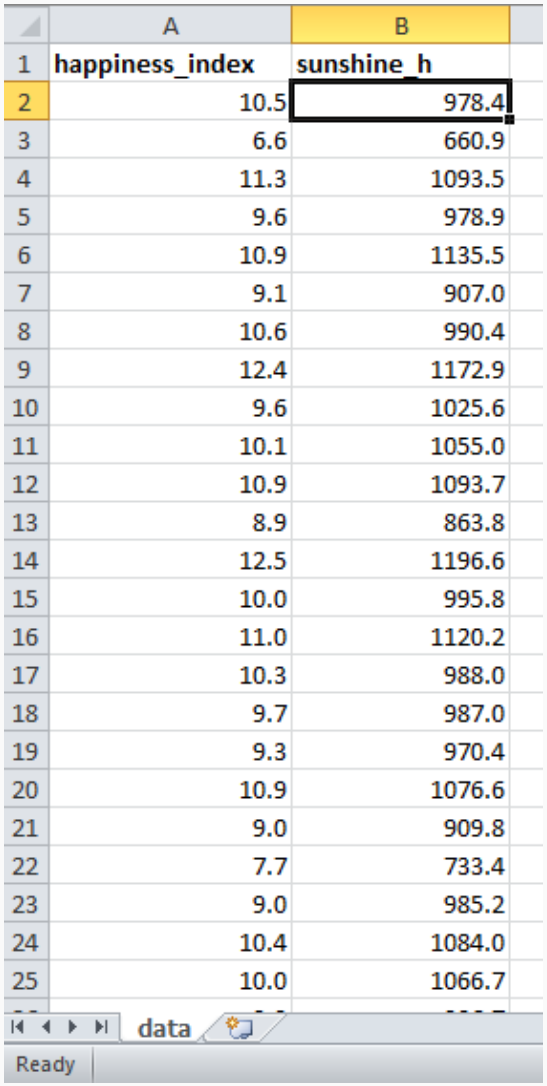
Doing reproducible science: from your hard-won data to a publishable manuscript without going mad

Francisco Rodriguez-Sanchez

@frod_san

A typical research workflow

1. Prepare data (**EXCEL**)



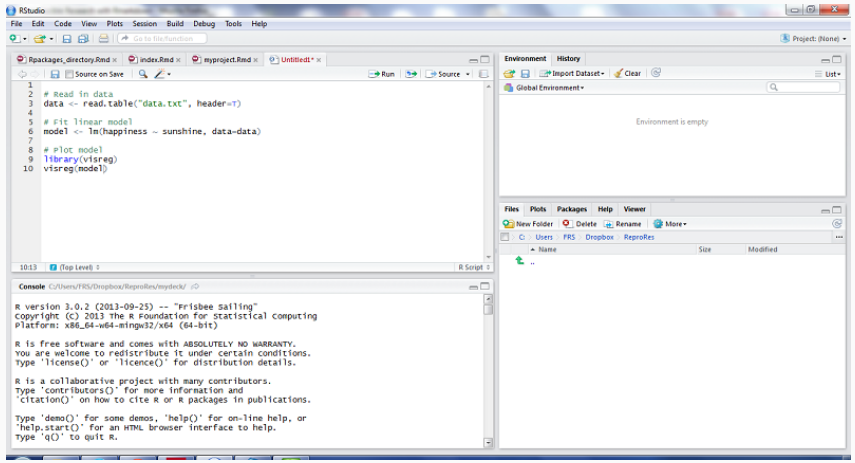
	A	B
1	happiness_index	sunshine_h
2	10.5	978.4
3	6.6	660.9
4	11.3	1093.5
5	9.6	978.9
6	10.9	1135.5
7	9.1	907.0
8	10.6	990.4
9	12.4	1172.9
10	9.6	1025.6
11	10.1	1055.0
12	10.9	1093.7
13	8.9	863.8
14	12.5	1196.6
15	10.0	995.8
16	11.0	1120.2
17	10.3	988.0
18	9.7	987.0
19	9.3	970.4
20	10.9	1076.6
21	9.0	909.8
22	7.7	733.4
23	9.0	985.2
24	10.4	1084.0
25	10.0	1066.7

data

Ready

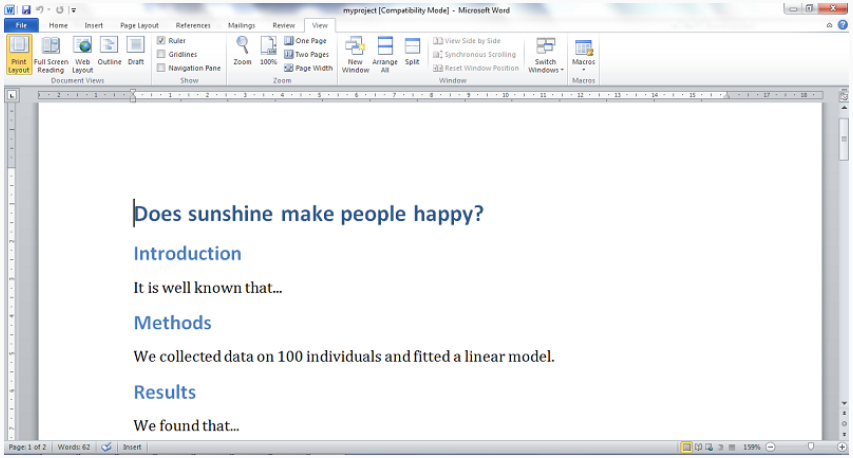
A typical research workflow

1. Prepare data (**EXCEL**)
2. Analyse data (**R**)



A typical research workflow

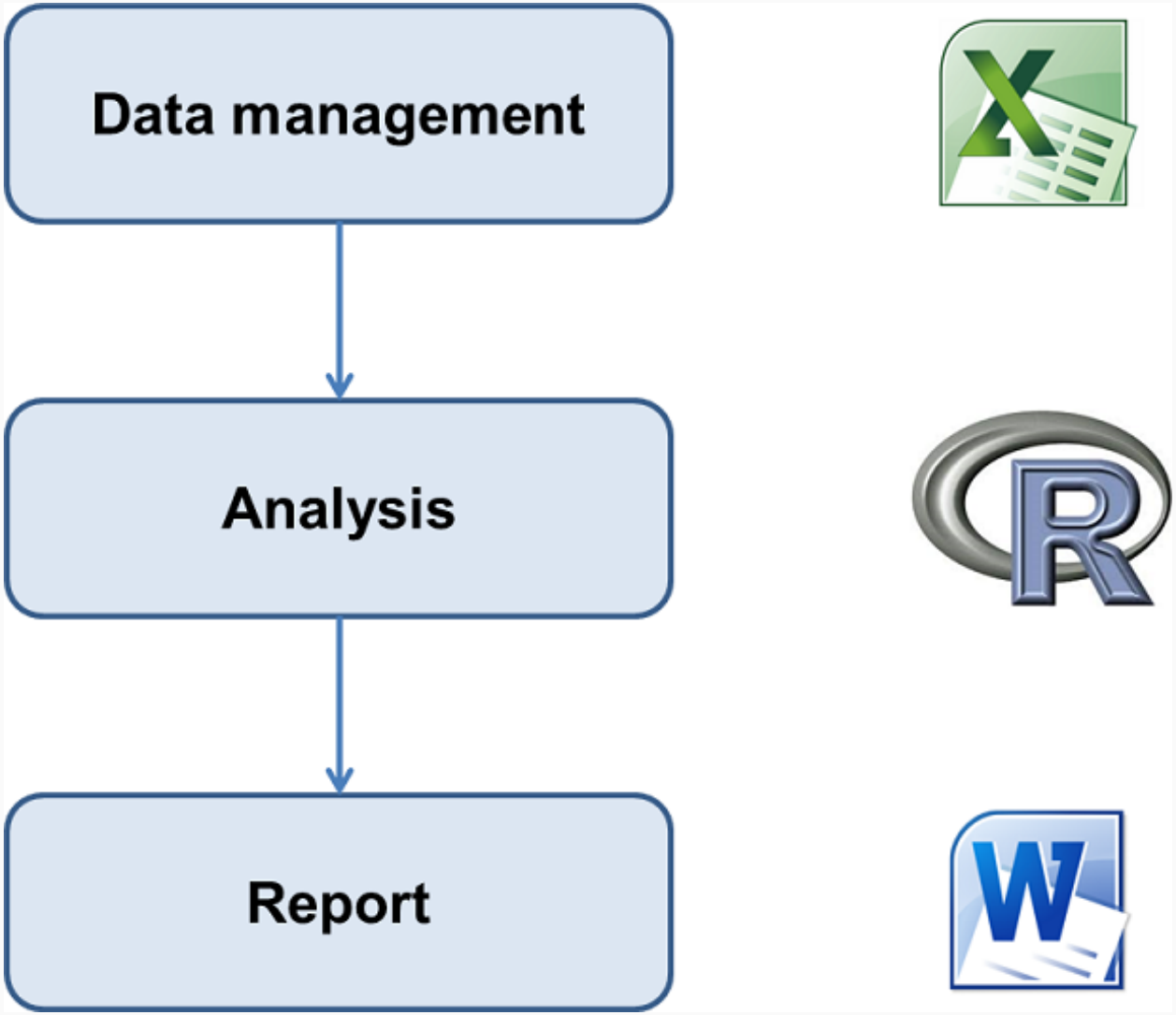
1. Prepare data (**EXCEL**)
2. Analyse data (**R**)
3. Write report/paper (**WORD**)



A typical research workflow

1. Prepare data (**EXCEL**)
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

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- What dataset was used? Which individuals were left out? Where is the clean dataset?

