

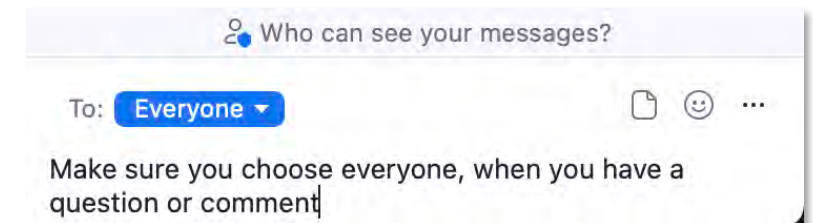
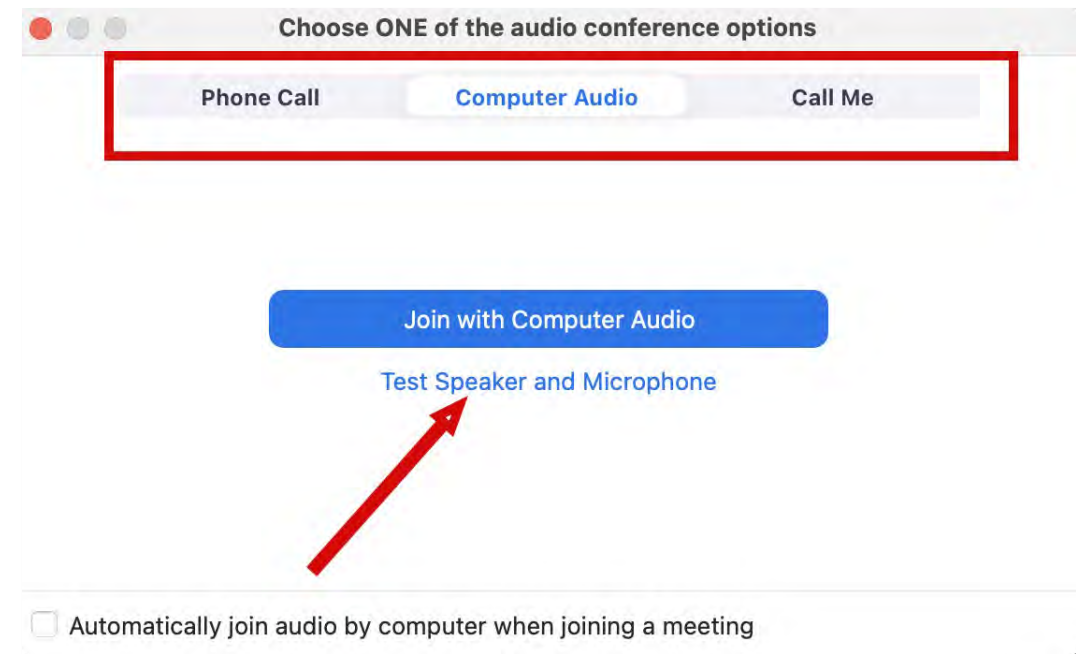
You will not hear any sound until the webinar starts.

## Connect Audio

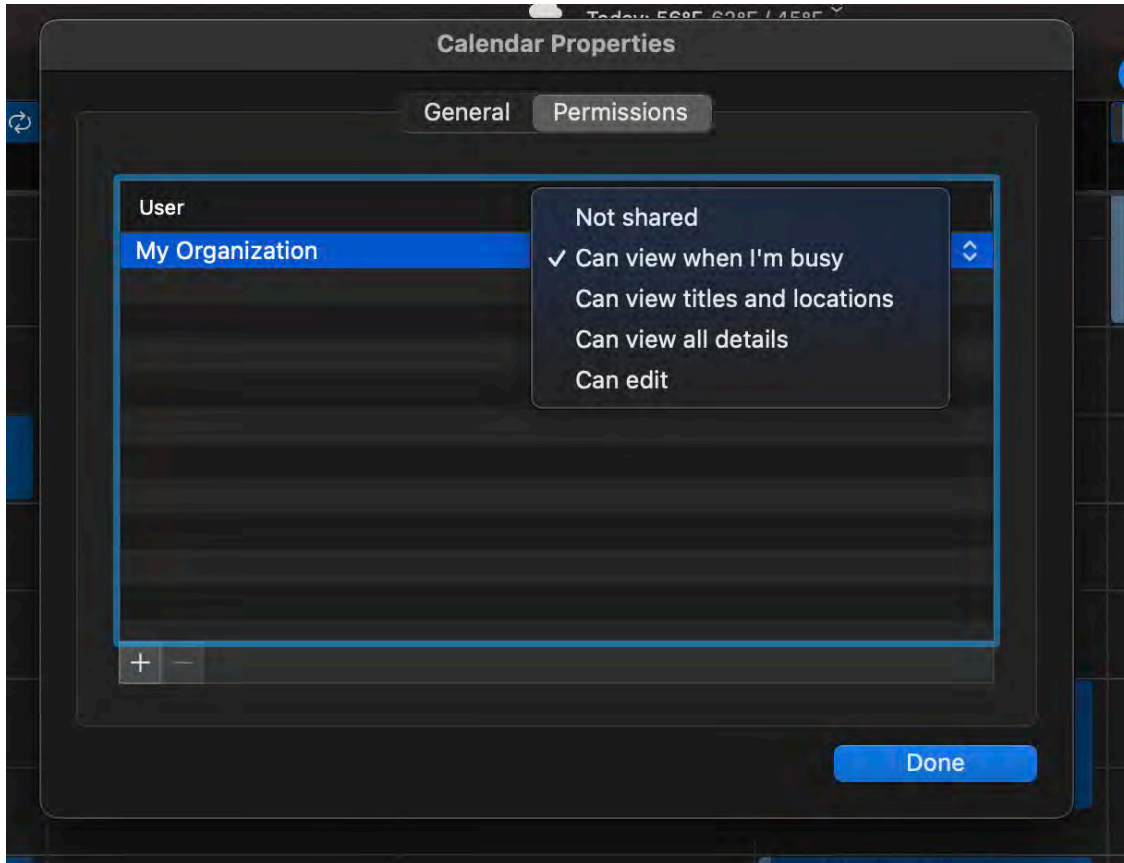
1. When you join Zoom, the **Join Audio** preferences box pops-up (Phone Call, Computer Audio, or Call Me)
2. Choose an option that works best for you
3. Join using that option
4. Use Test Speakers and Microphone option to optimize your webinar experience

## Chat

Please send your chat to **Everyone** to make sure the monitor sees your question



# Resources from PowerPoint



Please rename yourself, so we can:

