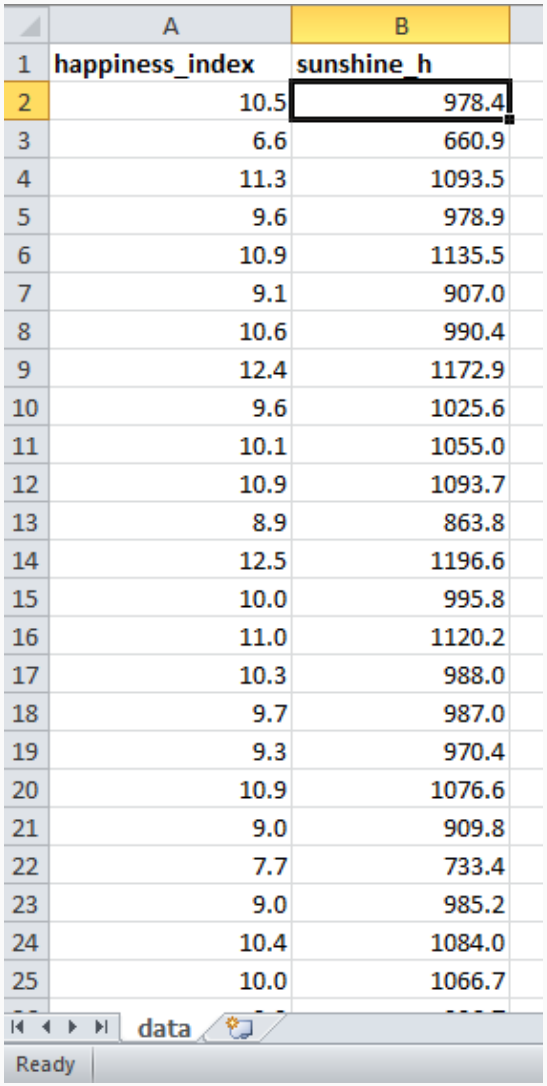
Doing reproducible science: from your hard-won data to a publishable manuscript without going mad

Francisco Rodriguez-Sanchez

@frod_san

A typical research workflow

1. Prepare data (**EXCEL**)



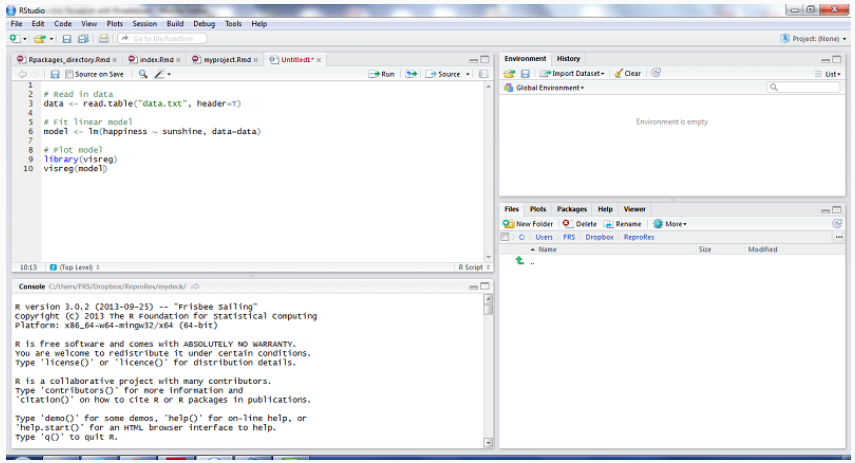
	A	B
1	happiness_index	sunshine_h
2	10.5	978.4
3	6.6	660.9
4	11.3	1093.5
5	9.6	978.9
6	10.9	1135.5
7	9.1	907.0
8	10.6	990.4
9	12.4	1172.9
10	9.6	1025.6
11	10.1	1055.0
12	10.9	1093.7
13	8.9	863.8
14	12.5	1196.6
15	10.0	995.8
16	11.0	1120.2
17	10.3	988.0
18	9.7	987.0
19	9.3	970.4
20	10.9	1076.6
21	9.0	909.8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

