Digital badge - Reproducible research

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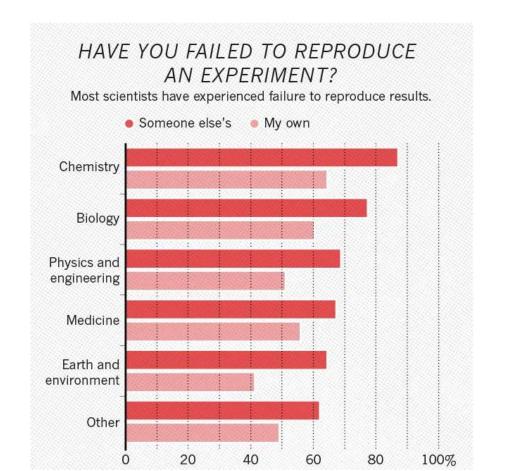




1,500 scientists lift the lid on reproducibility

Survey sheds light on the 'crisis' rocking research.

Monya Baker



Vol 435|9 June 2005

COMMENTARY

Scientists behaving badly

To protect the integrity of science, we must look beyond falsification, fabrication and plagiarism, to a wider range of questionable research practices, argue **Brian C. Martinson**, **Melissa S. Anderson** and **Raymond de Vries**.

Table 1 Percentage of scientists who say that they engaged in the behaviour listed within the previous three years $(n = 3,247)$			
Top ten behaviours	All	Mid-career	Early-career
Falsifying or 'cooking' research data	0.3	0.2	0.5
2. Ignoring major aspects of human-subject requirements	0.3	0.3	0.4
Not properly disclosing involvement in firms whose products are based on one's own research	0.3	0.4	0.3
 Relationships with students, research subjects or clients that may be interpreted as questionable 	1.4	1.3	1.4
5. Using another's ideas without obtaining permission or giving due credit	1.4	1.7	1.0
 Unauthorized use of confidential information in connection with one's own research 	1.7	2.4	0.8 ***
7. Failling to present data that contradict one's own previous research	6.0	6.5	5.3
8. Circumventing certain minor aspects of human-subject requirements	7.6	9.0	6.0 **
Overlooking others' use of flawed data or questionable interpretation of data	12.5	12.2	12.8
10. Changing the design, methodology or results of a study in response to pressure from a funding source	15.5	20.6	9.5***
Other behaviours			
11. Publishing the same data or results in two or more publications	4.7	5.9	3.4**
12. Inappropriately assigning authorship credit	10.0	12.3	7.4 ***
3. Withholding details of methodology or results in papers or proposals	10.8	12.4	8.9 **
4. Using inadequate or inappropriate research designs	13.5	14.6	12.2
15. Dropping observations or data points from analyses based on a gut feeling that they were inaccurate	15.3	14.3	16.5
16. In adequate record keeping related to research projects	27.5	27.7	27.3

Who benefits most from reproducibility?



Reproducibility is important because the you of 3 months ago is terrible at answering email! - @tracykteal at #2016dssummit

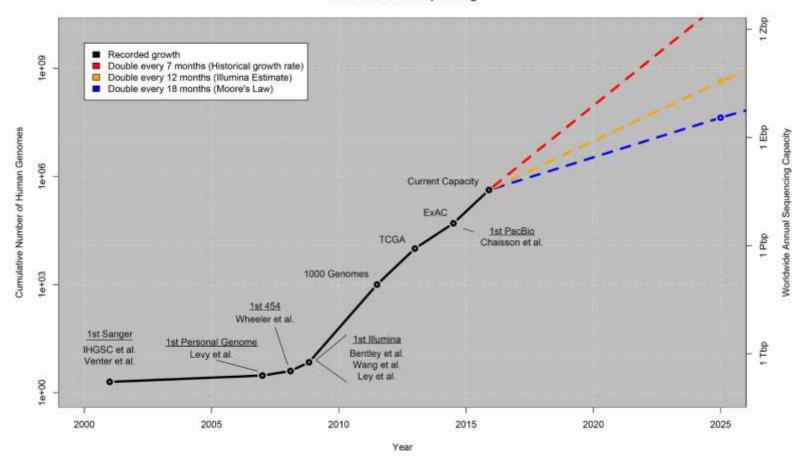
1:17 PM - 26 Oct 2016 from Manhattan, NY

Where to begin...



