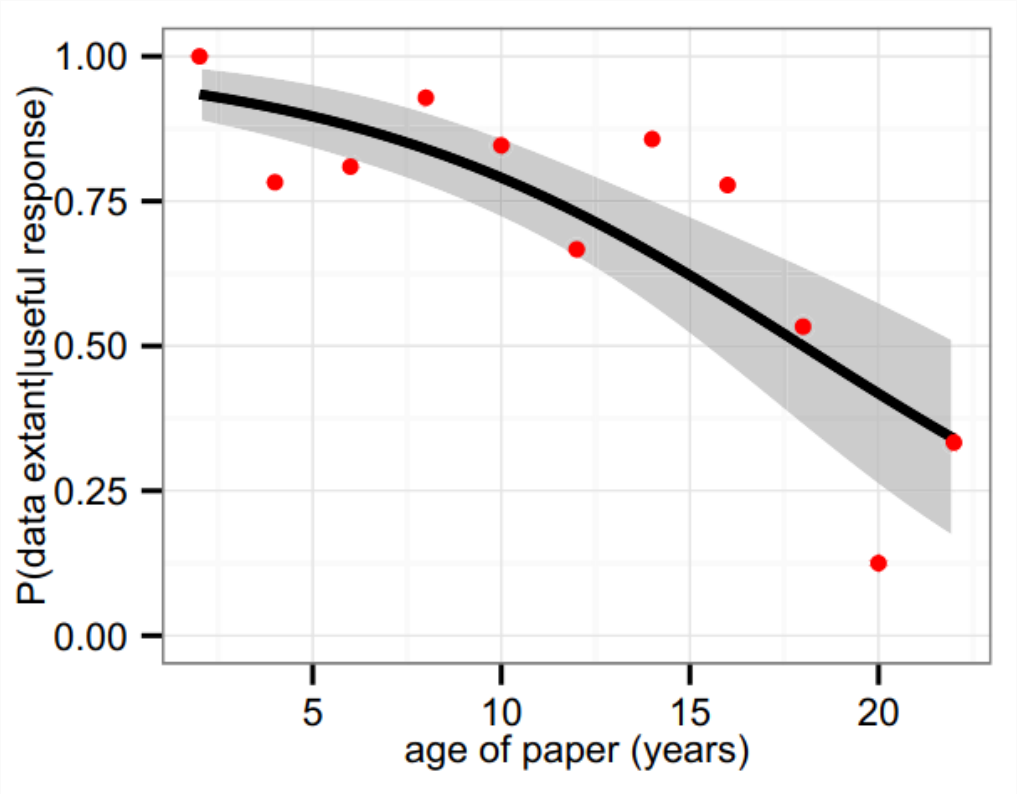
The citation advantage of linking publications to research data

Giovanni Colavizza[1,2], Iain Hrynaszkiewicz[3,4], Isla Staden[1,5], Kirstie Whitaker[1,6], Barbara McGillivray[1,6]*

Colavizza et al 2020

Let’s stop losing data & code

The Availability of Research Data Declines Rapidly with Article Age



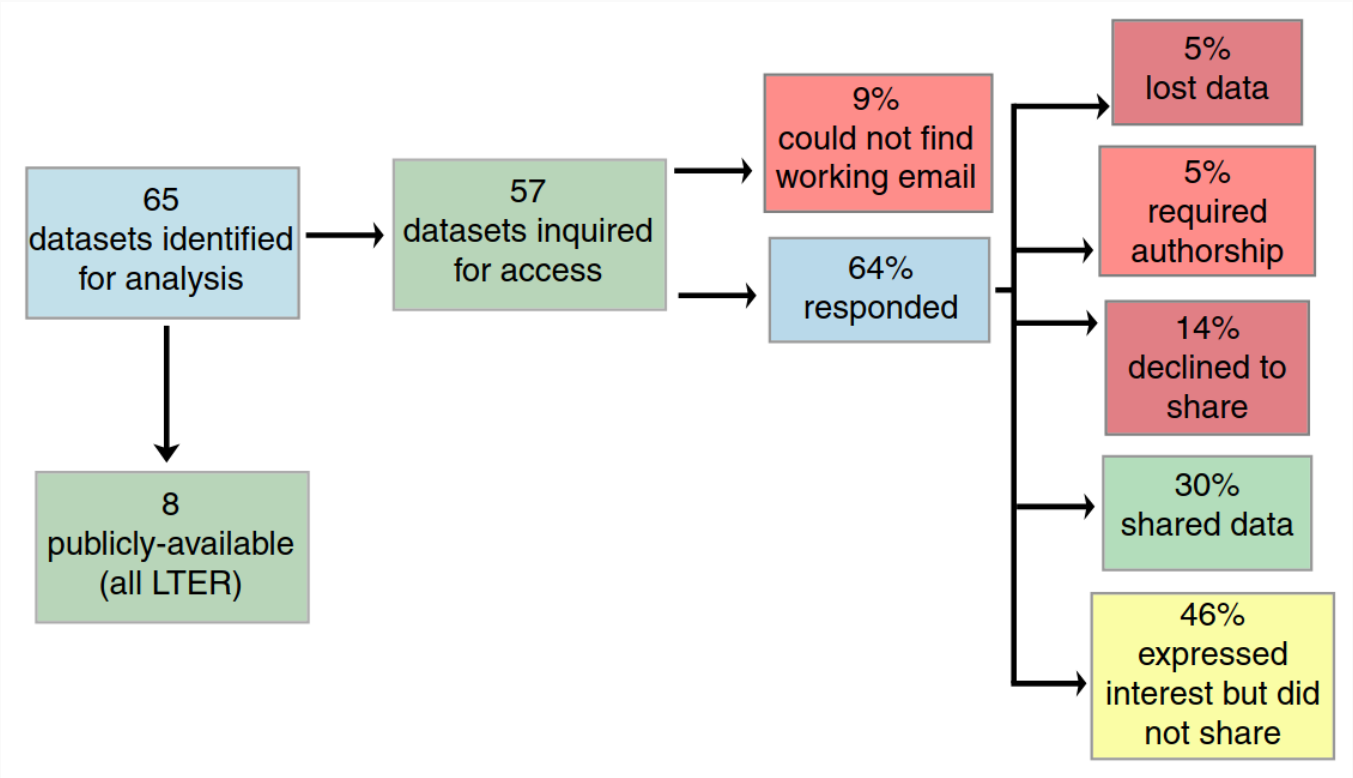
Vines et al 2014

Open data & code enable synthesis

REVIEW

Advances in global change research require open science by individual researchers

ELIZABETH M. WOLKOVICH*†, JAMES REGETZ‡ and MARY I. O'CONNOR†



Wolkovich et al 2012

Open data & code enable synthesis

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Advances in global change research require open science by individual researchers

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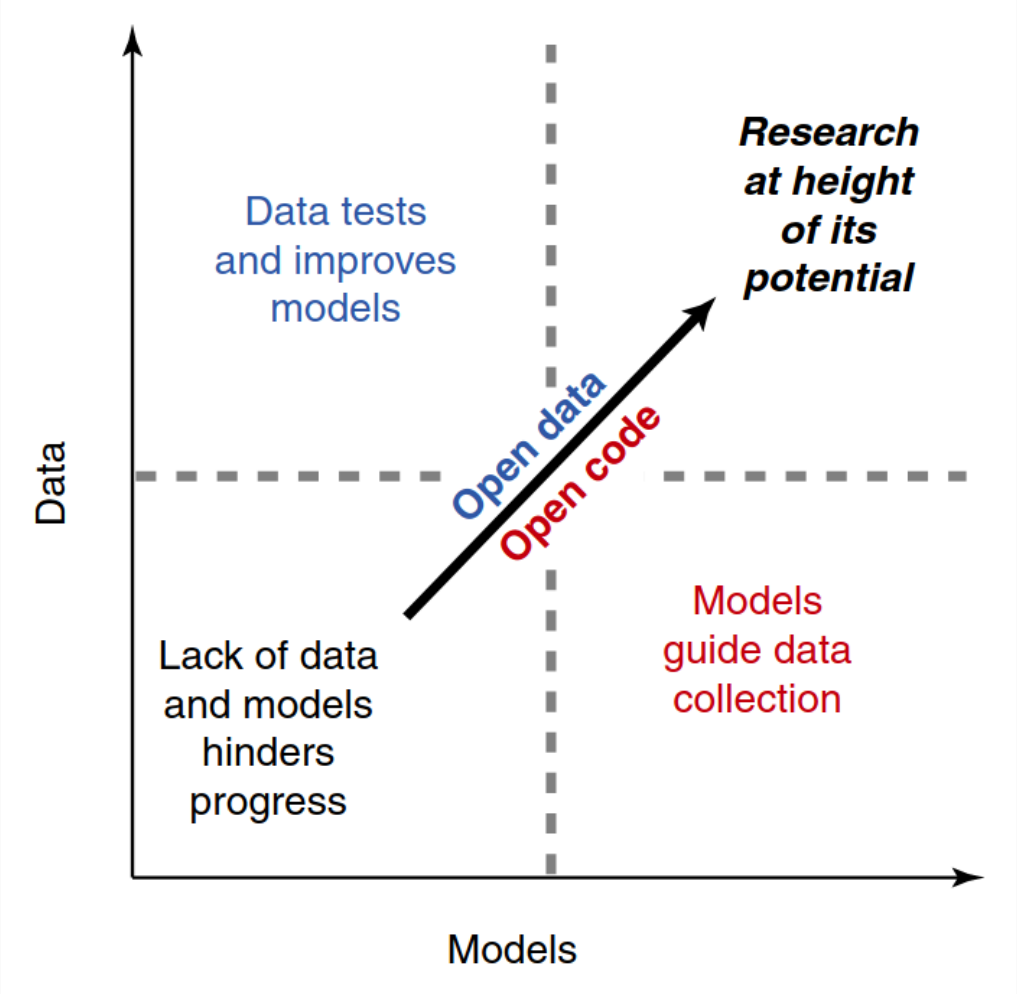


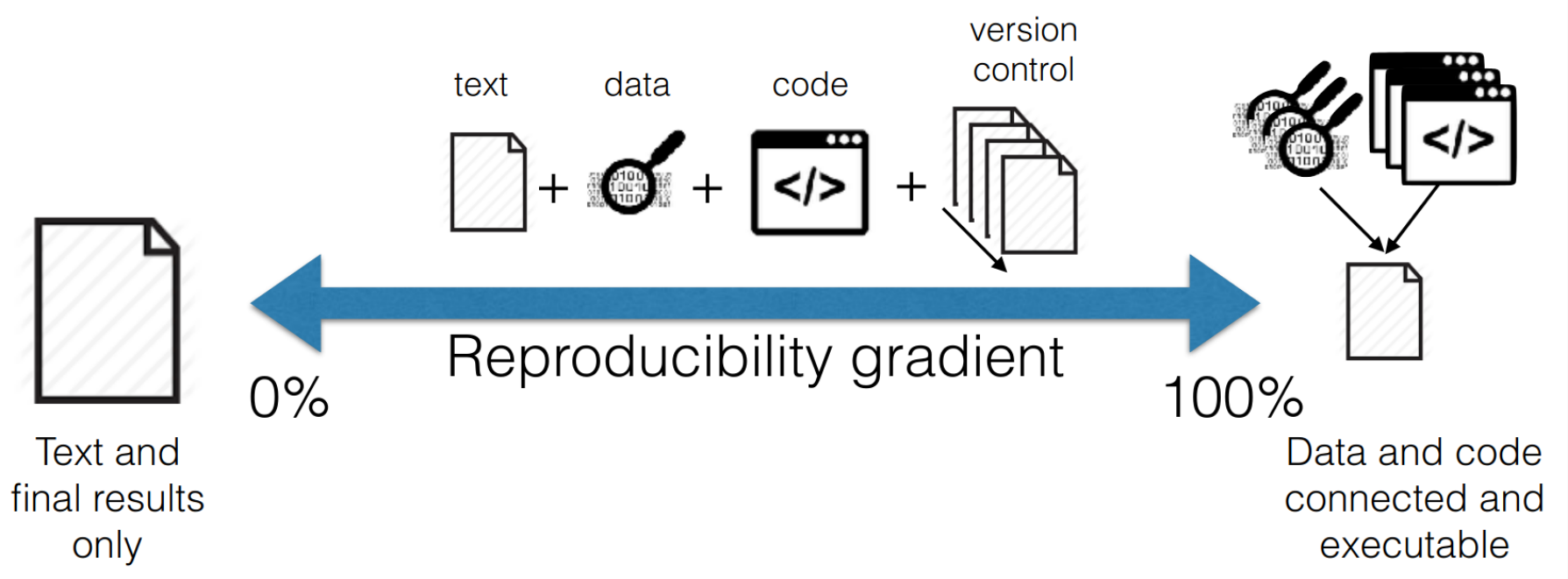
Wolkovich et al 2012

Reproducible workflows facilitate collaboration

and make everyone happier

How to do reproducible research

Reproducibility is a gradient



Rodríguez-Sánchez et al. 2016 (modif. Peng 2011)

Basic reproducibility

Basic reproducibility

- **MANUSCRIPT** (Text + Tables + Figures)
- **DATA** in permanent archive (see Tierney & Ram 2020)
- **CODE** in permanent archive (see Eglen et al 2016)

Permanent archive:

- Zenodo, Dryad, OSF, Figshare, Data Paper...
- NOT GitHub, website...

How to share data

- **Open** format (csv, txt)
- **README** (who, what, when, where, why, how)
- **Describe variables**
- **Licence** (CC0, CC-BY, ODbL)
- **Citation** (DOI)
- **Metadata** standardised (JSON, XML)

Tierney & Ram 2020

How to share code

- Scripts: **plain text** (`.R`)
- **Permanent archive** (eg. Zenodo) with **DOI (citable)**
- Licence
- README

Eglen et al 2016

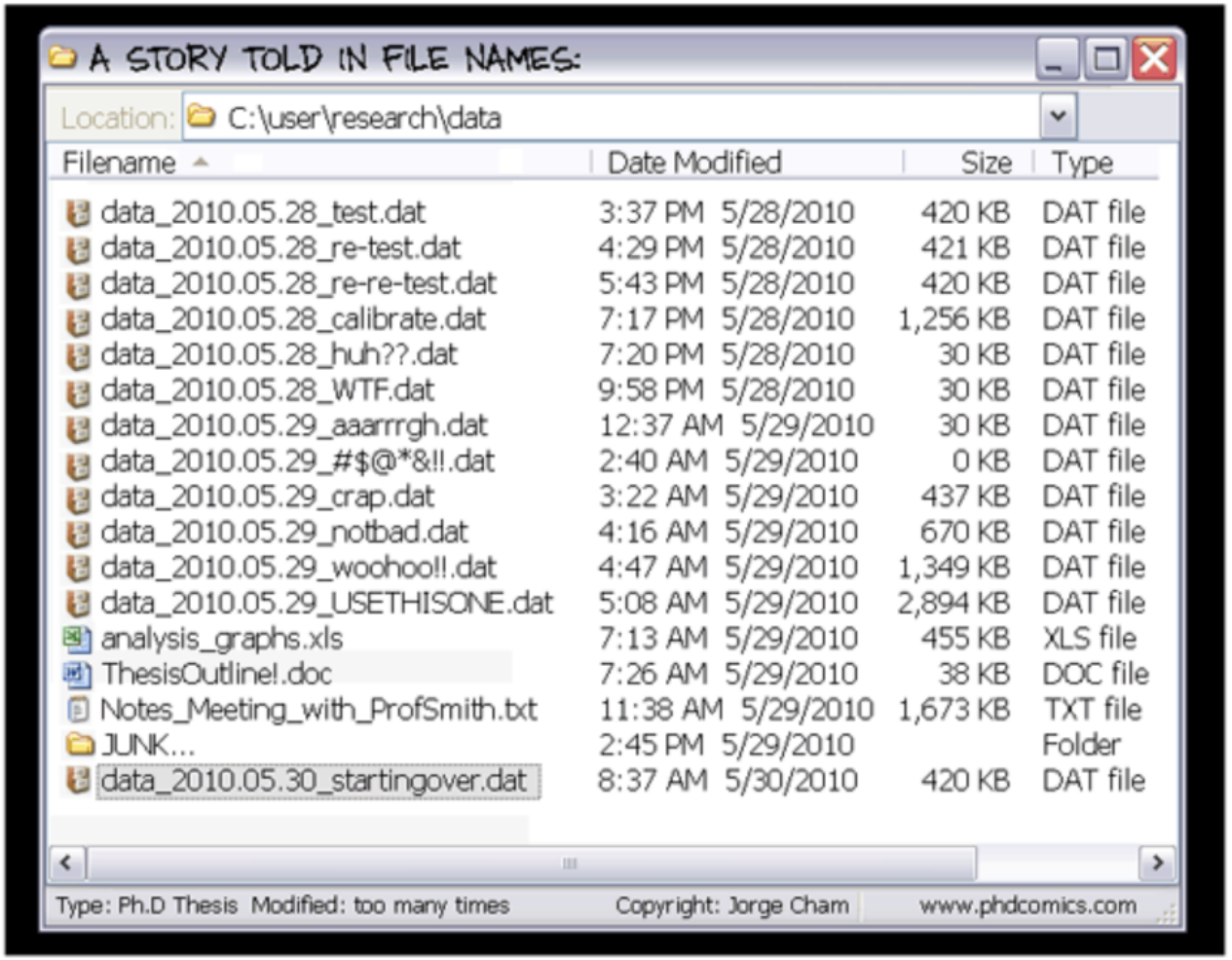
Basic reproducibility

DATA + CODE

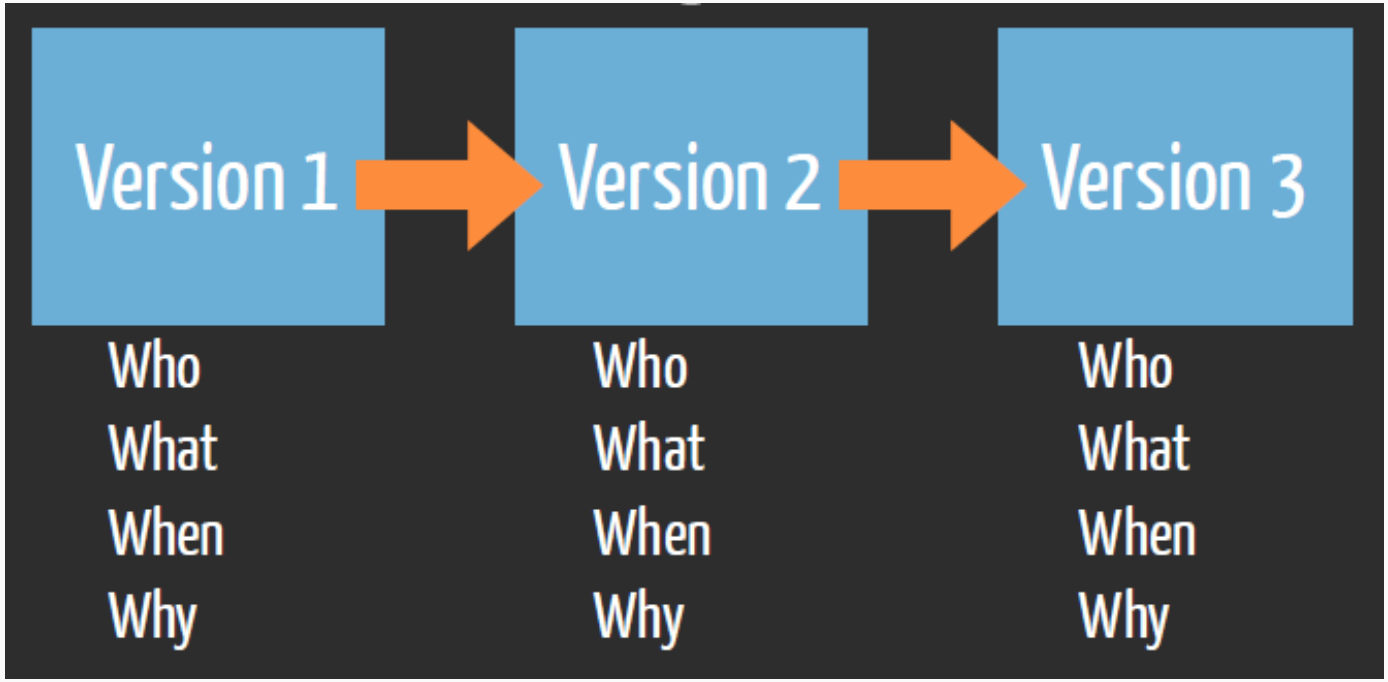
- analysis fully **traceable**
- results can be **regenerated**