data

Ready

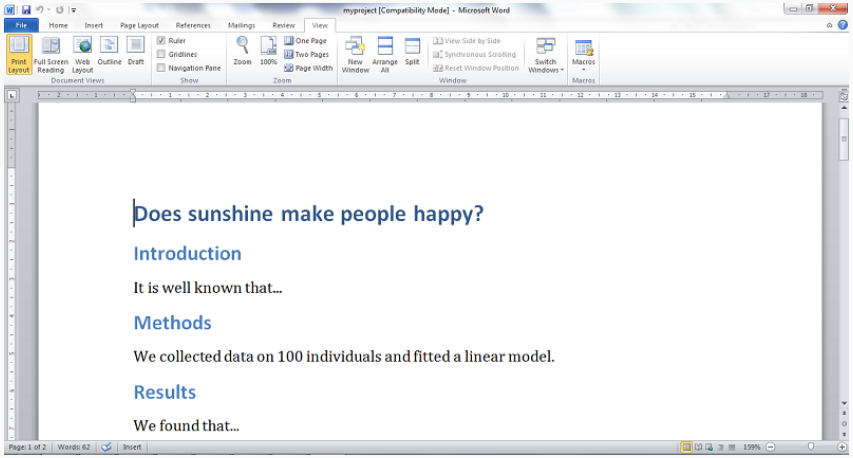
A typical research workflow

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



A typical research workflow

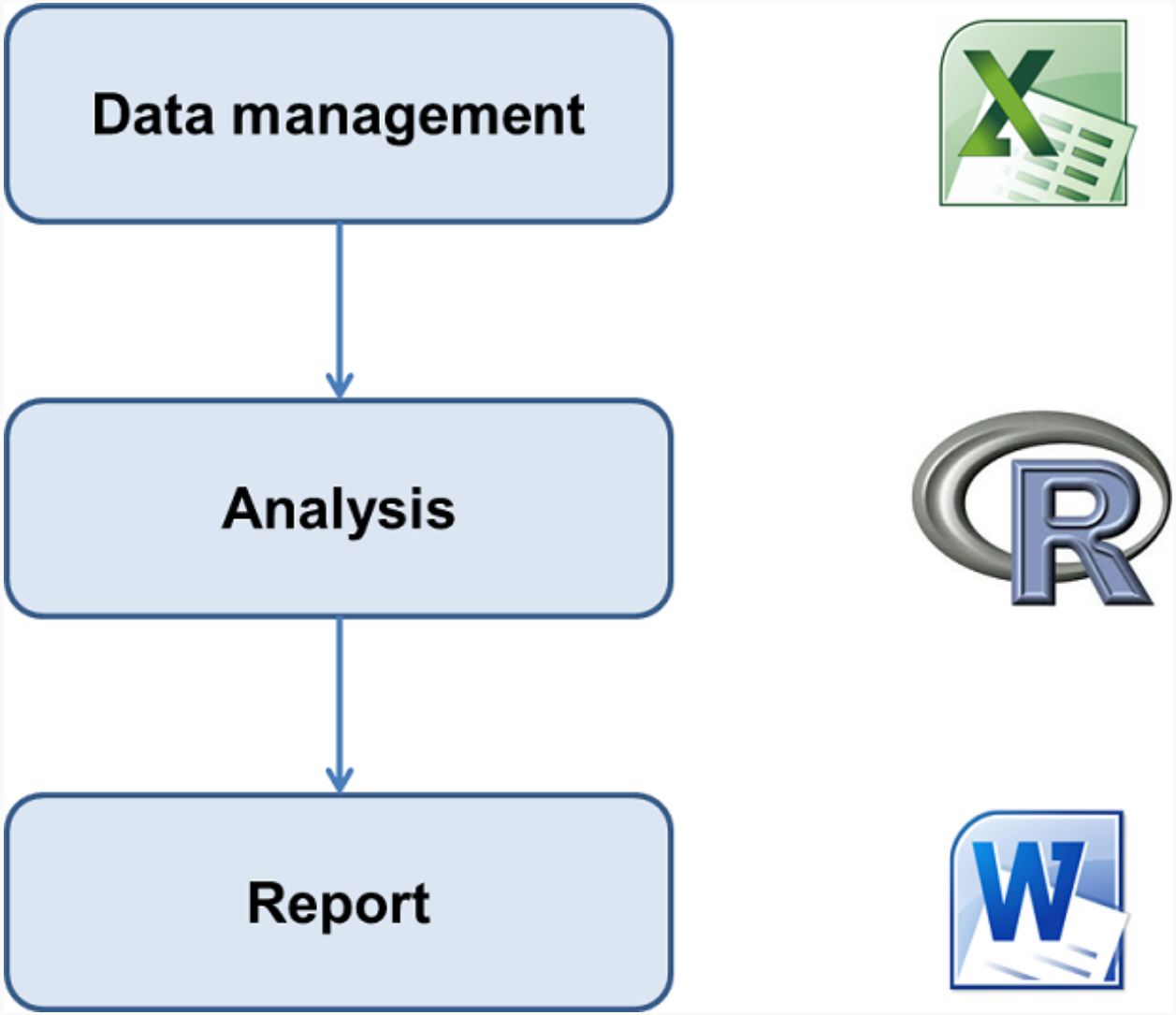
1. Prepare data (**EXCEL**)
2. Analyse data (**R**)
3. Write report/paper (**WORD**)



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 . . . ?

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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

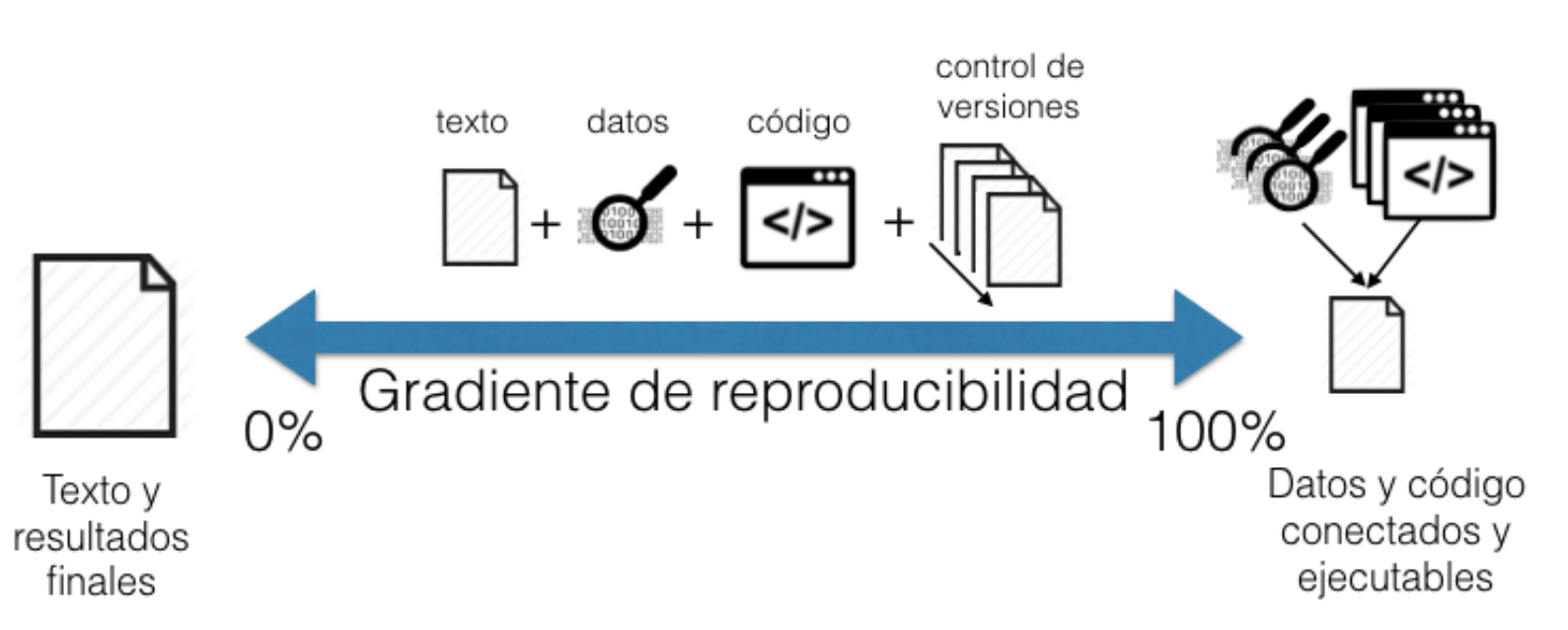
WHAT is Reproducible Science?