Problems of a broken workflow

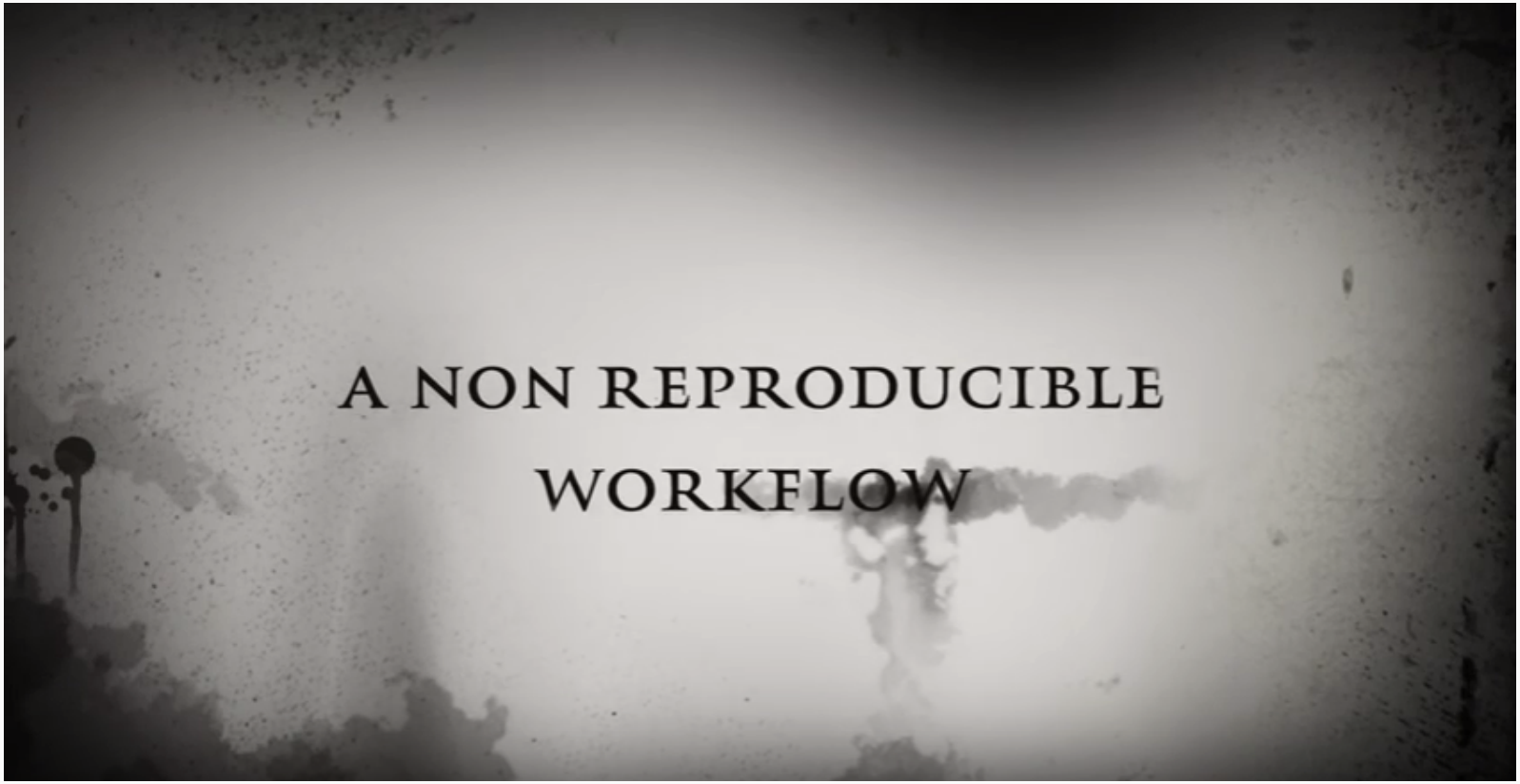
- How did you do this? What analysis is behind this figure? Did you account for . . . ?
- What dataset was used? Which individuals were left out? Where is the clean dataset?
- Oops, there is an error in the data. Can you repeat the analysis? And update figures/tables in Word!

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

Our everyday scary movie



https://youtu.be/s3JldKoA0zw

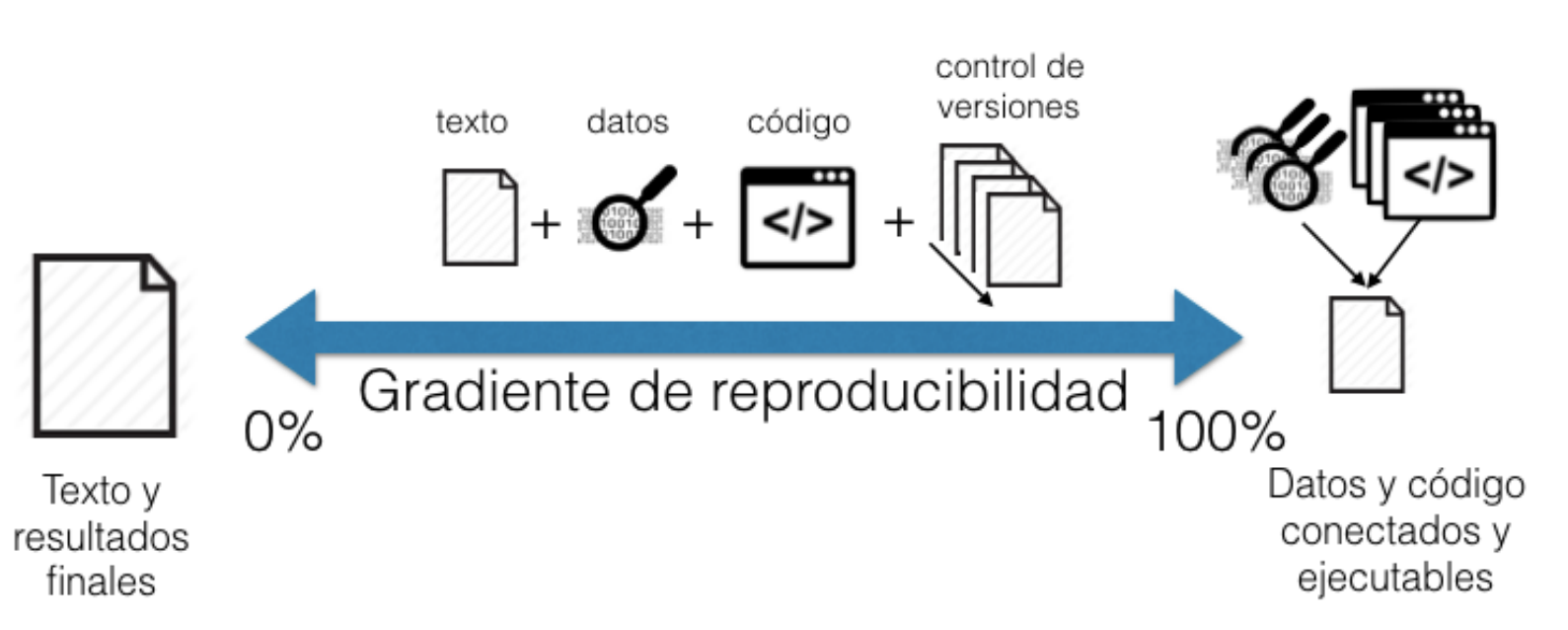
WHAT is Reproducible Science?

Reproducible Science: WHAT

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

- Transparent
- Traceable
- Comprehensive
- Useful

Most science is not reproducible

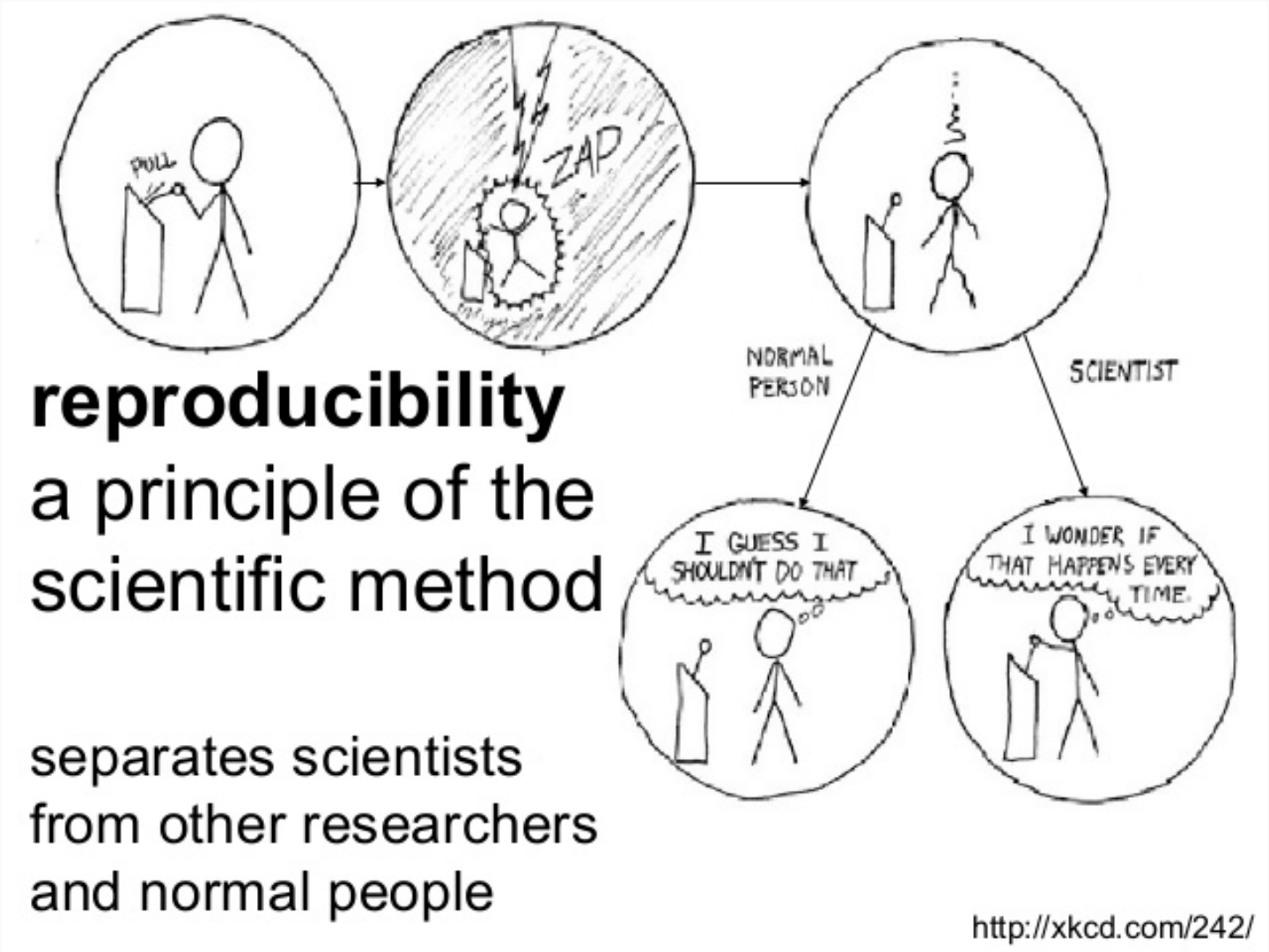


Even **you** will struggle to reproduce **your own results** from a few weeks/months ago.

You can't reproduce if you don't understand where a number came from. You can't reproduce what you don't remember. And trust me: you won't. You can't reproduce what you've lost. What if you need access to a file as it existed 1, 10, 100, or 1000 days ago?

Ben Bond-Lamberty

WHY Reproducible Science?



Carole Goble http://www.slideshare.net/carolegoble/ismb2013-keynotecleangoble

Noam Ross
@noamross

Follow

Gelman: "Reproducible research is even better when you're wrong" #stancon2017

Reproducible Science: WHY

- Fundamental pillar of **scientific method**

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- **Code reuse** & sharing accelerates scientific progress
- Increasingly required by **journals**
- Higher publication **impact** (citations, future collaborations, etc)

HOW TO DO Reproducible Science?

Reproducible Science: HOW

1. File **organisation**.
2. **Data management**. Spreadsheet good practices.
3. **Code-based** data analysis. **Rmarkdown**
4. Software **dependencies**.
5. **Version control** & collaborative writing.

File organisation

- All files in **same directory** (Rstudio project).

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- Derived, **clean data** in another folder.
- Figures, code, etc also have their own folder.

File organisation example

```
|- README          # general info about the project

|- analysis.R      # master script that executes everything

|- data-raw/       # original raw data

|- data/           # clean data (produced w/ script)

|- R/              # functions definitions

|- doc/            # manuscript files

|- figs/           # final figures

|- output/         # other code output
```

Data management

Data management

See https://www.dataone.org/best-practices

.