Version control

Piled Higher and Deeper *by Jorge Cham* **www.phdcomics.com**



Version control with `git`

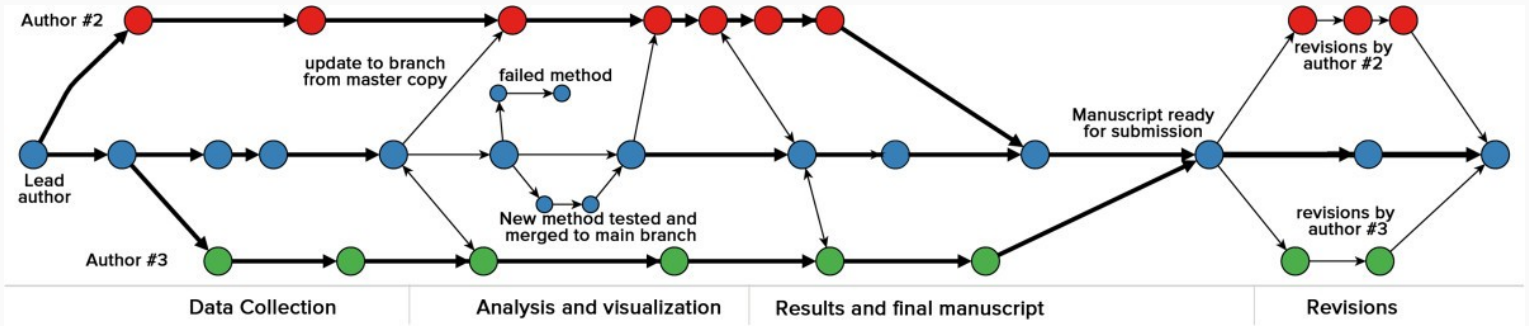


R. Fitzjohn

Much to learn from software engineering

Git can facilitate greater reproducibility and increased transparency in science

Karthik Ram

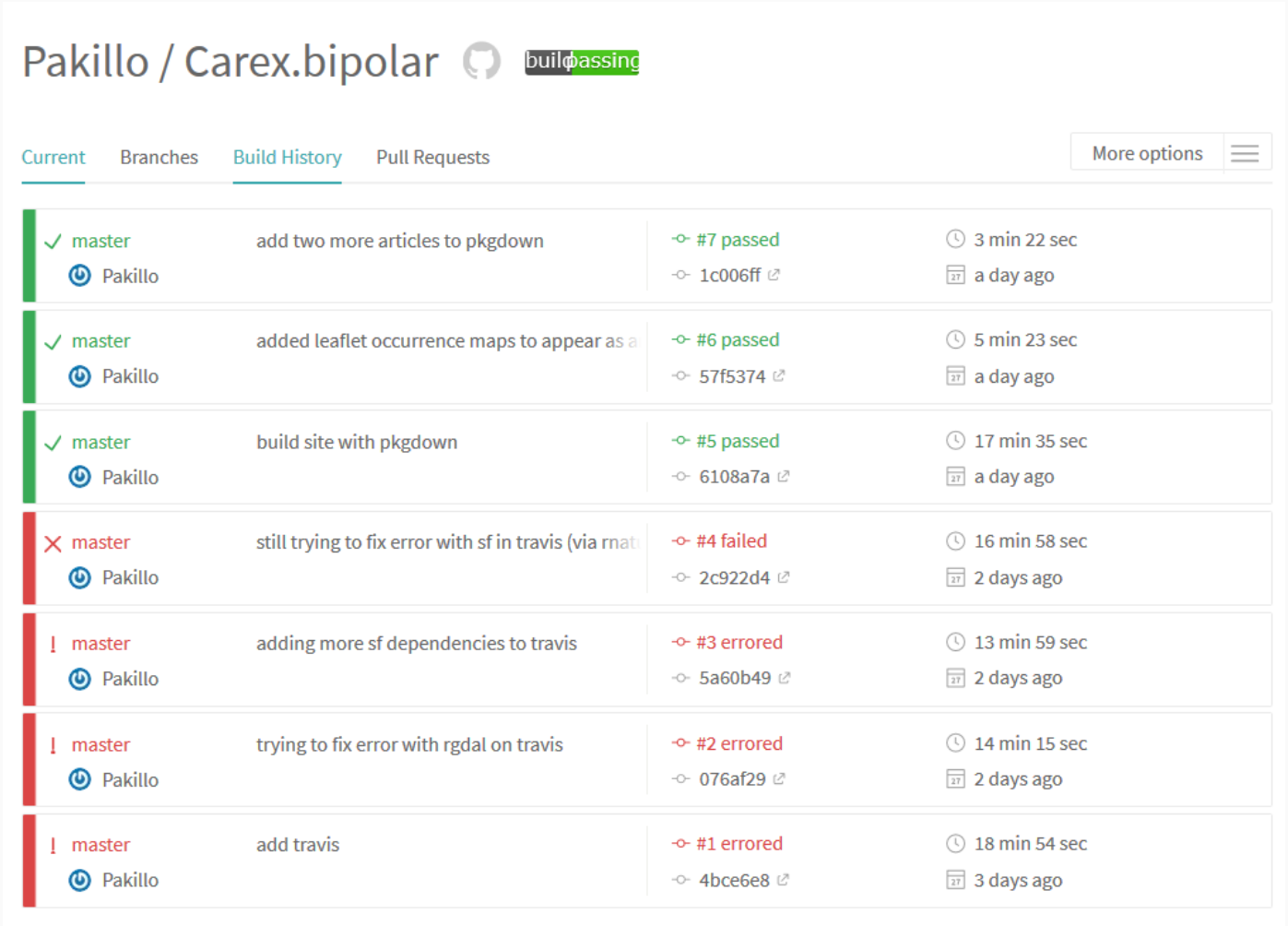


Ram 2013

Automatic checks with Continuous Integration

Reproducibility of computational workflows is automated using continuous analysis

Brett K Beaulieu-Jones[1] & Casey S Greene[2]



Structuring projects

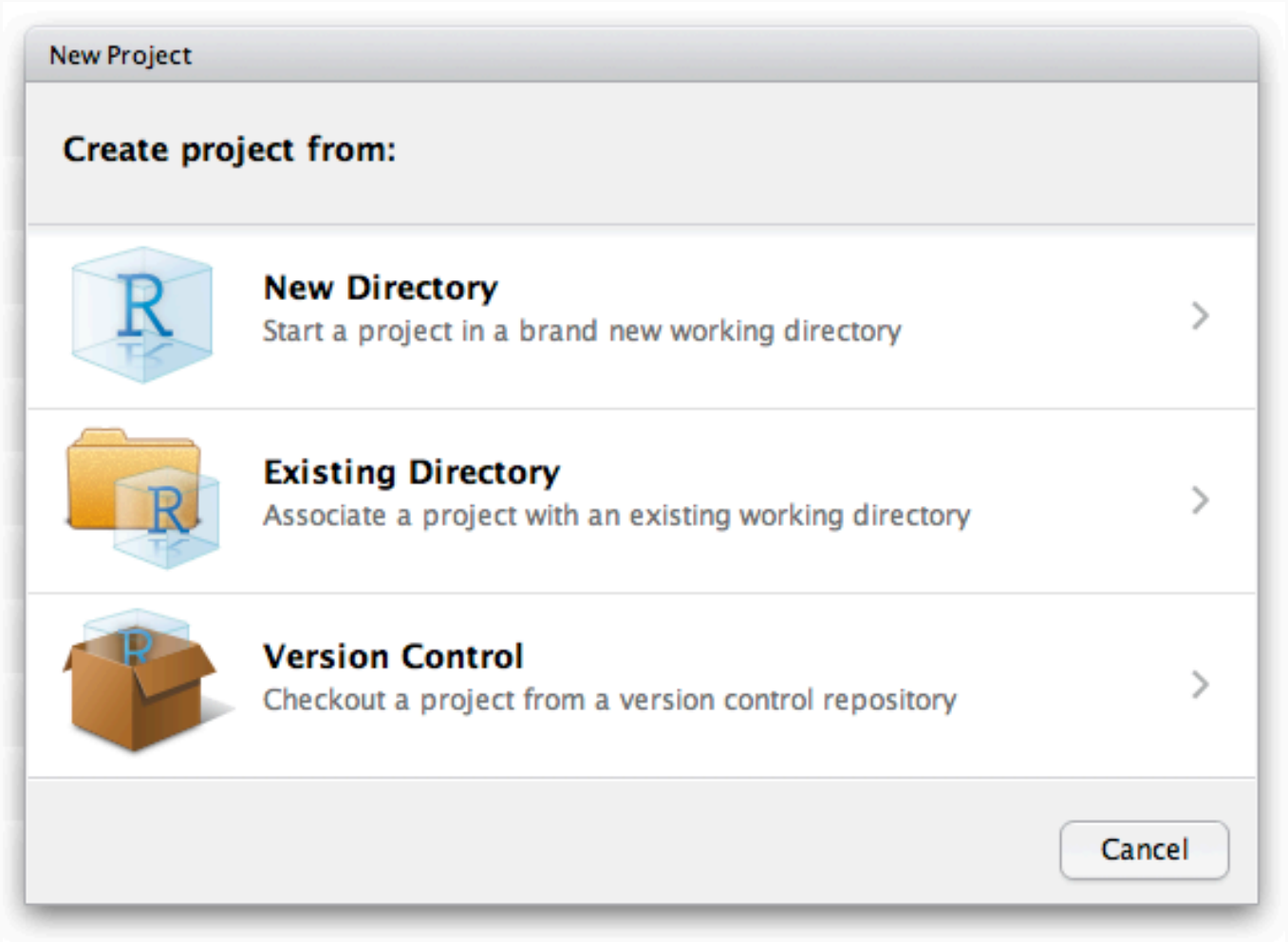
One Project = One Folder

```
myproject
  |
  |- data
  |
  |- code
  |
  |- output (figures etc)
  |
  |- manuscript
```

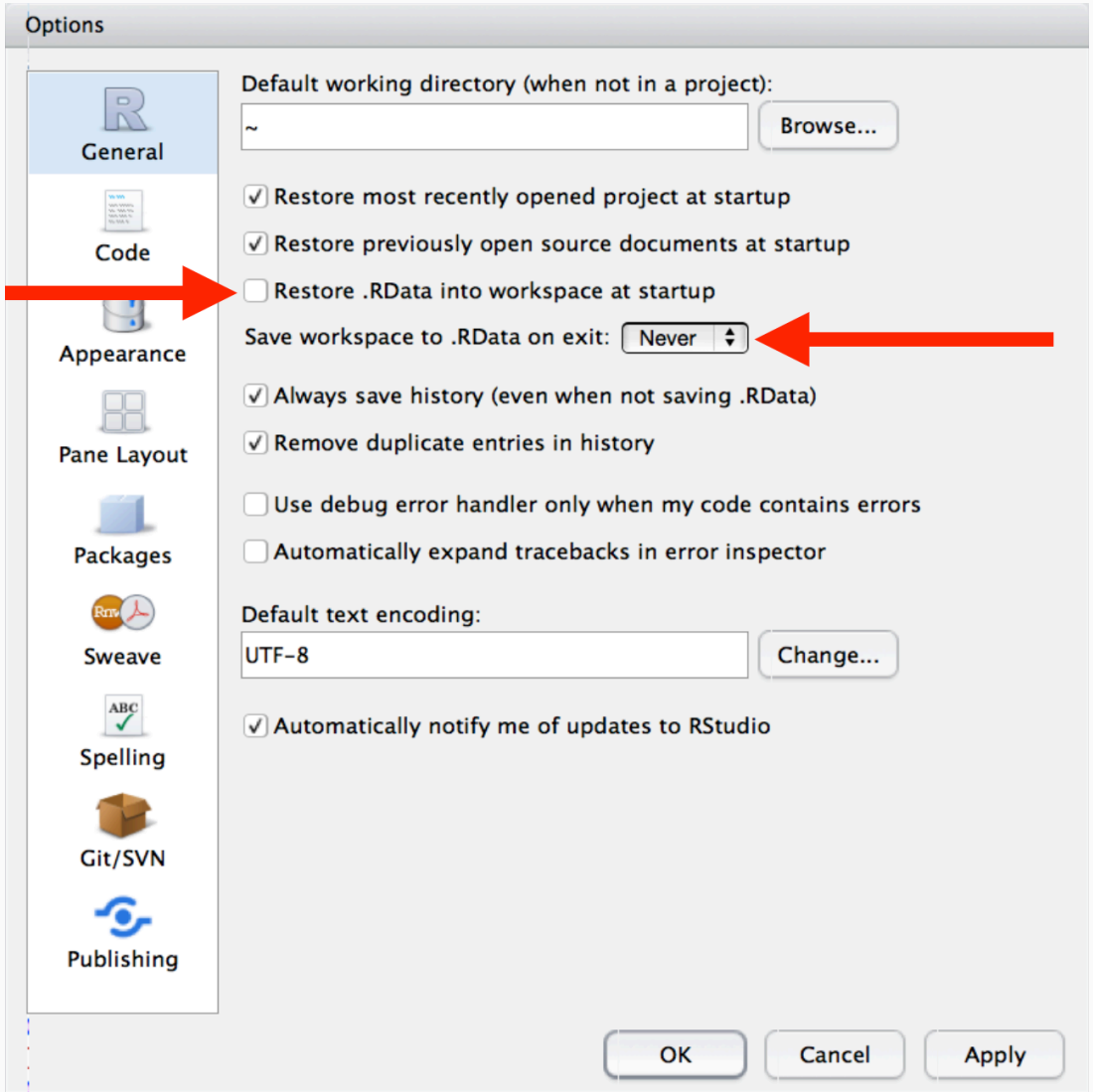
Project-Oriented Workflow: advantages

- Self-contained
- Easy to navigate (file paths)
- Easy to share

Rstudio projects

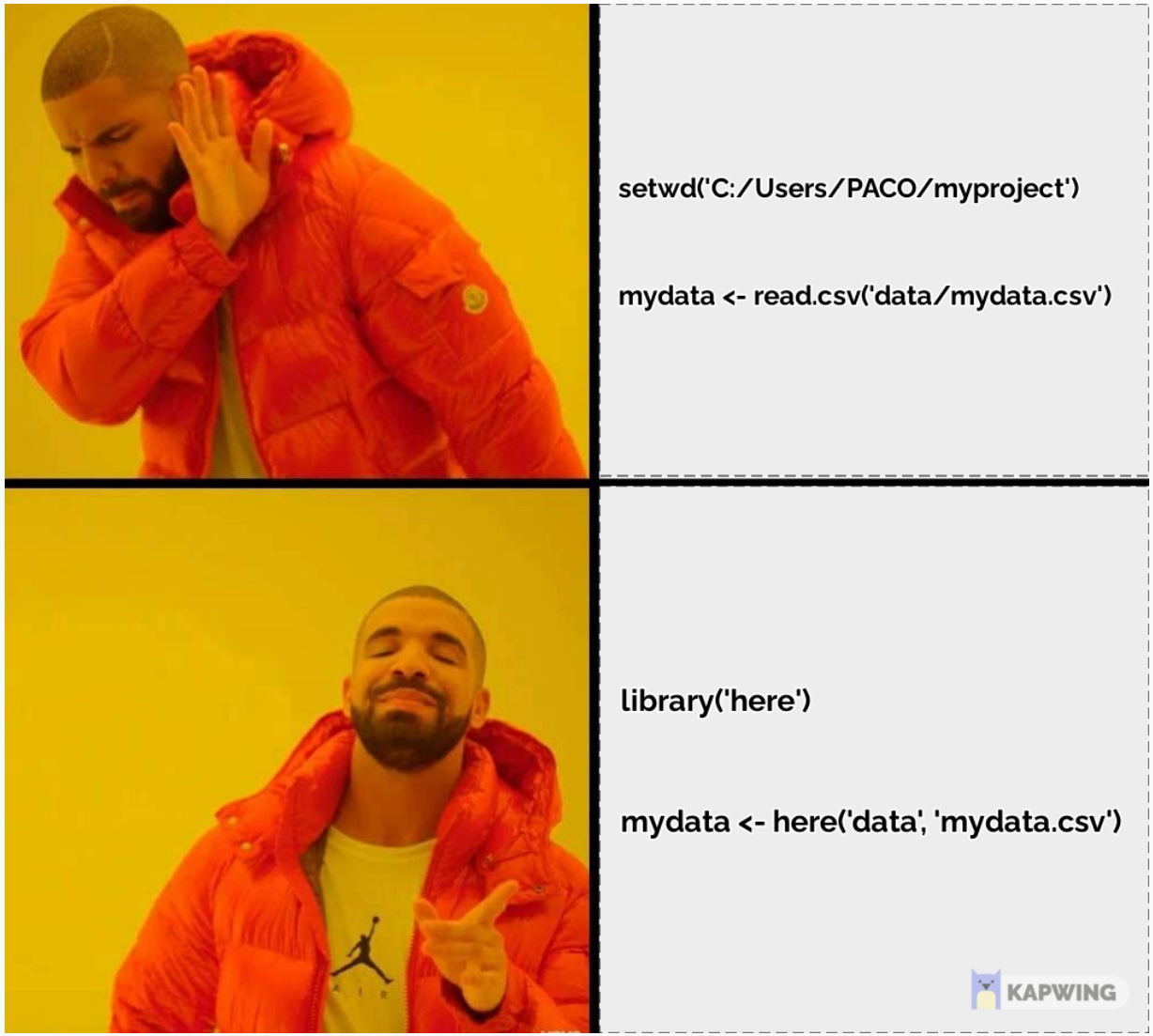


Avoid saving workspace



https://rstats.wtf

Use `here` for file paths



`fertile` package: real-time feedback on reproducibility

```
library('fertile')

setwd("C:/Users/FRS")
```

Error: setwd() is likely to break reproducibility. Use here::here() instead.

https://github.com/baumer-lab/fertile

Structuring projects: guidelines

Guidelines for structuring projects

- All files in **same directory**

Noble 2009, Rodriguez-Sanchez et al 2016, Wilson et al 2017

Guidelines for structuring projects

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- **Raw data** separate from **clean data**

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Noble 2009, Rodriguez-Sanchez et al 2016, Wilson et al 2017

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- README
- License

Noble 2009, Rodriguez-Sanchez et al 2016, Wilson et al 2017

Project organisation example

```
myproject

- data
  - data-raw
  - data-clean

- code

- output (figures etc)

- manuscript

- README
- License
- Makefile
```

README file

- What
- Who
- How
- Licence
- Citation
- etc

README.md

pandanusisotopes

launch binder

This repository contains the data and code for our paper:

> Florin, A. et al. (2020). *Palaeoprecipitation data from Madjedbebe, northern Australia: A novel proxy from ancient pandanus.*

How to cite

Please cite this compendium as:

> Marwick, B., A. Florin et al., (2020). *Compendium of R code and data for Palaeoprecipitation data from Madjedbebe, northern Australia: A novel proxy from ancient pandanus.* Accessed 16 Oct 2020. Online at https://doi.org/xxx/xxx

How to download

You can download the compendium as a zip from from this URL: https://github.com/benmarwick/pandanusisotopes/archive/master.zip

Licenses

Text and figures : CC-BY-4.0

Code : See the DESCRIPTION file

Data : CC-0 attribution requested in reuse

Document your data

https://docs.ropensci.org/dataspice/

```
library("dataspice")
create_spice()   # create CSV templates for metadata

edit_creators()  # open Shiny apps to edit the CSVs
prep_access()
edit_access()
prep_attributes()
edit_attributes()
edit_biblio()

write_spice()  # write machine-readable metadata

build_site()  # build human-readable metadata report
```

Write modular code

Break up scripts

```
prepare_data.R

run_analysis.R

make_figures.R
```

(and `makefile` will run them in the right order)

`makefile` runs code in appropriate order

`makefile.R`

```
source("prepare_data.R")

source("run_analysis.R")

source("make_figures.R")
```

Don’t Repeat Yourself (DRY)

```
dataset %>%
  filter(species == "Laurus nobilis") %>%
  ggplot() +
  geom_point(aes(x, y))

dataset %>%
  filter(species == "Laurus azorica") %>%
  ggplot() +
  geom_point(aes(x, y))
```

Don’t Repeat Yourself

Write functions (documented + tested)

```
plot_species <- function(sp, data) {
  data %>%
    filter(species == sp) %>%
    ggplot() +
    geom_point(aes(x, y))
}
```

Don’t Repeat Yourself

Use functions

```
plot_species(sp = ”Laurus nobilis”, dataset)

plot_species(sp = ”Laurus azorica”, dataset)
```

Don’t Repeat Yourself

Use for loops

```
for (i in species) {
  plot_species(sp = i, dataset)
}
```

Don’t Repeat Yourself

Good ol’ `lapply`

```
lapply(species, plot_species, data = dataset)
```

Don’t Repeat Yourself

```
library("purrr")

map(species, plot_species, data = dataset)
```

Comment your code

Why rather than **What**

```
## Response is not linear, so fit gam rather than lm

model.height <- gam(height ~ s(diameter), data = trees)
```

Use meaningful names for objects

```
m1 <- lm(height ~ diameter, data = trees)
m2 <- gam(height ~ s(diameter), data = trees)
```

Use meaningful names for objects

```
m1 <- lm(height ~ diameter, data = trees)
m2 <- gam(height ~ s(diameter), data = trees)
```