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

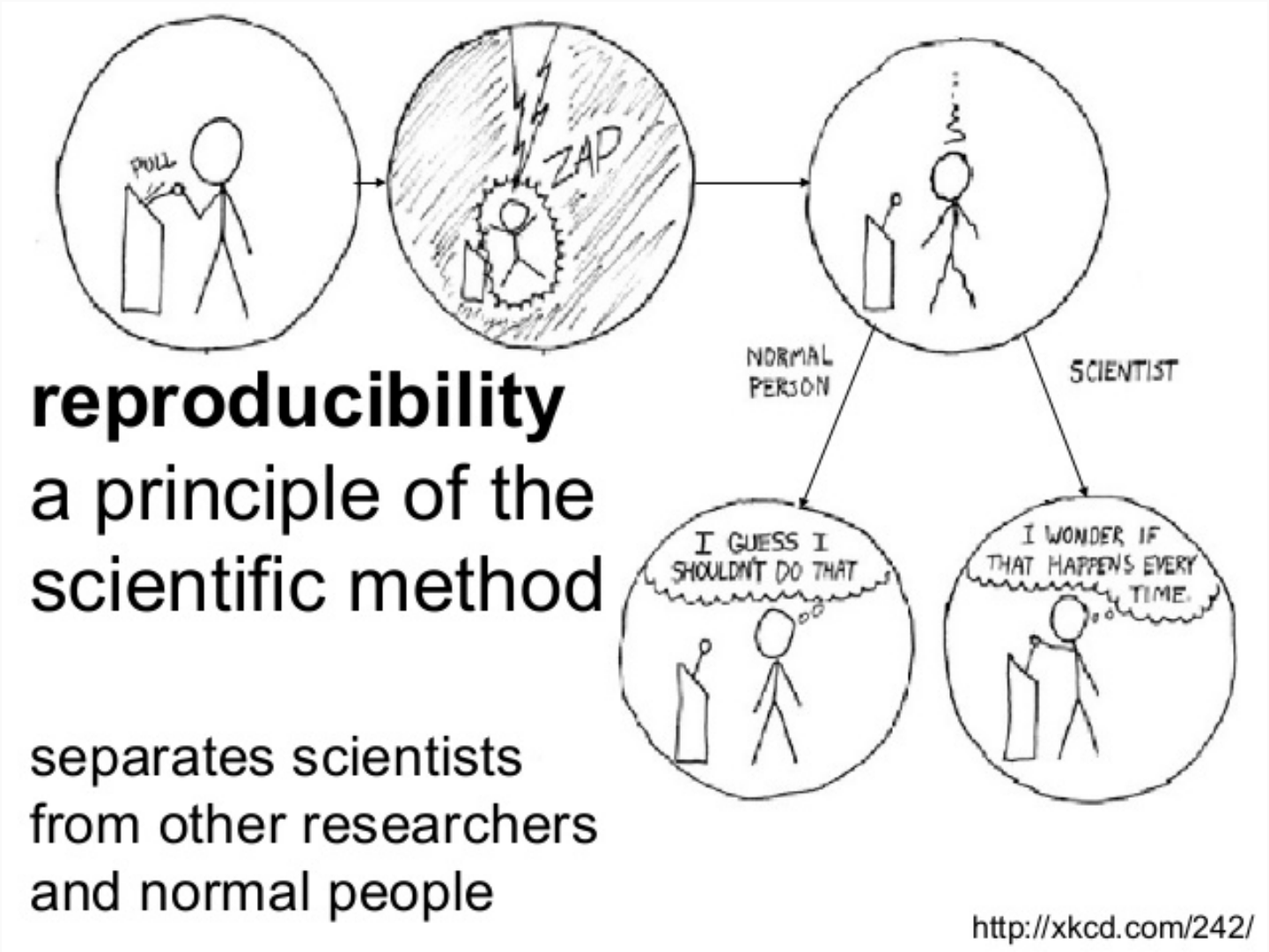


Even **you** will struggle to reproduce **your own results** from a few weeks/months ago.

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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- Fundamental pillar of **scientific method**
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- Regenerate results **automatically**
- **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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- **Raw data untouched** in independent folder.

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File organisation

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

File organisation example

```
myproject

|- 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
```

Data management

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

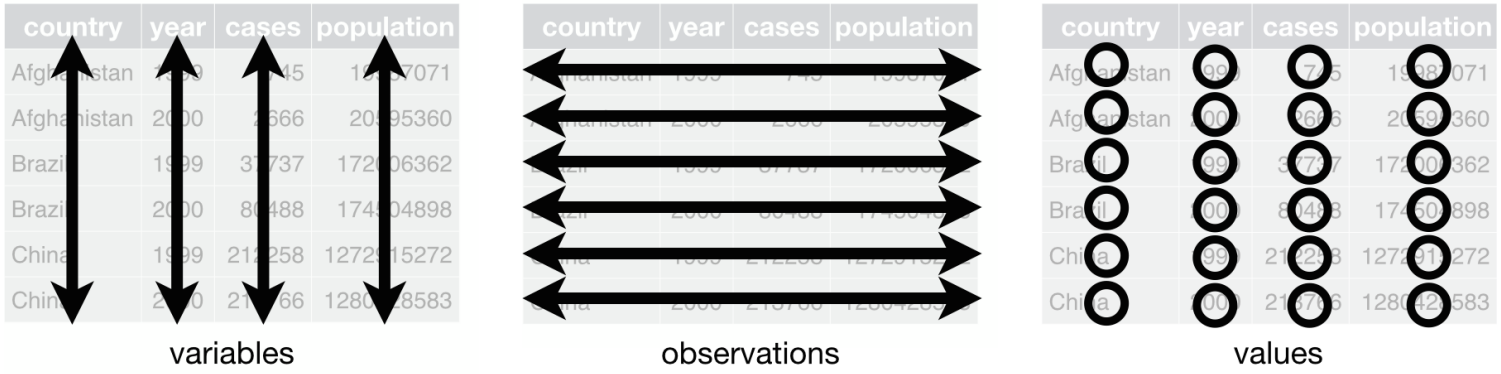
http://science.sciencemag.org/content/354/6317/1242.1

Storage

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

- Dropbox
- OSF
- Figshare, 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
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Afghanistan	745	2666
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table4

