

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

Francisco Rodriguez-Sanchez (@frod_san)

February 2017

A typical research workflow

1. Prepare data (**EXCEL**)

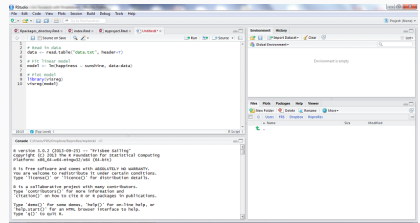
	A	B
1	happiness_index	sunshine_h
2	10.5	978.4
3	6.6	660.9
4	11.3	1093.5
5	9.6	978.9
6	10.9	1135.5
7	9.1	907.0
8	10.6	990.4
9	12.4	1172.9
10	9.6	1025.6
11	10.1	1055.0
12	10.9	1093.7
13	8.9	863.8
14	12.5	1196.6
15	10.0	995.8
16	11.0	1120.2
17	10.3	988.0
18	9.7	987.0
19	9.3	970.4
20	10.9	1076.6
21	9.0	909.8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

data

Ready

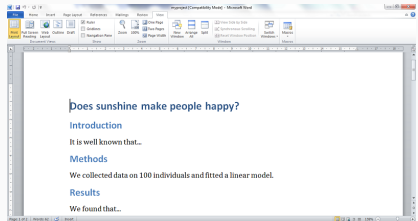
A typical research workflow

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



A typical research workflow

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

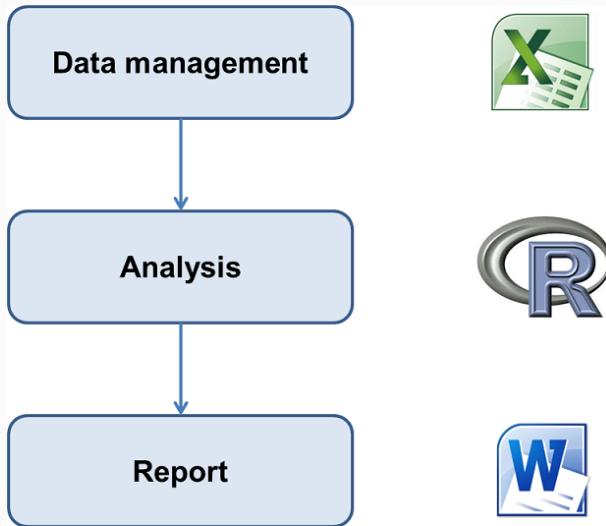


A typical research workflow

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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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

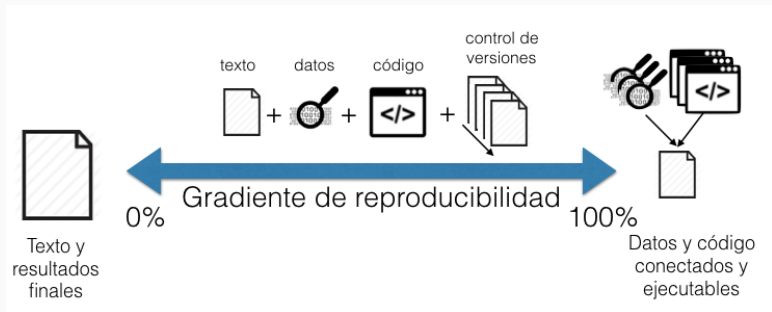
<https://youtu.be/s3JldKoA0zw>

WHAT is Reproducible Science?

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.

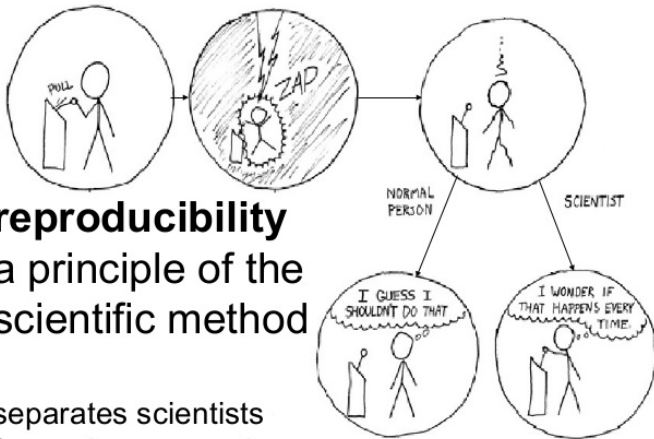
You can't reproduce if you don't understand where a number came from.