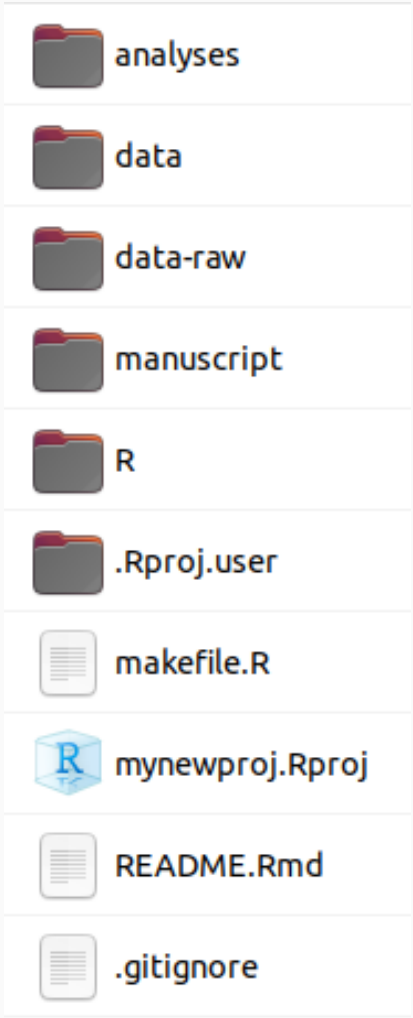
```
model.linear <- lm(height ~ diameter, data = trees)
model.gam <- gam(height ~ s(diameter), data = trees)
```

Project templates

Automatic project creation with `template`

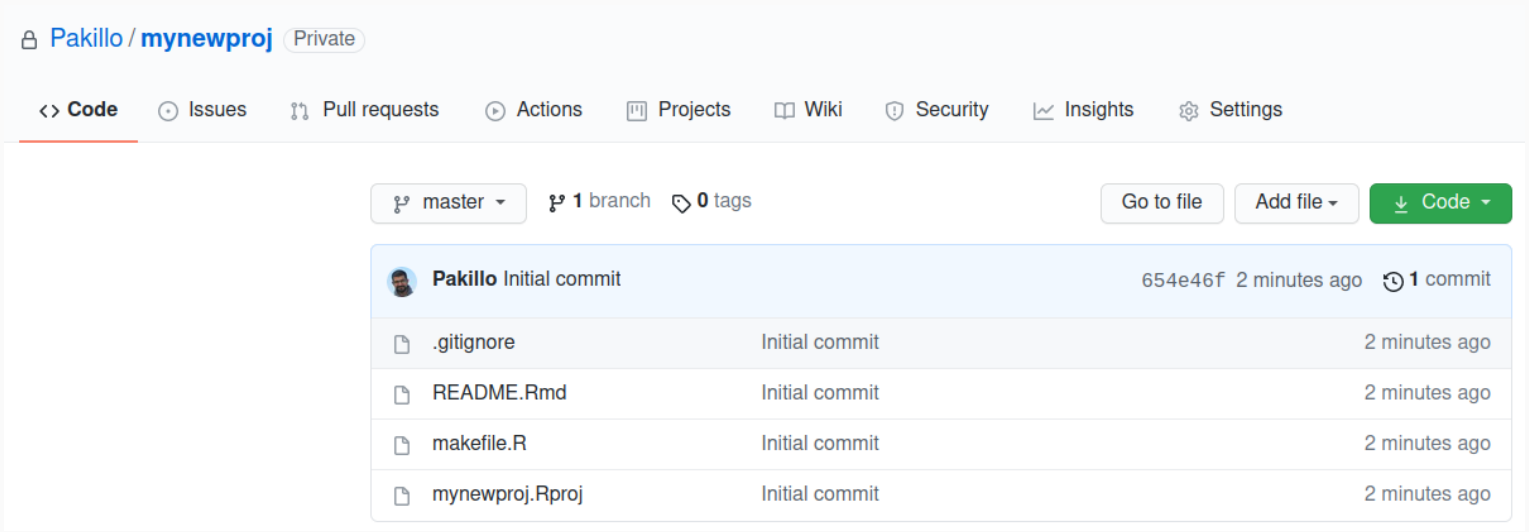
```
library('template')
```

```
new_project("mynewproj",
            package = FALSE)
```



`template`: New projects also on GitHub

```
new_project("mynewproj",
            package = FALSE,
            github = TRUE)
```



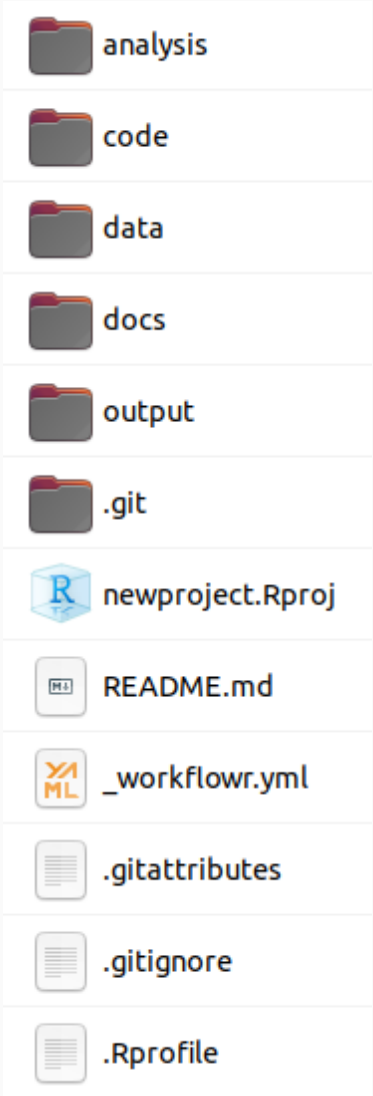
`workflowr`:

reproducible projects with website

`wflow_start` creates project scaffolding

```
library('workflowr')

wflow_start("newproject")
```



`wflow_open` starts new analysis

```
wflow_open("analysis/first-analysis.Rmd")
```

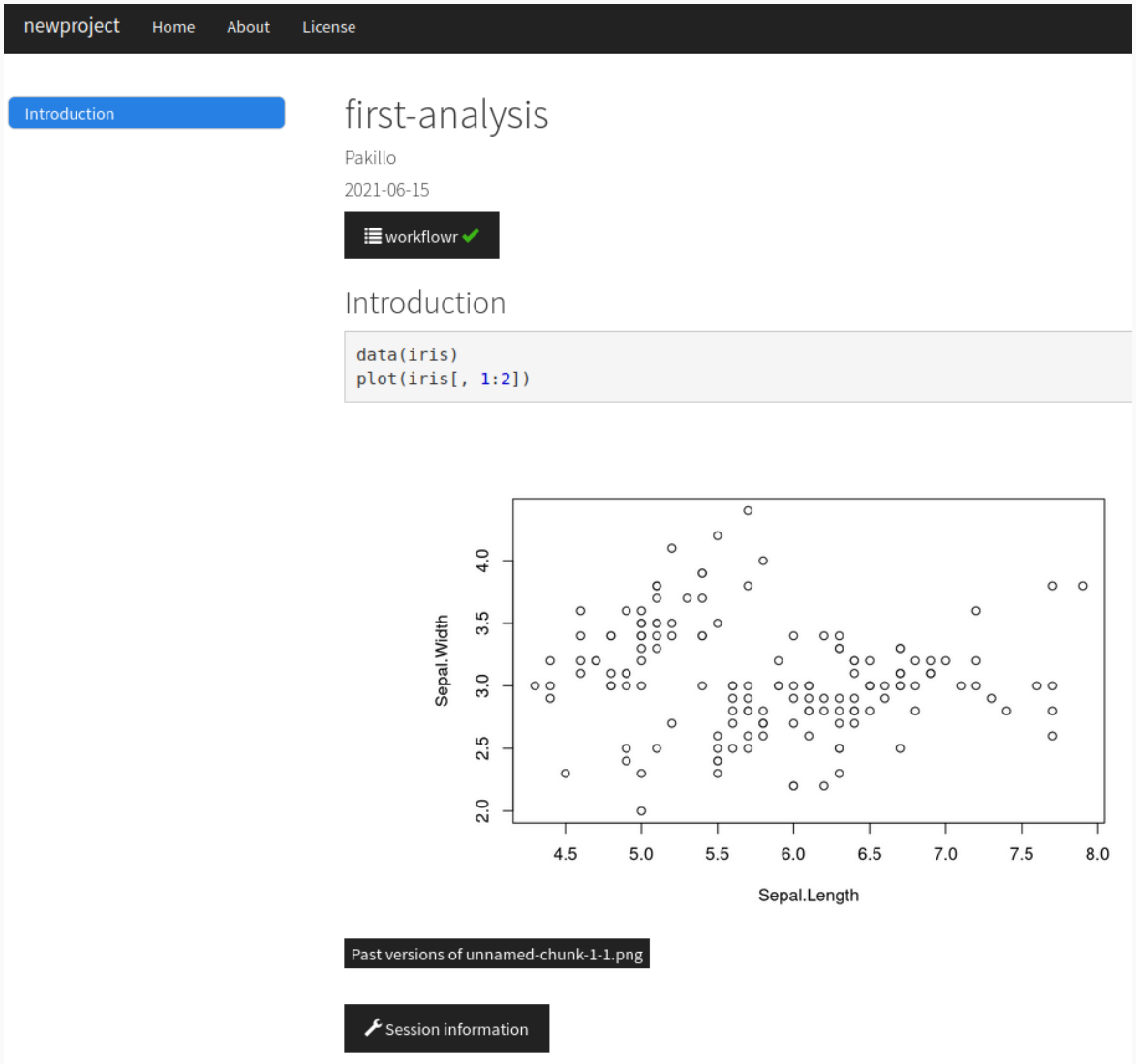
```
---
title: "first-analysis"
author: "Pakillo"
date: "2021-06-15"
output: workflowr::wflow_html
editor_options:
  chunk_output_type: console
---

## Introduction

```{r}
data(iris)
plot(iris)
```
```

`wflow_build` runs analyses and generates website

```
wflow_build()
```



`wflow_publish` commits changes & updates everything

```
wflow_publish(c("analysis/first-analysis.Rmd",
                "analysis/index.Rmd",
                "analysis/about.Rmd",
                "analysis/license.Rmd"),
              message = "Publish initial analyses")
```

Connect with GitHub/GitLab and deploy website

```
wflow_use_github("Pakillo")


wflow_git_push()
```

Research compendia: projects as packages

Projects as packages

- Standard structure

Rodríguez-Sánchez et al. 2016, Marwick et al 2018, but see McBain 2020

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- Promotes modular code, documented and tested

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- Automatic checks (Continuous Integration)

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- Automatic checks (Continuous Integration)
- Automatic code review (`goodpractice`)

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Projects as packages

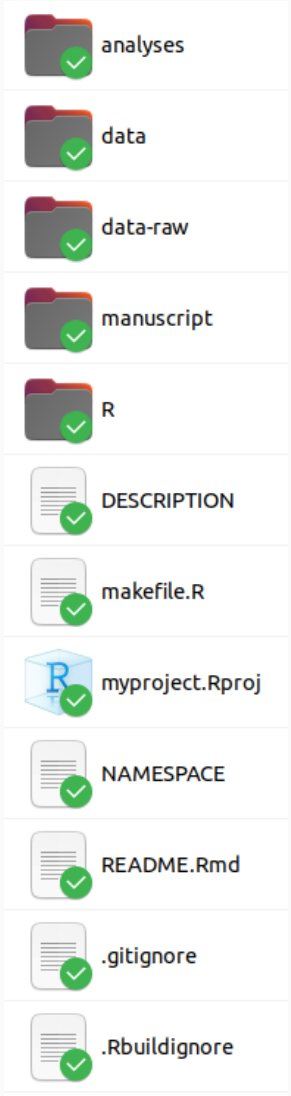
- Standard structure
- Promotes modular code, documented and tested
- Easy to share and run
- Automatic checks (Continuous Integration)
- Automatic code review (`goodpractice`)
- Easily create website with `pkgdown`

Rodríguez-Sánchez et al. 2016, Marwick et al 2018, but see McBain 2020

Creating package structure with `template`

```
library('template')
```

```
new_project("myproject",
            package = TRUE)
```



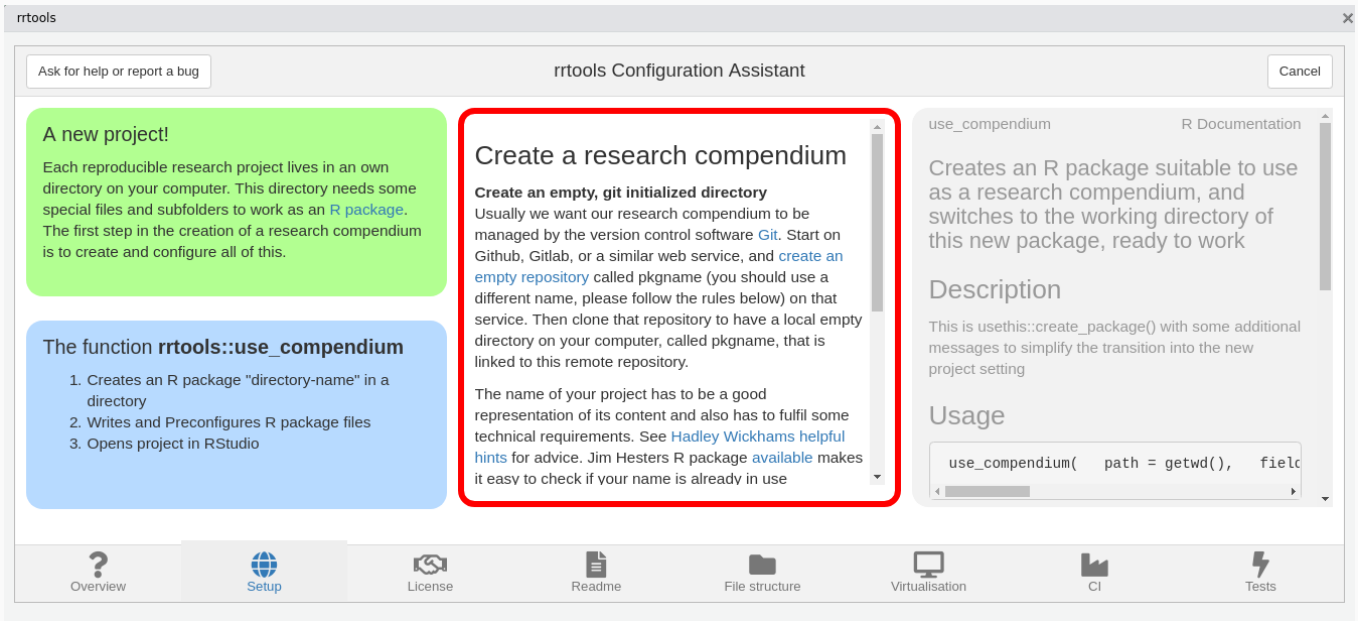
rrtools

`rrtools` creates research compendia

```
library("rrtools")

use_compendium("~/myproject/")
```

Rstudio addin: https://github.com/nevrome/rrtools.addin



`rrtools`: project structure

```
- README
- LICENSE
- DESCRIPTION
- travis.yml
- Dockerfile
- analysis/
  |
  |- paper/
      |- paper.Rmd
      |- references.bib
  |
  |- figures/
  |
  |- data/
      |- raw_data/
      |- derived_data/
```

rcompendium

`rcompendium` creates new project with all scaffolding

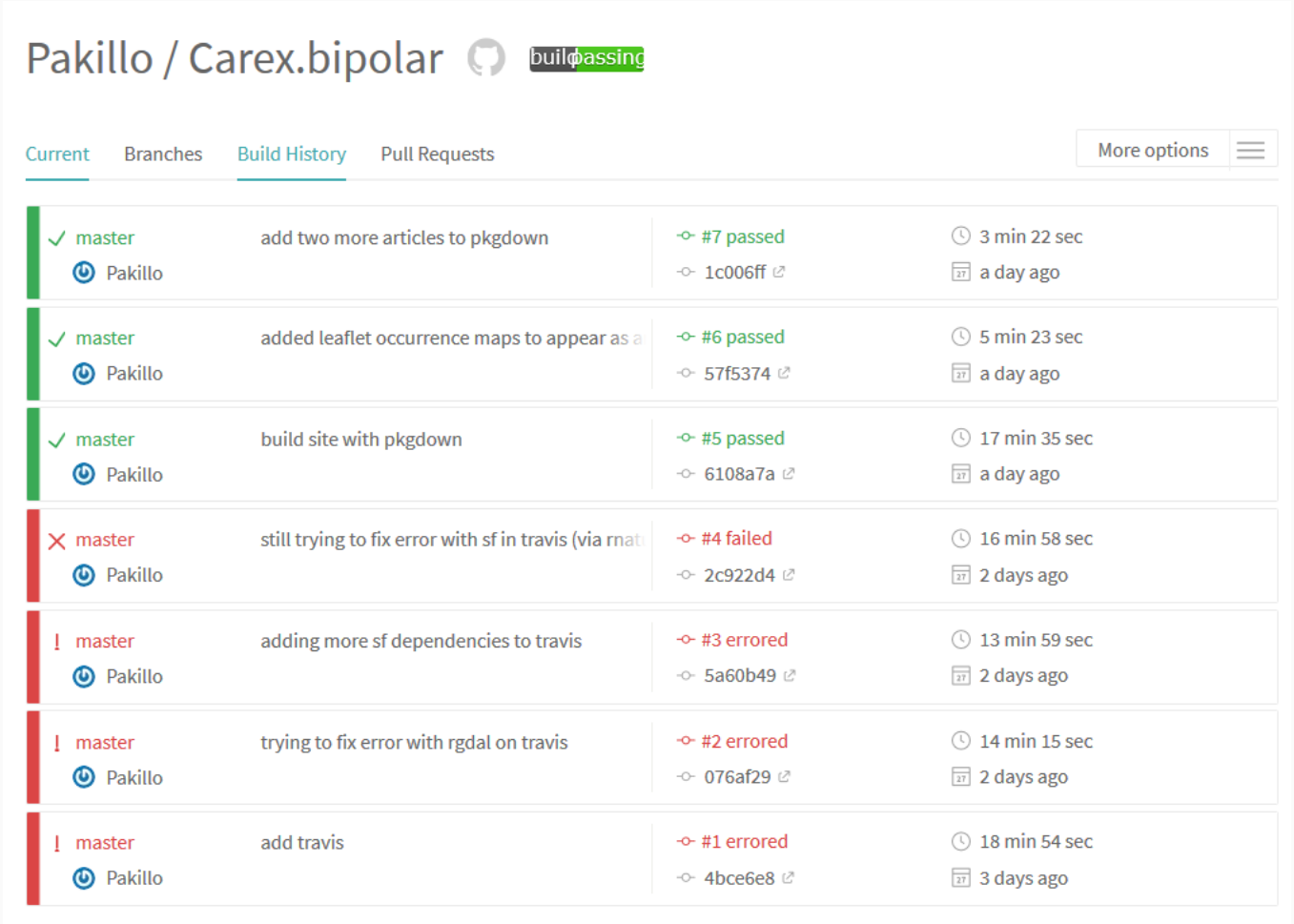
```
library('rcompendium')

new_compendium()
```

- R package structure
- GitHub repository
- Automatic testing & website update

Continuous Integration (GitHub Actions, GitLab CI...)

Automatic testing with every commit!



Minimalistic compendium

https://github.com/cboettig/compendium

- DESCRIPTION (dependencies)
- Manuscript (Rmd)
- GitHub Actions

Data management

Data management

See https://dataoneorg.github.io/Education/bestpractices/

.

1. Planification (e.g. DMPTool)
2. Collection
3. Metadata description (dataspice, EML, Data Packages, DataPackageR)
4. Quality control (e.g. assertr, validate, pointblank)
5. Storage

Document your data

https://docs.ropensci.org/dataspice/

```
library("dataspice")
create_spice()   # create CSV templates for metadata

edit_creators()  # open Shiny apps to edit the CSVs
prep_access()
edit_access()
prep_attributes()
edit_attributes()
edit_biblio()

write_spice()  # write machine-readable metadata

build_site()  # build human-readable metadata report
```

Check data before analysis

```
library("assertr")

dataset %>%
  assert(within_bounds(0, 0.20), fruit.weight) %>%
  assert(in_set("black", "red"), colour)
```

Check out also `pointblank`

Editorial expression of concern

IN THE 3 June issue, *Science* published the Report "Environmentally relevant concentrations of microplastic particles influence larval fish ecology" by Oona M. Lönnstedt and Peter Eklöv (*1*). The authors have notified *Science* of the theft of the computer on which the raw data for the paper were stored. These data were not backed up on any other device nor deposited in an appropriate repository. *Science* is publishing this Editorial Expression of Concern to alert our readers to the fact that no further data can be made available, beyond those already presented in the paper and its supplement, to enable readers to understand, assess, reproduce, or extend the conclusions of the paper.