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

Spreadsheet good practices

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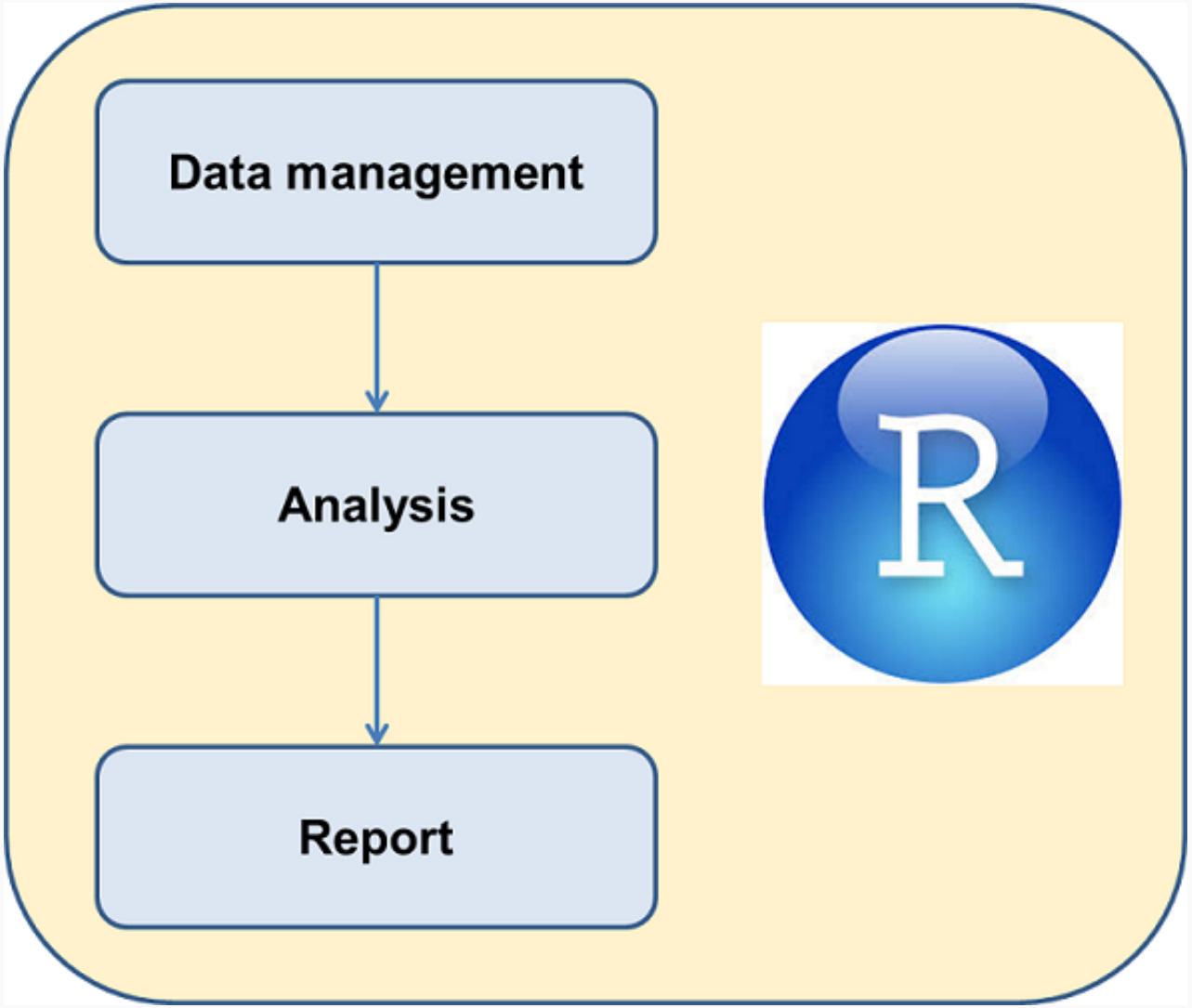
- http://kbroman.org/dataorg/

Data analysis

Always use code

- Reproducible
- Reusable

Dynamic reports



Rmarkdown documents

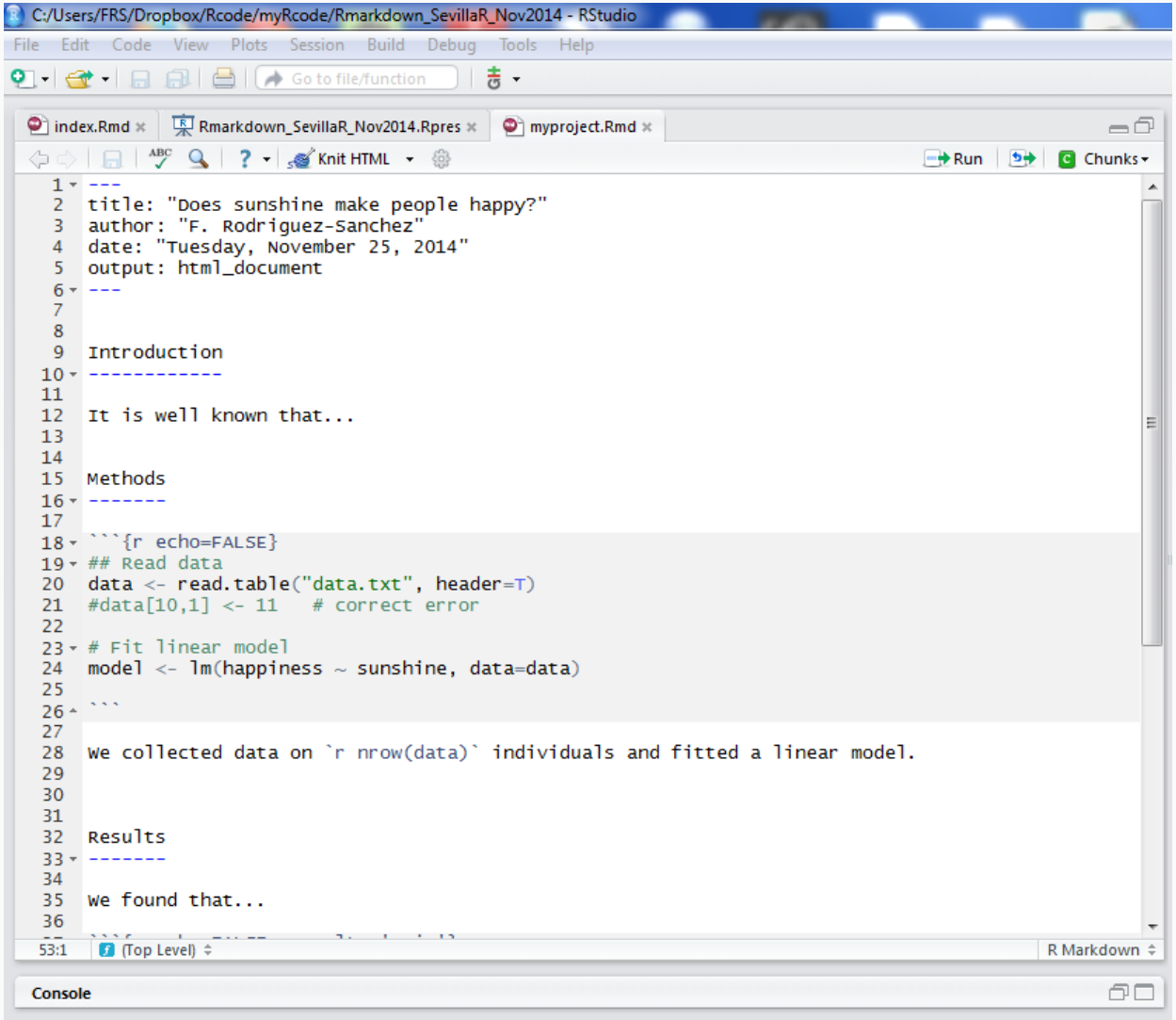
- Fully reproducible (trace all results inc. tables and plots)
- Dynamic (regenerate with 1 click)
- Suitable for
  - documents (Word, PDF, etc)
  - presentations
  - books
  - websites
  - ...