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

Storage

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

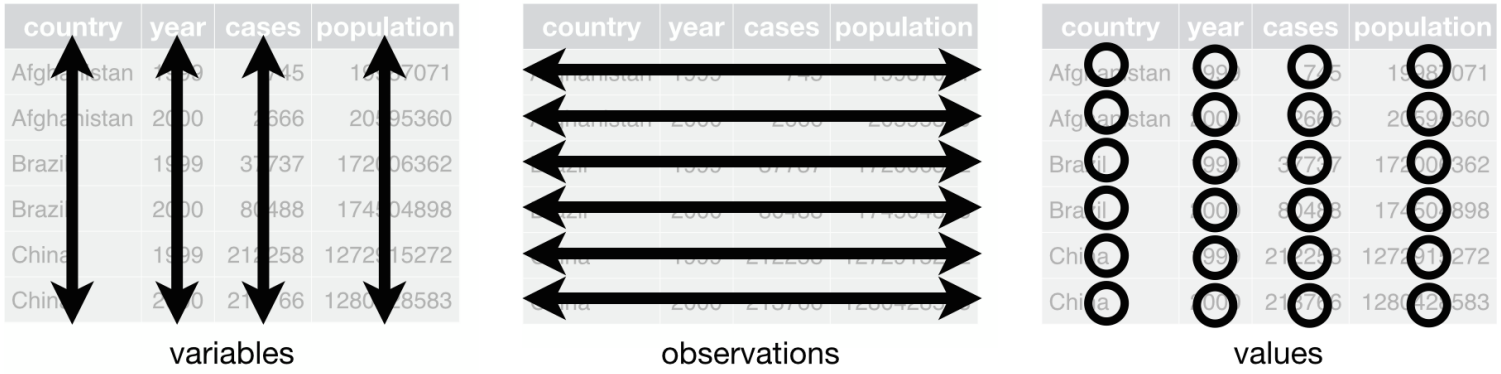
http://science.sciencemag.org/content/354/6317/1242.1

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



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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table4

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

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

Common spreadsheet errors

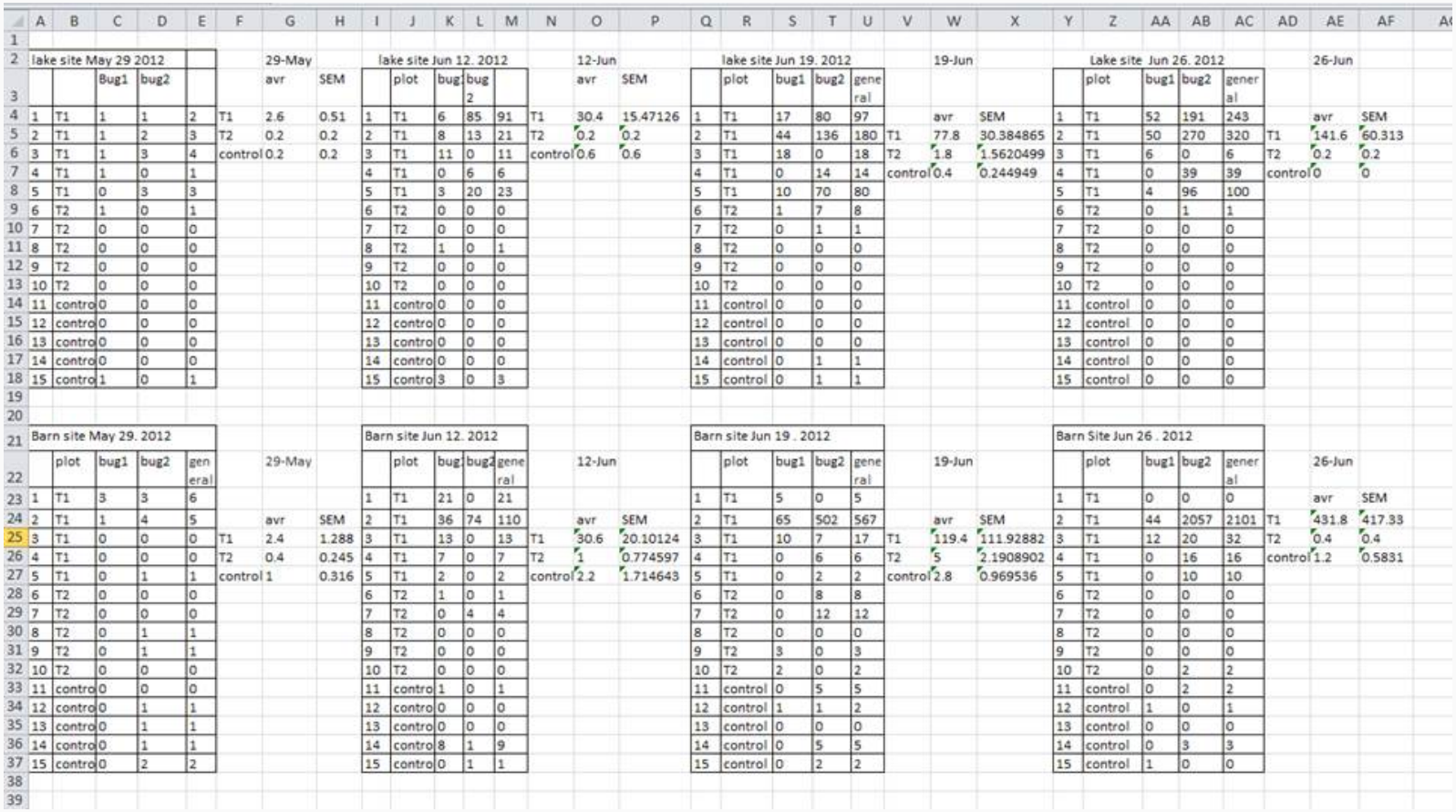
More than one variable per column

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

Source: Data Carpentry

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

Multiple tables



| | | |

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

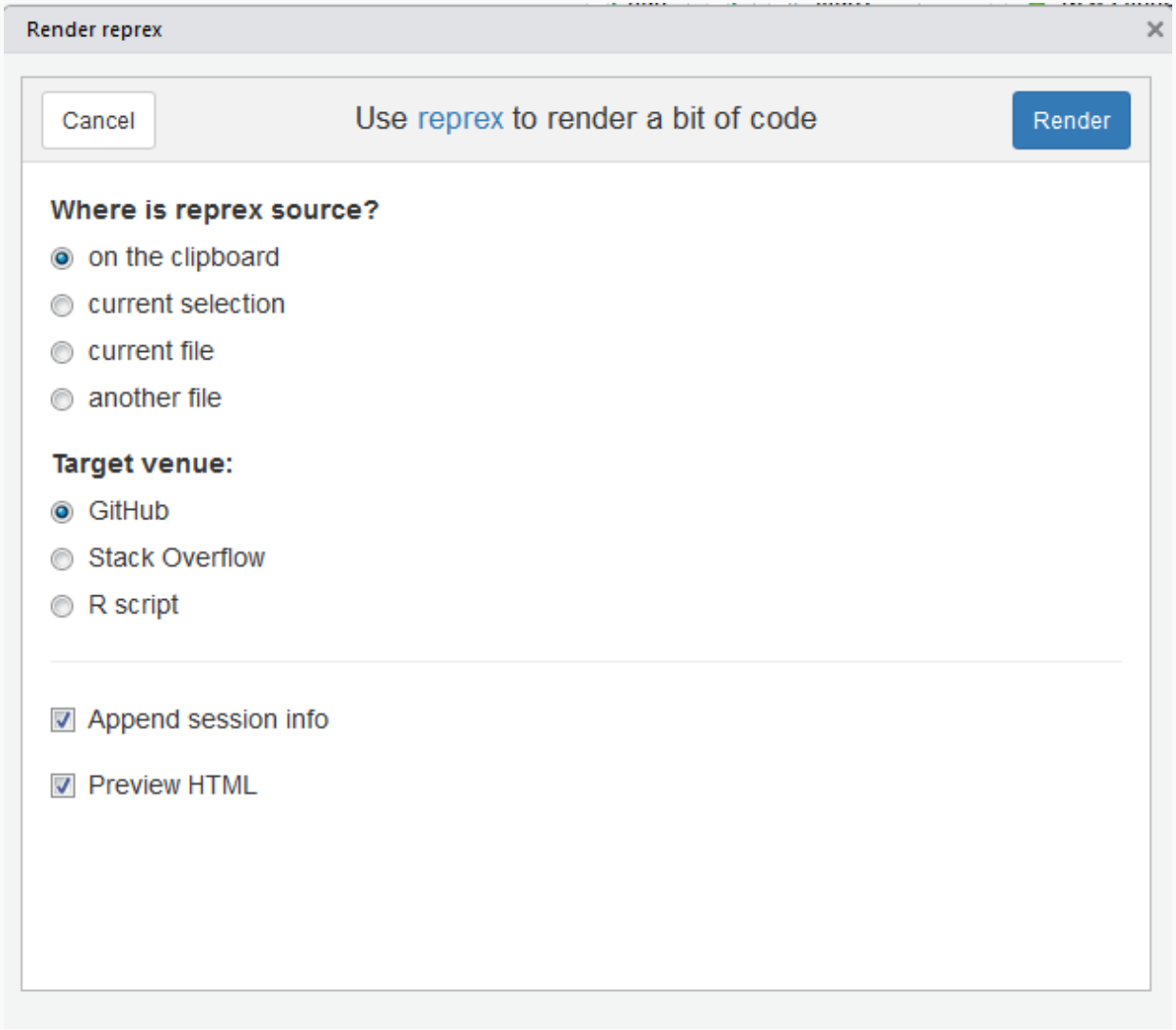
https://ndownloader.figshare.com/files/2252083