Jeremy Berg

Editor in Chief

http://science.sciencemag.org/content/354/6317/1242.1

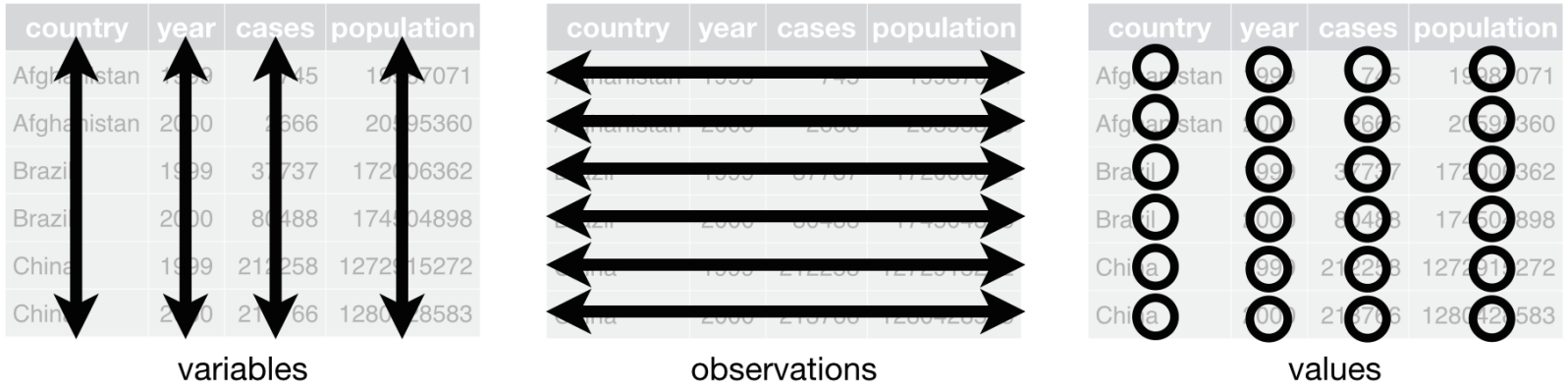
Storage

Use the **cloud**: safe, persistent, easy to share

- Open Science Framework
- GitHub
- Dropbox
- Figshare, Zenodo, etc
- See all data repositories in www.re3data.org

Tidy data

Tidy data



country	year	cases
Afghanistan	1999	745
Afghanistan	2000	2666
Brazil	1999	37737
Brazil	2000	80488
China	1999	212258
China	2000	213766

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Afghanistan	745	2666
Brazil	37737	80488
China	212258	213766

table4

http://r4ds.had.co.nz/tidy.html

Be careful with data entry and management in Excel!

COMMENT Open Access

Gene name errors are widespread in the scientific literature

Mark Ziemann[1], Yotam Eren[1,2] and Assam El-Osta[1,3*]

Abstract

The spreadsheet software Microsoft Excel, when used with default settings, is known to convert gene names to dates and floating-point numbers. A programmatic scan of leading genomics journals reveals that approximately one-fifth of papers with supplementary Excel gene lists contain erroneous gene name conversions.

frequently reused. Our aim here is to raise awareness of the problem.

We downloaded and screened supplementary files from 18 journals published between 2005 and 2015 using a suite of shell scripts. Excel files (.xls and.xlsx suffixes) were converted to tabular separated files (tsv) with ssconvert (v1.12.9). Each sheet within the Excel file was converted to a separate tsv file. Each column of data in the tsv file was screened for the presence of gene sym-

Spreadsheet good practices

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- Input dates as **year, month, day** in separate columns. Or **YYYY-MM-DD** as text.

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- `http://kbroman.org/dataorg/`
- Broman & Woo: Data organization in spreadsheets

Common spreadsheet errors

More than one variable per column

Date collected	Plot	Species-Sex	Weight
1/9/78	1	DM-M	40
1/9/78	1	DM-F	36
1/9/78	1	DS-F	135
1/20/78	1	DM-F	39
1/20/78	2	DM-M	43
1/20/78	2	DS-F	144
3/13/78	2	DM-F	51
3/13/78	2	DM-F	44
3/13/78	2	DS-F	146

Date collected	Plot	Species	Sex	Weight
1/9/78	1	DM	M	40
1/9/78	1	DM	F	36
1/9/78	1	DS	F	135
1/20/78	1	DM	F	39
1/20/78	2	DM	M	43
1/20/78	2	DS	F	144
3/13/78	2	DM	F	51
3/13/78	2	DM	F	44
3/13/78	2	DS	F	146

Source: Data Carpentry

Multiple tables

	A	B	C	D	E	F	G	H
1								
2	lake site May 29 2012						29-May	
3			Bug1	bug2			avr	SEM
4	1	T1	1	1	2	T1	2.6	0.51
5	2	T1	1	2	3	T2	0.2	0.2
6	3	T1	1	3	4	control	0.2	0.2
7	4	T1	1	0	1			
8	5	T1	0	3	3			
9	6	T2	1	0	1			
10	7	T2	0	0	0			
11	8	T2	0	0	0			
12	9	T2	0	0	0			
13	10	T2	0	0	0			
14	11	contro	0	0	0			
15	12	contro	0	0	0			
16	13	contro	0	0	0			
17	14	contro	0	0	0			
18	15	contro	1	0	1			
19								
20								
21	Barn site May 29. 2012							
22		plot	bug1	bug2	general		29-May	
23	1	T1	3	3	6			
24	2	T1	1	4	5		avr	SEM
25	3	T1	0	0	0	T1	2.4	1.288
26	4	T1	0	0	0	T2	0.4	0.245
27	5	T1	0	1	1	control	1	0.316
28	6	T2	0	0	0			
29	7	T2	0	0	0			
30	8	T2	0	1	1			
31	9	T2	0	1	1			
32	10	T2	0	0	0			
33	11	contro	0	0	0			
34	12	contro	0	1	1			
35	13	contro	0	1	1			
36	14	contro	0	1	1			
37	15	contro	0	2	2			
38								
39								

	I	J	K	L	M	N	O	P
1								
2	lake site Jun 12. 2012						12-Jun	
3		plot	bug1	bug 2			avr	SEM
4	1	T1	6	85	91	T1	30.4	15.47126
5	2	T1	8	13	21	T2	0.2	0.2
6	3	T1	11	0	11	control	0.6	0.6
7	4	T1	0	6	6			
8	5	T1	3	20	23			
9	6	T2	0	0	0			
10	7	T2	0	0	0			
11	8	T2	1	0	1			
12	9	T2	0	0	0			
13	10	T2	0	0	0			
14	11	contro	0	0	0			
15	12	contro	0	0	0			
16	13	contro	0	0	0			
17	14	contro	0	0	0			
18	15	contro	3	0	3			
19								
20								
21	Barn site Jun 12. 2012							
22		plot	bug1	bug2	general		12-Jun	
23	1	T1	21	0	21			
24	2	T1	36	74	110		avr	SEM
25	3	T1	13	0	13	T1	30.6	20.10124
26	4	T1	7	0	7	T2	1	0.774597
27	5	T1	2	0	2	control	2.2	1.714643
28	6	T2	1	0	1			
29	7	T2	0	4	4			
30	8	T2	0	0	0			
31	9	T2	0	0	0			
32	10	T2	0	0	0			
33	11	contro	1	0	1			
34	12	contro	0	0	0			
35	13	contro	0	0	0			
36	14	contro	8	1	9			
37	15	contro	0	1	1			
38								
39								

	Q	R	S	T	U	V	W	X
1								
2		lake site Jun 19. 2012					19-Jun	
3		plot	bug1	bug2	general			
4	1	T1	17	80	97		avr	SEM
5	2	T1	44	136	180	T1	77.8	30.384865
6	3	T1	18	0	18	T2	1.8	1.5620499
7	4	T1	0	14	14	control	0.4	0.244949
8	5	T1	10	70	80			
9	6	T2	1	7	8			
10	7	T2	0	1	1			
11	8	T2	0	0	0			
12	9	T2	0	0	0			
13	10	T2	0	0	0			
14	11	control	0	0	0			
15	12	control	0	0	0			
16	13	control	0	0	0			
17	14	control	0	1	1			
18	15	control	0	1	1			
19								
20								
21	Barn site Jun 19 . 2012							
22		plot	bug1	bug2	general		19-Jun	
23	1	T1	5	0	5			
24	2	T1	65	502	567		avr	SEM
25	3	T1	10	7	17	T1	119.4	111.92882
26	4	T1	0	6	6	T2	5	2.1908902
27	5	T1	0	2	2	control	2.8	0.969536
28	6	T2	0	8	8			
29	7	T2	0	12	12			
30	8	T2	0	0	0			
31	9	T2	3	0	3			
32	10	T2	2	0	2			
33	11	control	0	5	5			
34	12	control	1	1	2			
35	13	control	0	0	0			
36	14	control	0	5	5			
37	15	control	0	2	2			
38								
39								

	Y	Z	AA	AB	AC	AD	AE	AF
1								
2		Lake site Jun 26. 2012					26-Jun	
3		plot	bug1	bug2	general			
4	1	T1	52	191	243		avr	SEM
5	2	T1	50	270	320	T1	141.6	60.313
6	3	T1	6	0	6	T2	0.2	0.2
7	4	T1	0	39	39	control	0	0
8	5	T1	4	96	100			
9	6	T2	0	1	1			
10	7	T2	0	0	0			
11	8	T2	0	0	0			
12	9	T2	0	0	0			
13	10	T2	0	0	0			
14	11	control	0	0	0			
15	12	control	0	0	0			
16	13	control	0	0	0			
17	14	control	0	0	0			
18	15	control	0	0	0			
19								
20								
21	Barn Site Jun 26 . 2012							
22		plot	bug1	bug2	general		26-Jun	
23	1	T1	0	0	0		avr	SEM
24	2	T1	44	2057	2101	T1	431.8	417.33
25	3	T1	12	20	32	T2	0.4	0.4
26	4	T1	0	16	16	control	1.2	0.5831
27	5	T1	0	10	10			
28	6	T2	0	0	0			
29	7	T2	0	0	0			
30	8	T2	0	0	0			
31	9	T2	0	0	0			
32	10	T2	0	2	2			
33	11	control	0	2	2			
34	12	control	1	0	1			
35	13	control	0	0	0			
36	14	control	0	3	3			
37	15	control	1	0	0			
38								
39								

Multiple tabs

Could you avoid new tab by adding a column to original spreadsheet?

Using formatting, comments, etc to convey information

Plot: 2			
Date collecte	Species	Sex	Weight
1/8/14	NA		
1/8/14	DM	M	44
1/8/14	DM	M	38
1/8/14	OL		
1/8/14	PE	M	22
1/8/14	DM	M	38
1/8/14	DM	M	48
1/8/14	DM	M	43
1/8/14	DM	F	35
1/8/14	DM	M	43
1/8/14	DM	F	37
1/8/14	PF	F	7
1/8/14	DM	M	45
1/8/14	OT		
1/8/14	DS	M	157
1/8/14	OX		
2/18/14	NA	M	218
2/18/14	PF	F	7
2/18/14	DM	M	52

measurement device not calibrated

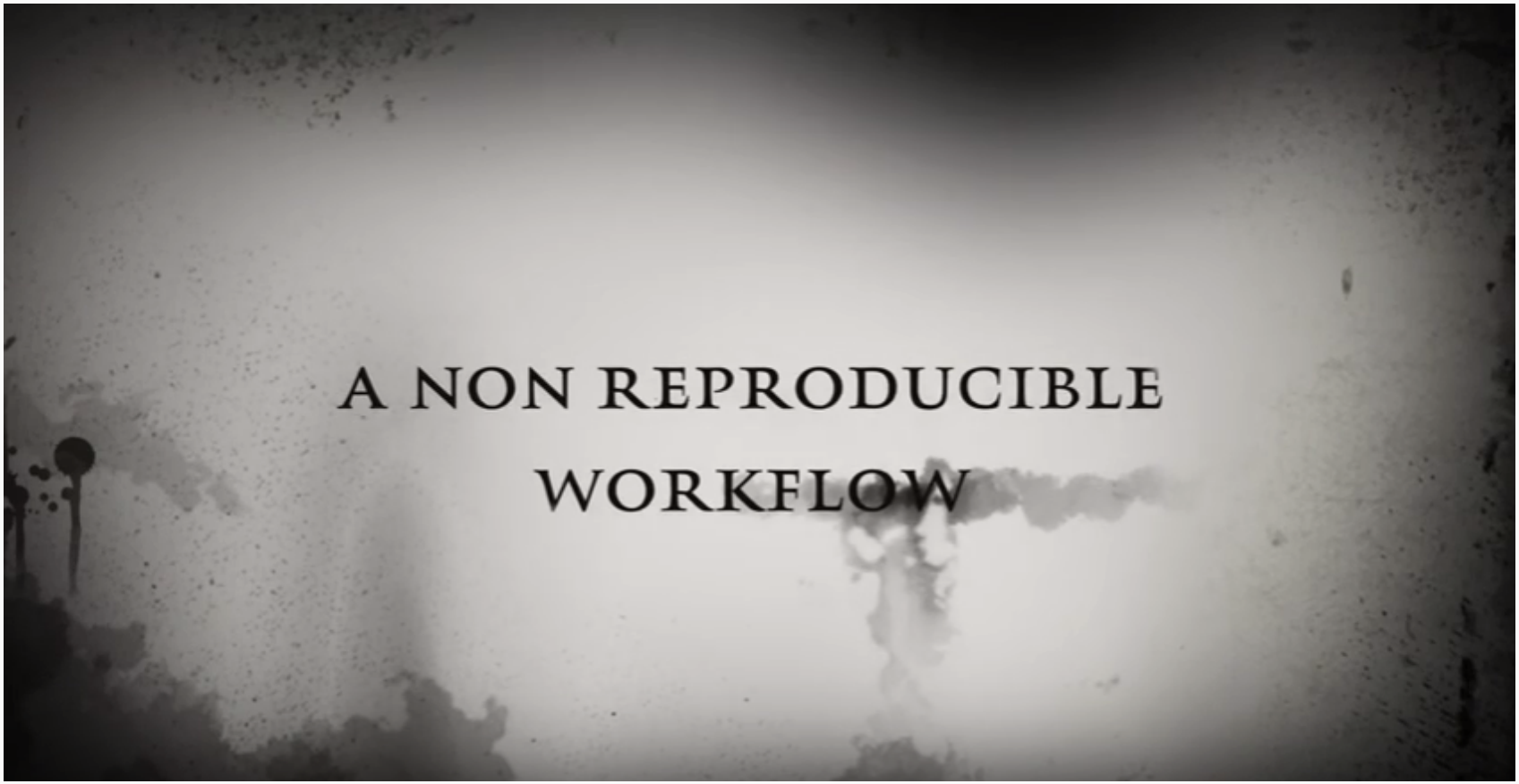
Date collecte	Species	Sex	Weight	Calibrated
1/8/14	NA			
1/8/14	DM	M	44	Y
1/8/14	DM	M	38	Y
1/8/14	OL			
1/8/14	PE	M	22	Y
1/8/14	DM	M	38	Y
1/8/14	DM	M	48	Y
1/8/14	DM	M	43	Y
1/8/14	DM	F	35	Y
1/8/14	DM	M	43	Y
1/8/14	DM	F	37	Y
1/8/14	PF	F	7	Y
1/8/14	DM	M	45	Y
1/8/14	OT			
1/8/14	DS	M	157	N
1/8/14	OX			
2/18/14	NA	M	218	N
2/18/14	PF	F	7	Y
2/18/14	DM	M	52	Y

Your turn: tidy up this messy dataset

https://ndownloader.figshare.com/files/2252083

Reproducible dynamic documents with Rmarkdown

A scary movie... with happy ending

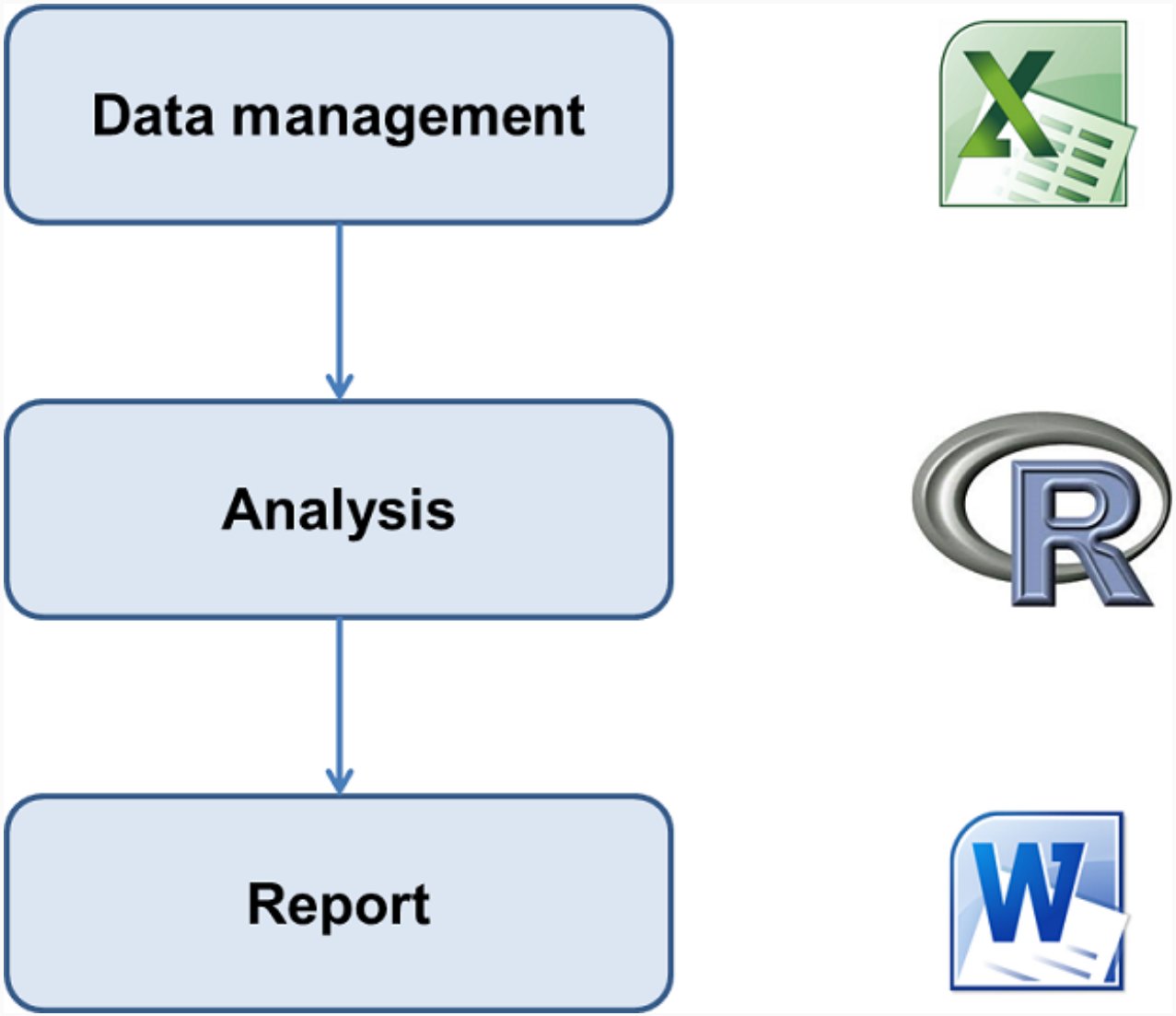


https://youtu.be/s3JldKoA0zw

A typical research workflow

1. Prepare data (**spreadsheet**)
2. Analyse data (**R**)
3. Write report/paper (**Word**)
4. Start the email attachments nightmare...

This workflow is broken



Problems of a broken workflow

- How did you do this? What analysis is behind this figure? Did you account for ...?

Problems of a broken workflow

- How did you do this? What analysis is behind this figure? Did you account for ...?
- What dataset was used? Which individuals were left out? Where is the clean dataset?

Problems of a broken workflow

- How did you do this? What analysis is behind this figure? Did you account for ...?
- What dataset was used? Which individuals were left out? Where is the clean dataset?
- Oops, there is an error in the data. Can you repeat the analysis? And update figures/tables in Word!

Manual copy-paste is tedious & problematic

```
Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept) -0.0651657  0.4264970  -0.153    0.879
sunshine     0.0100228  0.0004232  23.683   <2e-16
```

'Transcribing numbers **from stats software by hand** was the largest source of errors'

(Eubank 2016)

Trevor A. Branch
@TrevorABranch

Follow

My rule of thumb: every analysis you do on a dataset will have to be redone 10–15 times before publication. Plan accordingly. #Rstats

Your **closest collaborator** is you 6 months ago,

and you don’t respond to emails.

(P. Wilson)

Even **you** will struggle to reproduce

your own results from a few weeks/months ago.