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|)
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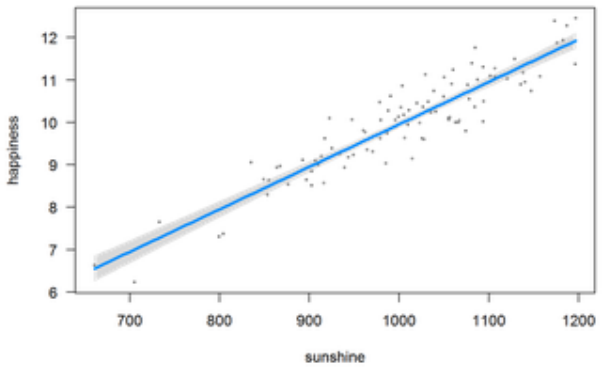
sunshine	0.0100228	0.0004232	23.6833264	0.0000000



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!**

Other formats: PDF, Word

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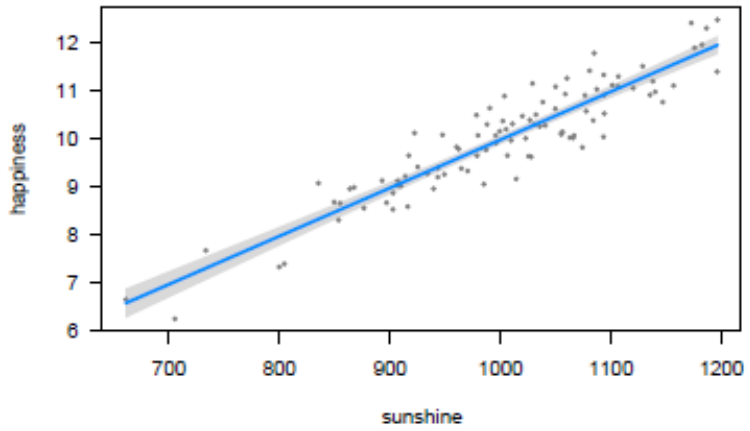

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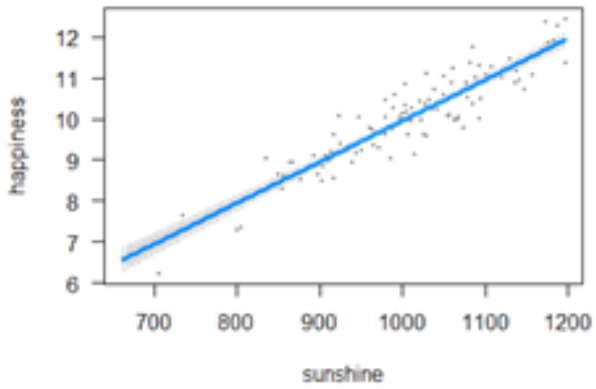
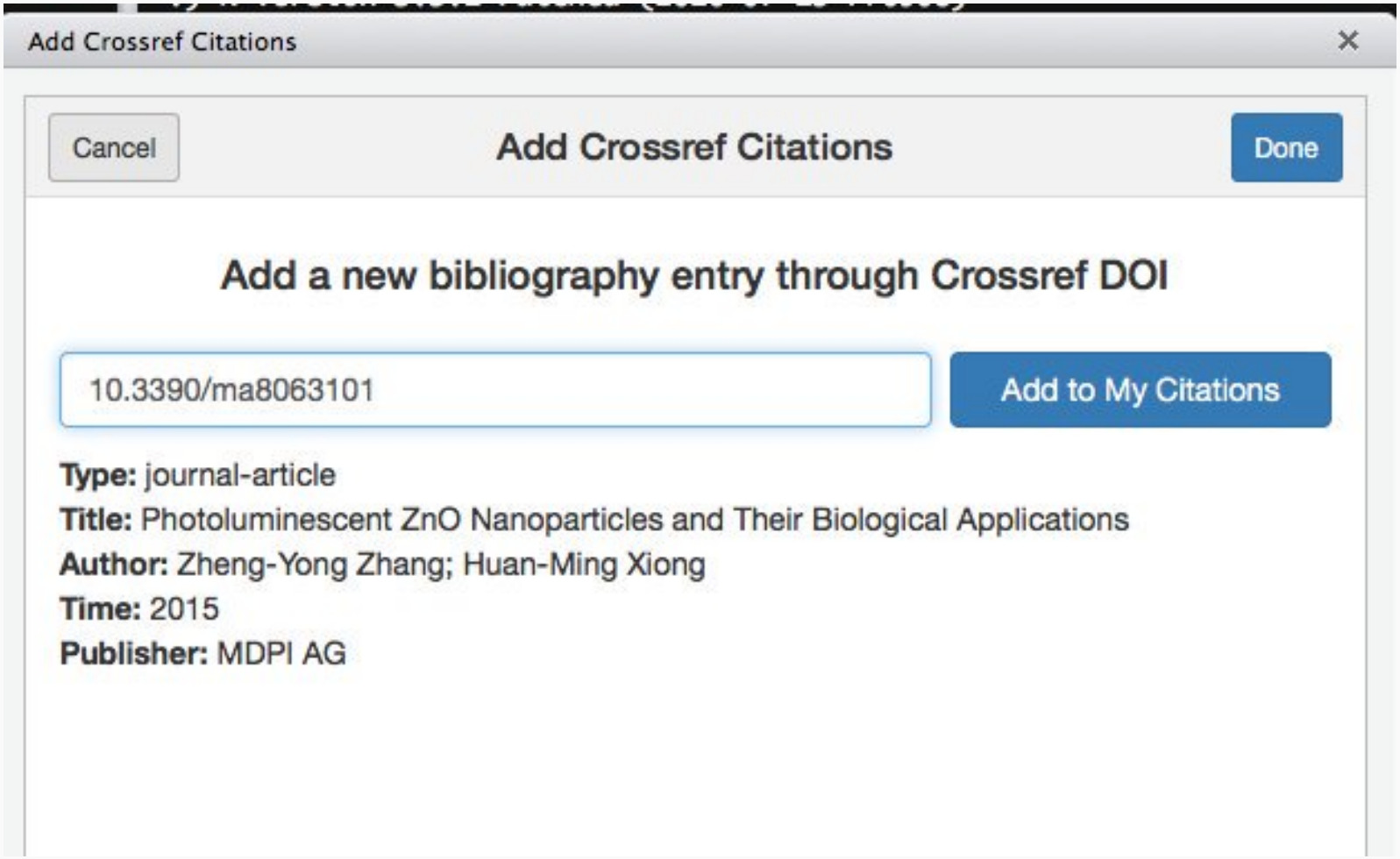


