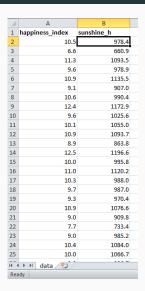
Doing reproducible science: from your hard-won data to a publishable manuscript without going mad

Francisco Rodriguez-Sanchez @frod\_san

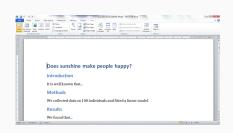
1. Prepare data (EXCEL)



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



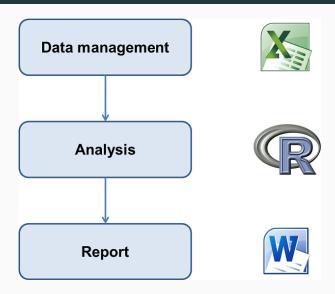
- 1. Prepare data (EXCEL)
- 2. Analyse data (R)
- Write report/paper (WORD)



- 1. Prepare data (EXCEL)
- 2. Analyse data (R)
- 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!





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/s3JldKoAOzw

# 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.

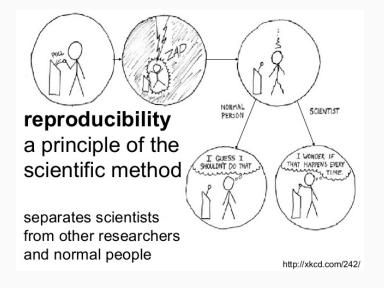
You can't reproduce if you don't understand where a number came from.

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





N

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

Fundamental pillar of scientific method

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

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- Regenerate results **automatically**

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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?**

- 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).

- All files in same directory (Rstudio project).
- Raw data untouched in independent folder.

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- Derived, clean data in another folder.

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

### File organisation example

- figs/

```
myproject
I - README
          # general info about the project
|- data/
          # clean data (produced w/ script)
I- R/
          # functions definitions
l- doc/
          # manuscript files
```

# 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.

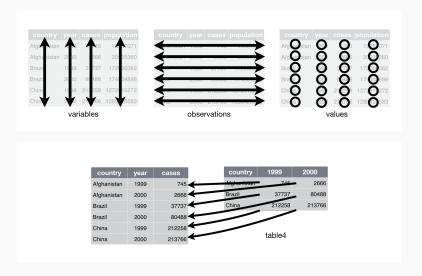
> Jeremy Berg Editor in Chief

#### Storage

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

- Dropbox
- OSF
- Figshare, etc
- See all data repositories in www.re3data.org

#### Tidy data



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

#### **Spreadsheet good practices**

• Put variables in columns (things you are measuring: height, weight, sex)

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- http://www.datacarpentry.org/spreadsheet-ecology-lesson/

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- http://kbroman.org/dataorg/

# **Common spreadsheet errors**

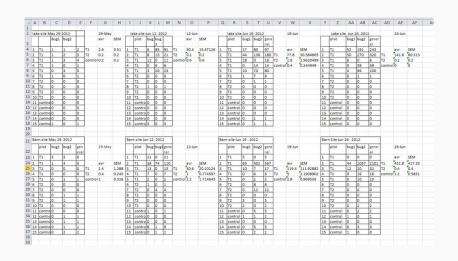
### More than one variable per column

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

DI . 1		0	147-1-1-1
Plot	Species	Sex	Weight
1	DM	M	40
1	DM	F	36
1	DS	F	135
1	DM	F	39
2	DM	M	43
2	DS	F	144
2	DM	F	51
2	DM	F	44
2	DS	F	146
	1 2 2 2 2	1 DM 1 DM 1 DS	1 DM M 1 DM F 1 DS F 1 DM F 2 DM M 2 DS F 2 DM F 2 DM F

Source: Data Carpentry

### 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				
1/8/14	PE	M	22	
1/8/14	DM	M	38	
1/8/14	DM	М	48	
1/8/14		М	43	
1/8/14	DM	F	35	
1/8/14	DM	М	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		М	218	
2/18/14		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	Υ
1/8/14	DM	M	38	Υ
1/8/14				
1/8/14		M	22	
1/8/14		M	38	
1/8/14		M	48	
1/8/14		M	43	
1/8/14		F	35	
1/8/14		M	43	
1/8/14		F	37	
1/8/14		F		Υ
1/8/14		M	45	Υ
1/8/14				
1/8/14		М	157	N
1/8/14				
2/18/14		M	218	
2/18/14		F		Υ
2/18/14	DM	M	52	Υ

Your turn: tidy up this messy dataset

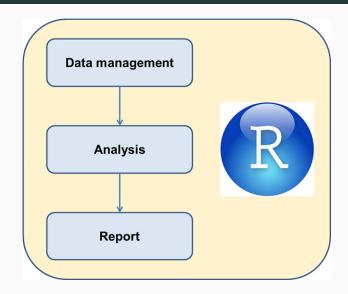
https://ndownloader.figshare.com/files/2252083

# **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
  - ...

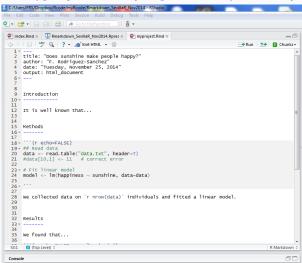


### Let's see Rmarkdown in action

In Rstudio, create new Rmarkdown document and click on  ${\tt Knit}$  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

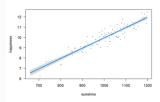
It is well known that individual well-being can be influenced by climatic conditions. However, ...