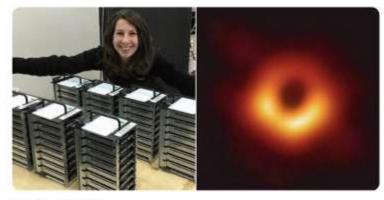
The challenge

Growth of DNA Sequencing





Congratulations to Dr Katie Bouman!
This is the woman who created the algorithm to crunch the 5 petabytes of data from 500 kg of hard drives from 8 radio telescopes to make the first image of the #EHTBlackHole #BlackHole



2:55 PM - 10 Apr 2019

Fundamental problem



I'm not in the office at the moment. Send any work to be translated

Beware of default settings

Ziemann et al. Genome Biology (2016) 17:177 DOI 10.1186/s13059-016-1044-7

Genome Biology

COMMENT

Open Access

Gene name errors are widespread in the scientific literature



Mark Ziemann¹, Yotam Eren^{1,2} and Assam El-Osta^{1,3*}

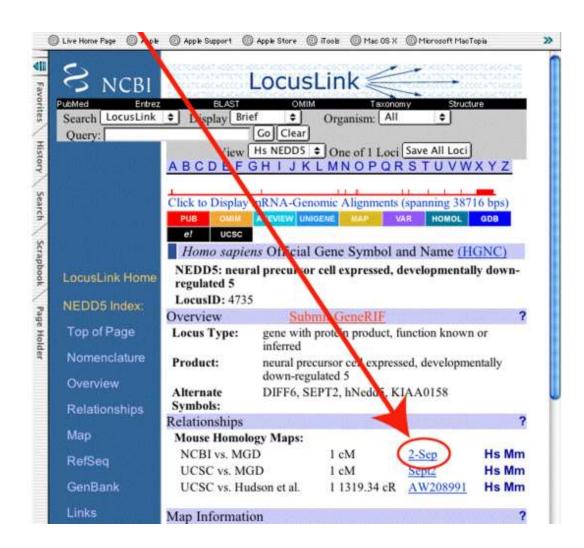
Abstract

conversions.

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

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-



Beware of default settings

Print



Data and computer code should be made publicly available at an early stage - or else ... esarastudillo

Last week we learned a famous 2010 academic paper, relied on by political big-hitters to

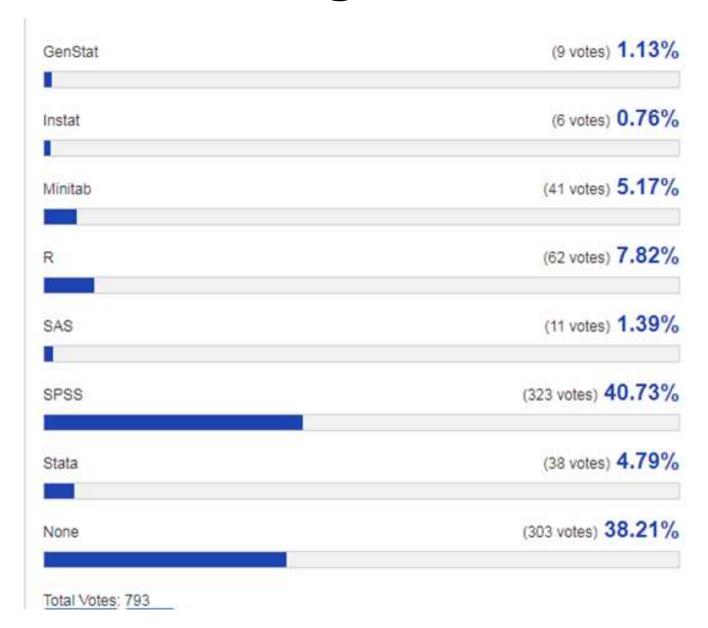
bolster arguments for austerity cuts, contained significant errors; and that those errors came
down to misuse of an Excel spreadsheet.