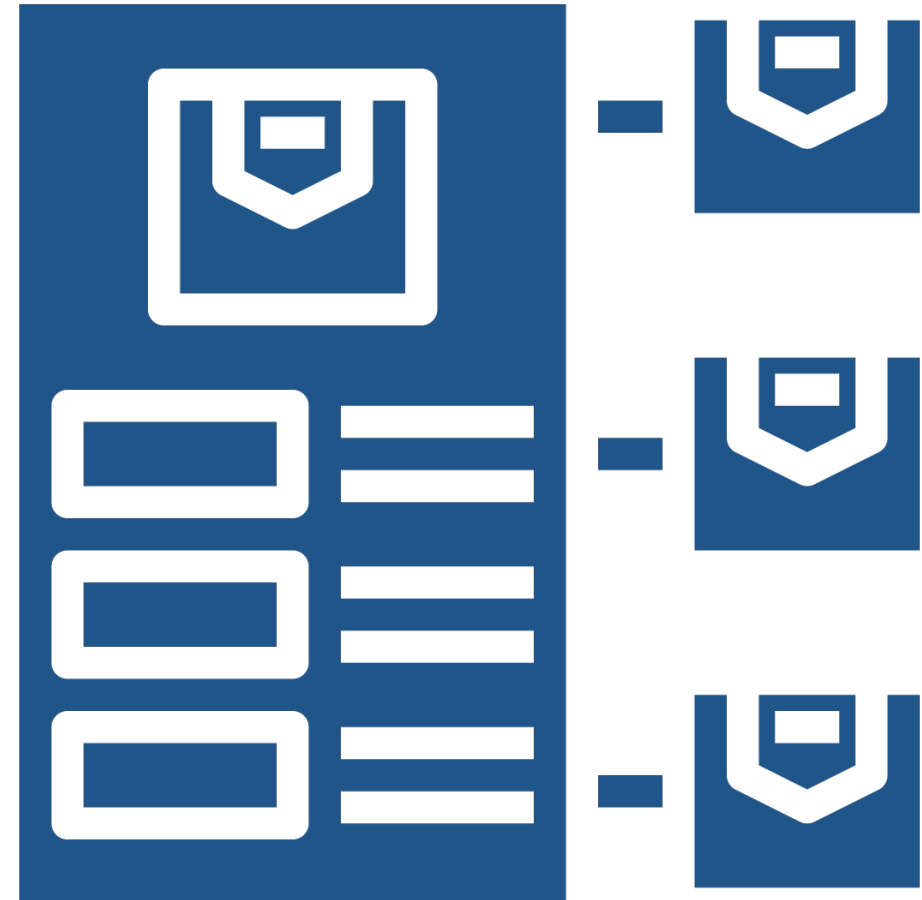
- Send you the student version of the PowerPoint
- Send your training certificate
- Add you to our list-serve

# Project Management and Reproducibility In RStudio

**Doug Joubert**  
**2023-02-28**

# Class Description

- Focuses on data and project management using R and Rstudio
- Some familiarity or experience in R and RStudio is recommended but not required



- Define scientific reproducibility
- Discuss best practices for organizing data in an RStudio project
- Discuss the importance of using a data dictionary and read me files
- Ensure that their data is machine readable

# Configuration for Exercises

- R is a programming language that is especially powerful for data exploration, visualization
- RStudio is an integrated development environment (IDE) that makes using R easier
- R and RStudio are two separate pieces of software
- **Must install R before you install RStudio**

1. Download R from the [CRAN website](https://cran.r-project.org/)
2. Run the .exe file that was just downloaded





1. Go to the RStudio [download page](#)
2. Under Installers select RStudio x.yy.zzz - Windows Vista/7/8/10 (where x, y, and z represent version numbers)
3. Double click the file to install it



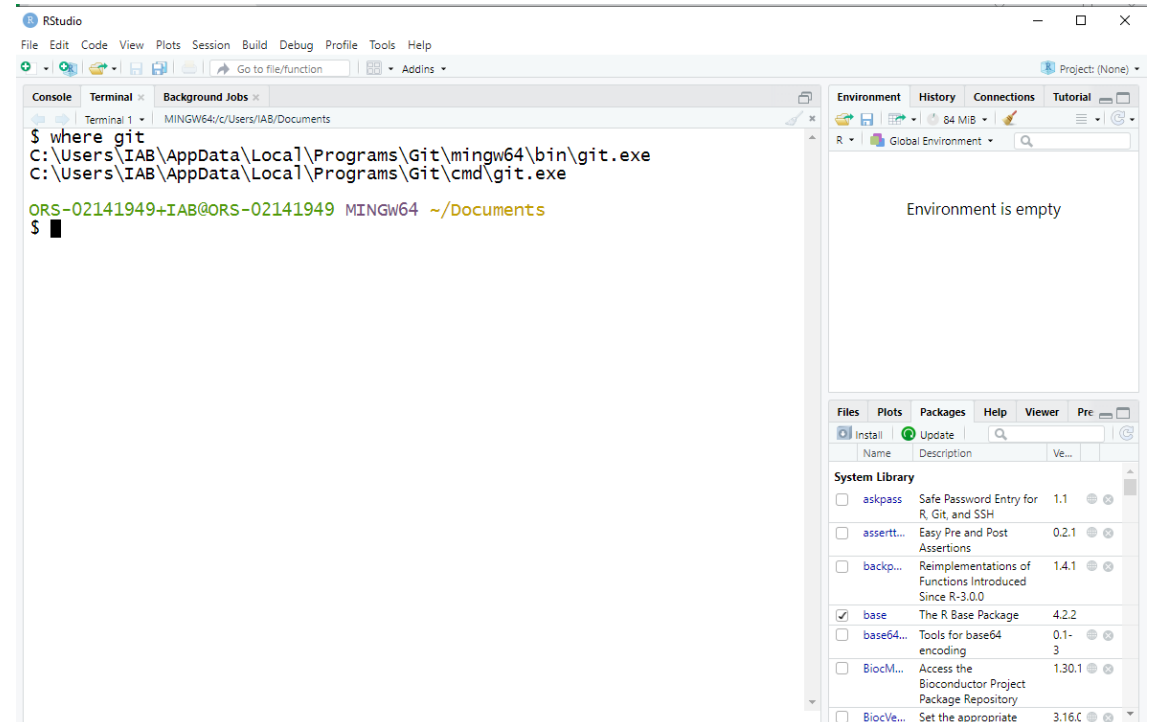
1. Download R from the [CRAN website](https://cran.r-project.org/)
2. Select the .pkg file for the latest R version
3. Double click on the downloaded file to install R
4. It is also a good idea to install XQuartz (needed by some packages)



1. Go to the RStudio [download page](#)
2. Under Installers select RStudio x.yy.zzz - Mac OS X 10.6+ (64-bit) (where x, y, and z represent version numbers)
3. Double click the file to install RStudio