Adding citations by DOI

rcrossref addin



Adding citations from BibTeX file

citr addin

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

Manuscript templates

- rticles
- rmdTemplates

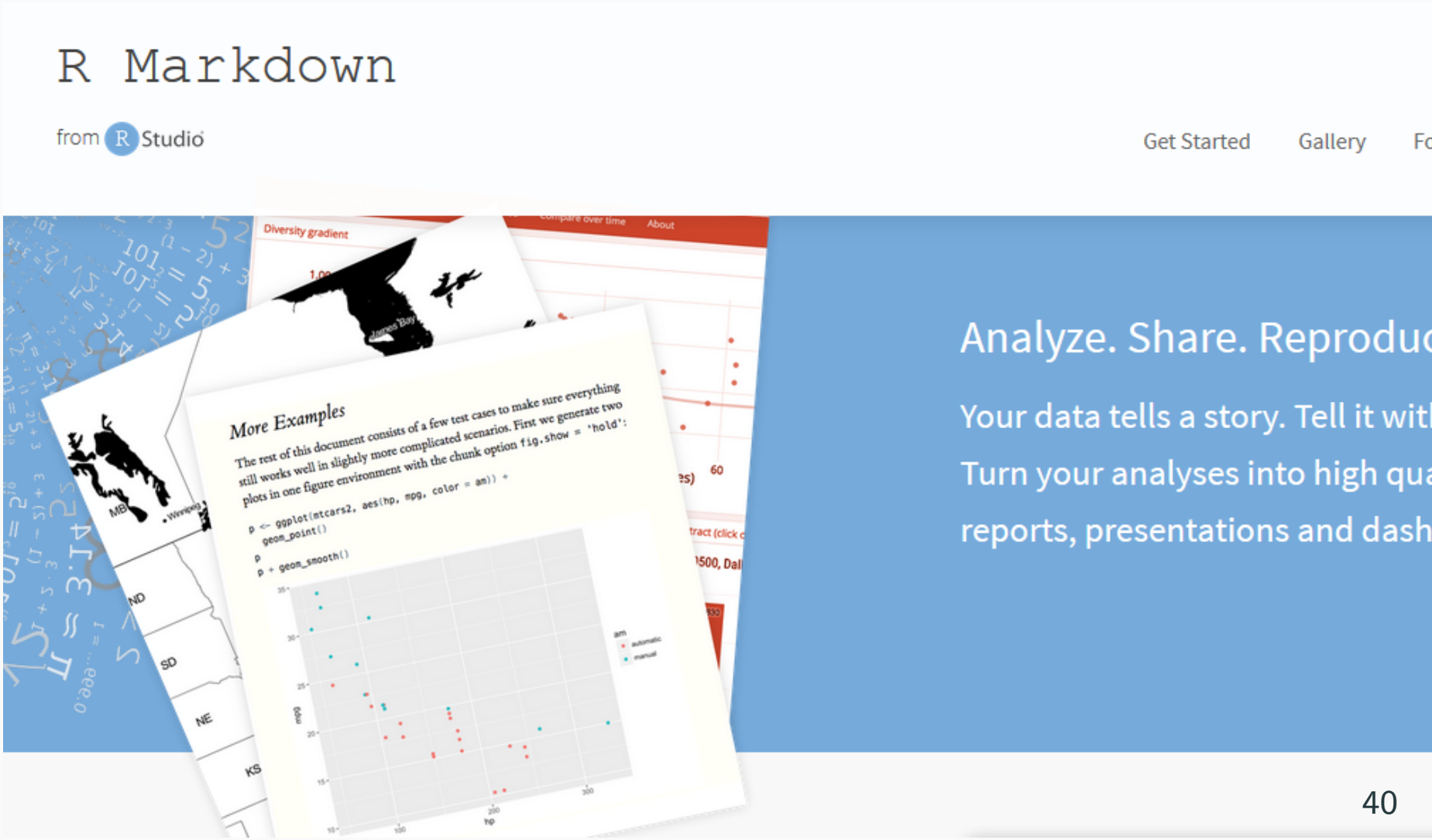
Can write full thesis in Rmarkdown!

See `thesis.Rmd`.

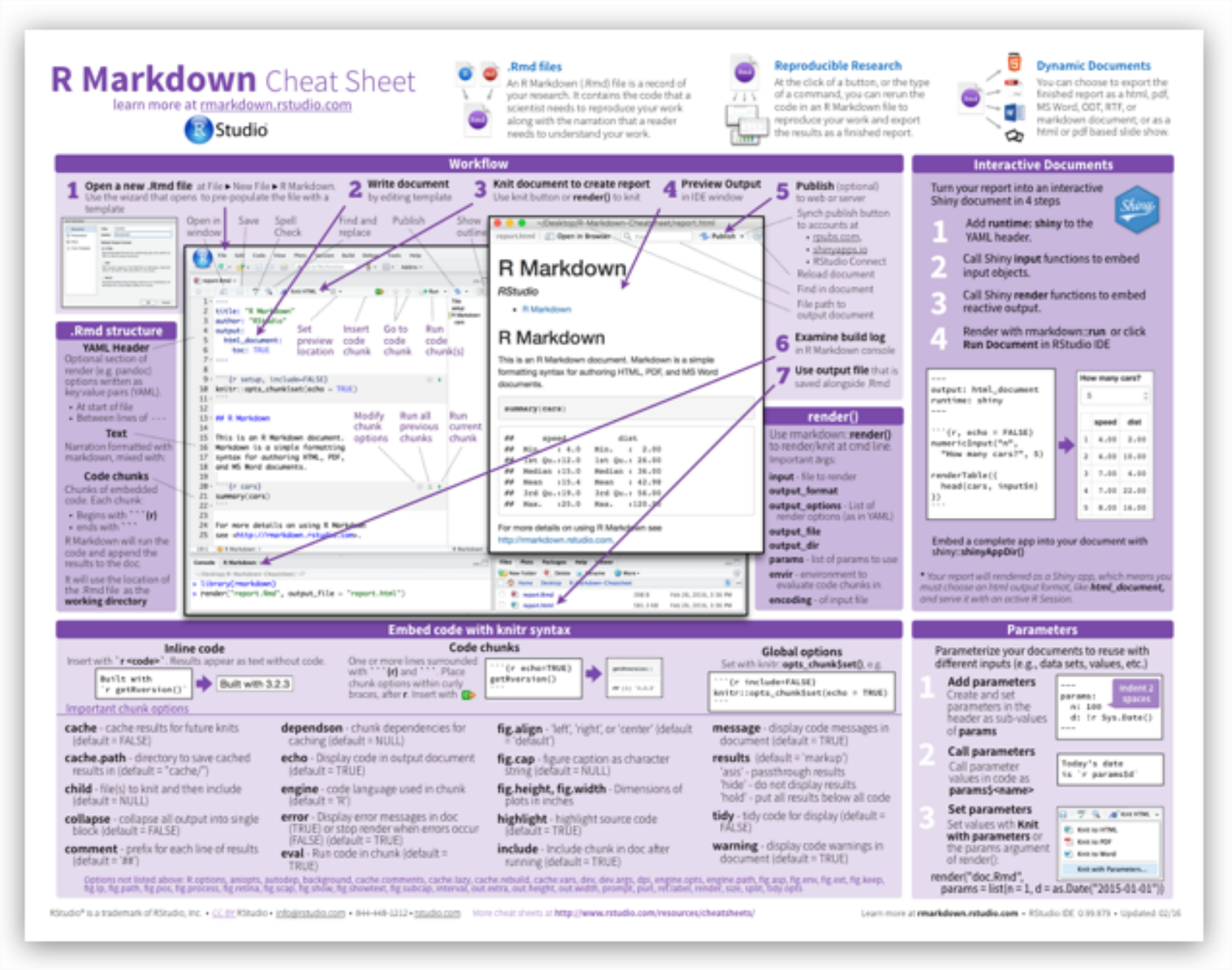
See `thesis.pdf`.