LinkedIn

Sadly, these are not the first mistakes of this size and nature when handling data. So what on Earth went wrong, and can we fix it?

Harvard's <u>Carmen Reinhart</u> and <u>Kenneth Rogoff</u> are two of the most respected and influential academic economists active today.

Where are we all coming from?



Putting the pieces together

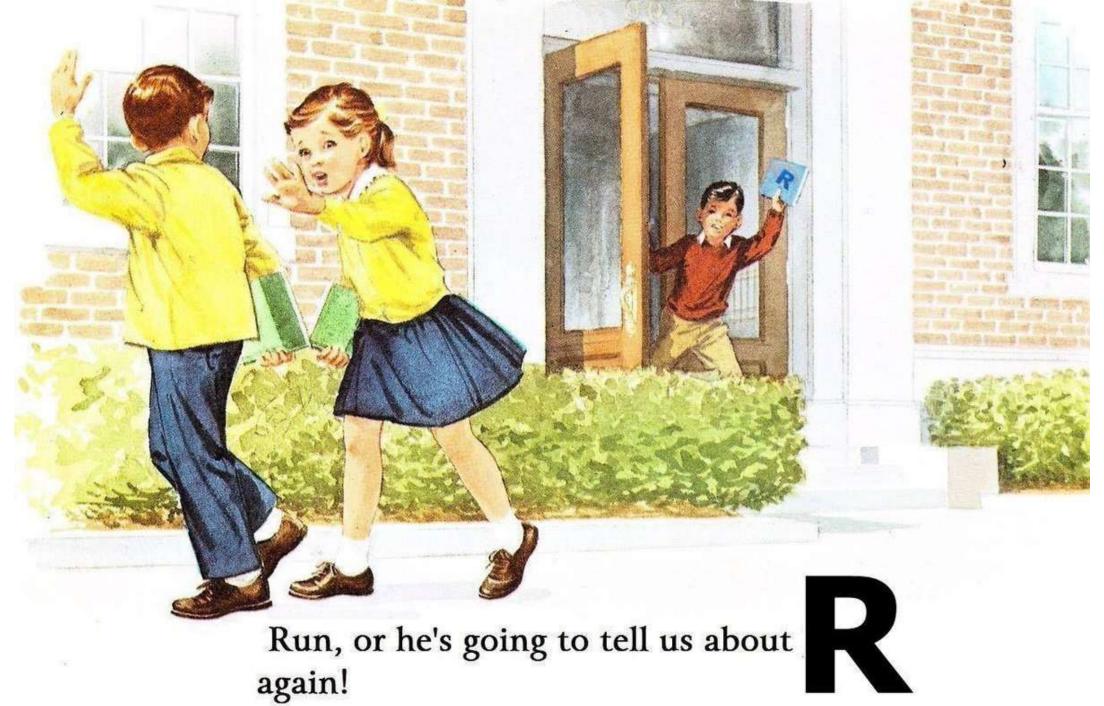
A: Define a project structure

B: Set a naming convention

C: Use scripted workflows

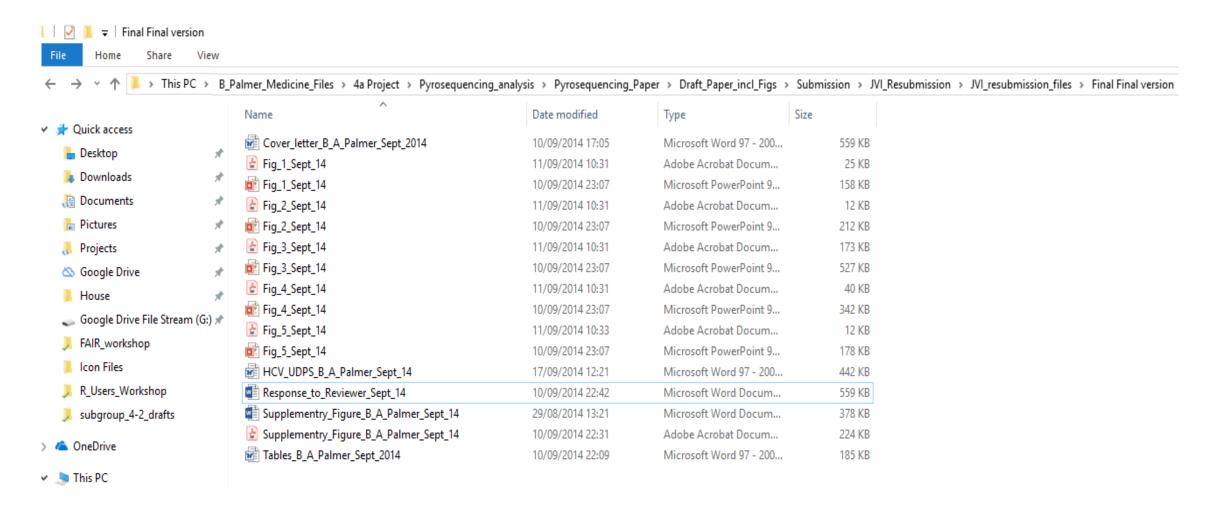
D: Digital notebooks

Reproducible research

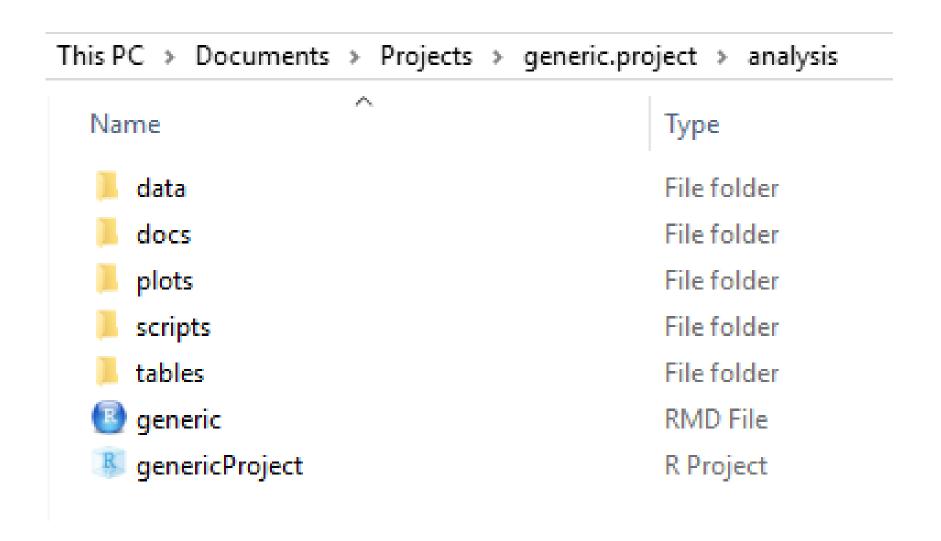


Still haven't found what I'm looking for

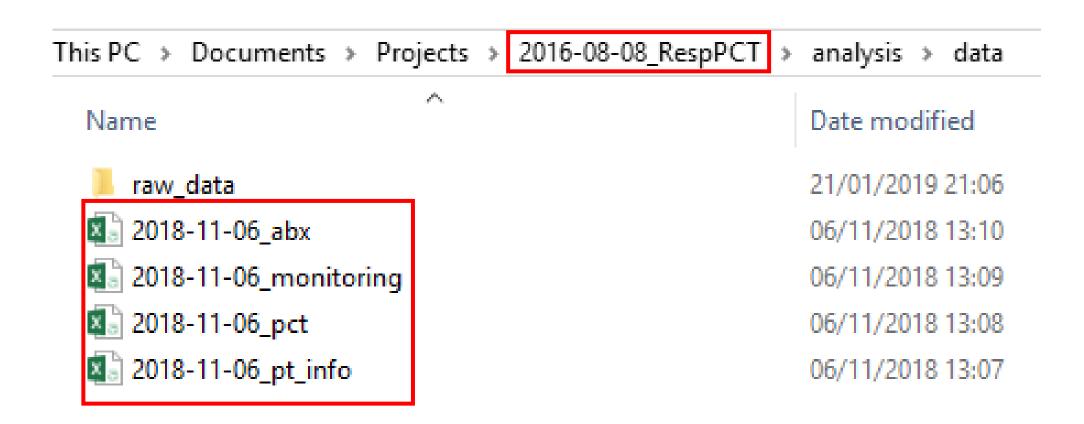
Help your future-self



A: Define a generic project structure



B: Give your files and folders informative names



Outline a file naming convention

Machine readable:

- Inherent order
- Avoid spaces