- Open Power Shell on Windows or Terminal in RStudio
- type: `where git`

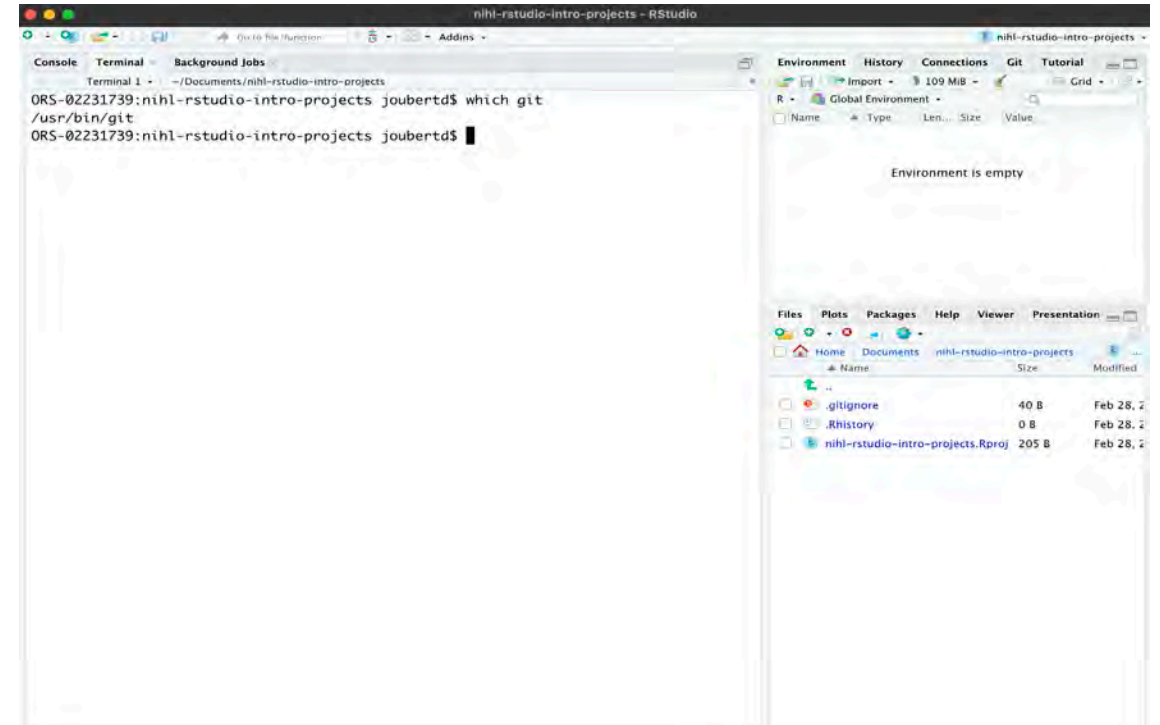


The screenshot shows the RStudio interface with the Terminal pane open. The command `where git` has been executed, and the output shows the path to the Git executable: `C:\Users\IAB\AppData\Local\Programs\Git\mingw64\bin\git.exe`. The prompt indicates the user is in a MINGW64 environment at `~/Documents`.

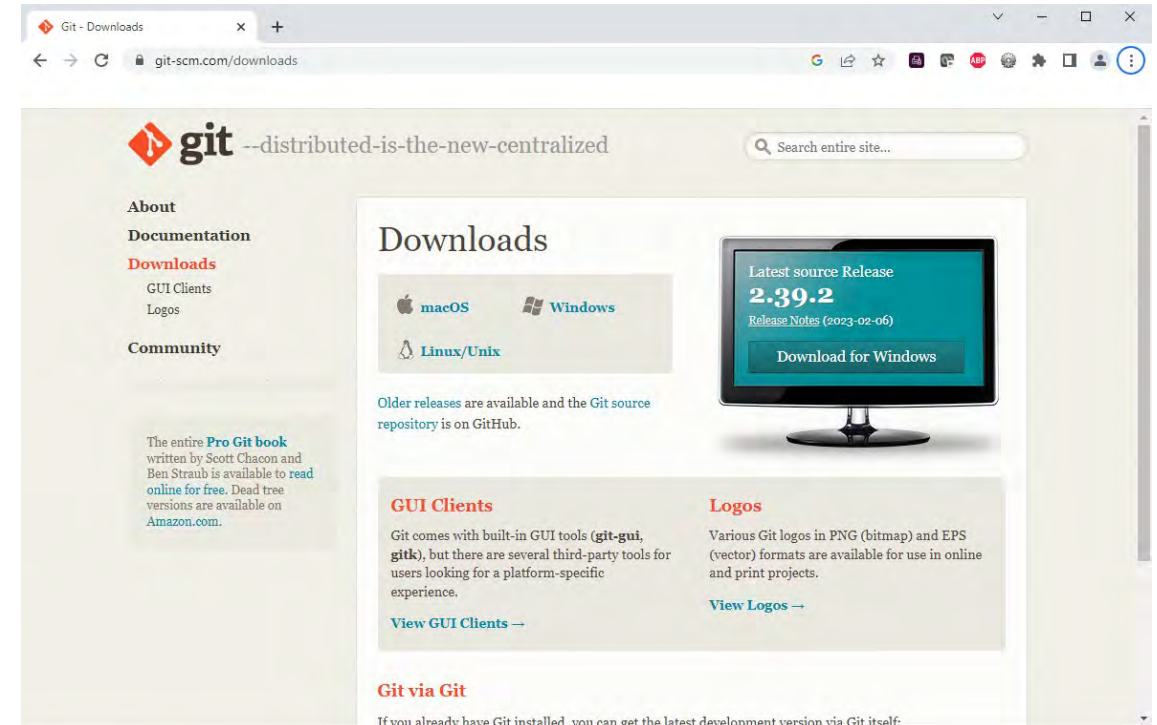
```
$ where git
C:\Users\IAB\AppData\Local\Programs\Git\mingw64\bin\git.exe
C:\Users\IAB\AppData\Local\Programs\Git\cmd\git.exe

ORS-02141949+IAB@ORS-02141949 MINGW64 ~/Documents
$
```

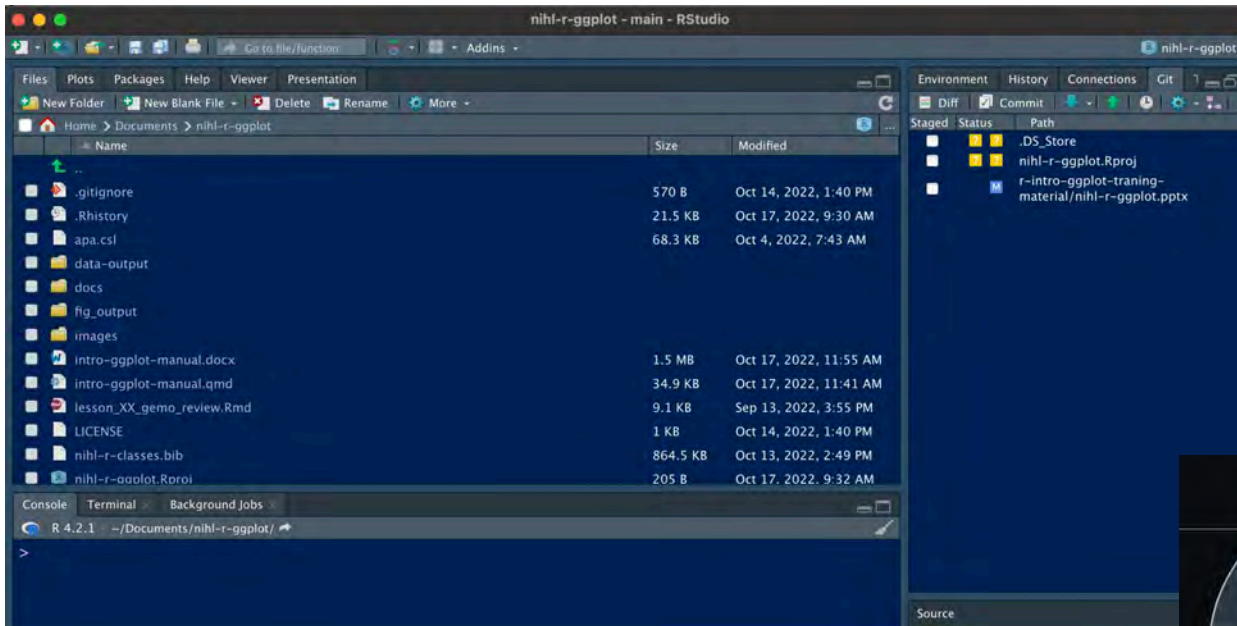
- Open Power Shell on Windows or Terminal in RStudio
- type: `which git`