Rmarkdown website

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



Rmarkdown cheat sheet



https://www.rstudio.com/wp-content/uploads/2016/03/

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 © 2014 RStudio, Inc. All rights reserved.

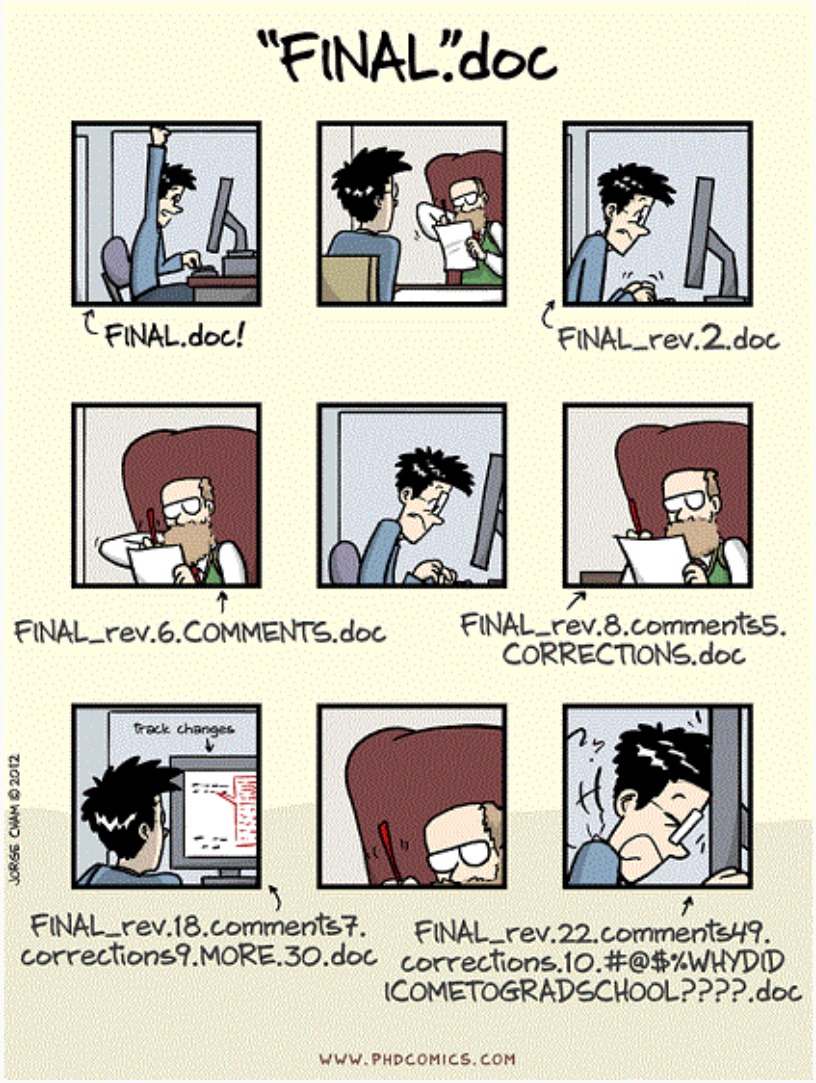
2

Managing software dependencies

Managing package dependencies in R

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

Version control

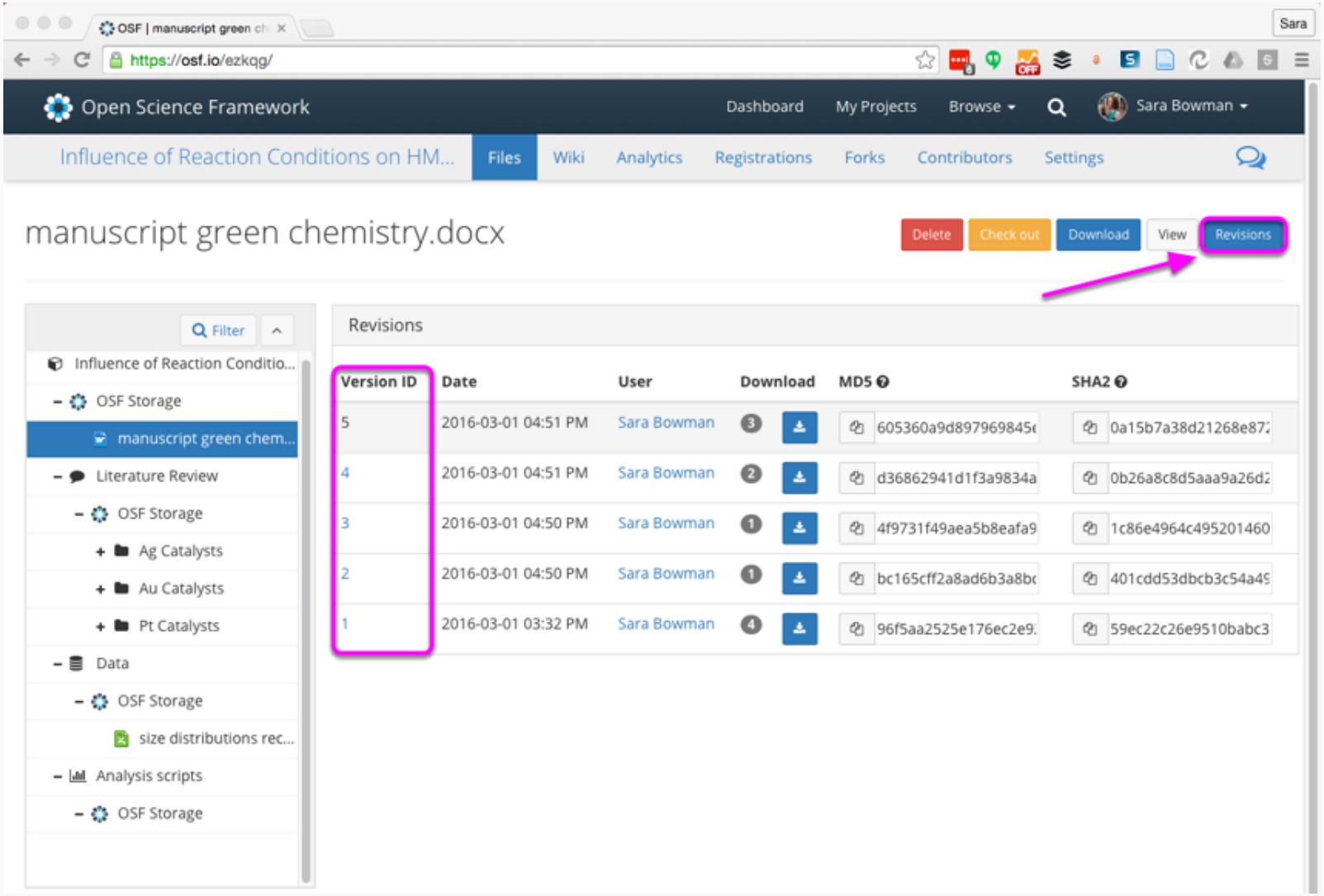

"FINAL".doc
FINAL.doc!
FINAL_rev.2.doc
FINAL_rev.6.COMMENTS.doc
FINAL_rev.8.comments5.
CORRECTIONS.doc
track changes
FINAL_rev.18.comments7.
corrections9.MORE.30.doc
FINAL_rev.22.comments49.
corrections.10.#@$%WHYDID
ICOMETOGRADSCHOOL????.doc
JORGE CHAM © 2012
WWW.PHDCOMICS.COM