Methods

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

Results
We found that...

	Estimate	\$td. Error	t value	Pr(> t
(Intercept)	-0.0651657	0.4264970	-0.1527928	0.878875
sunshine	0.0100228	0.0004232	23.6833264	0.000000



#### Discussion

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

#### Acknowledgements

Y. Xie, J. MacFarlane, Retudio...

## Spotted error in the data? No problem!

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

### Other formats: PDF, Word

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,  $\dots$ 

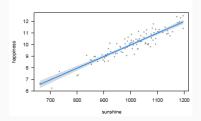
#### Methods

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We found that...

	Estimate	Std. Error	t value	Pr(> t
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sunshine	0.0100228	0.0004232	23.6833264	0.00000000



#### Does sunshine make people happy?

F. Rodriguez-Sanchez Tuesday, November 25, 2014

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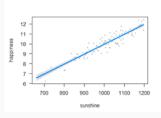
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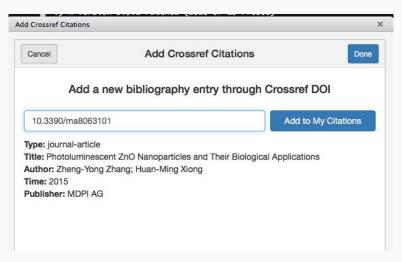
We found that...

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



## Adding citations by DOI

### rcrossref addin



## Adding citations from BibTeX file

citr addin

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

## Manuscript templates

- rticles
- rmdTemplates

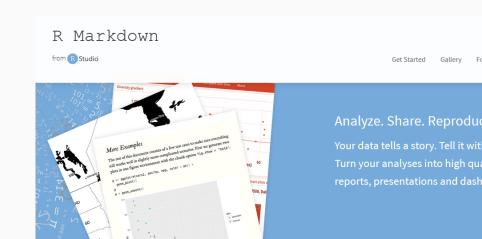
### Can write full thesis in Rmarkdown!

See thesis.Rmd.

See thesis.pdf.

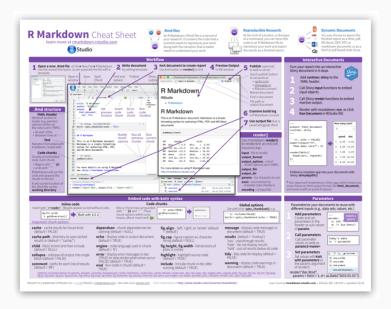
### Rmarkdown website

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



### Rmarkdown cheat sheet

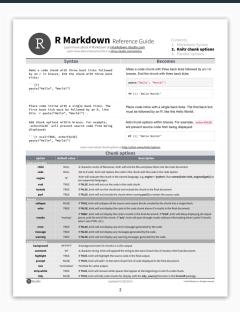
. . .



47

. / . . . / . . / . . / . . /

### Rmarkdown reference guide



48

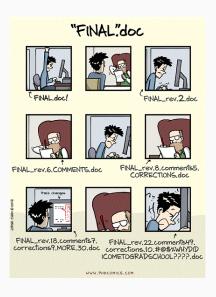
. . / . . . / . . / . . / . . /

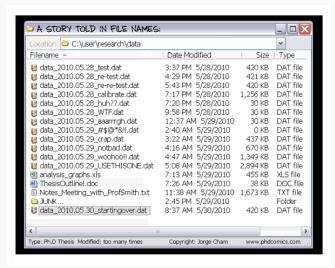
# Managing software dependencies

## Managing package dependencies in R

- sessionInfo (or session\_info)
- checkpoint
- packrat
- docker
- switchr
- rctrack