- [Git installation instructions](#) to install Git, if not on your computer

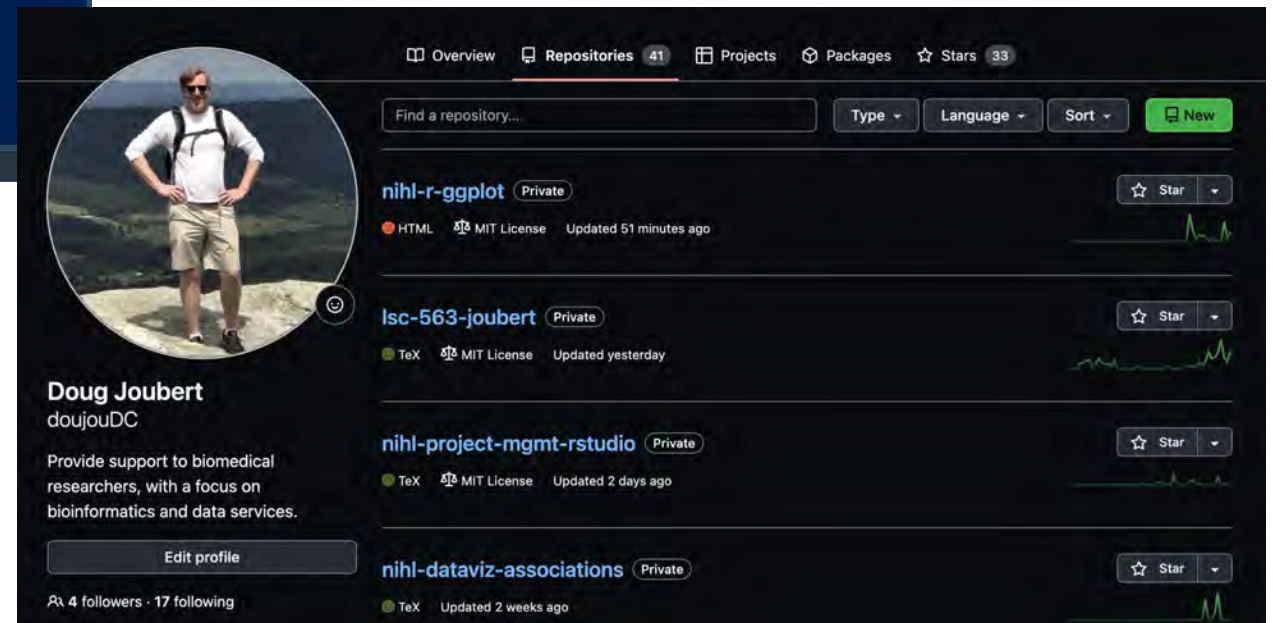


# Project Configuration



- Follows RStudio project framework
- Code in .qmd file
- Wilson, G., Bryan, J., Cranston, K., Kitze, J., Nederbragt, L., & Teal, T. K. (2017). Good enough practices in scientific computing. PLOS Computational Biology, 13(6), e1005510-e1005510.

- All class repos sync'd to GitHub
- Includes:
  - Class data
  - Folder structure
  - Training material
  - Exercises





# NIH Library R Classes: Basics

- Introduction to R and RStudio
- Introduction to R Data Types
- Data Wrangling in R
- Introduction to Project Management in RStudio (A)
- Reproducibility in RStudio: Basic Markdown
- Introduction to Data Visualization in R: ggplot (A)

The screenshot displays the NIH Library R Classes calendar for January 2023. On the left, a 'Training Category' sidebar lists various class categories with checkboxes: Bibliometrics Classes, Bioinformatics Classes, BTRIS Classes, CMS Training Classes, Data Services Classes, Databases and Searching Classes, Special Events, Systematic Reviews Classes, Technology Classes, and Writing and Editing Classes. An 'Apply' button is located at the bottom of this list. The main calendar view shows a grid for January 2023, with days of the week (Mon-Fri) and dates (1-31). The calendar is color-coded by day: Monday (light blue), Tuesday (light green), Wednesday (light orange), Thursday (light yellow), and Friday (light pink). The following table summarizes the classes scheduled for each day:

Day	Date	Class Title
Monday	2	
Tuesday	3	
Wednesday	4	Introduction to Scopus
Thursday	5	Visualizing Relationships in ggplot
Friday	6	
Monday	9	
Tuesday	10	Introduction to EndNote 20
Wednesday	11	Copyright and Plagiarism: What Authors Need to Know
Thursday	12	
Friday	13	
Monday	16	
Tuesday	17	Python for Data Science: How to Get Started, What to Learn, and Why
Wednesday	18	Introduction to R and RStudio
Thursday	19	
Friday	20	Introduction to PubMed
Monday	23	
Tuesday	24	Data Types in R and RStudio
Wednesday	25	
Thursday	26	Data Management and Sharing: Part 1
Friday	27	Data Management and Sharing: Part 2
Monday	30	
Tuesday	31	



- Reproducibility in RStudio:  
Advanced Markdown
- Working with Git in RStudio
- Introduction to Data  
Visualization in R:  
Customization in ggplot

The screenshot shows the NIH Library Course Catalog interface. On the left, there is a sidebar with two main sections: 'Training Types' and 'Training Category'. The 'Training Types' section includes links for 'Classes', 'Course Catalog' (which is highlighted), 'Events', 'Online Tutorials', and 'Request a Tutorial'. The 'Training Category' section includes links for 'Bibliometrics Classes', 'Bioinformatics Classes', 'BTRIS Classes', 'CMS Training Classes', and 'Data Services Classes'. The main content area is titled 'Course Catalog' and contains a paragraph explaining that the following topics are taught by the NIH Library, with a link to the full training catalog. Below this, it states that NIH Library classes are taught in-person in the NIH Library training rooms, Building 10, Clinical Center, near the South Entrance or virtually, and that self-paced online tutorials are available through a variety of vendors and library staff. A specific course, '3D Printing and Modeling Fundamentals', is listed under the 'Technology Classes' category. The description for this course mentions that 3D printing is revolutionizing biomedical research and that participants will learn about the NIH Library's free 3D Printing service, how to use it, and how to design a simple personalized keychain.

**Training Types**

- Classes
- Course Catalog**
- Events
- Online Tutorials
- Request a Tutorial

**Course Catalog**

Below are topic or subject areas taught by the NIH Library. Click the topic to see a list of upcoming classes or other related content. To view our full training catalog, visit [the library training calendar](#). We are open to your feedback and suggestions related to our training program. Please [suggest a class](#) if you do not see it listed.

NIH Library classes are taught in-person in the NIH Library training rooms, Building 10, Clinical Center, near the South Entrance or virtually. In addition to classes, [self-paced online tutorials](#) are available through a variety of vendors and our library staff.