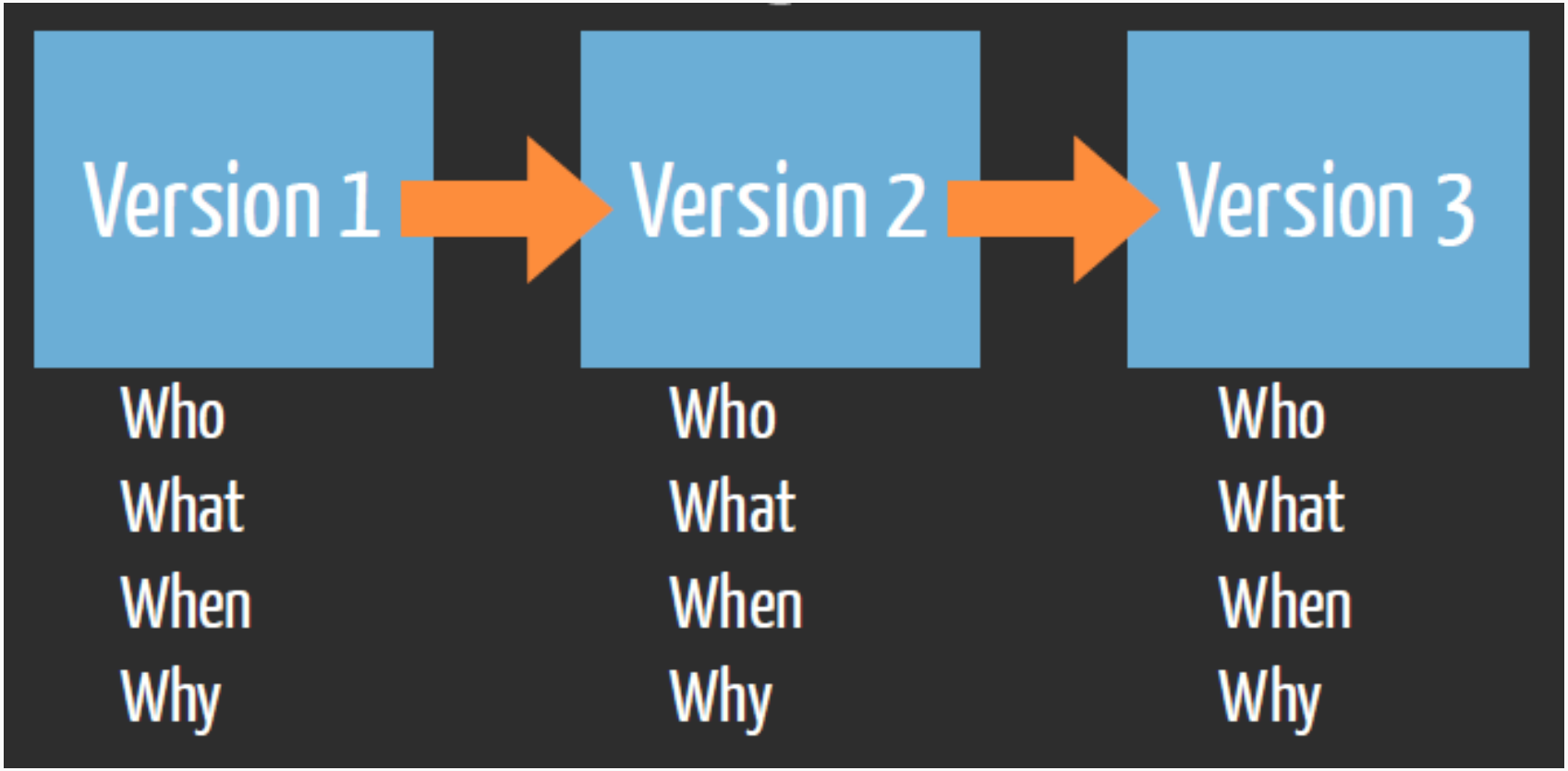
Dropbox

Dropbox keeps record of deleted/edited files for 30 days

Open Science Framework

Automatic version control, no time limit.

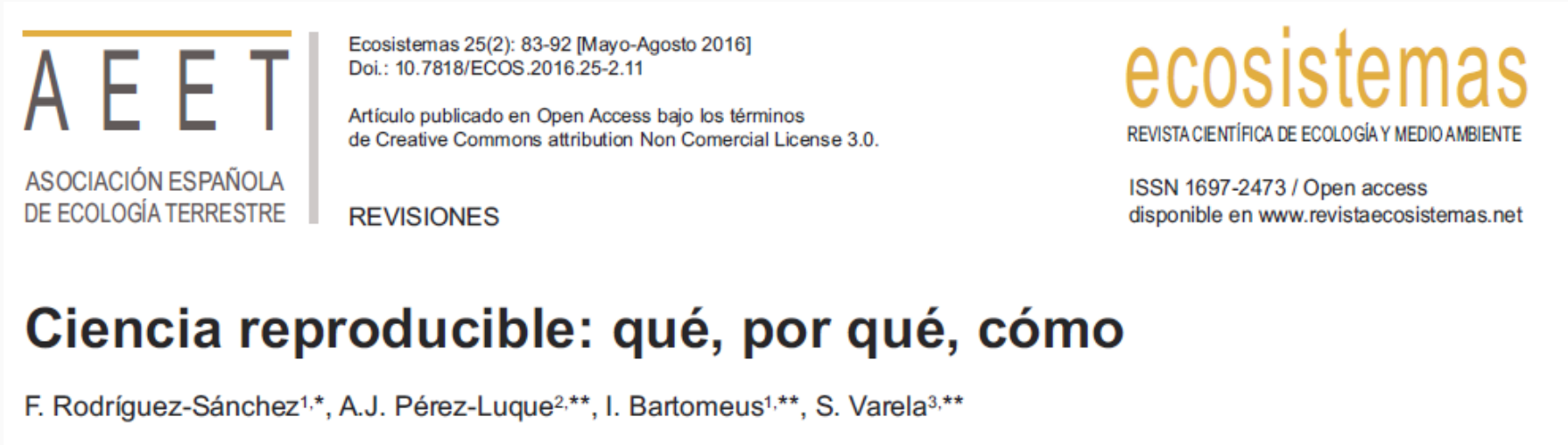




R. Fitzjohn

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

To read more



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Happy writing!

Slides and source code available at

https://github.com/Pakillo/ReproducibleScience