# **Version control**





Coordinates_rawdata.csv	18/05/2015 19:0
(S) coords_2015-09-09.csv	23/09/2015 17:1
Coords_2015-09-09_modif.csv	05/11/2015 15:2
Coords_2015-10-11_modif_YC.csv	17/11/2015 13:4
Coords_2015-10-18_modif_YC.csv	18/11/2015 17:2
Coords_2015-12-26_modif_YC.csv	28/12/2015 13:3
Coords_2015-12-26_modif_YC_years.csv	30/03/2016 19:3
Pulido et al_SM1_Data.csv	20/10/2015 11:5
Pulido et al_SM1_Data_modif_YC_2015-12-26.csv	28/12/2015 13:3
qualitative_data.csv	04/07/2016 15:5
cleandata.xlsx	25/06/2015 01:1
(I) cleandata_YC.xlsx	30/06/2015 16:2
COORDENADAS PACO_20-05-2016 CON REVIEWS.xlsx	20/05/2016 16:2
COORDENADAS PACO_20-05-2016 CON REVIEWS_FRS.xlsx	27/05/2016 19:4
COORDENADAS_paper195(Girella_elevata).xlsx	08/06/2016 13:0
coordenadas_raw_2016-06-08.xlsx	09/06/2016 15:5
(in coordenadas_raw_2016-06-08_old.xisx	08/06/2016 16:0
coordenadas_raw_2016-06-21.xlsx	21/06/2016 16:1
coords_2015-09-09_modif.xlsx	05/11/2015 15:2
coords_2015-10-11_modif_VC.xlsx	17/11/2015 13:3
Coords_2015-10-11_modif_YC_PACO.xlsx	17/11/2015 17:0
Coords_2015-10-18_modif_YC.xlsx	18/11/2015 17:2
coords_2015-12-26_modif_YC.xlsx	30/03/2016 19:3
(I) coords_2016-04-02.xlsx	05/04/2016 17:4
(I) coords_2016-04-02_VC.xlsx	06/04/2016 18:0
@_coords_2016-04-08_YC.xlsx	11/04/2016 13:5
dataset_y_coords_09_09_15.xlsx	23/09/2015 17:1
Datos metaanalisis_18-04-2016.xlsx	19/04/2016 16:2
FINAL METAANALISYS_14-6-2016_WITH REVIEWS.xisx	21/06/2016 16:1
FINAL METAANALISYS_16-6-2016_WITH REVIEWS.xlsx	21/06/2016 16:1
FINAL METAANALISYS_2016-04-27_WITH REVIEWS.xisx	25/05/2016 18:0
FINAL METAANALISYS_2016-04-27_WITH REVIEWS_FRS.xlsx	27/05/2016 18:4
FINAL METAANALISYS_2016-04-29_EXCLUDING REVIEWS.xlsx	08/06/2016 13:0
FINAL VOTECOUNTING_1-7-2016.xlsx	04/07/2016 15:4
fitnessdata_2016-06-22.xlsx	22/06/2016 21:0
IFs for Bastien_19-3-2016_YC.xlsx	28/03/2016 19:2
Metaanalysis final_01-05-2015 with coordinates.xlsx	18/05/2015 19:2
Metaanalysis final_22-05-2015 coords.xlsx	24/06/2015 15:5
Metaanalysis final_25-06-2015.xdsx	30/06/2015 16:5
Metaanalysis y coords revisadas_05-08-2015_AH_JE.xlsx	23/09/2015 12:5
Dulido et al_SM1_Data_2016-05-27.xlsx	27/05/2016 18:4
Min. Co. and Cast Day, 2015 OF 27 DACO. de.	00.000/2016 16:2

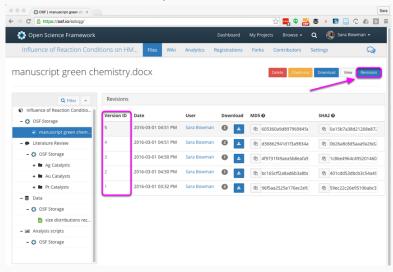
04/07/2016 21:21
04/07/2016 20:49
04/07/2016 20:42
30/06/2016 20:03
05/07/2016 15:53

## **Dropbox**

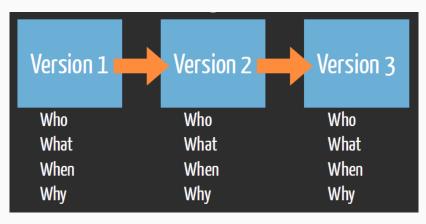
Dropbox keeps record of deleted/edited files for 30 days

### **Open Science Framework**

Automatic version control, no time limit.



### Git & GitHub



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



Ecosistemas 25(2): 83-92 [Mayo-Agosto 2016] Doi.: 10.7818/ECOS.2016.25-2.11

Artículo publicado en Open Access bajo los términos de Creative Commons attribution Non Comercial License 3.0.

**REVISIONES** 



ISSN 1697-2473 / Open access disponible en www.revistaecosistemas.net

### Ciencia reproducible: qué, por qué, cómo

F. Rodríguez-Sánchez<sup>1,\*</sup>, A.J. Pérez-Lugue<sup>2,\*\*</sup>, I. Bartomeus<sup>1,\*\*</sup>, S. Varela<sup>3,\*\*</sup>

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

## Happy writing!



Slides and source code available at

 $\verb|https://github.com/Pakillo/ReproducibleScience|\\$