**Training Category**

- Bibliometrics Classes
- Bioinformatics Classes
- BTRIS Classes
- CMS Training Classes
- Data Services Classes

- **3D Printing and Modeling Fundamentals**

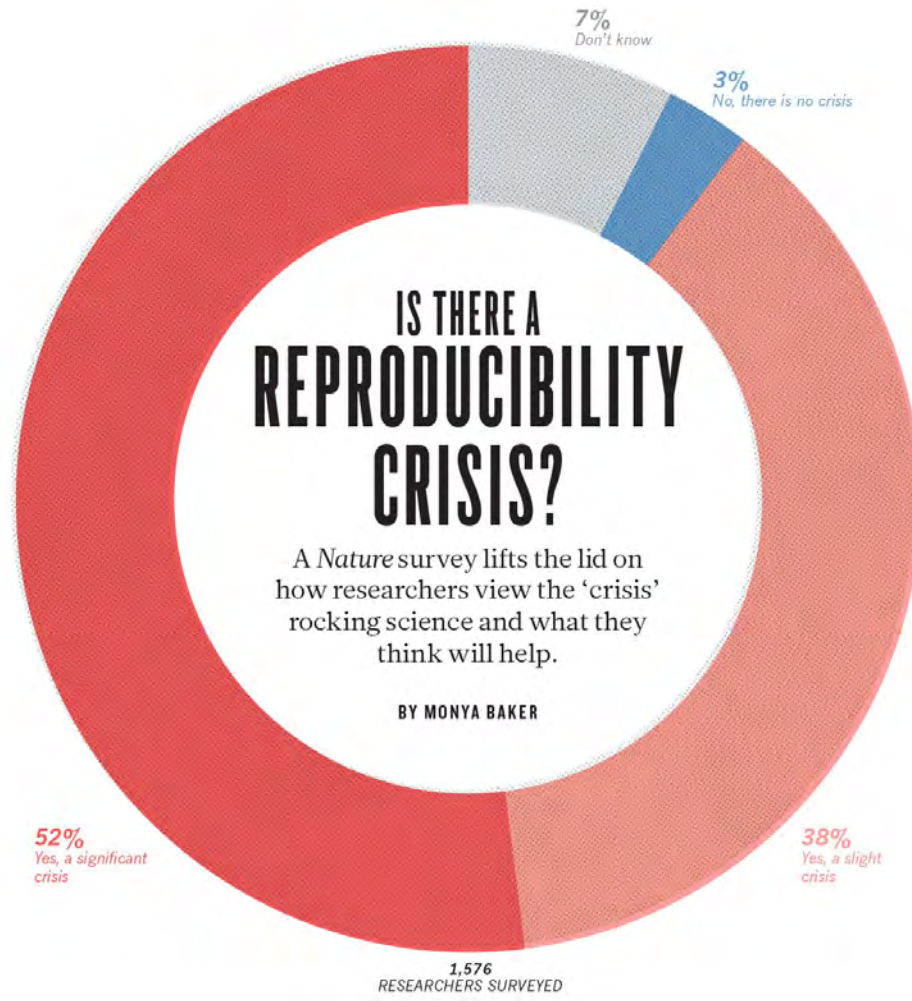
3D printing is revolutionizing biomedical research by enabling scientists to engage in creative problem solving, build customized solutions, and develop faster prototypes of their ideas. Join us to learn about the NIH Library's free 3D Printing service and how you can utilize it by printing free online models or designing your own. Participants will understand how 3D printers work and how this technology is being applied at NIH, locate resources for 3D printing software and models, and manipulate shapes to create a basic design using TinkerCAD, a free online tool. Beginners and interested individuals with no previous experience in this area are highly encouraged to attend. Upon completion of this hands-on workshop participants will design a simple personalized keychain that they can queue for printing.

Training Category: [Technology Classes](#)

According to the [U.S. National Science Foundation \(NSF\)](#) subcommittee on replicability in science (2015):

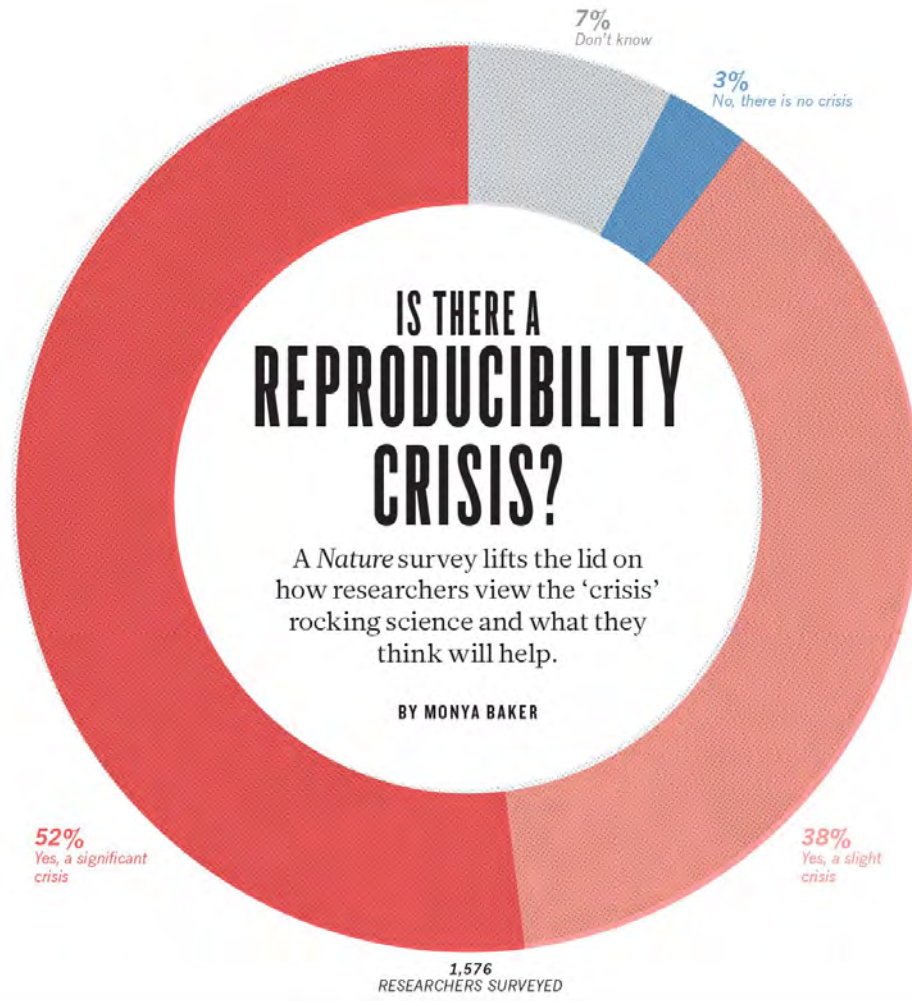
Science should routinely evaluate the reproducibility of findings that enjoy a prominent role in the published literature. To make reproduction possible, efficient, and informative, **researchers should sufficiently document the details of the procedures used to collect data, to convert observations into analyzable data, and to perform data analysis.**

Bollen, K., et al (2015)



- 1,576 researchers took online questionnaire
- More than 70% of researchers have tried and failed to reproduce another scientist's experiments
- More than half have failed to reproduce their own experiments
- Specific factors in handout

Baker, M. (2016).



