

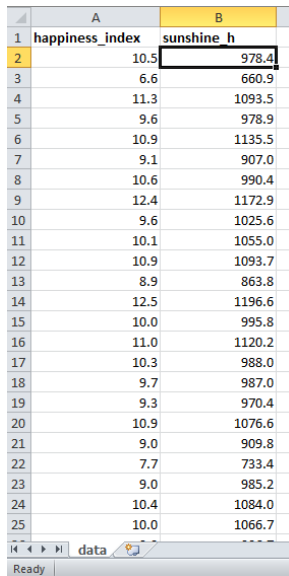
Doing reproducible science:  
from your hard-won data  
to a publishable manuscript  
without going mad

Francisco Rodriguez-Sanchez

[http://bit.ly/frod\\_san](http://bit.ly/frod_san)

# A typical research workflow

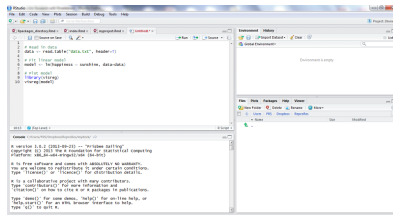
## 1. Prepare data (**EXCEL**)



	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

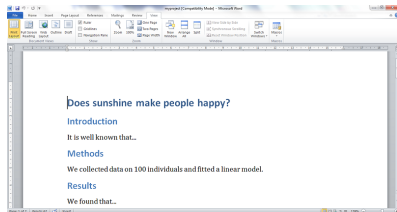
# A typical research workflow

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**)



This workflow is broken

**Data management**



**Analysis**



**Report**



# Problems of a broken workflow

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

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- ▶ 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!



Every analysis you do on a dataset will have to be redone 10–15 times before publication. Plan accordingly.

*Trevor A. Branch*

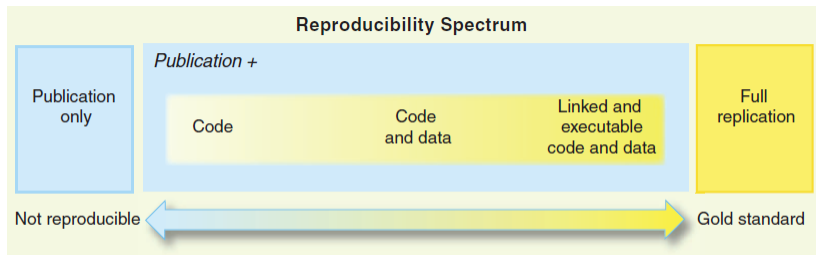
# WHAT is Reproducible Science?

# 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



Peng (2011) *Science*

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?

# Reproducible Science: WHY

- ▶ Fundamental pillar of scientific method

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- ▶ Much less prone to errors
- ▶ Automatically regenerate results
- ▶ 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.

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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  
  