Data analysis

Always use code

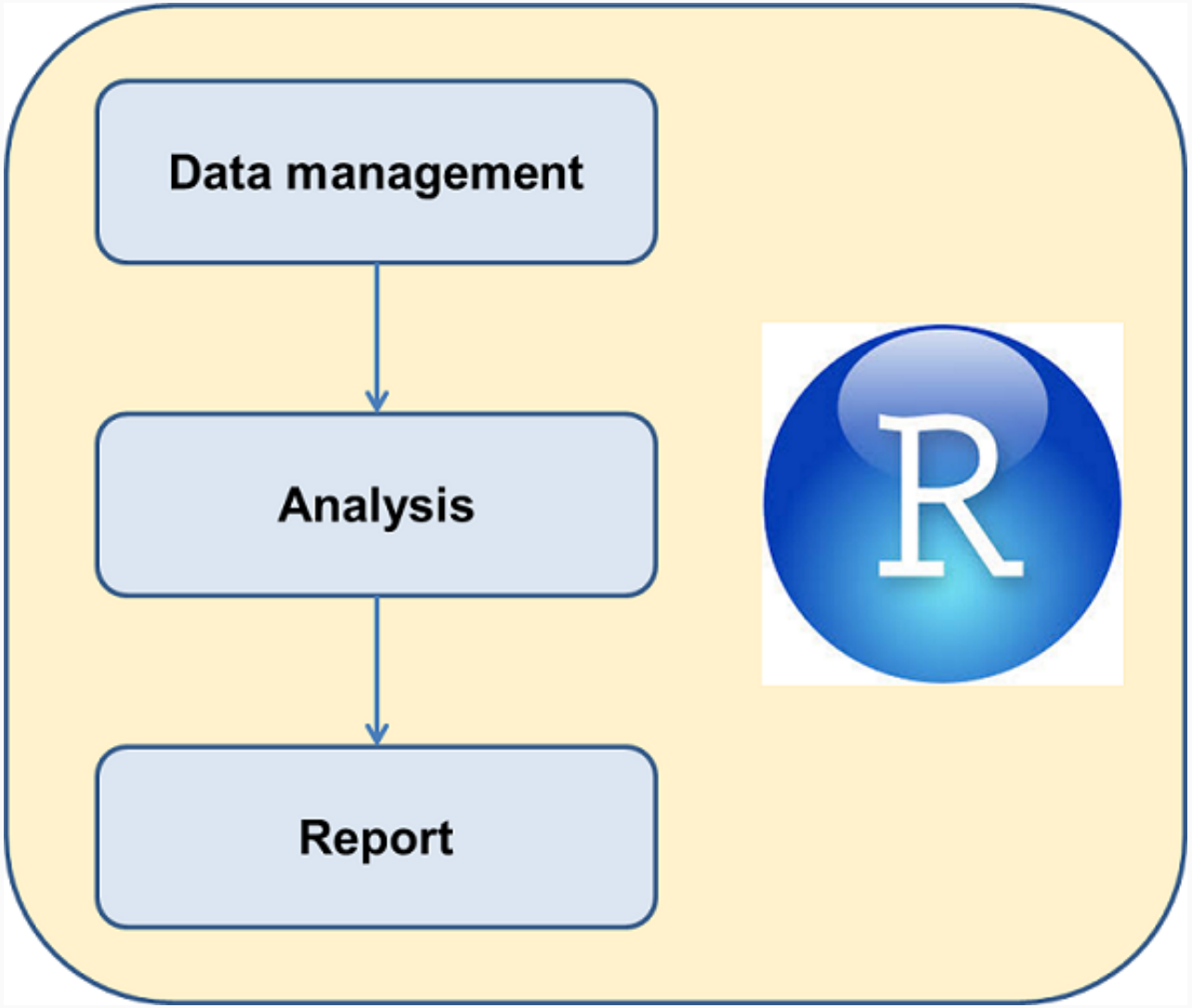
- Reproducible
- Reusable

Stuck with error / Found bug? Use `reprex`



https://reprex.tidyverse.org/

Dynamic reports



Rmarkdown documents

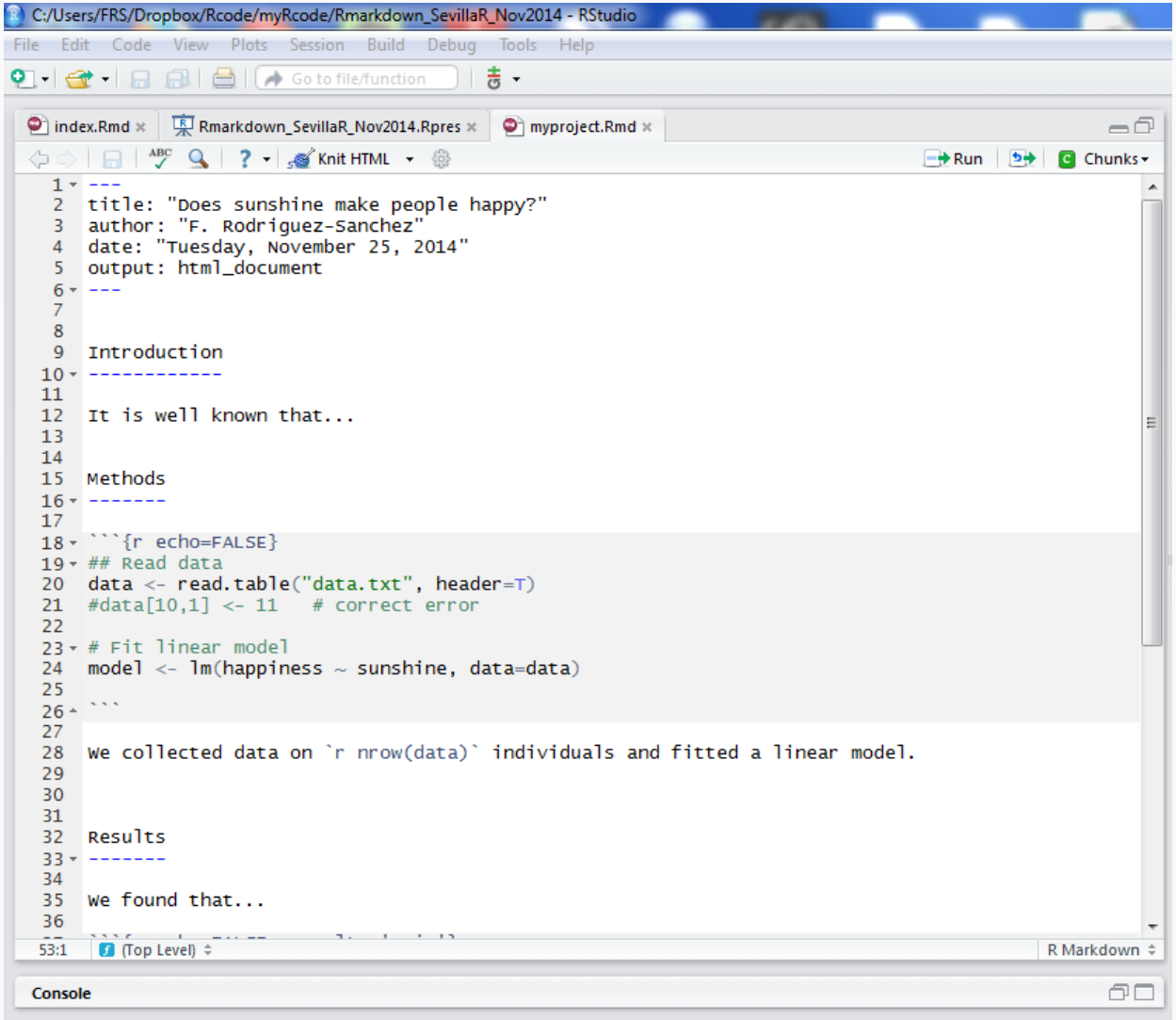
- Fully reproducible (trace all results inc. tables and plots)
- Dynamic (regenerate with 1 click)
- Suitable for
  - documents (HTML, Word, PDF)
  - presentations (HTML, PDF, PowerPoint)
  - books
  - websites
  - ...

Let's see Rmarkdown in action

In Rstudio, create new Rmarkdown document and click on `Knit HTML`.

Example: Does sunshine influence happiness?

See myproject.Rmd (http://bit.ly/rmdsun)



HTML output includes text, plot and formatted table

Does sunshine make people happy?

F. Rodriguez-Sanchez

Tuesday, November 25, 2014

Introduction

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

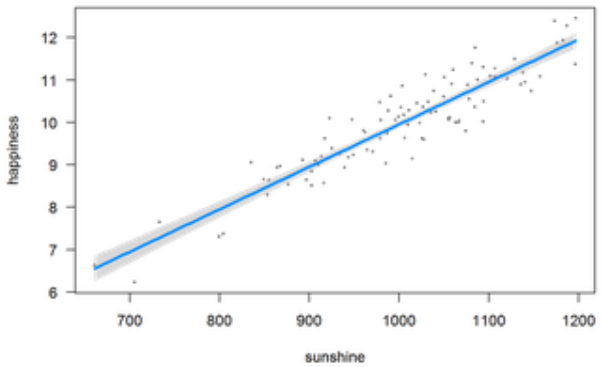
Methods

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

Results

We found that...

	Estimate	Std. Error	t value	Pr(>|t|)
(Intercept)	-0.0651657	0.4264970	-0.1527928	0.8788758
sunshine	0.0100228	0.0004232	23.6833264	0.0000000



Discussion

These results confirm that sunshine is good for happiness (slope = 0.0100228).

Acknowledgements

Y. Xie, J. MacFarlane, Rstudio...

Spotted error in the data? No problem!

Make changes in Rmarkdown document, click `knit` and report will **update automatically!**

Why Rmarkdown?

Convince me to start using R Markdown

R Markdown rmarkdown

Darren_Dahly

1. Start using R Markdown to generate reports of your data analyses.
2. If the data changes, rerun the report with a click of the mouse.
3. Take 3 days off of work.
4. On the 4th day, tell your collaborators that the re-analysis is complete.
5. Be hailed as a hero.

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

Other formats: PDF, Word, PowerPoint...

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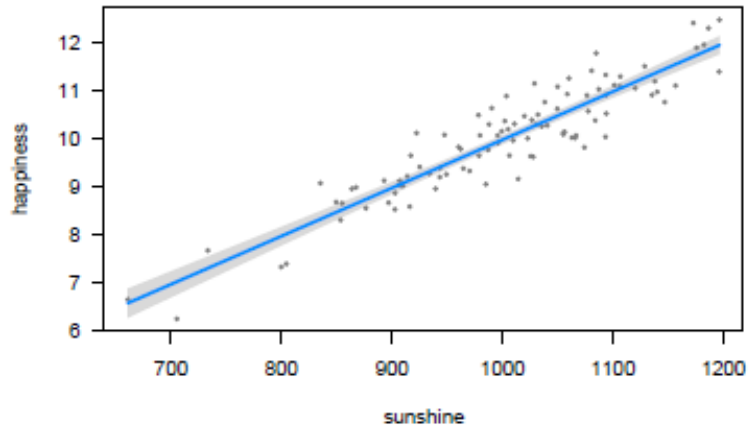