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](#)

- Fundamental pillar of **scientific method**

Reproducible Science: WHY

- Fundamental pillar of **scientific method**
- Much less prone to **errors**

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- Increasingly required by **journals**
- Higher publication **impact** (citations, future collaborations, etc)

HOW TO DO Reproducible Science?

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

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

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- 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>

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	population
Afghanistan	1999	745	19987071
Afghanistan	2000	2666	20065360
Brazil	1999	37737	17206362
Brazil	2000	80488	17404898
China	1999	212258	127205272
China	2000	213766	128053583

variables

country	year	cases	population
Afghanistan	1999	745	19987071
Afghanistan	2000	2666	20065360
Brazil	1999	37737	17206362
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China	1999	212258	127205272
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observations

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table4

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

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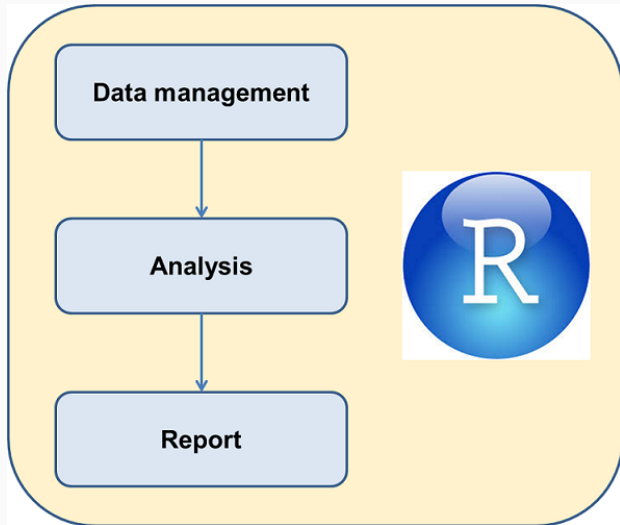
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- <http://kbroman.org/dataorg/>

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
 - ...

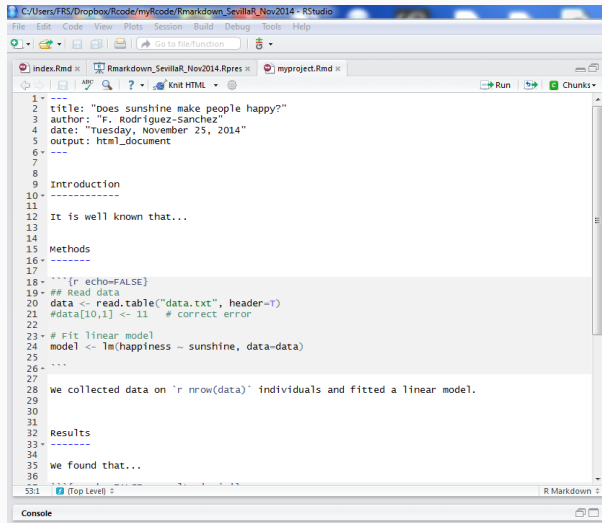


Let's see Rmarkdown in action

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

Example: Does sunshine influence happiness?