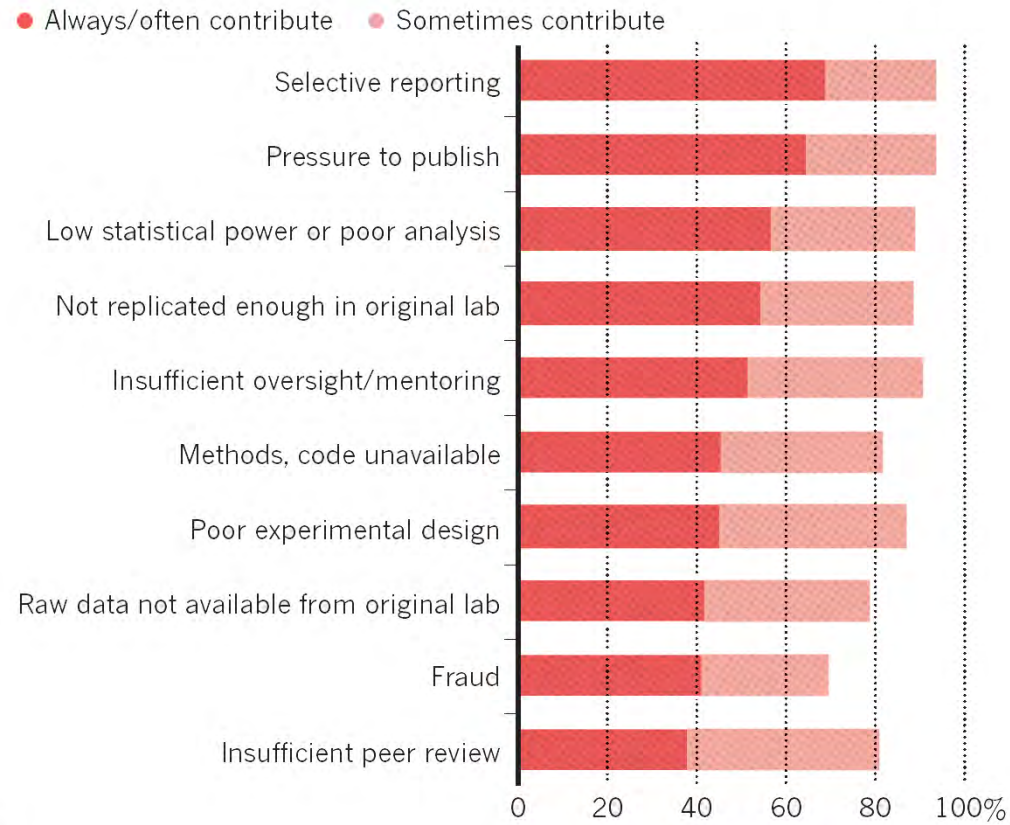
- Sometimes-contradictory attitudes towards reproducibility:
  - > 52% agree that there is a significant crisis
  - < 31% think that failure to reproduce published results means results are wrong
  - Most still trust the published literature

Baker, M. (2016).



## WHAT FACTORS CONTRIBUTE TO IRREPRODUCIBLE RESEARCH?

Many top-rated factors relate to intense competition and time pressure.



5  
Baker, M. (2016).

- > 60% said that two factors were problems:
  - Pressure to publish
  - Selective reporting
- > 50% pointed to:
  - Insufficient replication in the lab
  - Poor oversight
  - Low statistical power

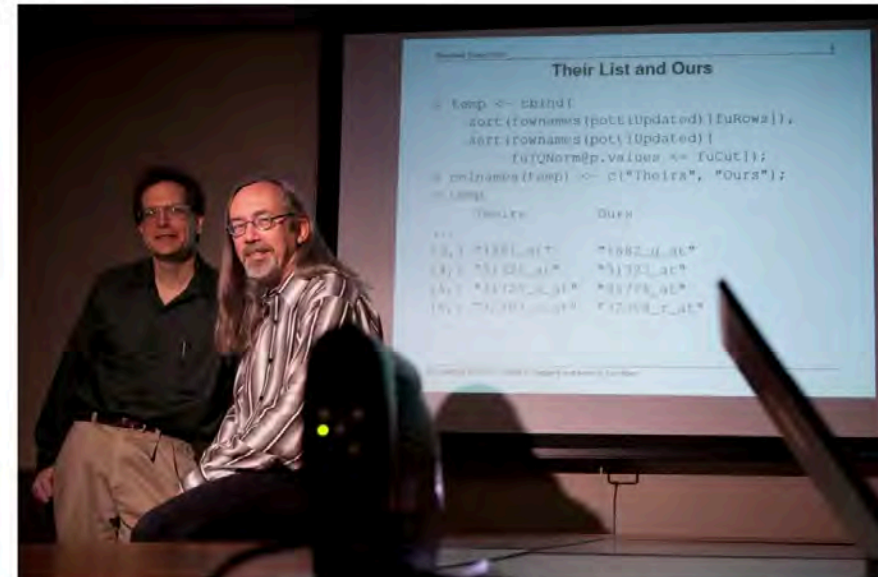
- 5 selfish reasons to use reproducibility practices:
  - Helps to avoid data loss and disaster
  - Makes it easier to write papers
  - Helps reviewers see it your way
  - Enables continuity of your work
  - Helps to build your reputation

## How Bright Promise in Cancer Testing Fell Apart

Give this article



75



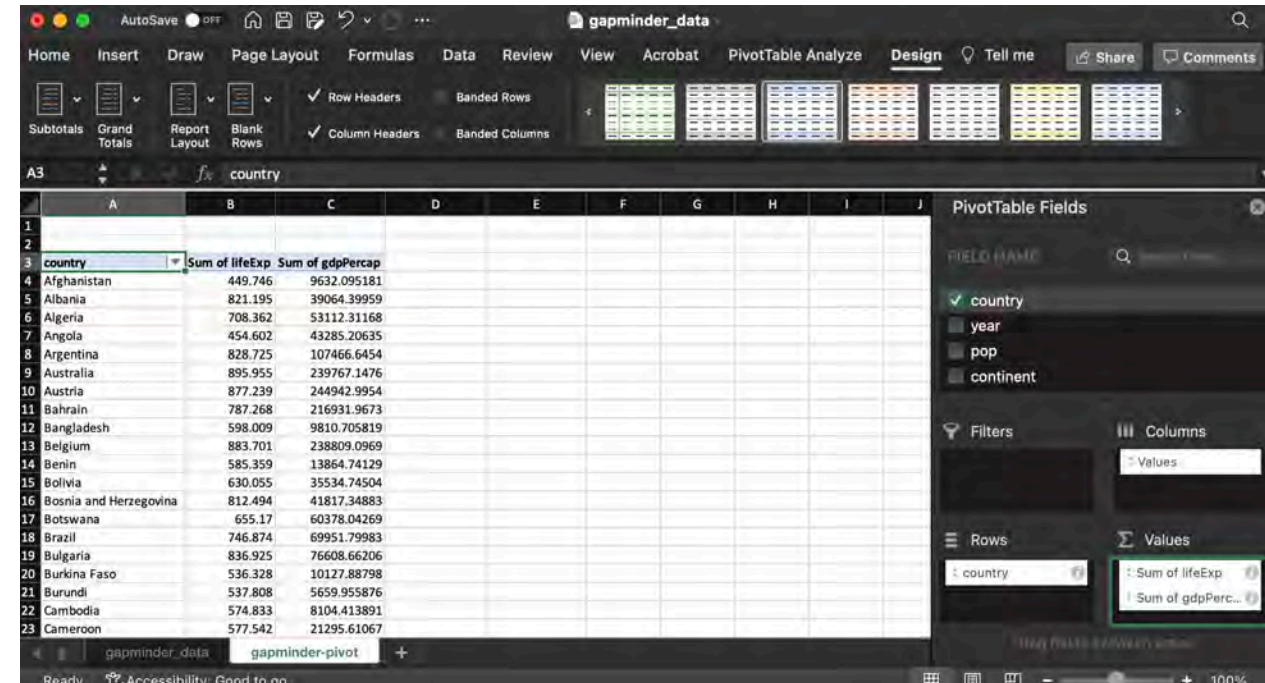
Keith Baggerly, left, and Kevin Coombes, statisticians at M. D. Anderson Cancer Center, found flaws in research on tumors. Michael Stravato for The New York Times

Markowetz, F. (2015).