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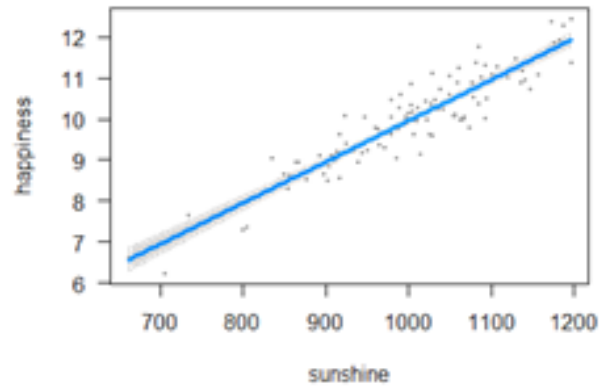
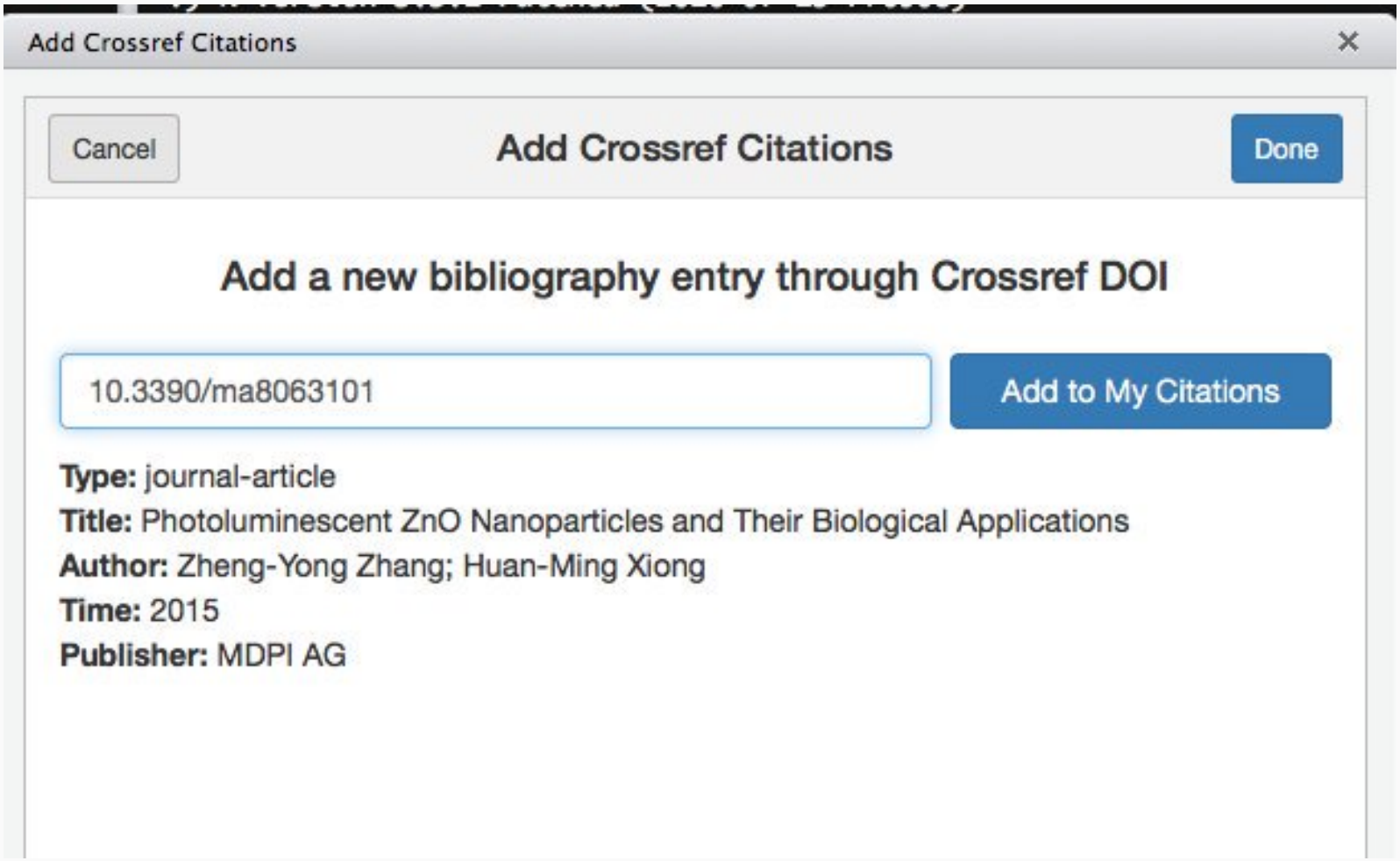
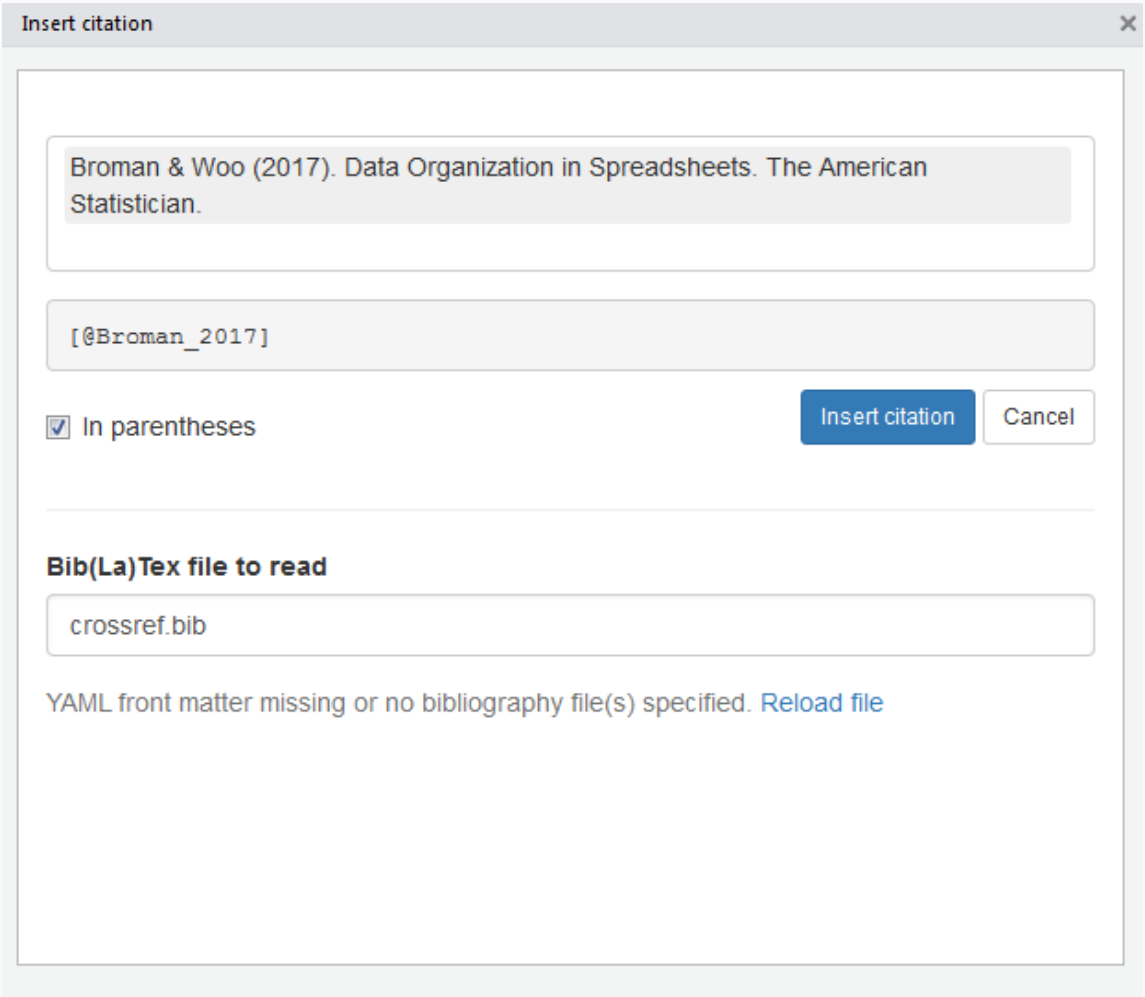


Adding citations by DOI: rcrossref



Adding citations from BibTeX file (or Zotero): citr

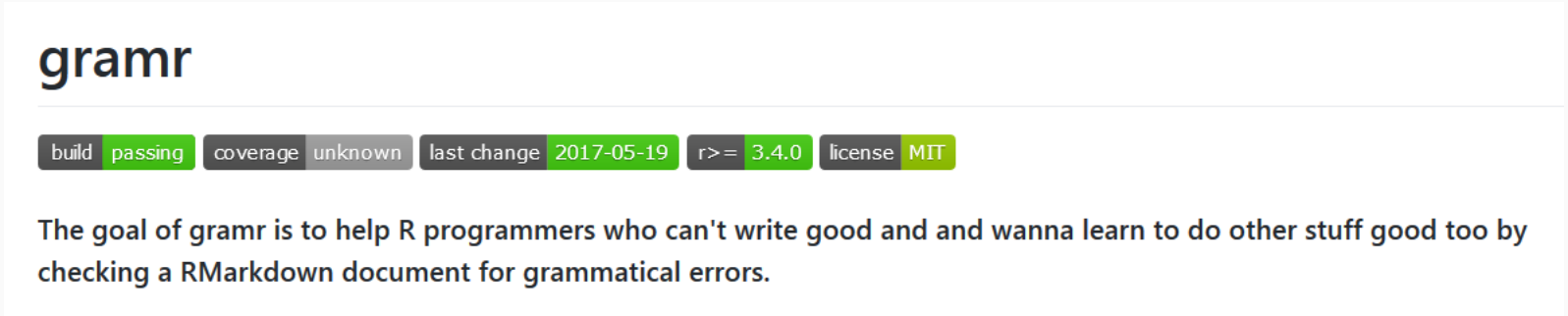


https://github.com/crsh/citr/

Insert equations

- Using LaTeX ($ or $$)
- bookdown:::mathquill
- mathpix: https://github.com/jonocarroll/mathpix

Revise writing style: gramr

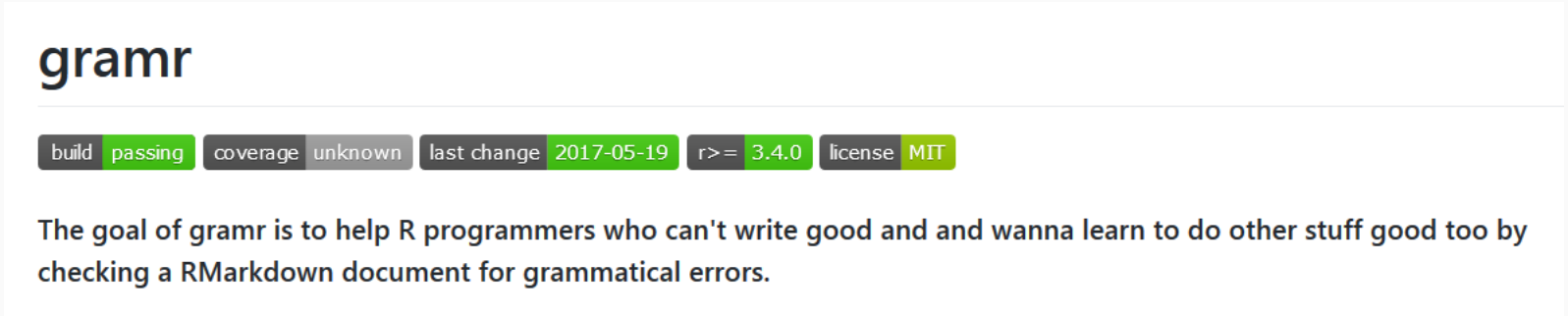


https://github.com/ropenscilabs/gramr

Spell and grammar checking

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

Find synonyms



https://github.com/gadenbuie/synamyn

Word count and readability

https://github.com/benmarwick/wordcountaddin

Manuscript templates

- rticles: Elsevier, Springer, PeerJ, PNAS, PLoS...
- rmdTemplates
- Check out GitHub for Rmarkdown templates...

Write your next PNAS/PLoS/PeerJ/whatever in Rmarkdown!

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 19, 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.

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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.

DRAFT

Some real examples

Impactos de la herbivoría por ungulados en las comunidades de plantas leñosas del Parque Natural Los Alcornocales

Francisco Rodríguez-Sánchez[1,4], Virginia Luque-Oliva[1,2], Vicente Jurado[3]

1. Departamento de Ecología Integrativa, Estación Biológica de Doñana, Consejo Superior de Investigaciones Científicas, Avda. Américo Vespucio 26, 41092 Sevilla, España.

1. Universidad Pablo de Olavide, Ctra. de Utrera s/n, Dos Hermanas, Sevilla, España.

1. Facultad de Geografía e Historia, C/ Doña María de Padilla s/n, 41004 Sevilla, España.

1. Autor para correspondencia [frodriguez.work@gmail.com]

Resumen

Las poblaciones de ciervos y otros ungulados se han incrementado enormemente en muchas áreas mediterráneas en las últimas décadas. Los impactos del incremento de la presión de herbivoría en las comunidades de plantas y la eficacia de distintas medidas de conservación están aún poco claras. En este trabajo se evalúan los efectos de la herbivoría en comunidades arbustivas del Campo de Gibraltar y Parque Natural de Los Alcornocales. Se ha comparado la diversidad de plantas, la cobertura, la altura y la intensidad de daños dentro y fuera de un total de 20 cercados de exclusión de herbívoros establecidos hace 10-15 años para favorecer la regeneración del bosque. Aunque la composición de la comunidad de plantas (riqueza de especies y diversidad) fue similar en las zonas cercadas y no cercadas, la altura de los arbustos y su cobertura fueron mayores dentro de los cercados de protección. En contraste, el daño de herbivoría fue

https://github.com/Pakillo/exclosures-Almoraima/

Can write full thesis in Rmarkdown!