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



```
1 ---
2 title: "Does sunshine make people happy?"
3 author: "F. Rodríguez-Sánchez"
4 date: "Tuesday, November 25, 2014"
5 output: html_document
6 ---
7
8
9 Introduction
10 ---
11
12 It is well known that...
13
14
15 Methods
16 ---
17
18 ```{r echo=FALSE}
19 ## Read data
20 data <- read.table("data.txt", header=T)
21 #data[10,1] <- 11 # correct error
22
23 # Fit linear model
24 model <- lm(happiness ~ sunshine, data=data)
25
26 ```
27
28 we collected data on `r nrow(data)` individuals and fitted a linear model.
29
30
31
32 Results
33 ---
34
35 we found that...
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```

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, ...

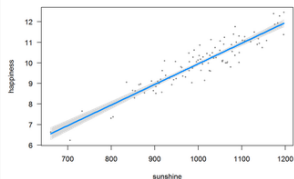
Methods

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!**

Other formats: PDF, Word

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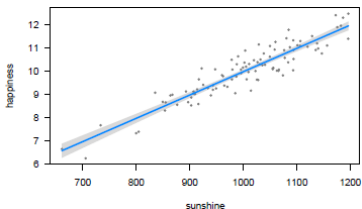
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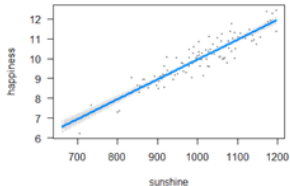
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Adding citations by DOI

rcrossref addin

Add Crossref Citations

Cancel Add Crossref Citations Done

Add a new bibliography entry through Crossref DOI

10.3390/ma8063101 Add to My Citations

Type: journal-article
Title: Photoluminescent ZnO Nanoparticles and Their Biological Applications
Author: Zheng-Yong Zhang; Huan-Ming Xiong
Time: 2015
Publisher: MDPI AG

Adding citations from BibTeX file

citr addin

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

- `rticles`
- `rmdTemplates`

Can write full thesis in Rmarkdown!

See `thesis.Rmd`.

See `thesis.pdf`.

Rmarkdown website

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

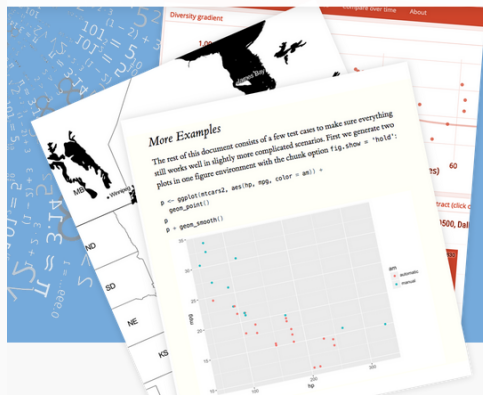
R Markdown

from  Studio

Get Started

Gallery

For



Analyze. Share. Reproduce.

Your data tells a story. Tell it with R.

Turn your analyses into high quality

reports, presentations and dashboards.

Rmarkdown cheat sheet

R Markdown Cheat Sheet

learn more at rmarkdown.rstudio.com



.Rmd files

An R Markdown (.Rmd) file is a record of your research. It contains the code that a scientist needs to reproduce your work along with the narration that a reader needs to understand your work.

Reproducible Research

At the click of a button, or the type of a command, you can rerun the code in an R Markdown file to reproduce your work and export the results as a finished report.

Dynamic Documents

You can choose to export the finished report as a HTML, pdf, MS Word, ODT, RTF, or markdown document, or as a text or pdf based slide show.

Workflow

- 1 Open a new .Rmd file: File > New File > R Markdown. Use the wizard that opens to prepopulate the file with a template.
- 2 Write document by editing template.
- 3 Knit document to create report by clicking button or `knitr::render()` to knit.
- 4 Preview output in IDE window.
- 5 Publish (optional) to web or server. Sync publish button to accounts at:
 - pubs.rstudio.com
 - slideshows.rstudio.com
 - RStudio Connect
- 6 Examine build log in R Markdown console.
- 7 Use output file that is saved alongside .Rmd.

Interactive Documents

Turn your report into an interactive Shiny document in 4 steps

- 1 Add runtime: shiny to the YAML header.
- 2 Call Shiny input functions to embed input objects.
- 3 Call Shiny render functions to embed reactive output.
- 4 Render with `markdown::run` or click Run Document in RStudio IDE.

.Rmd structure

YAML Header
Optional section of header (e.g. pandoc) options written as key-value pairs (NAME, value).
• At start of file.
• Between lines of ---

Text
Narration formatted with markdown, mixed with code chunks.

Code chunks
Chunks of embedded code. Each chunk:
• Begins with ````` [R]
• Ends with `````
• R Markdown will run the code and append the results to the doc.
• It will use the location of the .Rmd file in the working directory.

Embed code with knitr syntax

Inline code

Insert with `<code>`. Usually appear as text without code.

Built with `<code>` (built with 3.2.3)

Code chunks

One or more lines surrounded with ````` [R] and `````. Place chunk options within curly braces, after ````` insert with `<code>` (built with 3.2.3)

Global options

Set with `knitr::opts_chunk$set()`, e.g.