Image: NY Times

# Why Learn R? – It is More Powerful

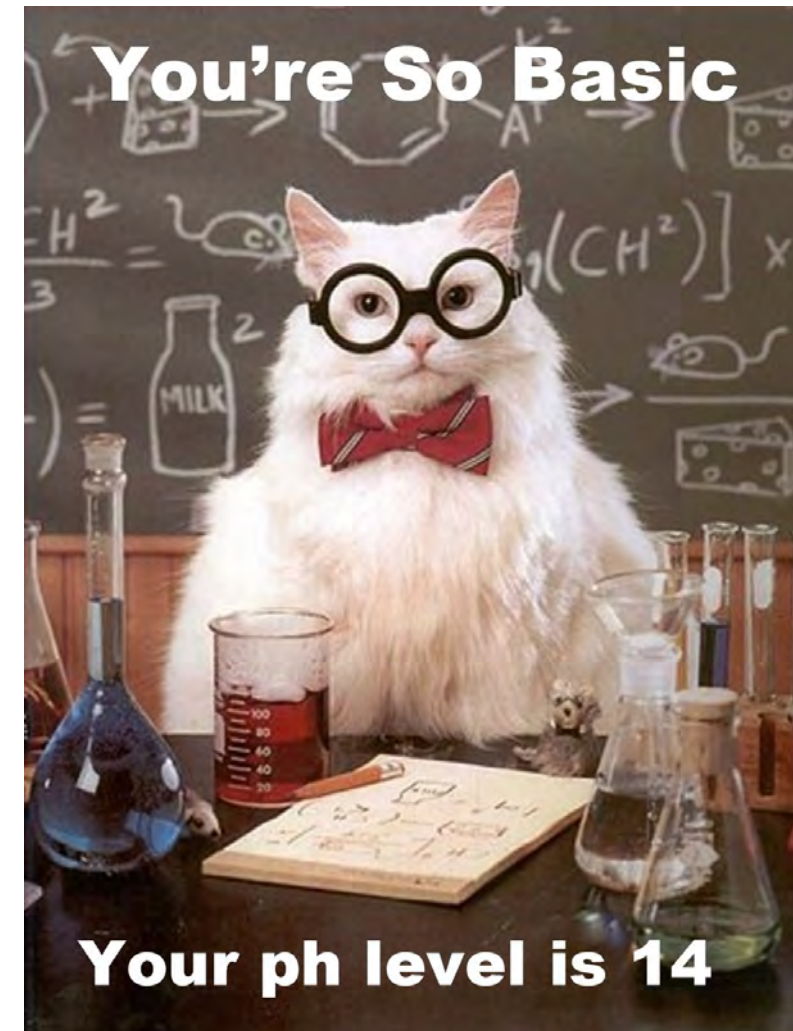
- Why should I learn R when Pivot Tables do the same thing?
- For example, Figure 4 is showing a Pivot Table for [gapminder](#) data
  - Mean
  - Median
  - Min value
  - Max value



country	Sum of lifeExp	Sum of gdpPercap
Afghanistan	449.746	9632.095181
Albania	821.195	39064.39959
Algeria	708.362	53112.31168
Angola	454.602	43285.20635
Argentina	828.725	107466.6454
Australia	895.955	239767.1476
Austria	877.239	244942.9954
Bahrain	787.268	216931.9673
Bangladesh	598.009	9810.705819
Belgium	883.701	238809.0969
Benin	585.359	13864.74129
Bolivia	630.055	35534.74504
Bosnia and Herzegovina	812.494	41817.34883
Botswana	655.17	60378.04269
Brazil	746.874	69951.79983
Bulgaria	836.925	76608.66206
Burkina Faso	536.328	10127.88798
Burundi	537.808	5659.955876
Cambodia	574.833	8104.413891
Cameroon	577.542	21295.61067

# Why Learn R? – It is More Powerful

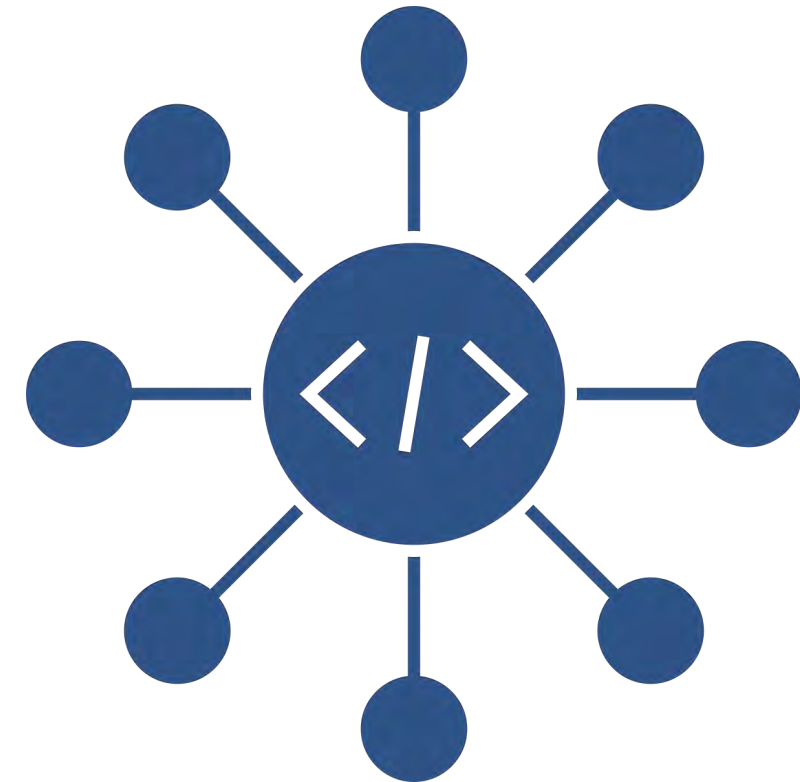
- With R, using 2 lines of code
  - Group data by country and run one regression model
  - Display statistics like the coefficients or the R2 value
  - I agree with Chemistry Cat, Excel is so basic