- Avoid punctuation
- Remove case-sensitivity

Human readable:

- Contains info on content
- Avoid spaces
- Avoid punctuation
- Remove case sensitivity

Metadata:

Separate with underscores ("_")

- Avoid punctuation
- Remove case-sensitivity

```
01 marshal-data.r
02 pre-dea-filtering.r
03 dea-with-limma-voom.r
04 explore-dea-results.r
90 limma-model-term-name-fiasco.r
helper01 load-counts.r
helper02_load-exp-des.r
helper03 load-focus-statinf.r
helper04 extract-and-tidy.r
```

Outline a file naming convention

Chronological order:

```
2013-06-26_BRAFWTNEGASSAY_Plasmid-Cellline-100-1MutantFraction_H01.csv
2013-06-26_BRAFWTNEGASSAY_Plasmid-Cellline-100-1MutantFraction_H02.csv
2013-06-26_BRAFWTNEGASSAY_Plasmid-Cellline-100-1MutantFraction_H03.csv
2013-06-26_BRAFWTNEGASSAY_Plasmid-Cellline-100-1MutantFraction_platefile.csv
2014-02-26_BRAFWTNEGASSAY_FFPEDNA-CRC-1-41_A01.csv
2014-02-26_BRAFWTNEGASSAY_FFPEDNA-CRC-1-41_A02.csv
2014-02-26_BRAFWTNEGASSAY_FFPEDNA-CRC-1-41_A03.csv
2014-02-26_BRAFWTNEGASSAY_FFPEDNA-CRC-1-41_A03.csv
```

Logical order:

```
01_marshal-data.r
02_pre-dea-filtering.r
03_dea-with-limma-voom.r
04_explore-dea-results.r
90_limma-model-term-name-fiasco.r
helper01_load-counts.r
helper02_load-exp-des.r
helper03_load-focus-statinf.r
helper04_extract-and-tidy.r
```

Everything in its right place

- Make your file names:
 - 1. Machine readable
 - 2. Human readable
 - 3. Work with default ordering

NO

Name

- All unique 4a amino acid Sequences (B-N).fas
- 📄 All unique 4a amino acid Sequences (B-N).meg
- All_AA_haplotypes.meg
- All_AA_haplotypes_with_clonal_sequences.meg
- BS100_AA_with_clones
- BS100_AA_with_clones.nwk
- BS1000_AA_pyro&clones
- BS1000_AA_pyro&clones.nwk
- BS1000_AA_pyro_only
- BS1000_AA_pyro_only.nwk
- BS1000_Unique_Clonal_AA