```
knitr::opts_chunk$set(
  echo = FALSE,
  message = FALSE,
  results = "markup",
  tidy = TRUE,
  warning = TRUE
)
```

Important chunk options

cache - cache results for future knits (default = FALSE)

cache.path - directory to save cached results (default = "cache/")

child - file(s) to knit and then include (default = NULL)

collapse - collapse all output into single block (default = FALSE)

comment - prefix for each line of results (default = "#")

dependson - chunk dependencies for caching (default = NULL)

echo - Display code in output document (default = TRUE)

engine - code language used in chunk (default = "R")

error - Display error messages in doc (TRUE) or stop render when error occurs (FALSE) (default = TRUE)

eval - Run code in chunk (default = TRUE)

fig.align - "left", "right", or "center" (default = "center")

fig.cap - Figure caption as character string (default = NULL)

fig.height, **fig.width** - Dimensions of plots in inches

highlight - highlight source code (default = TRUE)

include - include chunk in doc after running (default = TRUE)

Parameters

Parameterize your documents to reuse with different inputs (e.g. data sets, values, etc.)

- 1 Add parameters: Create and set parameters in the header as sub-values of `params`
- 2 Call parameters: Call parameter values in code as `params$parameter-name`
- 3 Set parameters: Set values with `knitr::params()` or the `params` argument of `render()`

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Learn more at rmarkdown.rstudio.com | RStudio® © 2016 RStudio | updated 02/16

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

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

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

8 Studio

Updated 10/30/2014

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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



FINAL_rev.18.comments7.
corrections9.MORE_30.doc



FINAL_rev.22.comments49.
corrections.10. #@\$%WHYDID
ICOMETOGRADSCHOOL?????.doc

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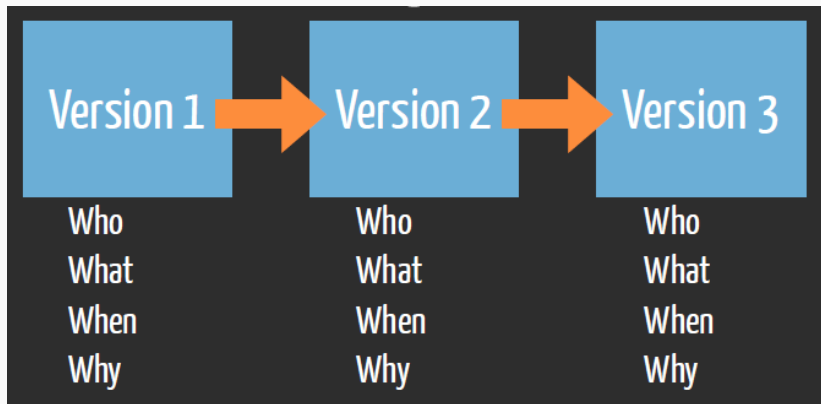
Dropbox keeps record of deleted/edited files for 30 days

Open Science Framework

Automatic version control, no time limit.

The screenshot displays the Open Science Framework (OSF) web interface. At the top, the browser address bar shows the URL <https://osf.io/ezkqg/>. The OSF logo and navigation menu are visible, including links to Dashboard, My Projects, Browse, Registrations, Forks, Contributors, and Settings. The current project is titled "Influence of Reaction Conditions on HM...". Below the project title, the file "manuscript green chemistry.docx" is listed. To the right of the file name are buttons for "Delete", "Check out", "Download", "View", and "Revisions". A pink arrow points to the "Revisions" button. The "Revisions" table shows a list of five revisions, with the "Version ID" column highlighted by a pink box. The table columns are Version ID, Date, User, Download, MD5, and SHA2.

Version ID	Date	User	Download	MD5	SHA2
5	2016-03-01 04:51 PM	Sara Bowman	3	605360a9d897969845e	0a15b7a38d21268e87;
4	2016-03-01 04:51 PM	Sara Bowman	2	d36862941d1f3a9834a	0b26a8c8d5aaa9a26d2
3	2016-03-01 04:50 PM	Sara Bowman	1	4f9731f49aea5b8eafa9	1c86e4964c495201460
2	2016-03-01 04:50 PM	Sara Bowman	1	bc165cff2a8ad6b3a8bc	401cdd53dbcb3c54a45
1	2016-03-01 03:32 PM	Sara Bowman	4	96f5aa2525e176ec2e9;	59ec22c26e9510bac3



R. Fitzjohn

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



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REVISIONES

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

Happy writing!



Slides and source code available at

<https://github.com/Pakillo/ReproducibleScience>