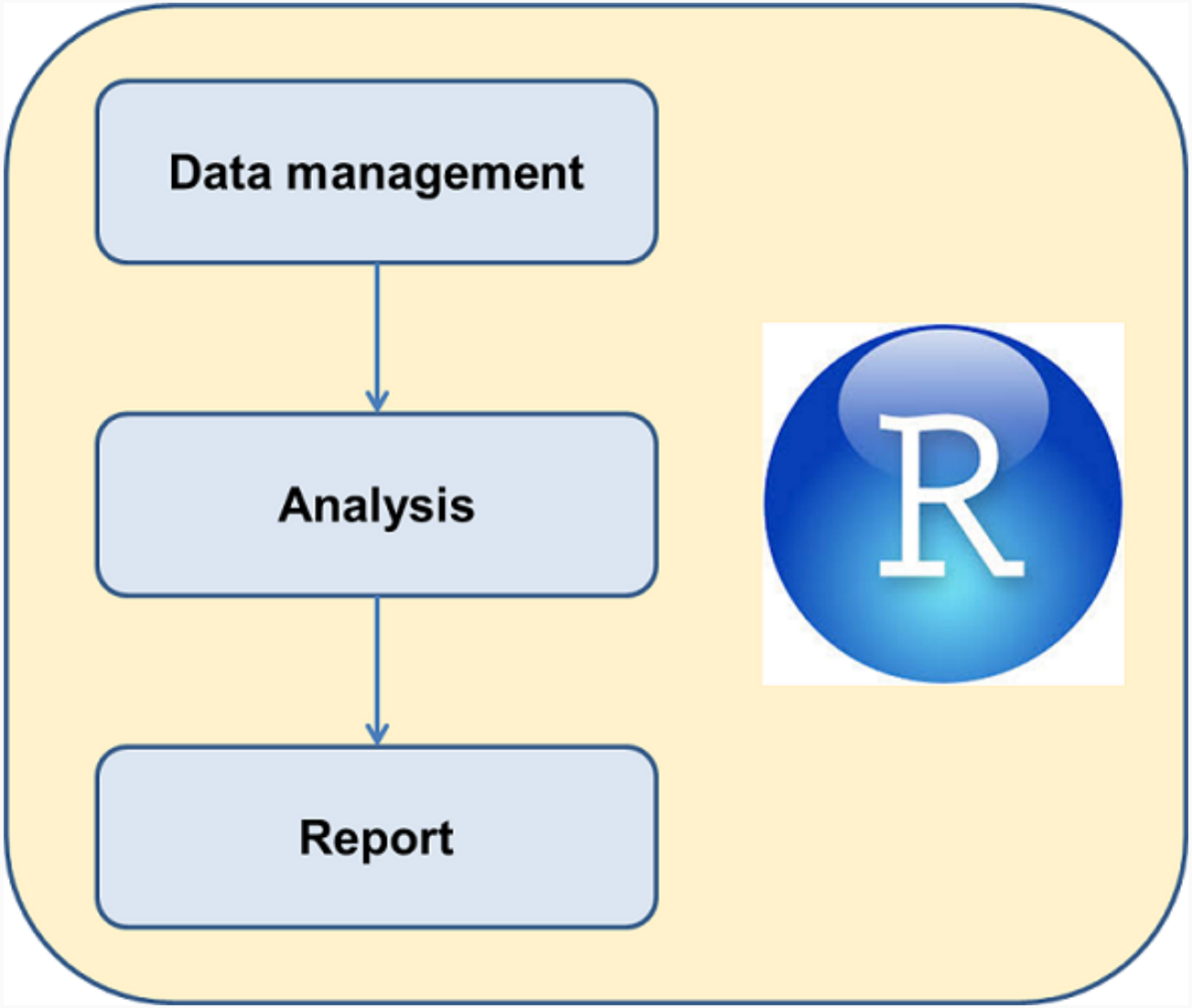
Writing reproducible manuscripts is hard

Revising non-reproducible manuscripts is even harder

.

Also, please note that because rev#1 asked to re-calculate effect sizes (...) we need to change every single number in the main text.

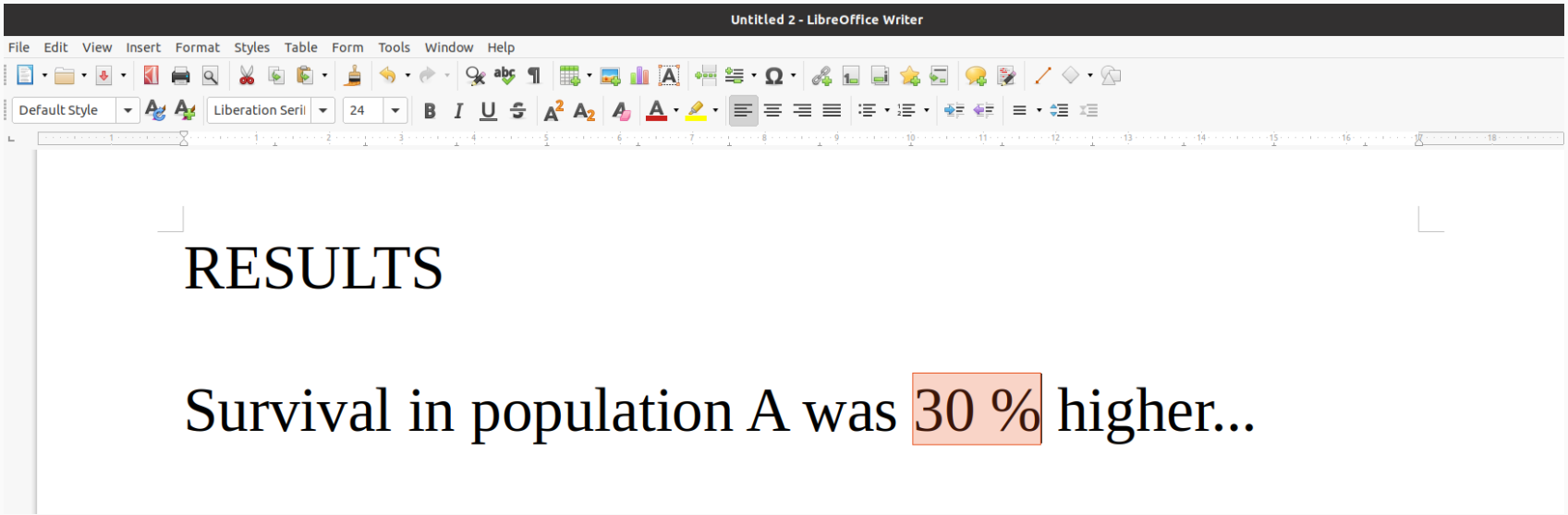
Dynamic reports



Rmarkdown documents

- **Fully reproducible** (trace all results inc. tables and plots)
- **Dynamic** (regenerate with 1 click)
- **Multiple outputs**:
  - documents (HTML, Word, PDF)
  - presentations (HTML, PDF, PowerPoint)
  - books
  - websites...

Where does this value come from?



Dynamic documents with Rmarkdown

Rmarkdown:

> Survival in population A was `` `r surv.diff` `` % higher

Output:

> Survival in population A was **30** % higher

Dynamic documents with Rmarkdown

```
mydata <- read.csv("data.txt")
```

Rmarkdown:

> We measured `` `r nrow(mydata)` `` individuals

Output:

> We measured **100** individuals

> *Much better than copy-paste!*

Rmarkdown: code (R, Python, etc) + text (Markdown)

````
---
title: "Does sunshine make people happy?"
author: "FRS"
output: word_document
---

## Introduction

It is well known that individual well-being can be influenced by climatic conditions.


## Methods

```{r echo=FALSE}
## Read data
data <- read.table("data.txt", header = TRUE)

# Fit linear model
model <- lm(happiness ~ sunshine, data = data)
```

We collected data on `r nrow(data)` individuals and fitted a linear model.
````

Metadata
(YAML)

Text
(Markdown)

Code
(R, Python...)

Code chunk options

````
```{r echo=FALSE, eval=TRUE, cache=TRUE, fig.height=3}
plot(iris)
```
````

https://yihui.org/knitr/options/

Code chunk options

````
```{r}
#| echo = FALSE
#| eval = TRUE
#| fig.cap = "My figure caption"
plot(iris)
```
````

Naming chunks helps debugging

```
processing file: test.Rmd
  |.........                                                       |  14%
  ordinary text without R code

  |.................                                               |  29%
label: setup (with options)
List of 1
 $ include: logi FALSE

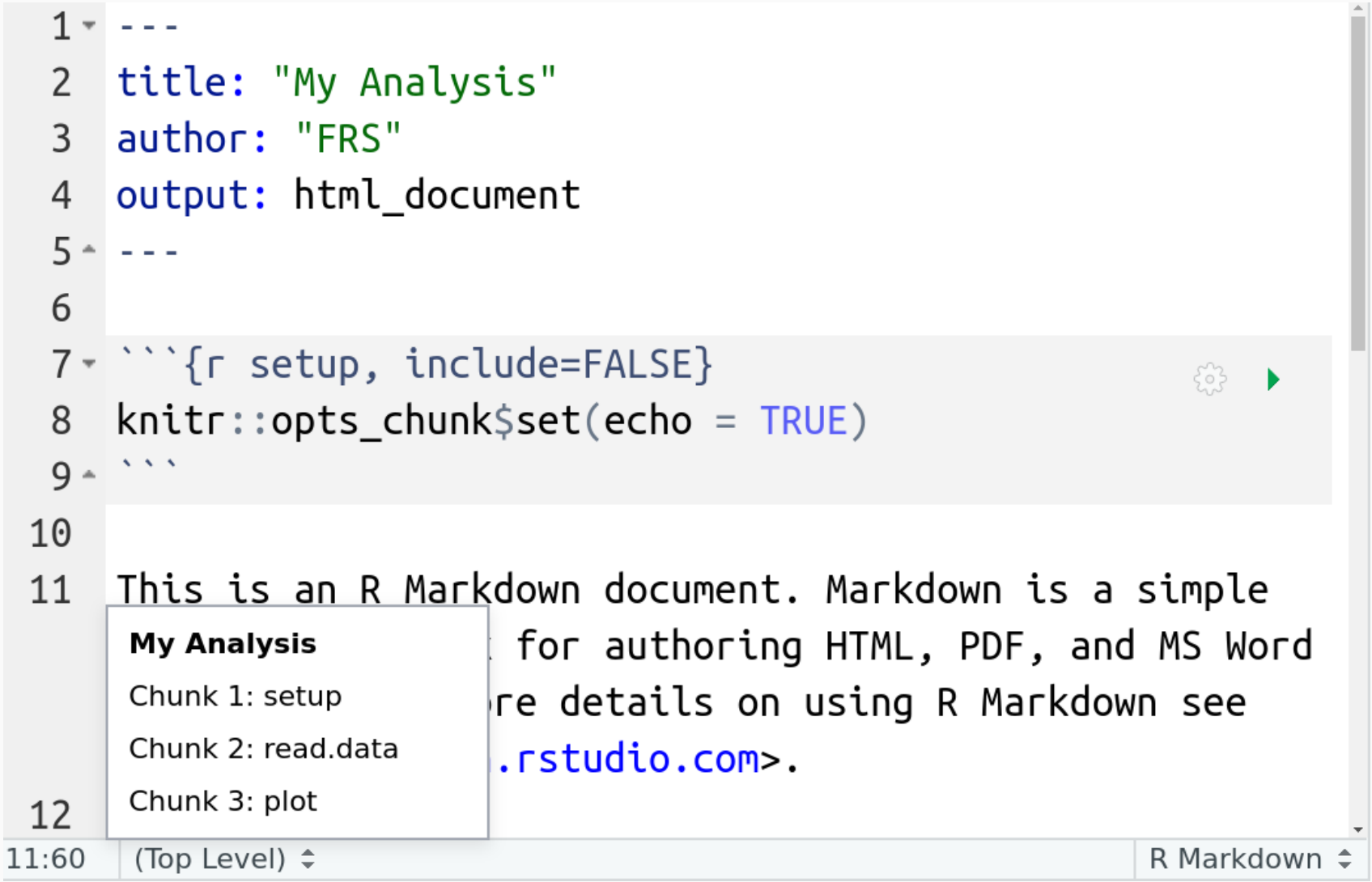
  |.........................                                       |  43%
  ordinary text without R code

  |.................................                               |  57%
label: read.data
  |.........................................                       |  71%
  ordinary text without R code

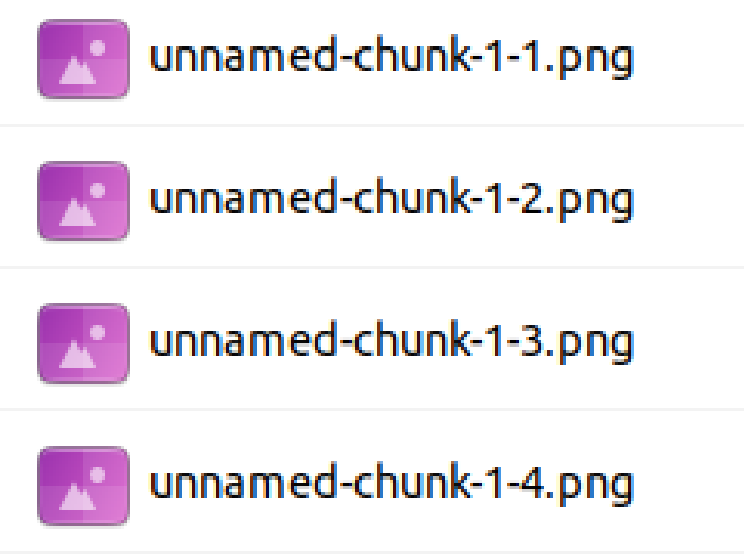
  |.................................................               |  86%
label: plot (with options)
List of 1
 $ echo: logi FALSE


Quitting from lines 28-29 (test.Rmd)
Error in eval(predvars, data, env) : object 'specie' not found
Calls: <Anonymous> ... plot.formula -> eval -> eval -> <Anonymous> -> eval -> eval
Execution halted
```

Naming chunks helps navigating long docs



Naming chunks: figure files take chunk name



¡Not only R! Python, Julia, C++, SQL, Stan, etc

`knitr` engines:

```
 [1] "asis"       "asy"        "awk"        "bash"       "block"      "block2"
 [7] "bslib"      "c"          "cat"        "cc"         "coffee"     "comment"
[13] "css"        "ditaa"      "dot"        "embed"      "eviews"     "exec"
[19] "fortran"    "fortran95"  "gawk"       "go"         "groovy"     "haskell"
[25] "highlight"  "js"         "julia"      "lein"       "mysql"      "node"
[31] "octave"     "perl"       "php"        "psql"       "python"     "R"
[37] "Rcpp"       "Rscript"    "ruby"       "sas"        "sass"       "scala"
[43] "scss"       "sed"        "sh"         "sql"        "stan"       "stata"
[49] "targets"    "tikz"       "verbatim"   "zsh"
```

Markdown: easy text formatting

```
# Header

## Subheader

*italic*

**bold**

[a link](https://example.com)
```

.

Handy: https://thinkr-open.github.io/remedy/

Or use Visual Markdown Editor

Regenerate Word/PDF/HTML with one click

a

```
---
title: "Does sunshine make people happy?"
output: pdf_document
bibliography: refs.bib
---

# Introduction

Climate influences individual well-being [@Rehdanz_2005].
However, ...

# Methods

```{r echo=FALSE}
# read data
data <- read.table("data.txt", header=T)
data[10,1] <- 11   # correct error

# fit linear model
model <- lm(happiness ~ sunshine, data=data)
```

We collected data on `r nrow(data)` individuals and fitted a
linear model.

Results

We found that...

```{r echo=FALSE, results='asis'}
# make table with model output
print(xtable::xtable(model), comment = FALSE)
```

```{r echo=FALSE, fig.height=3, fig.width=3, fig.align='center'}
visreg::visreg(model) # plot
```

Discussion

Our results confirm that happiness is related to
sunshine (slope = `r coef(model)[2]`).

References
```

b

Does sunshine make people happy?

Introduction

Climate influences individual well-being (Rehdanz and Maddison 2005). However, ...

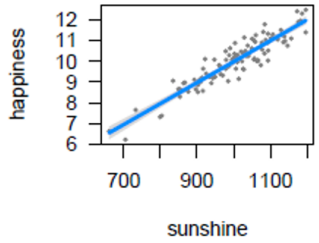
Methods

We collected data on 100 individuals and fitted a linear model.

Results

We found that...

	Estimate	Std. Error	t value	Pr(>|t|)
(Intercept)	-0.0986	0.4271	-0.23	0.8180
sunshine	0.0101	0.0004	23.75	0.0000



Discussion

Our results confirm that happiness is related to sunshine (slope = 0.0100652).

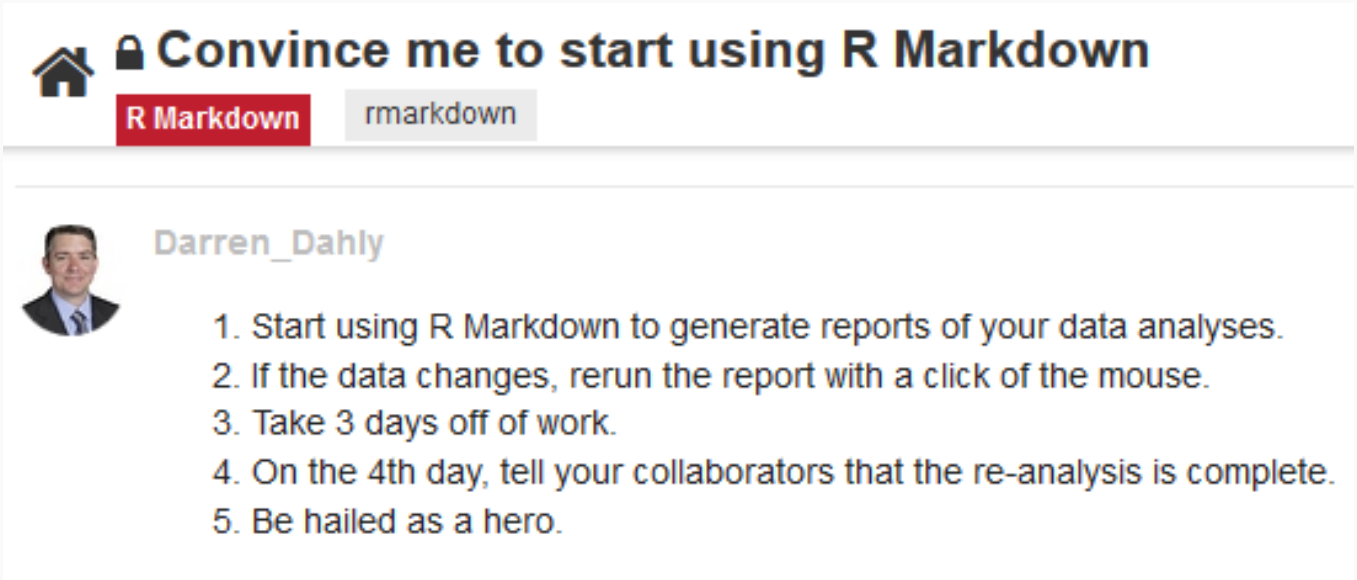
References

Rehdanz, Katrin, and David Maddison. 2005. "Climate and Happiness." *Ecological Economics* 52 (1). Elsevier BV: 111–25. doi:10.1016/j.ecolecon.2004.06.015.

Spotted error in the data? No problem!

- Make changes in Rmarkdown document
- Click `Knit` in Rstudio
- Report will **update automatically!**

Why Rmarkdown?



https://community.rstudio.com/t/convince-me-to-start-using-r-markdown/1636/12

Your turn

Create, edit and share Rmarkdown document

File > New File > Rmarkdown

Write text

Insert code chunks

Change chunk options (echo, eval, etc)

HTML/Word/PDF output

PDF generation requires LaTeX

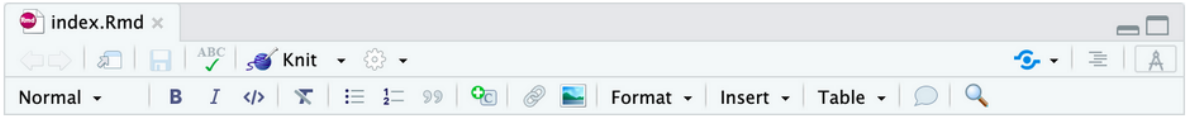
```
library('tinytex')

install_tinytex()
```

Rmarkdown bells and whistles

‘Visual Rmarkdown’: Rmd as in word processor

The editor toolbar includes buttons for the most commonly used formatting commands:



Additional commands are available on the **Format**, **Insert**, and **Table** menus:

Format

- Bold ⌘B
- Italic ⌘I
- Code ⌘D
- Text ▸
- Bullets & Numbering ▸
- Blockquote
- Line Block
- Div Block...
- Code Block...
- Raw ▸
- Clear Formatting ⌘\
- Edit Attributes... F4

Insert

- Rmd Chunk ⌥⌘I
- Image... ⇧⌘I
- Link... ⌘K
- Horizontal Rule ⌘_
- Definition ▸
- Inline Math
- Display Math
- Footnote ⇧⌘F7
- Citation...
- Div Block...
- Code Block...
- YAML Block
- Comment ⇧⌘C

Table

- Insert Table... ⌥⌘T
- ✓ Table Header
- Table Caption
- Align Column ▸
- Insert Row Above
- Insert Row Below
- Insert Column Left
- Insert Column Right
- Delete Row
- Delete Column
- Delete Table

https://rstudio.github.io/visual-markdown-editing

Automatic table generation

```
model <- lm(happiness ~ sunshine, data = mydata)
xtable(model)
```

	Estimate	Std. Error	t value	Pr(>|t|)
(Intercept)	-0.0652	0.4265	-0.15	0.8789
sunshine	0.0100	0.0004	23.68	0.0000

Many alternatives: `gtsummary`, `modelsummary`, `huxtable`, etc

`equatiomatic` describes model structure

We fitted a linear model:

```
library('equatiomatic')
model <- lm(happiness ~ sunshine, data = mydata)
extract_eq(model)
```

$$\text{happiness} = \alpha + \beta_1(\text{sunshine}) + \epsilon \tag{1}$$

Models that describe themselves!

```
library("report")
model <- lm(happiness ~ sunshine, data = mydata)
report(model)
```

We fitted a linear model (estimated using OLS) to predict happiness with sunshine (formula: happiness ~ sunshine). The model explains a statistically significant and substantial proportion of variance (R2 = 0.85, F(1, 98) = 560.90, p < .001, adj. R2 = 0.85). The model's intercept, corresponding to sunshine = 0, is at -0.07 (95% CI [-0.91, 0.78], t(98) = -0.15, p = 0.879). Within this model:

- The effect of sunshine is statistically significant and positive (beta = 0.01, 95% CI [9.18e-03, 0.01], t(98) = 23.68, p < .001; Std. beta = 0.92, 95% CI [0.85, 1.00])

Standardized parameters were obtained by fitting the model on a standardized version of the dataset. 95%

Confidence Intervals (CIs) and p-values were computed using a Wald t-distribution approximation.