See thesis.Rmd.

See thesis.pdf.

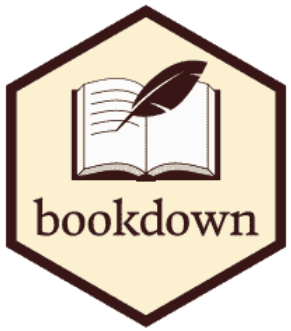
Bookdown

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: xaringan

https://github.com/yihui/xaringan

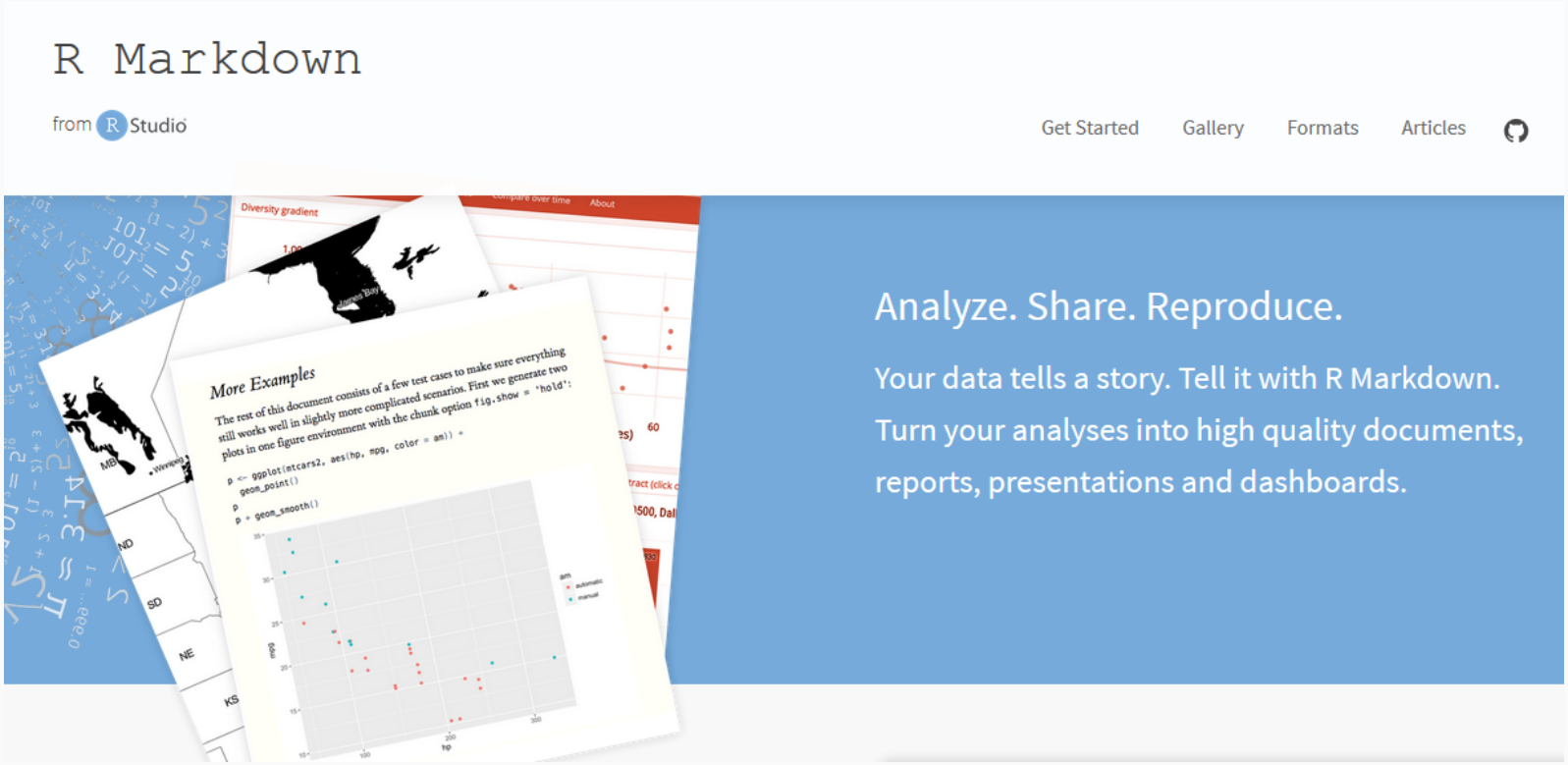
Parameterised reports

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

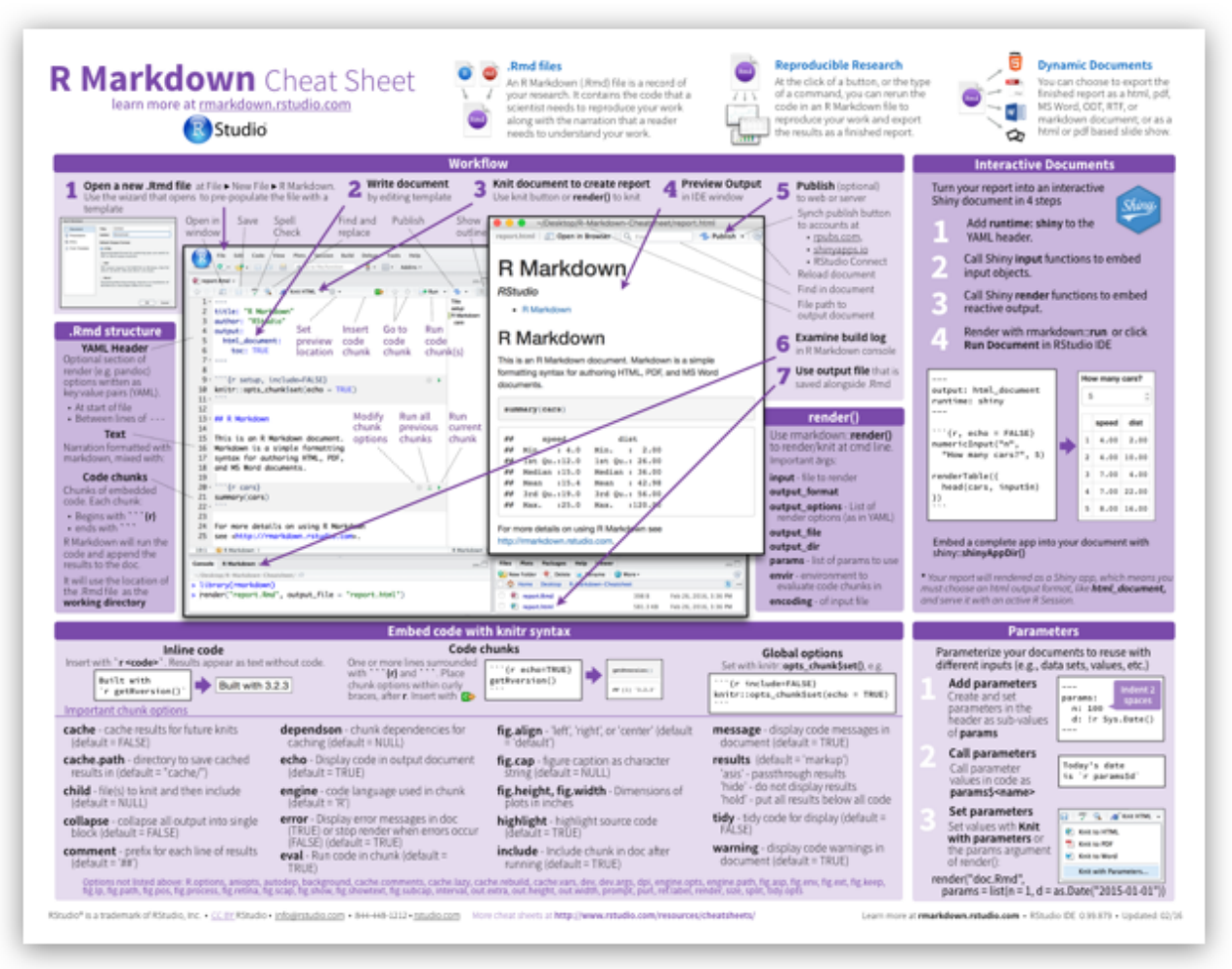
Resources

Rmarkdown website

http://rmarkdown.rstudio.com/index.html

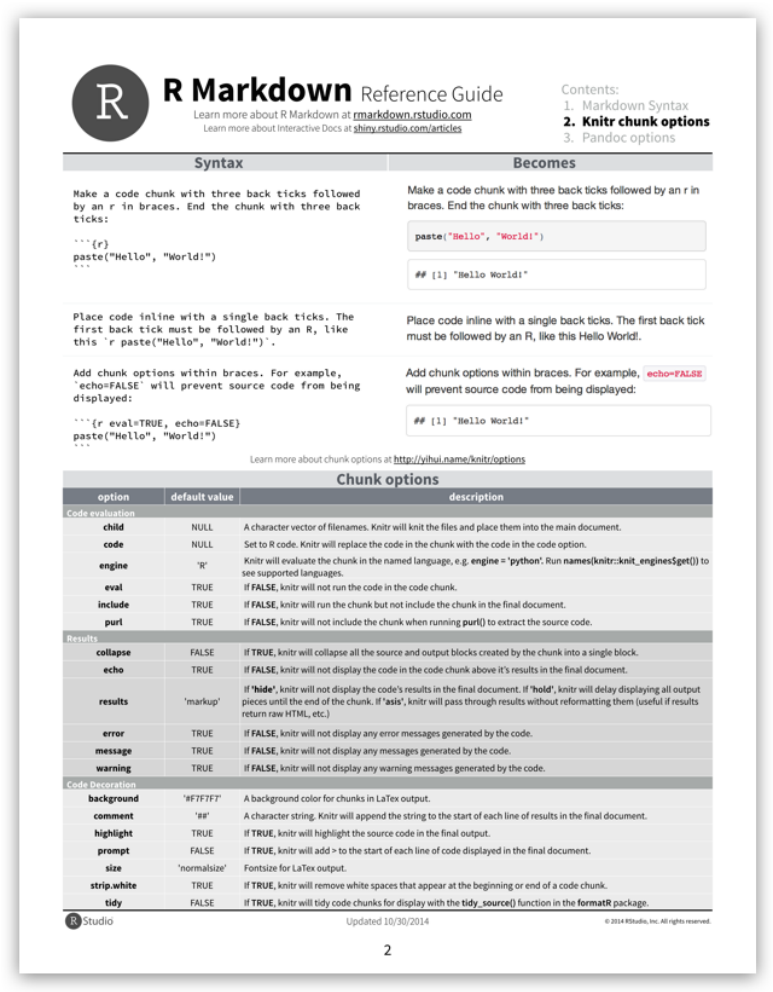


Rmarkdown cheat sheet



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.