| - output/         # other code output
```

# Data management

# Data management

1. Planification (e.g. DMPTool)
2. Collection
3. Metadata description (EML, Morpho)
4. Quality control
5. Storage

# Storage

Use the cloud: safe, persistent, easy to share

- ▶ Dropbox
- ▶ OSF
- ▶ Figshare, etc
- ▶ See all data repositories in [www.re3data.org](http://www.re3data.org)

# Spreadsheet good practices

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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

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	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y	Z	AA	AB	AC	AD	AE	AF	AG																			
1																																																				
2	lake site May 29 2012								29-May		lake site Jun 12 2012					12-Jun			lake site Jun 19 2012					19-Jun			Lake site Jun 26 2012					26-Jun																				
3	plot bug1 bug2					avr SEM			plot bug1 bug2 gene ral					avr SEM			plot bug1 bug2 gene ral					avr SEM			plot bug1 bug2 gene ral					avr SEM																						
4	1	T1	1	1	2	T1	2.6	0.51	1	T1	6	85	91	T1	30.4	15.47126	1	T1	17	80	97				avr	SEM	1	T1	52	191	243		avr	SEM																		
5	2	T1	1	2	3	T2	0.2	0.2	2	T1	8	13	21	T2	0.2	0.2	2	T1	44	136	180	T1	77.8	30.384865	2	T1	50	270	320	T2	0.2	0.2	0.2																			
6	3	T1	1	3	4	control 0.2		0.2	3	T1	11	0	11		control 0.6	0.6	3	T1	18	0	18	T2	1.8	1.5620499	3	T1	6	0	6		control 0	0	0																			
7	4	T1	1	0	1				4	T1	0	6	6				4	T1	0	14	14	control 0.4		0.244949	4	T1	0	39	39	control 0		0	0																			
8	5	T1	0	3	3				5	T1	3	20	23				5	T1	10	70	80				5	T1	4	96	100																							
9	6	T2	1	0	1				6	T2	0	0	0				6	T2	1	7	8				6	T2	0	1	1																							
10	7	T2	0	0	0				7	T2	0	0	0				7	T2	0	1	1				7	T2	0	0	0																							
11	8	T2	0	0	0				8	T2	1	0	1				8	T2	0	0	0				8	T2	0	0	0																							
12	9	T2	0	0	0				9	T2	0	0	0				9	T2	0	0	0				9	T2	0	0	0																							
13	10	T2	0	0	0				10	T2	0	0	0				10	T2	0	0	0				10	T2	0	0	0																							
14	11	control	0	0	0				11	control	0	0	0				11	control	0	0	0				11	control	0	0	0																							
15	12	control	0	0	0				12	control	0	0	0				12	control	0	0	0				12	control	0	0	0																							
16	13	control	0	0	0				13	control	0	0	0				13	control	0	0	0				13	control	0	0	0																							
17	14	control	0	0	0				14	control	0	0	0				14	control	0	1	1				14	control	0	0	0																							
18	15	control	1	0	1				15	control	3	0	3				15	control	0	1	1				15	control	0	0	0																							
19																																																				