Insert equations with LaTeX

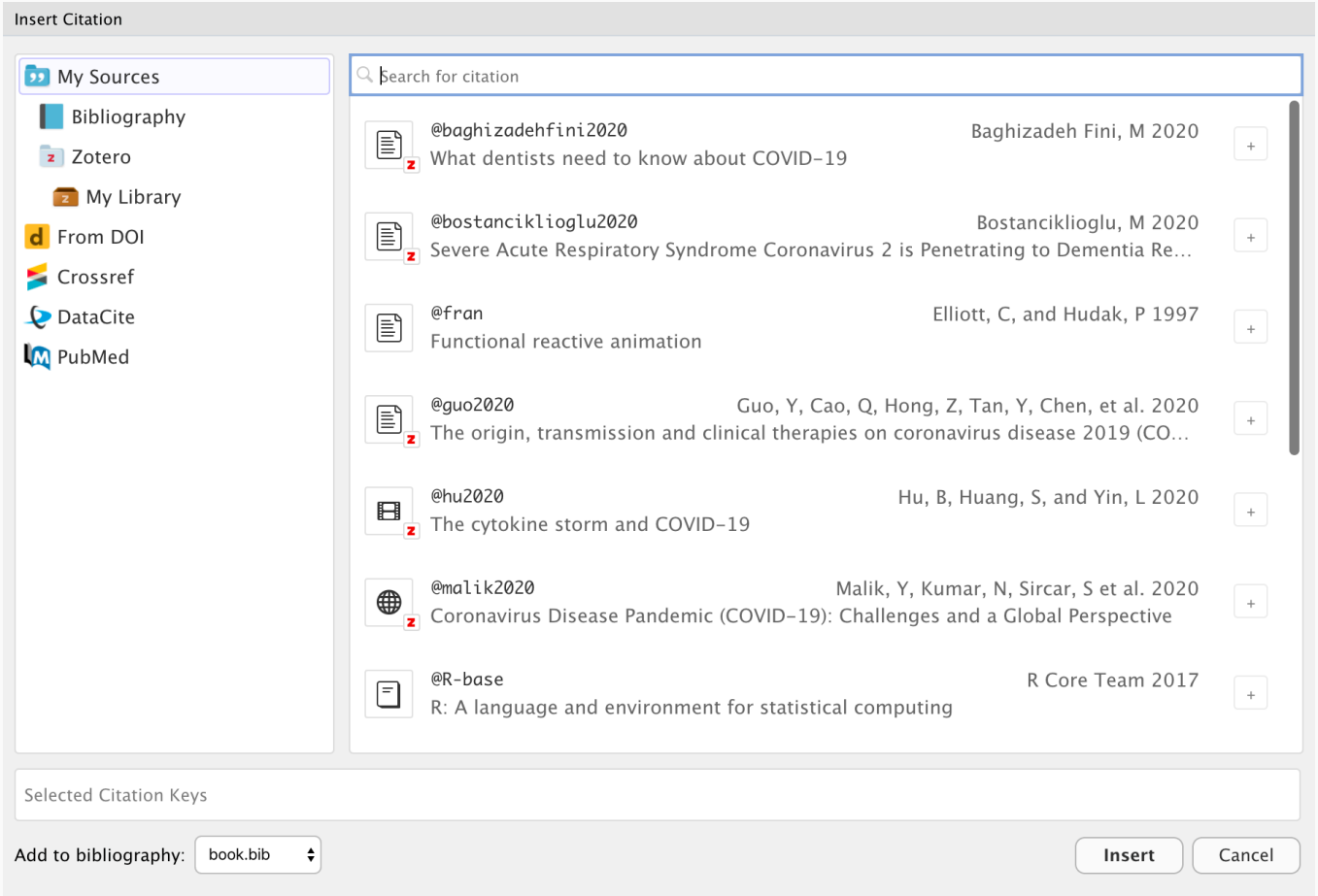
Using LaTeX:

```
$$
y \sim N(\mu, \sigma^2)
$$
```

$$y \sim N(\mu, \sigma^2)$$

- Mathpix: https://github.com/jonocarroll/mathpix

Citing bibliography



https://rstudio.github.io/visual-markdown-editing/#/citations

Using BibTeX file with references

```
---
title: "My awesome Rmd"
output: html_document
bibliography: references.bib
---
```

Format bibliography for any journal

```
---
title: "Does sunshine make people happy?"
author: "FRS"
output: word_document
bibliography: myrefs.bib
csl: ecology-letters.csl
---
```

Thousands of Citation Styles:

https://www.zotero.org/styles

https://github.com/citation-style-language/styles

Rmarkdown templates

- rticles
- papaja
- rrtools
- pinp
- rmdTemplates
- pagedreport
- GitHub!

My cool paper written in Rmarkdown

F. Rodriguez-Sanchez[a,1,2] and And Friends[a,b]

[a]Some Institute of Technology, Department, Street, City, State, Zip; [b]Another University Department, Street, City, State, Zip

This manuscript was compiled on September 18, 2018

Please provide an abstract of no more than 250 words in a single paragraph. Abstracts should explain to the general reader the major contributions of the article. References in the abstract must be cited in full within the abstract itself and cited in the text.

one | two | optional | optional | optional

This PNAS journal template is provided to help you write your work in the correct journal format. Instructions for use are provided below.

Note: please start your introduction without including the word "Introduction" as a section heading (except for math articles in the Physical Sciences section); this heading is implied in the first paragraphs.

Guide to using this template

Please note that whilst this template provides a preview of the typeset manuscript for submission, to help in this preparation, it will not necessarily be the final publication layout. For more detailed information please see the PNAS Information for Authors.

Author Affiliations. Include department, institution, and complete address, with the ZIP/postal code, for each author. Use lower case letters to match authors with institutions, as shown in the example. Authors with an ORCID ID may supply this information at submission.

Submitting Manuscripts. All authors must submit their articles at PNAScentral. If you are using Overleaf to write your article, you can use the "Submit to PNAS" option in the top bar of the editor window.

Format. Many authors find it useful to organize their manuscripts with the following order of sections; Title, Author Affiliation, Keywords, Abstract, Significance Statement, Results, Discussion, Materials and methods, Acknowledgments, and References. Other orders and headings are permitted.

Manuscript Length. PNAS generally uses a two-column format averaging 67 characters, including spaces, per line. The maximum length of a Direct Submission research article is six pages and a PNAS PLUS research article is ten pages including all text, spaces, and the number of characters displaced by figures, tables, and equations. When submitting tables, figures, and/or equations in addition to text, keep the text for your manuscript under 39,000 characters (including spaces) for Direct Submissions and 72,000 characters (including spaces) for PNAS PLUS.

References. References should be cited in numerical order as they appear in text; this will be done automatically via bibtex, e.g. (1) and (2, 3). All references, including for the SI, should be included in the main manuscript file. References appearing in both sections should not be duplicated. SI references

Fig. 1. Placeholder image of a frog with a longer example caption to show justification setting.

included in tables should be included with the main reference section.

Data Archival. PNAS must be able to archive the data essential to a published article. Where such archiving is not possible, deposition of data in public databases, such as GenBank, ArrayExpress, Protein Data Bank, UniData, and others outlined in the Information for Authors, is acceptable.

Language-Editing Services. Prior to submission, authors who believe their manuscripts would benefit from professional editing are encouraged to use a language-editing service (see list at www.pnas.org/site/authors/language-editing.xhtml). PNAS does not take responsibility for or endorse these services, and their use has no bearing on acceptance of a manuscript for publication.

Significance Statement

Authors must submit a 120-word maximum statement about the significance of their research paper written at a level understandable to an undergraduate educated scientist outside their field of speciality. The primary goal of the Significance Statement is to explain the relevance of the work in broad context to a broad readership. The Significance Statement appears in the paper itself and is required for all research papers.

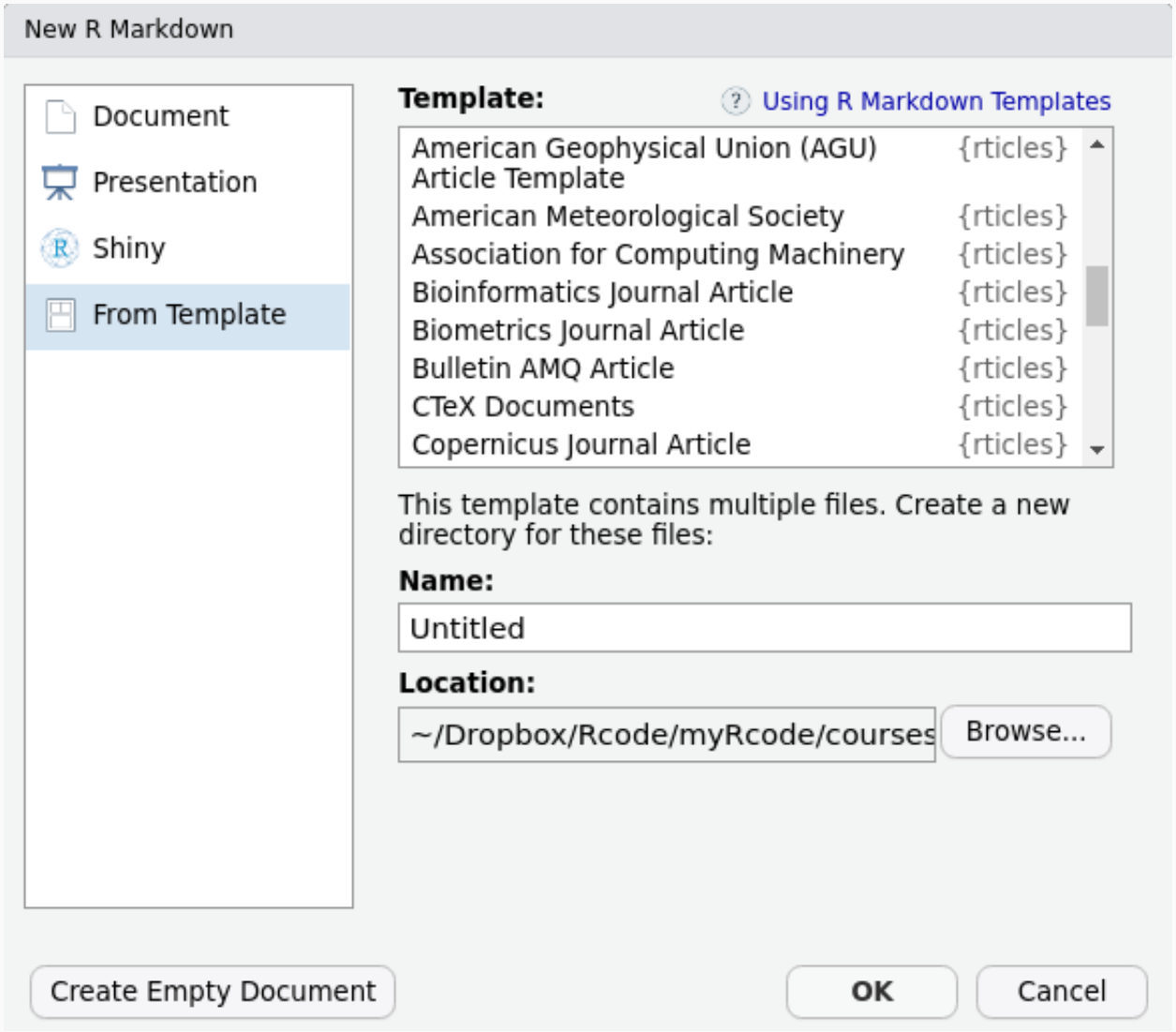
Please provide details of author contributions here.

Please declare any conflict of interest here.

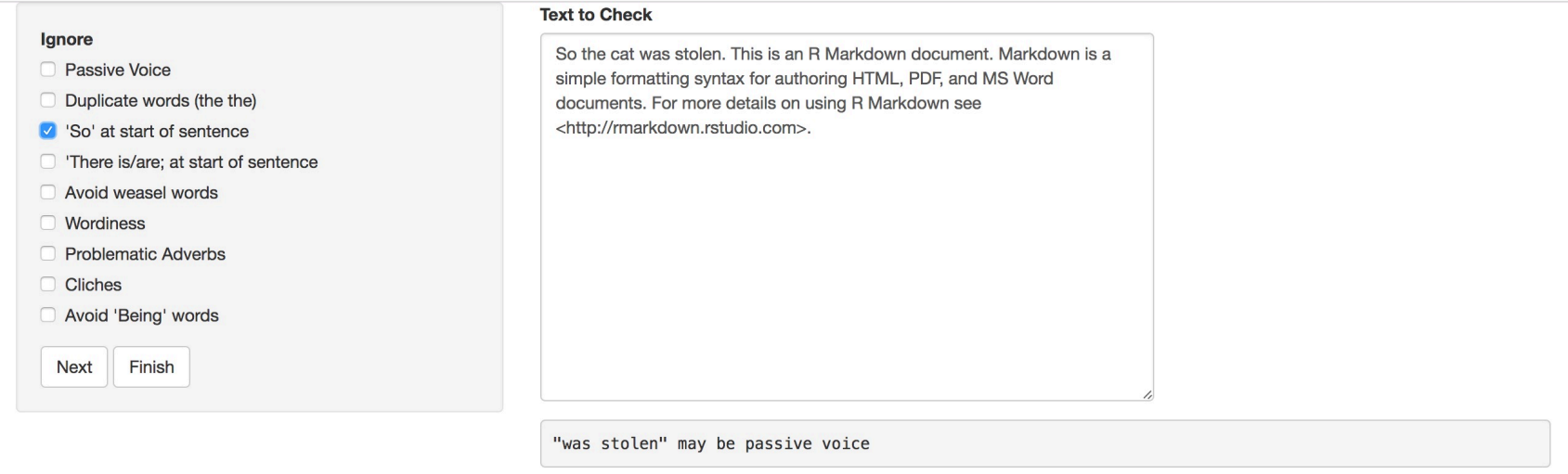
www.pnas.org/cgi/doi/10.1073/pnas.XXXXXXXXXX

PNAS | September 18, 2018 | vol. XXX | no. XX | 1–2

Accessing Rmd templates



Revise writing style: gramr

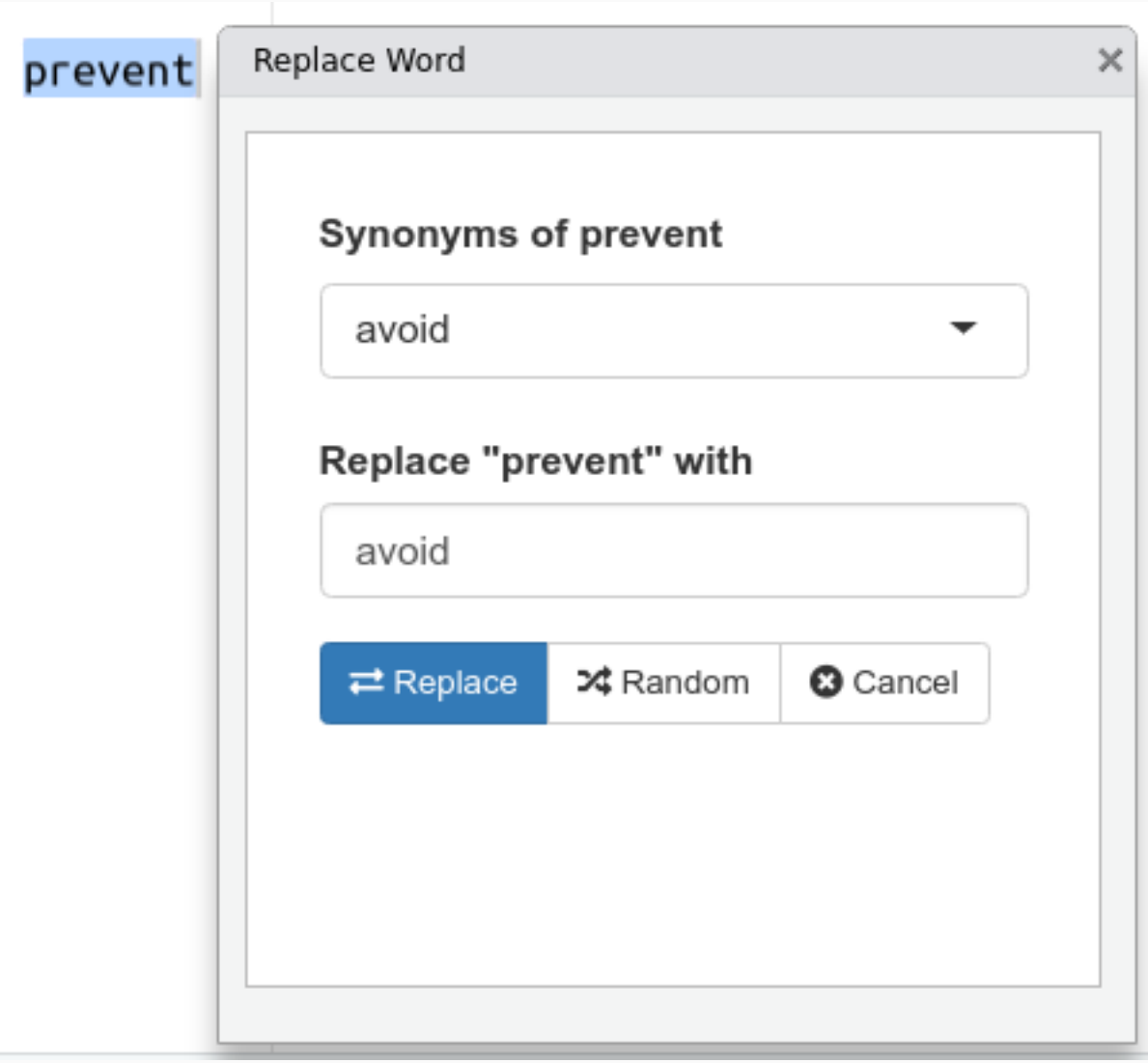


https://github.com/ropenscilabs/gramr

Spell and grammar checking

https://github.com/nevrome/wellspell.addin

Find synonyms



https://github.com/gadenbuie/synamyn

Word count and readability

Method	koRpus	stringi
Word count	107	104
Character count	604	603
Sentence count	10	Not available
Reading time	0.5 minutes	0.5 minutes

https://github.com/benmarwick/wordcountaddin

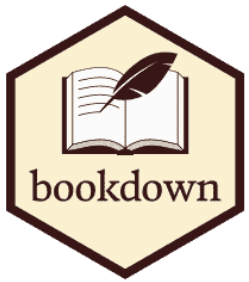
Write books, theses, with **bookdown**

BOOKDOWN

Write HTML, PDF, ePub, and Kindle books with R Markdown

The **bookdown** package is an open-source R package that facilitates writing books and long-form articles/reports with R Markdown. Features include:

- Generate printer-ready books and ebooks from R Markdown documents.
- A markup language easier to learn than LaTeX, and to write elements such as section headers, lists, quotes, figures, tables, and citations.
- Multiple choices of output formats: PDF, LaTeX, HTML, EPUB, and Word.
- Possibility of including dynamic graphics and interactive applications (HTML widgets and Shiny apps).
- Support a wide range of languages: R, C/C++, Python, Fortran, Julia, Shell scripts, and SQL, etc.
- LaTeX equations, theorems, and proofs work for all output formats.
- Can be published to GitHub, bookdown.org, and any web servers.
- Integrated with the RStudio IDE.
- One-click publishing to https://bookdown.org.