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2

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

Rmarkdown book

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* →

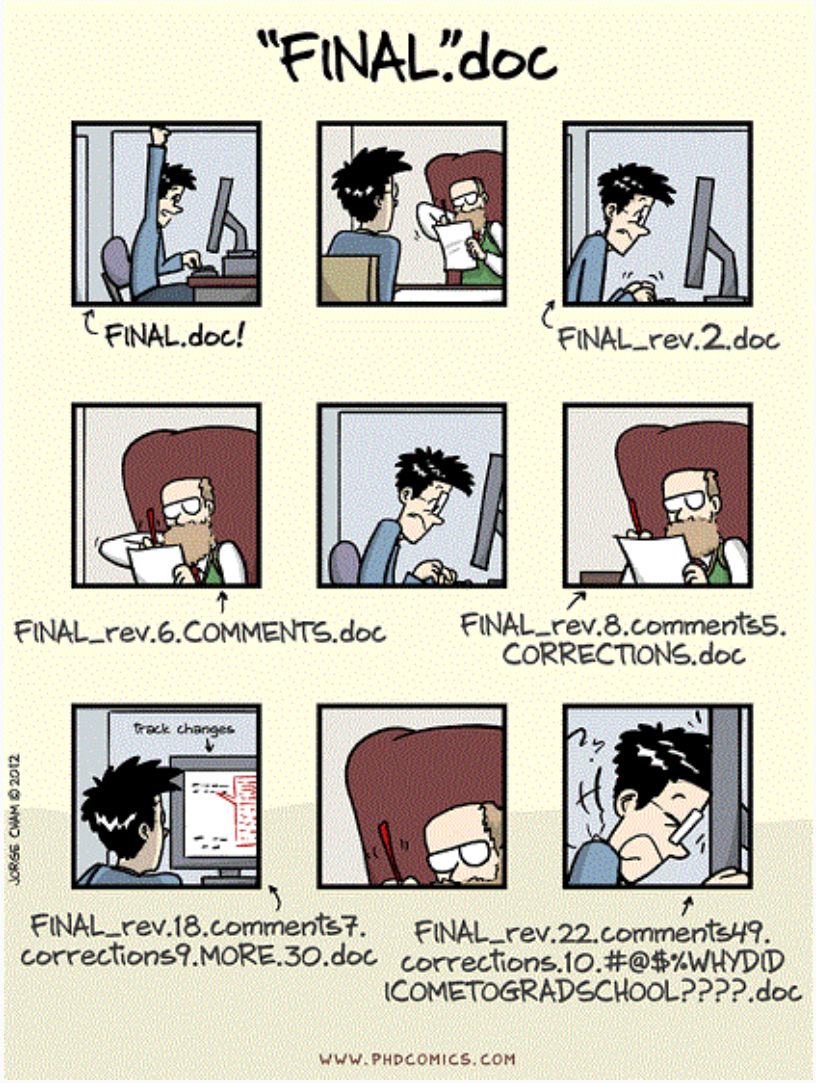
https://bookdown.org/yihui/rmarkdown/

Managing software dependencies

Managing package dependencies in R

- **sessionInfo** (or session_info)
- **checkpoint**
- packrat
- switchr
- docker

Version control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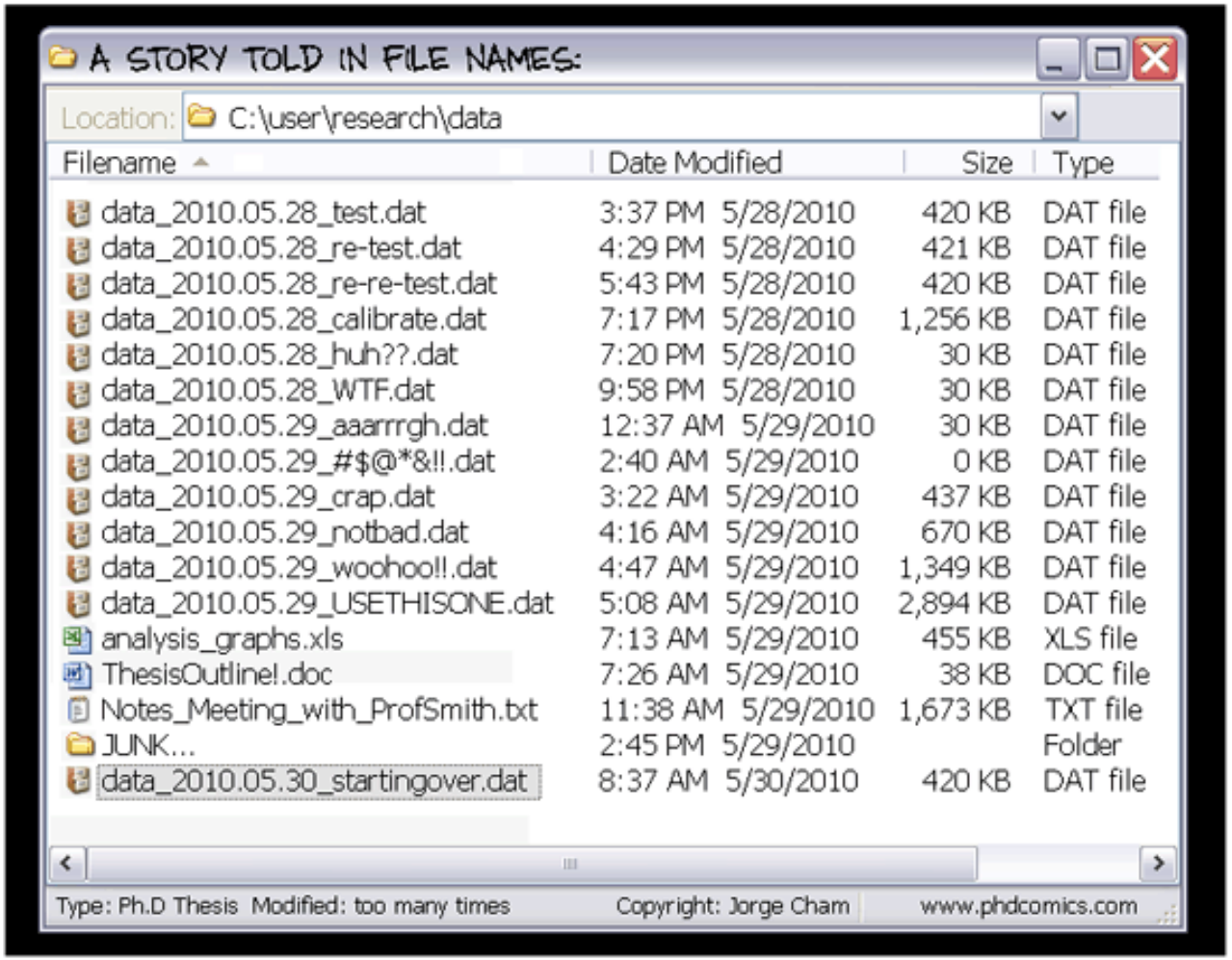
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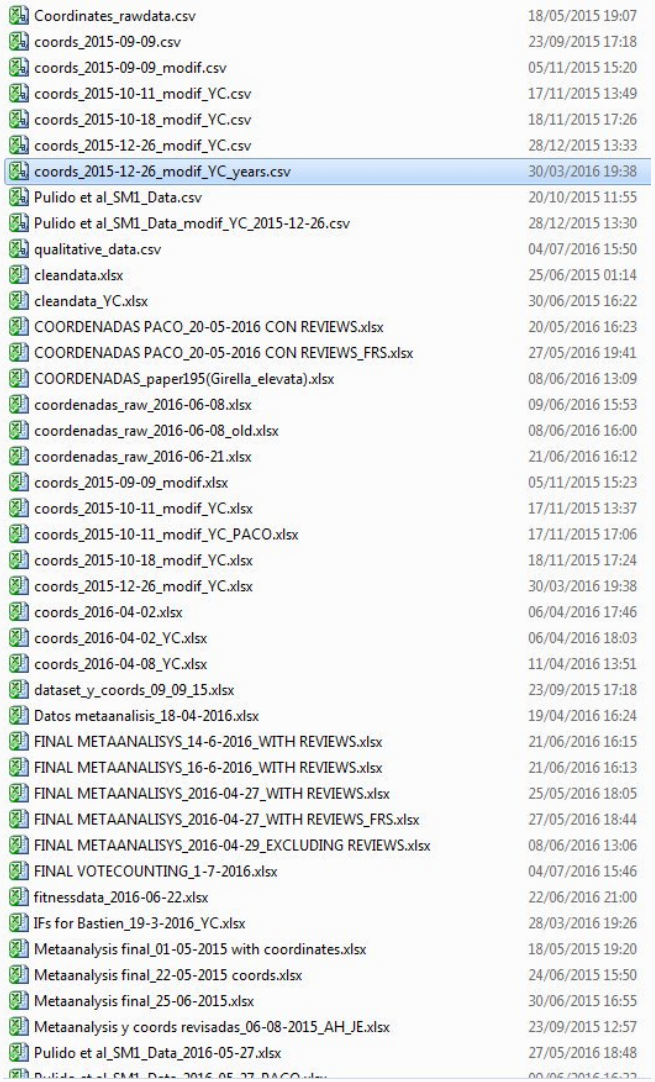
www.phdcomics.com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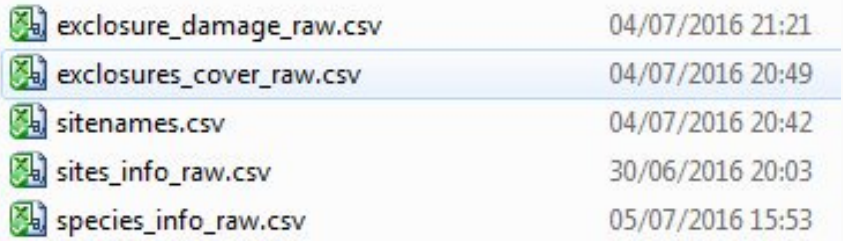
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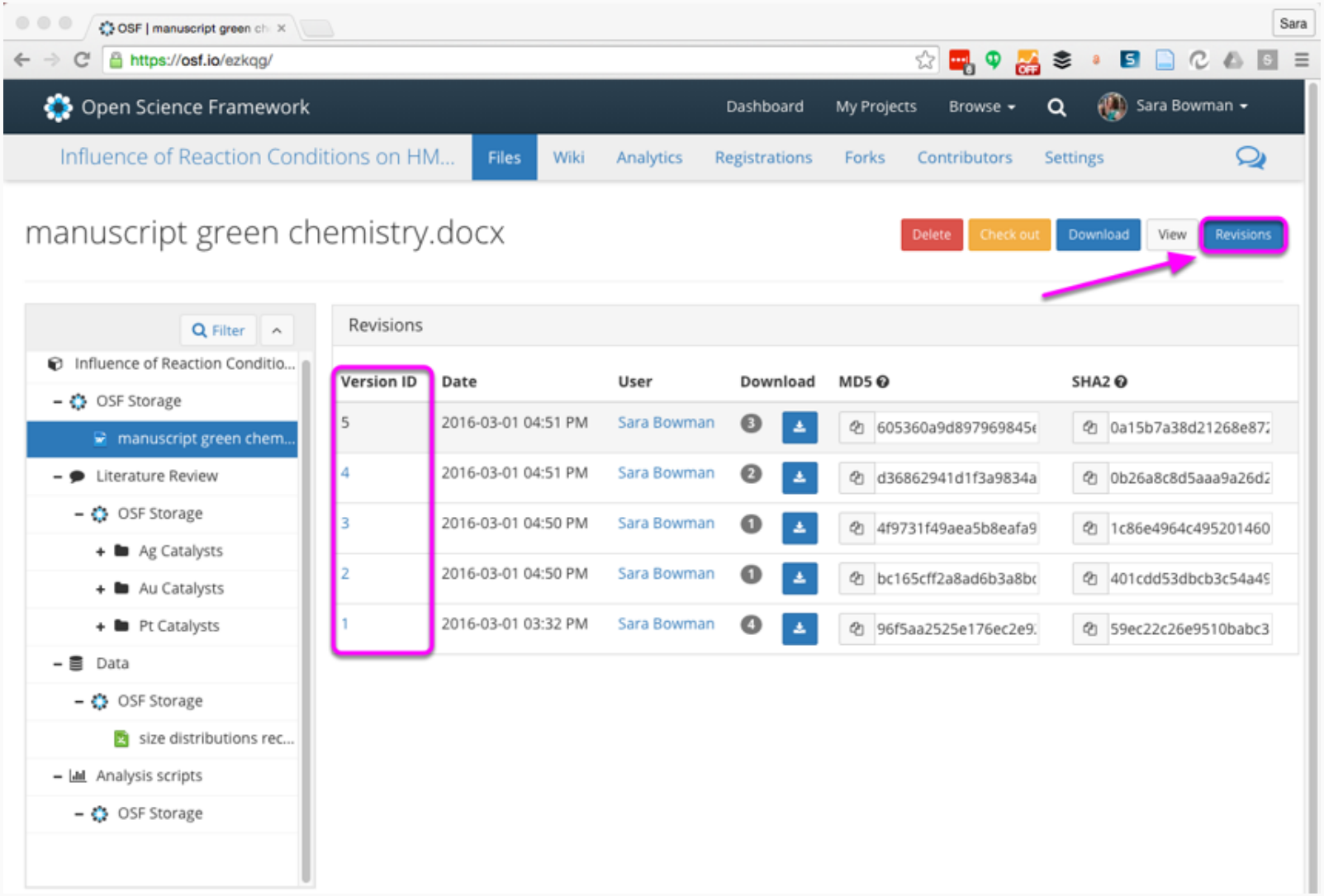
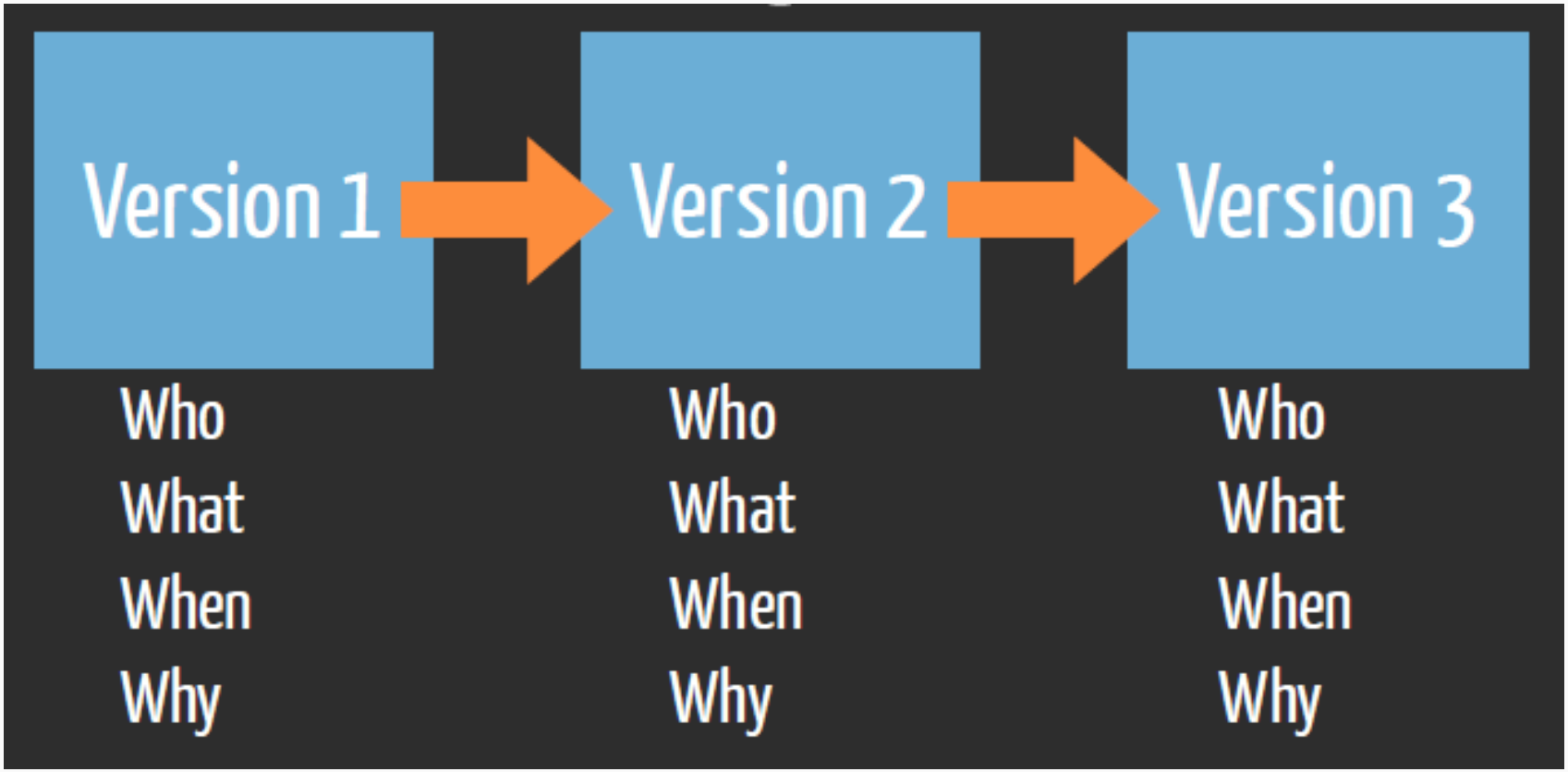
Automatic version control, no time limit.