20	Barn site May 29 2012																Barn site Jun 12 2012												Barn site Jun 19 2012												Barn Site Jun 26 2012											
21	plot bug1 bug2 gene ral					29-May			plot bug1 bug2 gene ral					12-Jun			plot bug1 bug2 gene ral					19-Jun			plot bug1 bug2 gene ral					26-Jun																						
22	1	T1	3	3	6				1	T1	21	0	21				1	T1	5	0	5						1	T1	0	0	0																					
23	2	T1	1	4	5		avr	SEM	2	T1	36	74	110		avr	SEM	2	T1	65	502	567		avr	SEM	2	T1	44	2057	2101	T1	avr	SEM	417.33																			
24	3	T1	0	0	0	T1	2.4	1.288	3	T1	13	0	13	T1	30.6	20.10124	3	T1	10	7	17	T1	19.4	11.92882	3	T1	12	20	32	T2	0.4	0.4	0.4																			
25	4	T1	0	0	0	T2	0.4	0.245	4	T1	7	0	7	T2	1	0.774597	4	T1	0	6	6	T2	5	1.908902	4	T1	0	16	16		control 1.2	0.5831																				
26	5	T1	0	1	1	control 1		0.316	5	T1	2	0	2	control 2.2		1.714643	5	T1	0	2	2	control 2.8		0.969536	5	T1	0	10	10																							
27	6	T2	0	0	0				6	T2	1	0	1				6	T2	0	8	8				6	T2	0	0	0																							
28	7	T2	0	0	0				7	T2	0	4	4				7	T2	0	12	12				7	T2	0	0	0																							
29	8	T2	0	1	1				8	T2	0	0	0				8	T2	0	0	0				8	T2	0	0	0																							
30	9	T2	0	1	1				9	T2	0	0	0				9	T2	3	0	3				9	T2	0	0	0																							
31	10	T2	0	0	0				10	T2	0	0	0				10	T2	2	0	2				10	T2	0	2	2																							
32	11	control	0	0	0				11	control	1	0	1				11	control	0	5	5				11	control	0	2	2																							
33	12	control	0	1	1				12	control	0	0	0				12	control	1	1	2				12	control	1	0	1																							
34	13	control	0	1	1				13	control	0	0	0				13	control	0	0	0				13	control	0	0	0																							
35	14	control	0	1	1				14	control	8	1	9				14	control	0	5	5				14	control	0	3	3																							
36	15	control	0	2	2				15	control	0	1	1				15	control	0	2	2				15	control	1	0	0																							
37																																																				
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 collect	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		

Plot: 2				
Date collect	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>

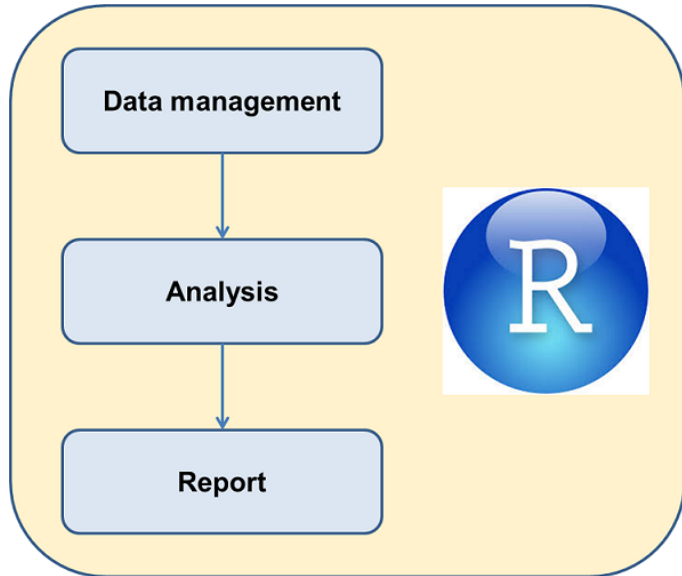


# Data analysis

# Always use code

- ▶ Reproducible
- ▶ Reusable

# Dynamic reports



# Rmarkdown documents

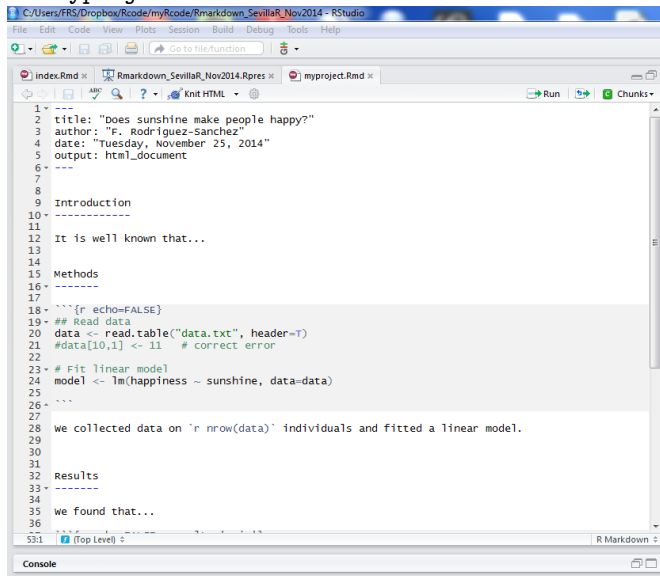
- ▶ Fully reproducible (trace all results inc. tables and plots)
- ▶ Dynamic (regenerate with 1 click)
- ▶ Suitable for
  - ▶ documents (Word, PDF, etc)
  - ▶ presentations
  - ▶ books
  - ▶ websites
  - ▶ ...

# 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`