https://bookdown.org/

Slide presentations with `xaringan`

https://slides.yihui.org/xaringan/

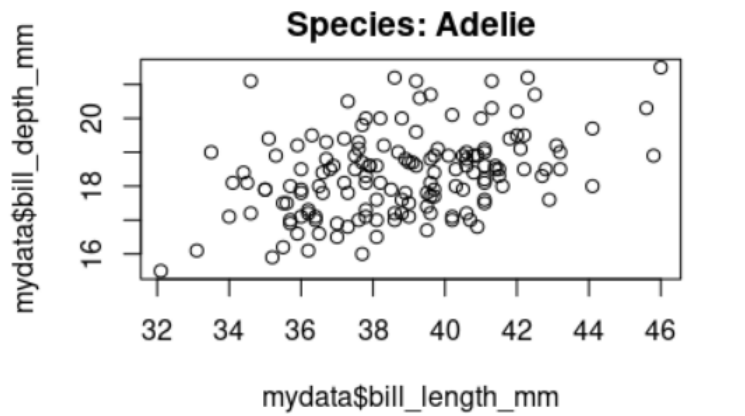
Parameterised reports

```
---
title: "My template report"
output: html_document
params:
  sp: Adelie
---
```

```{r}
library(palmerpenguins)
data("penguins")

mydata <- subset(penguins, species == params$sp)

plot(mydata$bill_length_mm, mydata$bill_depth_mm,
     main = paste0("Species: ", params$sp))
```



https://bookdown.org/yihui/rmarkdown/parameterized-reports.html

Render thousands of individual reports from Rmd template

```
library('rmarkdown')

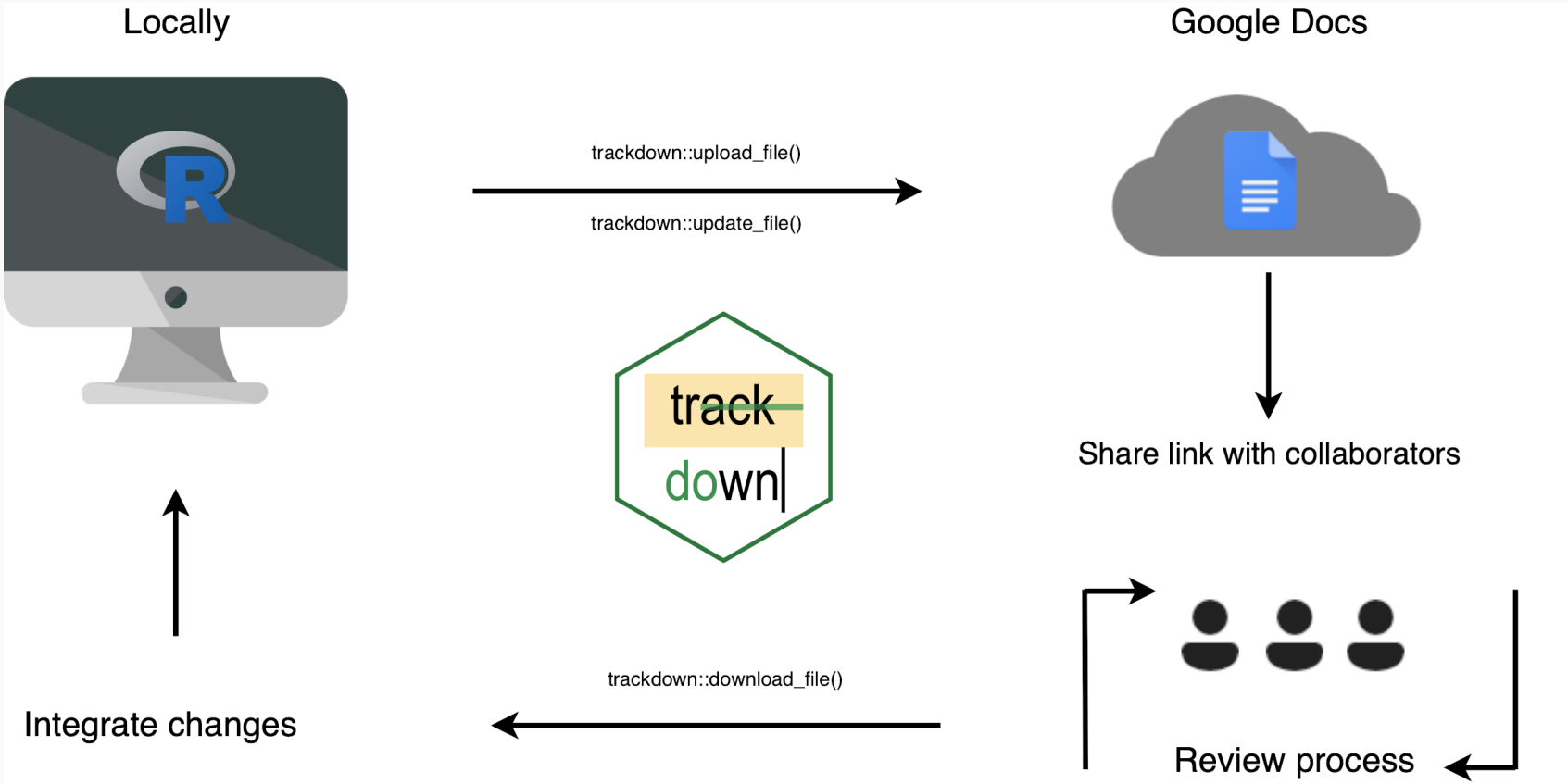
for (i in unique(penguins$species)) {

  render("template_report.Rmd",
         params = list(sp = i))

}
```

Collaborative writing

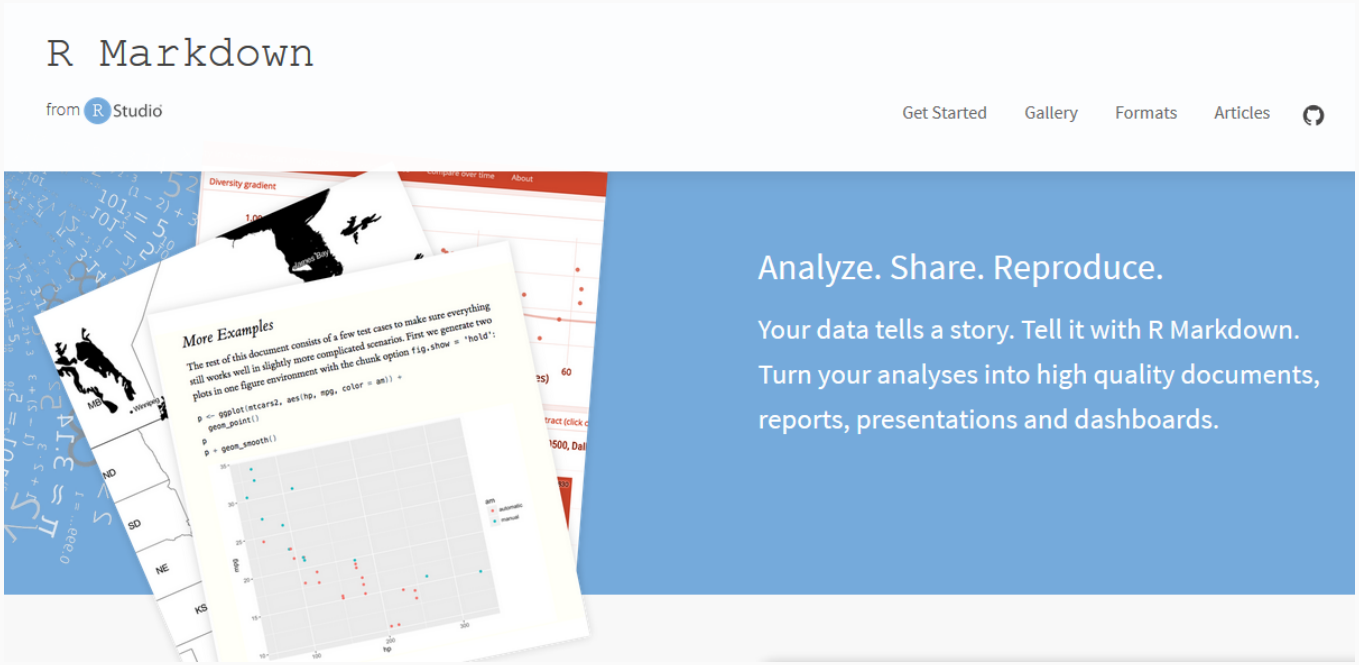
- GitHub, GitLab, etc
- Google Docs (trackdown)
- redoc



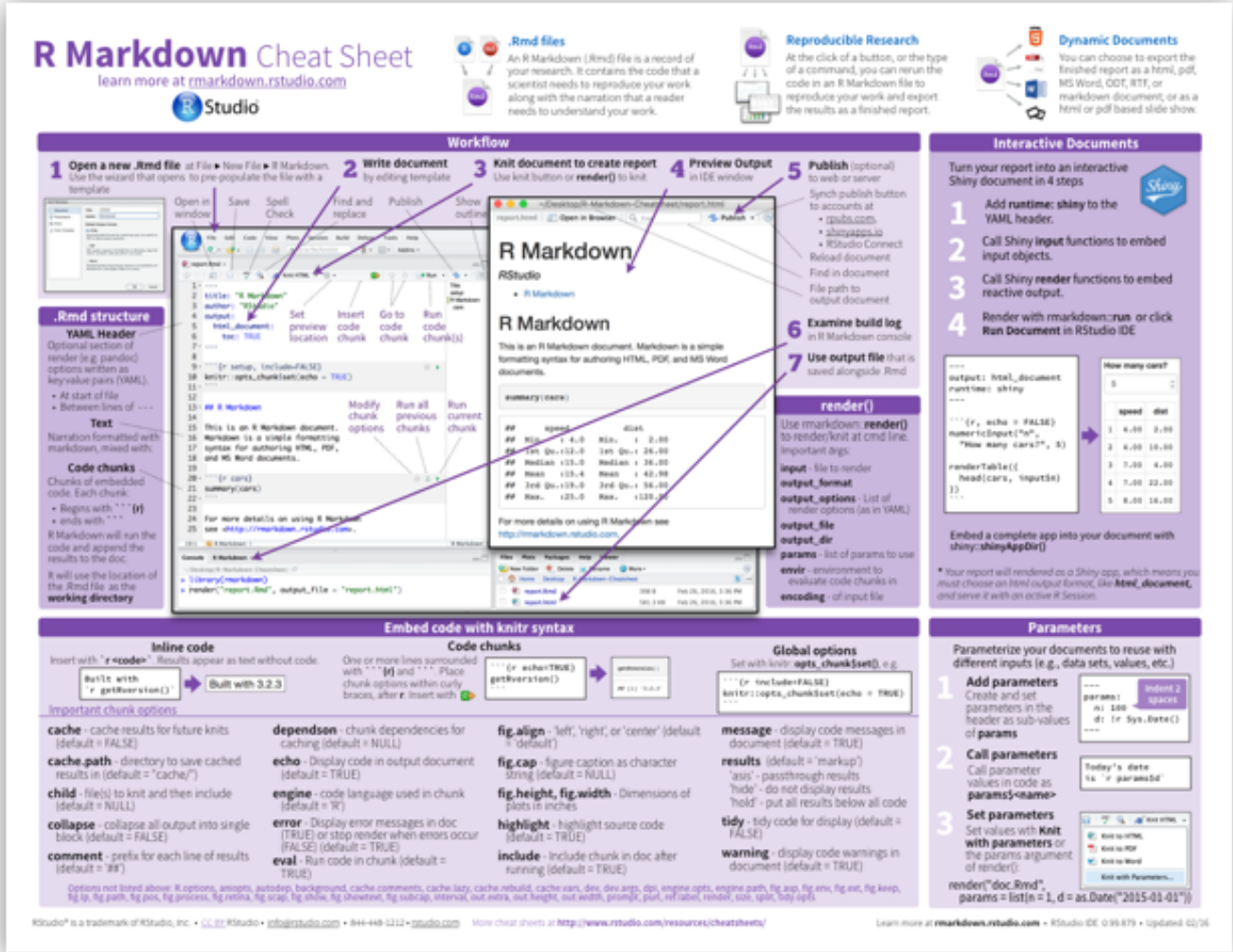
Rmarkdown resources

Rmarkdown website

http://rmarkdown.rstudio.com/



Rmarkdown cheat sheet



https://www.rstudio.org/links/r_markdown_cheat_sheet

Rmarkdown reference guide

R Markdown Reference Guide

Learn more about R Markdown at rmarkdown.rstudio.com
Learn more about Interactive Docs at shiny.rstudio.com/articles

Contents:
1. Markdown Syntax
2. **Knitr chunk options**
3. Pandoc options

Syntax	Becomes
Make a code chunk with three back ticks followed by an r in braces. End the chunk with three back ticks: ```{r} paste("Hello", "World!") ```	Make a code chunk with three back ticks followed by an r in braces. End the chunk with three back ticks: `paste("Hello", "World!")` `## [1] "Hello World!"`
Place code inline with a single back ticks. The first back tick must be followed by an R, like this `r paste("Hello", "World!")`.	Place code inline with a single back ticks. The first back tick must be followed by an R, like this Hello World!.
Add chunk options within braces. For example, `echo=FALSE` will prevent source code from being displayed: ```{r eval=TRUE, echo=FALSE} paste("Hello", "World!") ```	Add chunk options within braces. For example, `echo=FALSE` will prevent source code from being displayed: `## [1] "Hello World!"`

Learn more about chunk options at http://yihui.name/knitr/options

Chunk options

option	default value	description
Code evaluation		
child	NULL	A character vector of filenames. Knitr will knit the files and place them into the main document.
code	NULL	Set to R code. Knitr will replace the code in the chunk with the code in the code option.
engine	'R'	Knitr will evaluate the chunk in the named language, e.g. **engine = 'python'**. Run **names(knitr::knit_engines$get())** to see supported languages.
eval	TRUE	If **FALSE**, knitr will not run the code in the code chunk.
include	TRUE	If **FALSE**, knitr will run the chunk but not include the chunk in the final document.
purl	TRUE	If **FALSE**, knitr will not include the chunk when running **purl()** to extract the source code.
Results		
collapse	FALSE	If **TRUE**, knitr will collapse all the source and output blocks created by the chunk into a single block.
echo	TRUE	If **FALSE**, knitr will not display the code in the code chunk above it's results in the final document.
results	'markup'	If **'hide'**, knitr will not display the code's results in the final document. If **'hold'**, knitr will delay displaying all output pieces until the end of the chunk. If **'asis'**, knitr will pass through results without reformatting them (useful if results return raw HTML, etc.)
error	TRUE	If **FALSE**, knitr will not display any error messages generated by the code.
message	TRUE	If **FALSE**, knitr will not display any messages generated by the code.
warning	TRUE	If **FALSE**, knitr will not display any warning messages generated by the code.
Code Decoration		
background	'#F7F7F7'	A background color for chunks in LaTex output.
comment	'##'	A character string. Knitr will append the string to the start of each line of results in the final document.
highlight	TRUE	If **TRUE**, knitr will highlight the source code in the final output.
prompt	FALSE	If **TRUE**, knitr will add > to the start of each line of code displayed in the final document.
size	'normalsize'	Fontsize for LaTex output.
strip.white	TRUE	If **TRUE**, knitr will remove white spaces that appear at the beginning or end of a code chunk.
tidy	FALSE	If **TRUE**, knitr will tidy code chunks for display with the **tidy_source()** function in the **formatR** package.

RStudio Updated 10/30/2014

2

https://www.rstudio.org/links/r_markdown_reference_guide

Rmarkdown books

R Markdown: The Definitive Guide

by Yihui Xie, J. J. Allaire, Garrett Grolemund

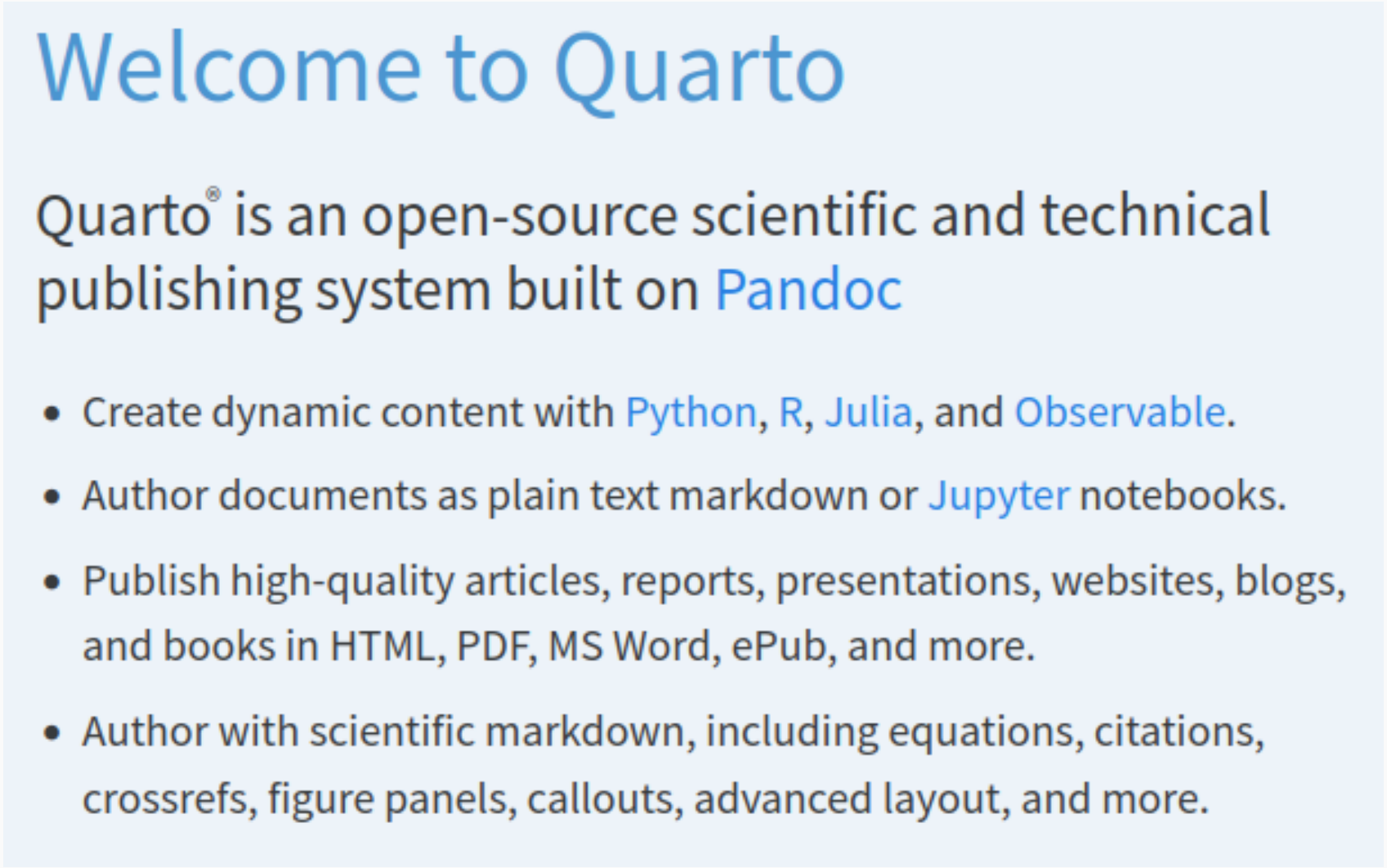
2018-09-11

Star 239

The first official book authored by the core R Markdown developers that provides a comprehensive and accurate reference to the R Markdown ecosystem. With R Markdown, you can easily create reproducible data analysis reports, presentations, dashboards, interactive applications, books, dissertations, websites, and journal articles, while enjoying the simplicity of Markdown and the great power of R and other languages. *Read more* →

https://bookdown.org/yihui/rmarkdown/

https://bookdown.org/yihui/rmarkdown-cookbook/



https://quarto.org/

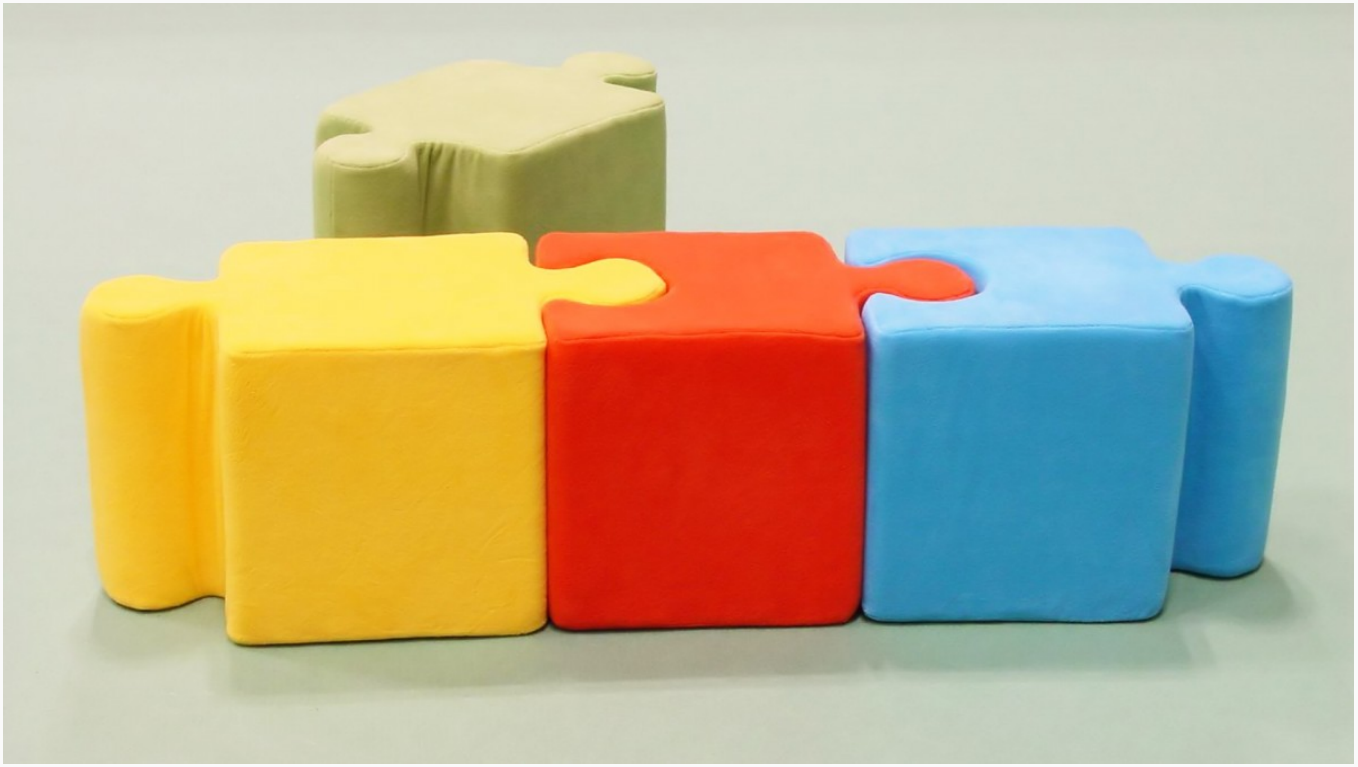
Your turn

Your turn

- Try visual markdown editor
- Add bibliography
- Try templates (rticles, rmdTemplates)
- Parameterised reports (e.g. different iris or penguin species)