Yes

Projects > 2016-08-08_RespPCT > analysis > scripts

Name

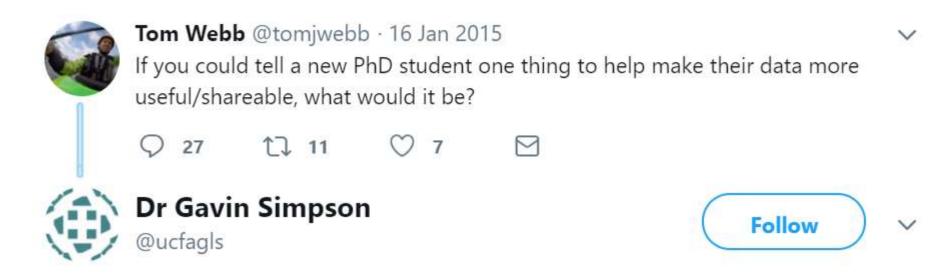
- 01_clean_data
- 02_plots
- 03_tables
- 04_stats_analysis
- 05_post_hoc_stats
- functions
- randomization
- tables

C: Joined up thinking

- The R scripts should also be human readable
 - Annotate the code
 - Break up the scripts into dedicated tasks
 - Interlink to other project scripts

```
1  # Data ----
2  # Eight tibbles returned from the 01_data_import_and_tidying_master_file.R
3  # 1. fgf23_data => FGF23 readings from study centres 01-03
4  # 2. food_level_data => Food diary entries
5  # 3. grouped_data => Dialysis and nondialysis diary entries by component
6  # 4. k_data => Serum potassium
7  # 5. master_data_clean => all the clean master file data if required
8  # 6. p_data => Serum phosphate
9  # 7. pth_data => Parathyroid hormone readings
10  # 8. pulses_nuts_data
11
12 source("scripts/01_data_import_and_tidying_master_file.R")
```

Work from the raw data ALWAYS!!



Replying to @tomjwebb

@tomjwebb don't, not even with a barge pole, not for one second, touch or otherwise edit the raw data files. Do any manipulations in script

D: R Markdown

- R Markdown combines the code you wrote, the output produced and you own comments
- You can view it as a digital lab notebook, where you are both recording what you're doing, and what you were thinking while you were doing it!
- R Markdown outputs can take many forms
 - Word documents, PDFs, slideshows etc.
- Once created the .Rmd file get sent to knitr, which executes the chunks of code and creates a new markdown document
 - this is then processed by pandoc which creates the finished file
 - knitr and pandoc are external websites

R Markdown

YAML header

Chunks of code

Plain text with data outputs from R code

Chunks of code

title: "This is a reproducible document" date: 19th June 2019 output: html document {r setup, include = FALSE} library(ggplot2) library(dplyr) smaller <- diamonds %>% filter(carat <= 2.5)</pre> We have data about `r nrow(diamonds)`

We have data about 'r nrow(diamonds)'
diamonds. Only
'r nrow(diamonds) - nrow(smaller)' are
larger than
2.5 carats. The distribution of the
remainder is shown below:

{r, echo = FALSE}
smaller %>%
ggplot(aes(carat)) +
geom_freqpoly(binwidth = 0.01)

Install the Chrome plugin PubPeer



Further reading





#PaperPerDayChallenge where I read at least one paper, well, per day for a whole year. To kick start, nature.com/articles/43573... inspired by @ukrepro Reproducibility Workshop @CumberlandLodge and a talk by @MarcusMunafo

Scientists behaving badly



In a questionnaire-based survey of US biomedical researchers, respondents admitted to a range of dubious practices. Transgressions included failing to present data

nature.com

Further reading





#119 I know I'm late to the party on this but Jesus! Pre-registration just tears up (inflated) effect sizes like a boss.

frontiersin.org/articles/10.33 ...