```
1 ---
2 title: "Does sunshine make people happy?"
3 author: "F. Rodriguez-Sanchez"
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...
36
37
38
39
40
41
42
43
44
45
46
47
48
49
50
51
52
53:1 (Top Level) | R Markdown
```

# HTML output

## 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, ...

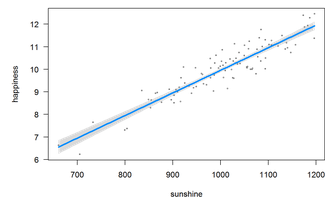
### Methods

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

## Does sunshine make people happy?

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Tuesday, November 25, 2014

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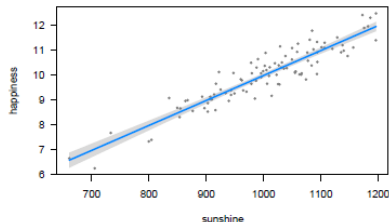
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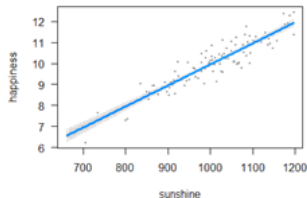
### Methods

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



# Adding citations

```
bibliography: references.bib
```

```
---{r citations_setup, include=FALSE}  
library(knitr)  
cite_options(citation_format = "pandoc")  
---
```

Introduction

It is well known that individual well-being can be influenced by climatic conditions ``r citep("10.1016/j.ecolecon.2004.06.015")``. However, ...

See output

## 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](https://doi.org/10.1016/j.ecolecon.2004.06.015).

# Can write full thesis in Rmarkdown!

See `thesis.Rmd`.

See `thesis.pdf`.

Your turn:

- ▶ Download [http://bit.ly/DEAD\\_datasets](http://bit.ly/DEAD_datasets)
- ▶ With dataset trees.txt, analyse relationship between DBH and height.

# Steps

- ▶ Create Rstudio project (in Dropbox folder)
- ▶ Create folder structure
- ▶ Save original data in data-raw folder.
- ▶ Set up OSF
- ▶ Data quality control in R
- ▶ Write report in rmarkdown.

# Managing software dependencies

# Managing package dependencies in R

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

# Version control

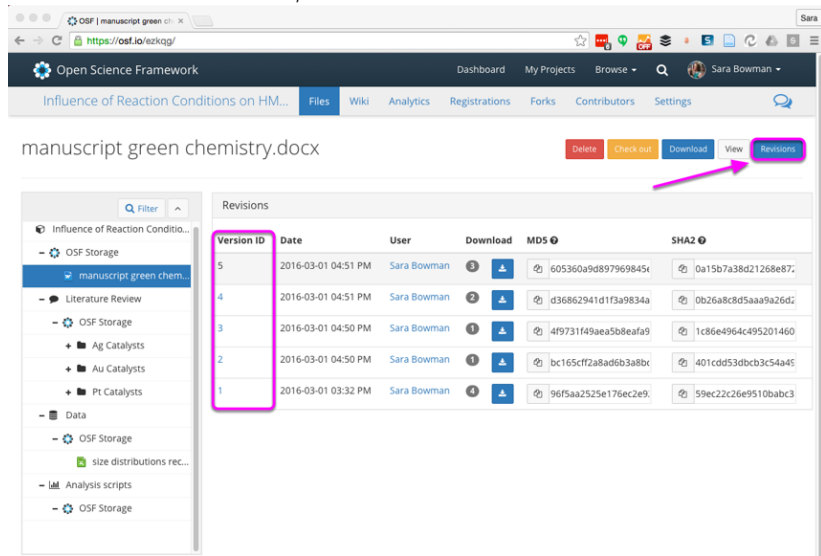


# Dropbox

Dropbox keeps record of deleted/edited files for 30 days

# Open Science Framework

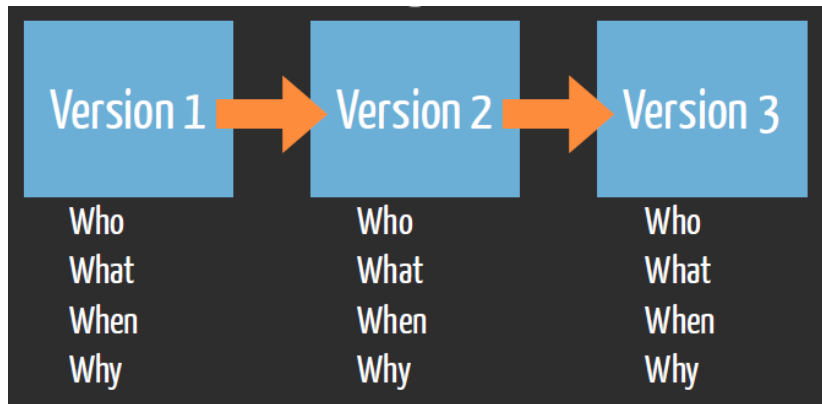
Automatic version control, no time limit.



The screenshot displays the Open Science Framework (OSF) interface. The top navigation bar includes links for Dashboard, My Projects, Browse, and a search bar. The project title is "Influence of Reaction Conditions on HM...". The file name "manuscript green chemistry.docx" is shown. A pink box highlights the "Revisions" button, with a pink arrow pointing to it. The "Revisions" table lists five versions, with the "Version ID" column highlighted by a pink box.

Version ID	Date	User	Download	MD5	SHA2
5	2016-03-01 04:51 PM	Sara Bowman	3	605360a9d897969845c	0a15b7a38d21268e87c
4	2016-03-01 04:51 PM	Sara Bowman	2	d3686294d1f3a9834a	0b26a8cd5aaa9a26d2
3	2016-03-01 04:50 PM	Sara Bowman	1	4f9731f49aea5b8eafa9	1c86e4964c495201460
2	2016-03-01 04:50 PM	Sara Bowman	1	bc165cfc2a8ad6b3a8bc	401cdd53dcb3c54a45
1	2016-03-01 03:32 PM	Sara Bowman	4	96f5aa2525e176ec2e9	59ec22c26e9510bac3

# Git & GitHub



R. Fitzjohn

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

# Collaborative writing

# Many alternatives

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

Happy writing!