R. Fitzjohn (https://github.com/richfitz/reproducibility-2014)

Git & GitHub

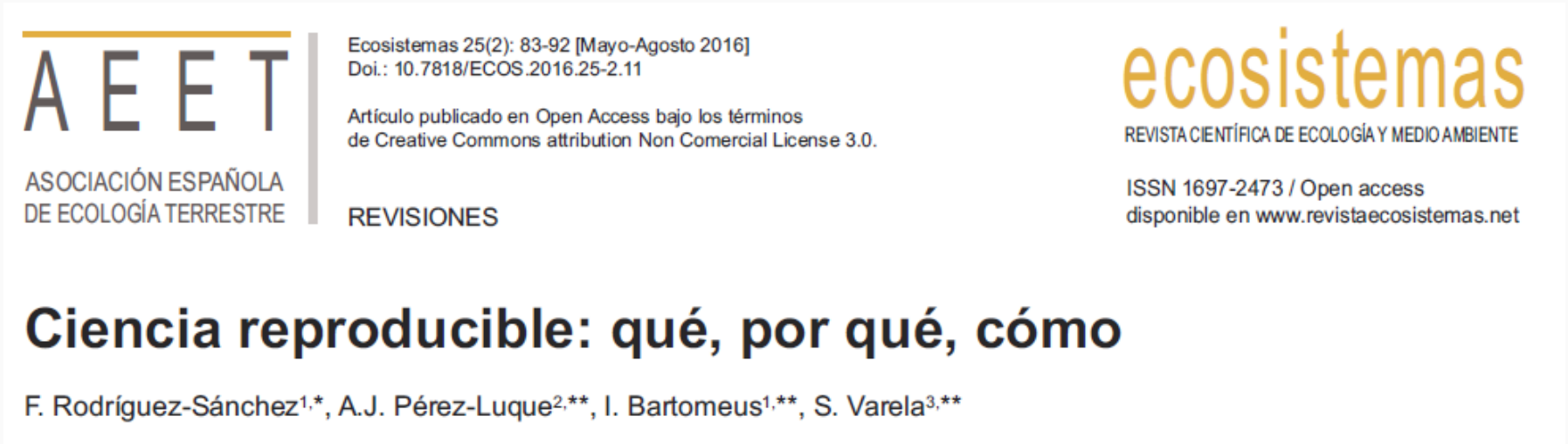
- Sign up for GitHub
- Install Git
- Introduce yourself
- Create repo on GitHub
- Clone repo in Rstudio
- Make changes, push, pull
- Collaboration

Collaborative writing

Many alternatives

- Rmarkdown + GitHub
- Word + Dropbox
- Google Docs
- Overleaf
- Authorea
- ...

To read more



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F. Rodríguez-Sánchez[1,*], A.J. Pérez-Luque[2,**], I. Bartomeus[1,**], S. Varela[3,**]

http://www.revistaecosistemas.net/index.php/ecosistemas/article/viewFile/1178/973

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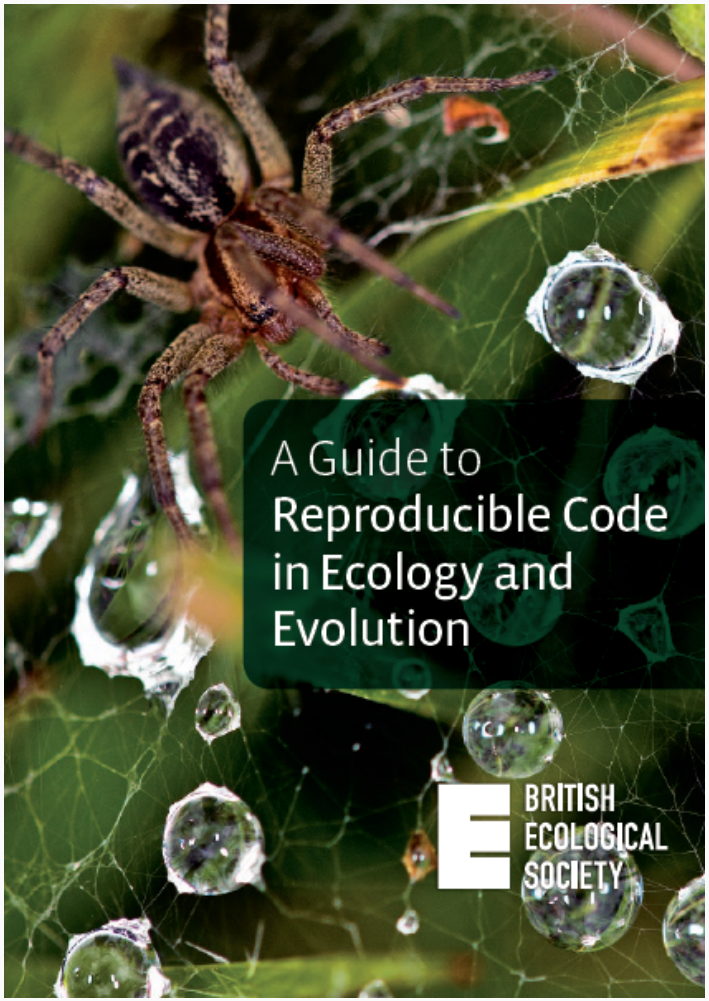

https://www.britishecologicalsociety.org/publications/guides-to/

Happy writing!

Slides and source code available at

https://github.com/Pakillo/ReproducibleScience