Workflow management

In complex projects we must **keep pieces organised**



`makefile` runs all code in right order

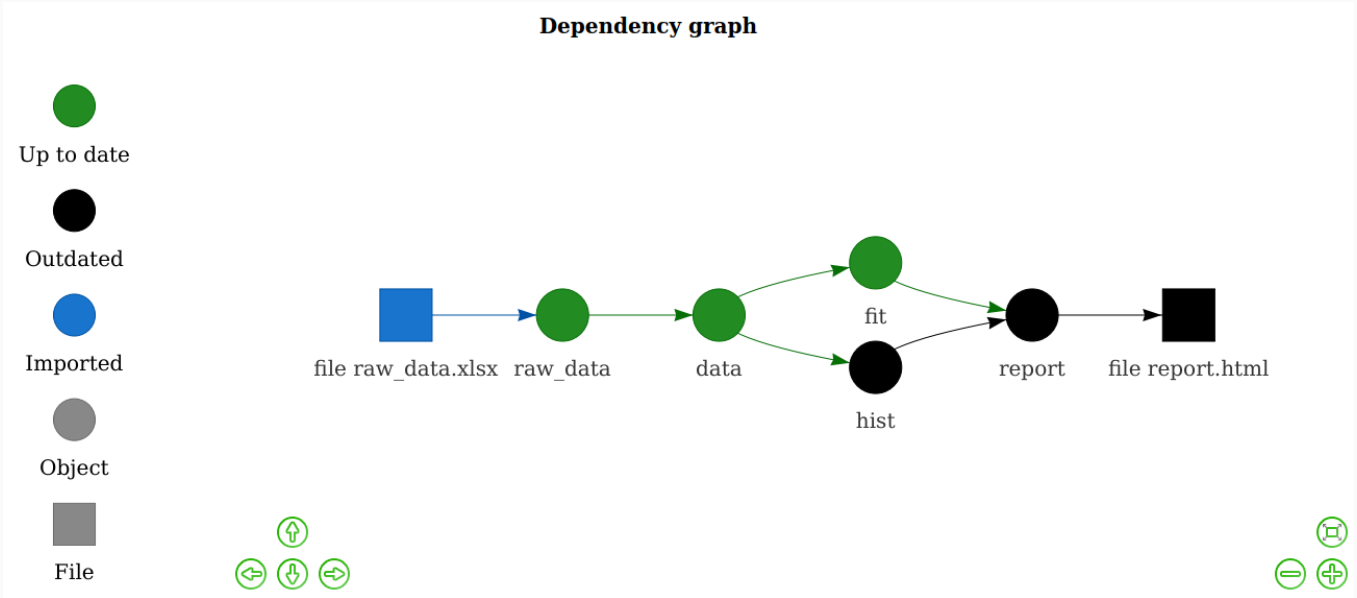
`makefile.R`

```
source("clean_data.R")

source("fit_model.R")

render("report.Rmd")
```

targets: advanced workflow management



https://docs.ropensci.org/targets/

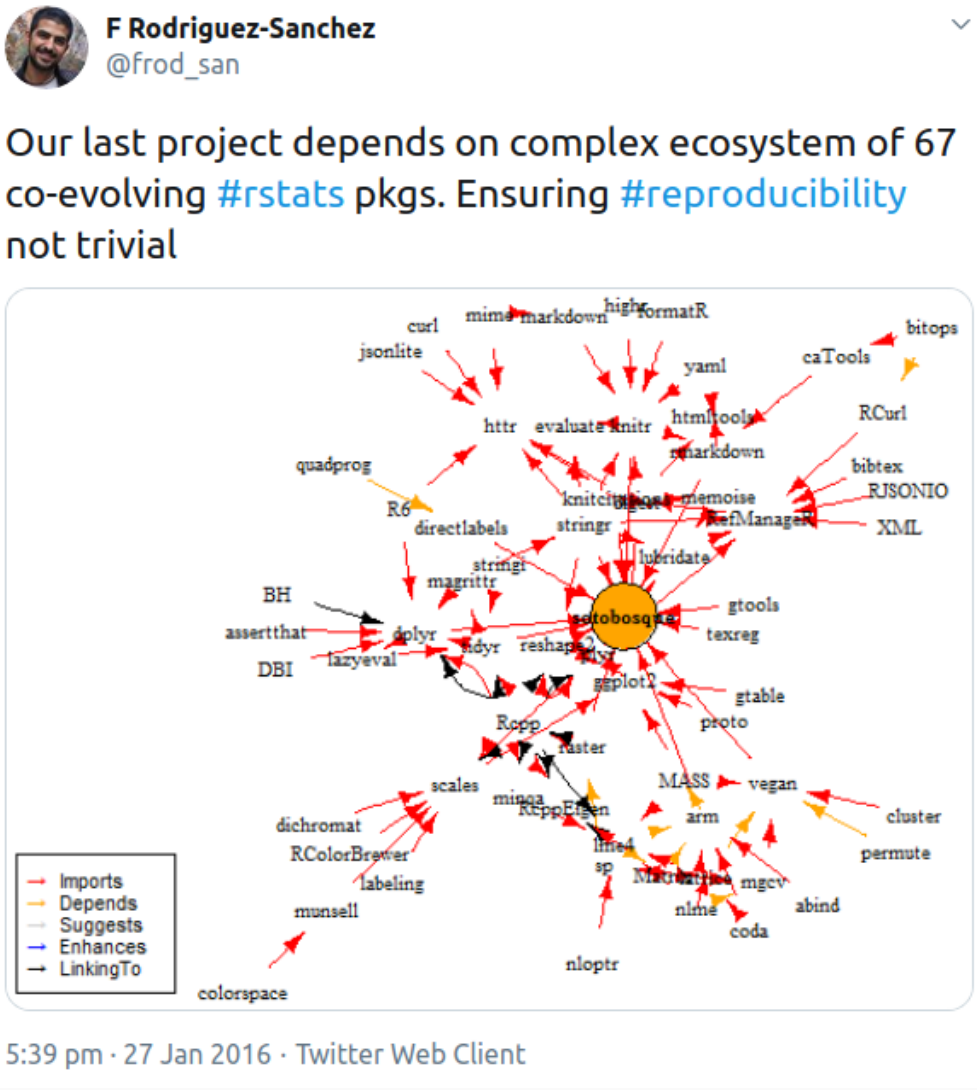
Your turn

Write makefile.R for your project

Try `targets` minimal example

https://github.com/wlandau/targets-minimal

Controlling software dependencies


F Rodriguez-Sanchez
@frod_san
Our last project depends on complex ecosystem of 67 co-evolving #rstats pkgs. Ensuring #reproducibility not trivial
curl
mime
markdown
highr
formatR
jsonlite
yaml
bitops
caTools
RCurl
httr
evaluate
knitr
htmltools
rmarkdown
quadprog
bibtex
RJSONIO
memoise
XML
R6
directlabels
stringr
lubridate
stringi
magrittr
BH
gtools
assertthat
dplyr
texreg
tidyr
reshape2
DBI
lazyeval
ggplot2
gtable
proto
Rcpp
raster
scales
MASS
vegan
cluster
dichromat
arm
permute
RColorBrewer
lme4
sp
labeling
mgcv
munsell
nlme
abind
coda
nloptr
colorspace
Imports
Depends
Suggests
Enhances
LinkingTo
5:39 pm · 27 Jan 2016 · Twitter Web Client

Package changes can break your analysis

How to reproduce your analysis in a year,

or different computer?

`sessionInfo` records OS & used packages

```
sessionInfo()
```

```
R version 4.2.0 (2022-04-22)
Platform: x86_64-pc-linux-gnu (64-bit)
Running under: Ubuntu 20.04.4 LTS

Matrix products: default
BLAS:   /usr/lib/x86_64-linux-gnu/blas/libblas.so.3.9.0
LAPACK: /usr/lib/x86_64-linux-gnu/lapack/liblapack.so.3.9.0

locale:
 [1] LC_CTYPE=en_GB.UTF-8       LC_NUMERIC=C
 [3] LC_TIME=es_ES.UTF-8        LC_COLLATE=en_GB.UTF-8
 [5] LC_MONETARY=es_ES.UTF-8    LC_MESSAGES=en_GB.UTF-8
 [7] LC_PAPER=es_ES.UTF-8       LC_NAME=C
 [9] LC_ADDRESS=C               LC_TELEPHONE=C
[11] LC_MEASUREMENT=es_ES.UTF-8 LC_IDENTIFICATION=C

attached base packages:
[1] stats     graphics  grDevices utils     datasets  methods   base

other attached packages:
[1] report_0.5.5       equatiomatic_0.3.1 xtable_1.8-4       knitr_1.40

loaded via a namespace (and not attached):
 [1] Rcpp_1.0.9          mvtnorm_1.1-3      lattice_0.20-45    tidyr_1.2.0
 [5] zoo_1.8-10          assertthat_0.2.1   digest_0.6.29      utf8_1.2.2
 [9] mime_0.12           R6_2.5.1           backports_1.4.1    evaluate_0.16
[13] coda_0.19-4         pillar_1.8.1       rlang_1.0.5        multcomp_1.4-20
[17] performance_0.9.2   rstudioapi_0.14    Matrix_1.4-1       effectsize_0.7.0.5
[21] rmarkdown_2.16      splines_4.2.0      stringr_1.4.1      shiny_1.7.2
[25] broom_1.0.1         compiler_4.2.0     httpuv_1.6.5       xfun_0.32
[29] pkgconfig_2.0.3     parameters_0.18.2  htmltools_0.5.3    insight_0.18.2
[33] tidyselect_1.1.2    tibble_3.1.8       codetools_0.2-18   fansi_1.0.3
```

`checkpoint` reconstructs packages in given date

```
library('checkpoint')

checkpoint("2019-10-08")

source("analysis.R")
```

1. Detects packages used
2. Installs version from given date (only CRAN)
3. Independent install (not messing w/ main library)

`automagic` records & install packages (CRAN + GitHub)

```
automagic::make_deps_file()
```

File `deps.yaml` records dependencies:

```
- Package: equatiomatic
  Repository: CRAN
  Version: 0.1.0

- Package: report
  GithubUsername: easystats
  GithubRepo: report
  GithubRef: HEAD
  GithubSHA1: c48a4bb0a40df7116bc502aa3ce2cbbc9d70b7e2
```

To install all those dependencies:

```
automagic()
```

renv also controls dependencies

```
renv::init()
# Create private package library for project

renv::snapshot()
# Capture dependencies in lockfile

renv::restore()
# Regenerate dependencies from lockfile
```

https://environments.rstudio.com/

To ensure reproducibility,

besides R packages

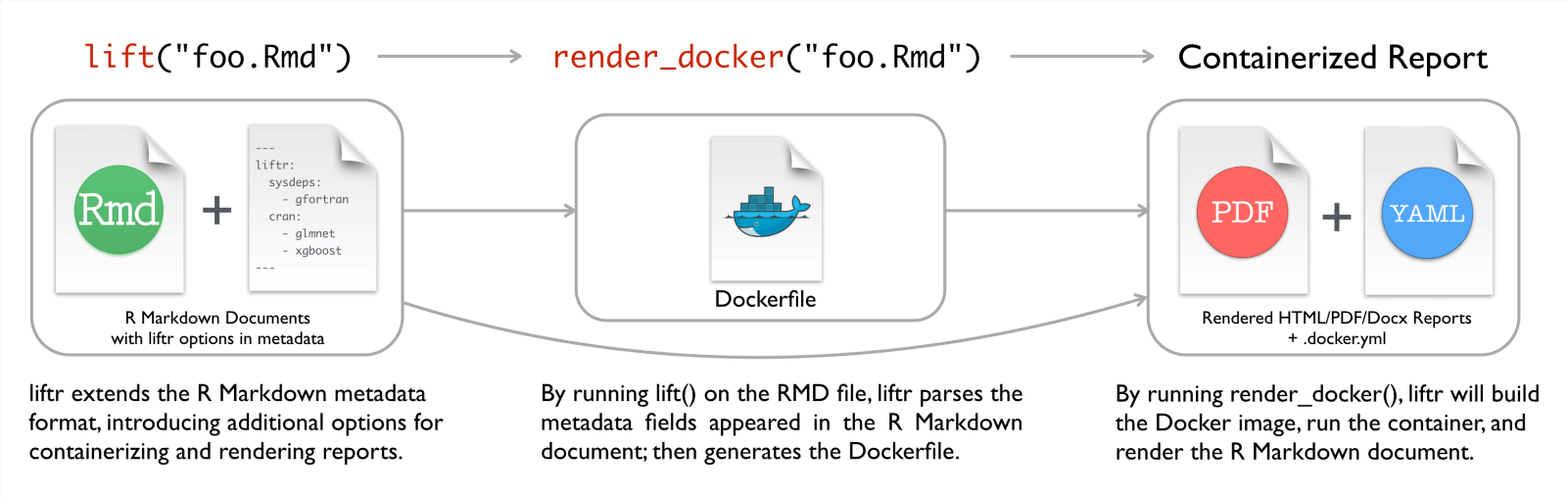
we also need to control

computational environment

`Docker` recreates virtual systems

from a `Dockerfile`

`liftr`: process Rmd in Docker container



https://liftr.me/

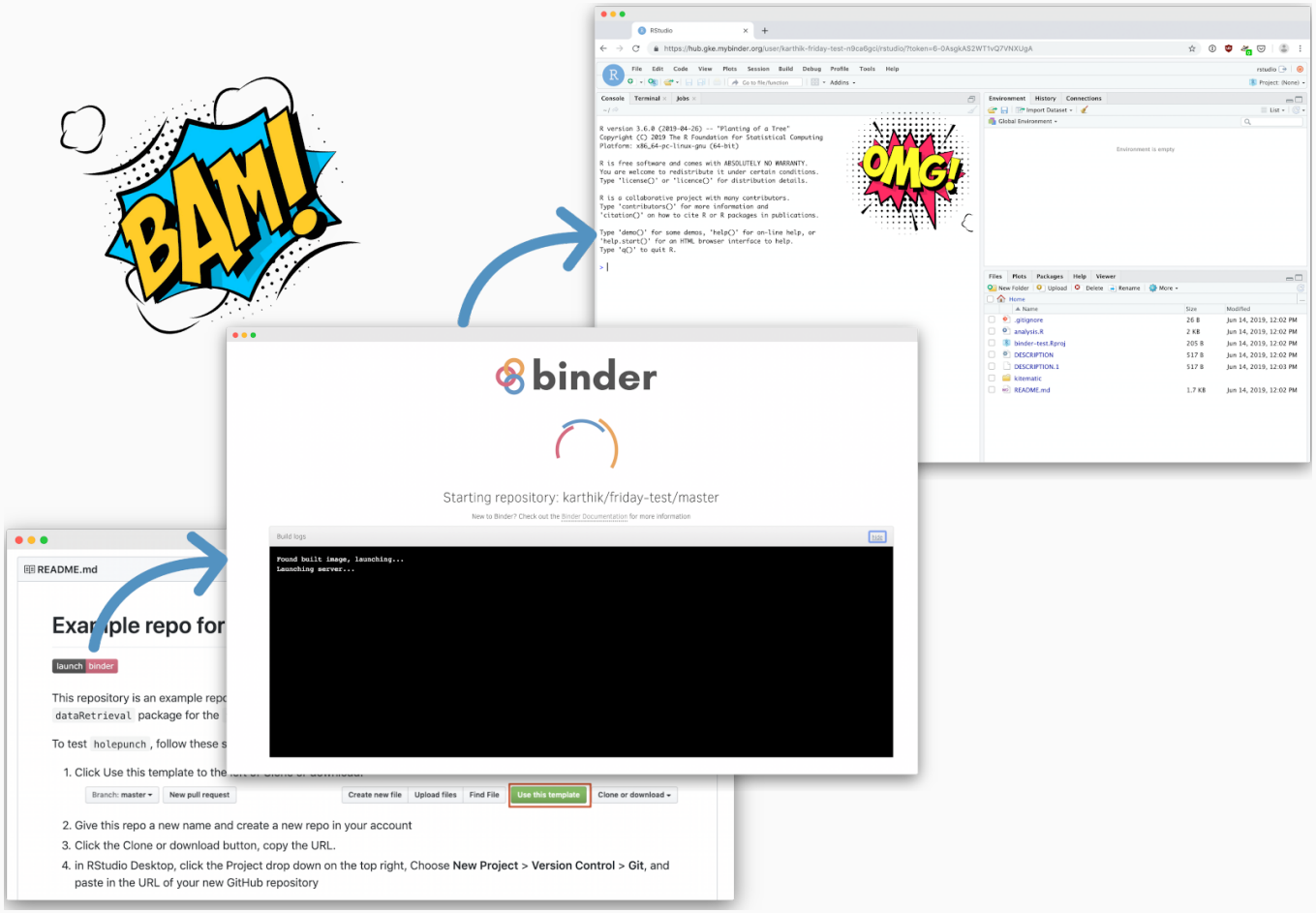
`containerit` creates Dockerfile

```
library("containerit")

dockfile <- dockerfile(from = "mypaper.Rmd")
```

https://o2r.info/containerit

holepunch: reproduce analysis in the cloud (Binder)



https://karthik.github.io/holepunch/

Your turn

Checkpoint

- Create script/Rmd using different packages
- Call `checkpoint` on former date

automagic/renv

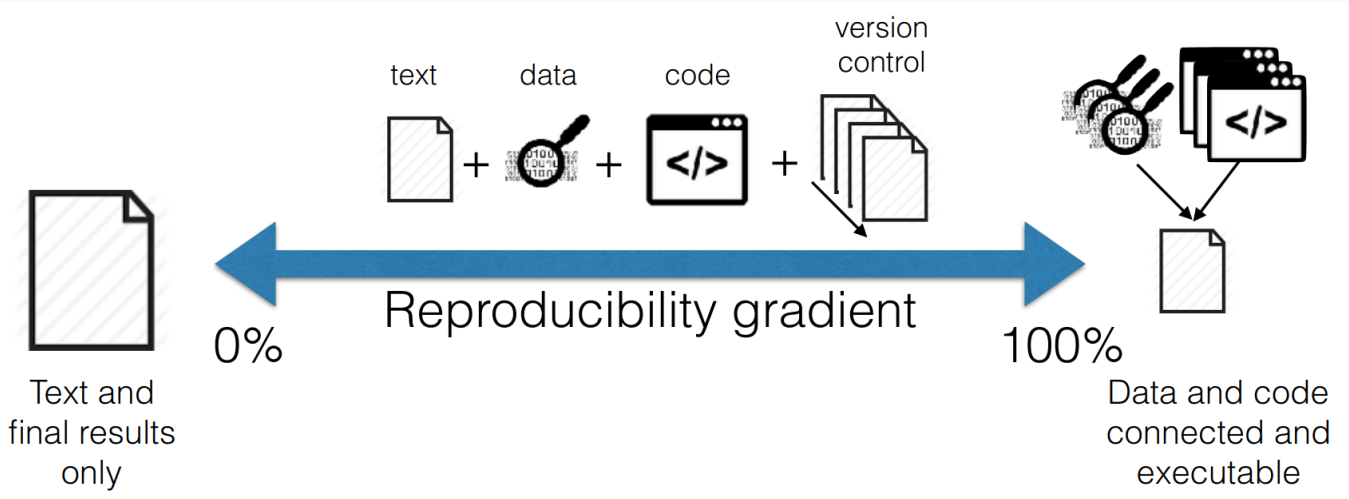
- Record dependencies:
  - `automagic::make_deps_file()`
  - `renv::snapshot`
- Recreate packages
  - `automagic()`
  - `restore()`

How to write more reproducible code

- BES guide to reproducible code
- Turing Way
- Good enough practices in scientific computing
- Ciencia reproducible: qué, por qué, cómo
- `https://rstats.wtf`
- `fertile` package
- CodeCheck

Reproducibility

- Good for you, good for science
- Requires systemic changes
- Reproducibility gradient: step by step



Happy collaboration!