# Why Learn R? – Free and Open Source

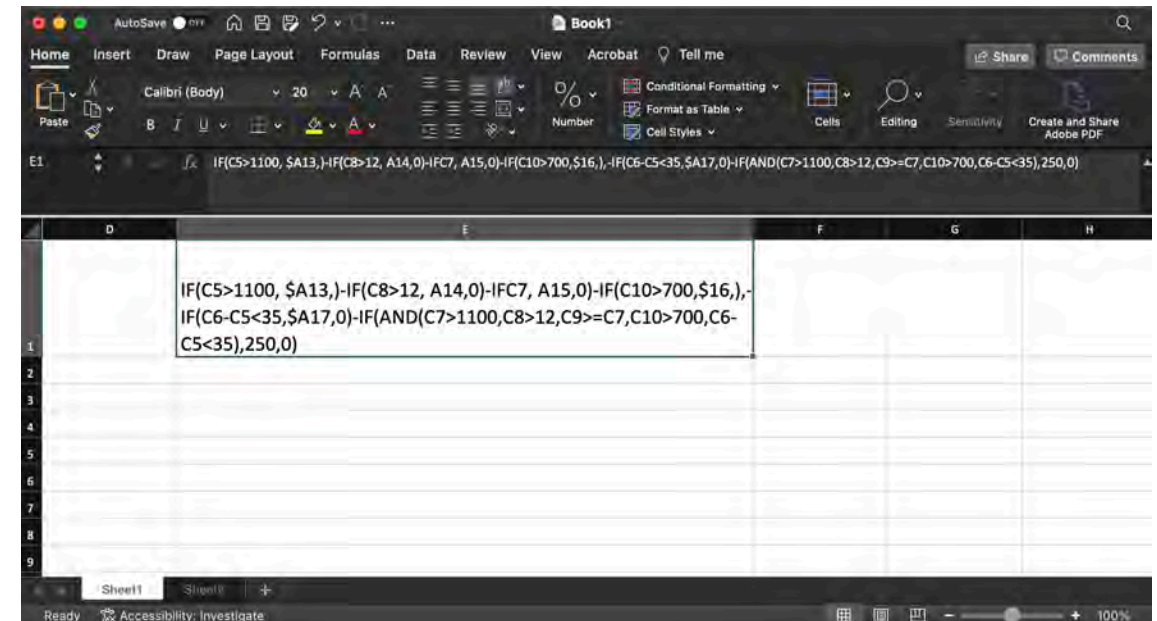
- This gets at a more philosophical reason for using R
- Not everyone has access to Office 365
- Tableau or Stata skills are great, but products are very expensive
- If sharing analysis results in Excel, not everyone will be able to open that file



(Heiss, 2022)

# Why Learn R? – Reproducibility

- Only way this would be reproducible is if you write down all the steps for:
  - Every menu you clicked
  - Every cell you clicked on to add a formula or changed the formatting
  - Have you ever seen an Excel spreadsheet with an accompanying set of instructions?



(Heiss, 2022)

- A 2016 study found gene name errors in 20% of the papers that they reviewed
- Web of Science search using the terms “Reproducible statistical analyses” OR “Reproducibility” resulted in over 7,000 published papers, in the last 10 years

Septin 2

Membrane-Associated Ring Finger (C3HC4) 1

2310009E13

	A	B
1	Actual value	What Excel turns it into
2	SEPT2	2-Sep
3	MARCH1	1-Mar
4	2310009E13	2.31E+19

(Ziemann, Eren, and EL-Osta)

- **Don't Touch the Raw Data:** no analysis on the original data, or, if you do, then explain what you did to the data.
- **Self-documenting and Reproducible Code:** consider writing your reports or papers in markdown. Markdown combines text with code.
- **Use Open Formats:** open formats as much as possible. That means sharing your data in csv or tab-delimited format.

(Heiss, 2022)



# RStudio Project Demo

- Creating a project in RStudio
- Brief discussion about “best practices”



# Best Practices for Managing Projects

- RStudio is an integrated development environment (IDE) for R and Python:
  - Free and open-source
  - Designed to make it easy to write and reuse code
  - Convenient to view and interact with the objects stored in your environment
  - Collaboration and Publishing Tools
  - Documents using R Markdown
- We have a separate [class](#) that focuses on Intro to R



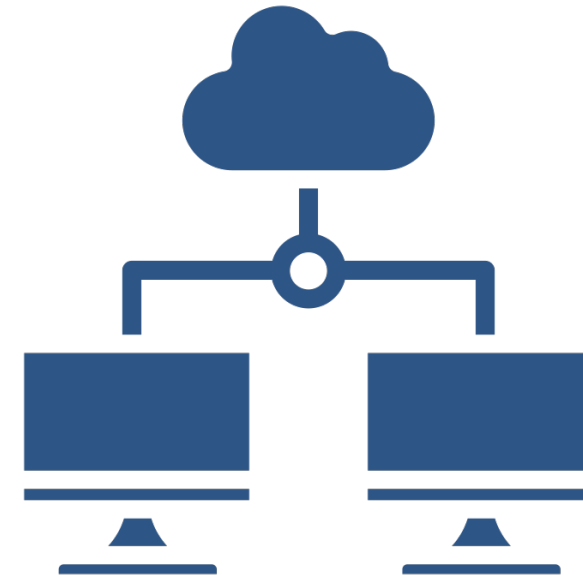
- Using the poll, list some problems that you have encountered when dealing with files and folders



- Cannot find your files on your computer (or your cloud storage)
- Multiple versions of files with names such as "finaldraft\_4.txt"
- Path issues when trying to run code
- Reviewers or colleagues cannot re-run your code/analyses



- Using the poll, list some problems that you have encountered when dealing with storage or sharing



- Files are only saved to your computer
- Collaborators don't share the files needed
- Files are shared via email attachments
- Difficult to know if you have the latest version of documents



OPEN ACCESS Freely available online

Community Page

## Best Practices for Scientific Computing

Greg Wilson<sup>1\*</sup>, D. A. Aruliah<sup>2</sup>, C. Titus Brown<sup>3</sup>, Neil P. Chue Hong<sup>4</sup>, Matt C Steven H. D. Haddock<sup>7</sup>, Kathryn D. Huff<sup>8</sup>, Ian M. Mitchell<sup>9</sup>, Mark D. Plumb Ethan P. White<sup>12</sup>, Paul Wilson<sup>13</sup>

<sup>1</sup> Mozilla Foundation, Toronto, Ontario, Canada, <sup>2</sup> University of Ontario Institute of Technology, Oshawa, Ontario, Canada, <sup>3</sup> University of Michigan, United States of America, <sup>4</sup> Software Sustainability Institute, Edinburgh, United Kingdom, <sup>5</sup> Space Telescope Science Institute, Baltimore, Maryland, United States of America, <sup>6</sup> University of Toronto, Toronto, Ontario, Canada, <sup>7</sup> Monterey Bay Aquarium Research Institute, Moss Landing, California, United States of America, <sup>8</sup> University of California Berkeley, Berkeley, California, United States of America, <sup>9</sup> University of British Columbia, Vancouver, British Columbia, Canada, <sup>10</sup> University of London, London, United Kingdom, <sup>11</sup> University College London, London, United Kingdom, <sup>12</sup> Utah State University, Logan, Utah, United States of America, <sup>13</sup> University of Wisconsin, Madison, Wisconsin, United States of America

### Introduction

Scientists spend an increasing amount of time building and using software. However, most scientists are never taught how to do this efficiently. As a result, many are unaware of tools and practices that would allow them to write more reliable and

error from another group's publication [6]. As with bench done to the most exacting standards, awareness of best practices both for reviewing computational science and for writing computational science. This paper describes a set

F1000Research

F1000

COMMENTARY

REVISED Software Carpentry: lessons learned

review: 3 approved]

Greg Wilson

Software Carpentry Foundation, Austin, TX, USA

**v2** First published: 19 Feb 2014, 3:62  
<https://doi.org/10.12688/f1000research.3-62.v1>  
Latest published: 28 Jan 2016, 3:62  
<https://doi.org/10.12688/f1000research.3-62.v2>

### Abstract

Since its start in 1998, Software Carpentry has evolved from a week-

Open P

Approv

version

## Good Enough Practices for Scientific Computing

Greg Wilson<sup>1</sup>, Jennifer Bryan<sup>2</sup>, Karen Cranston<sup>3</sup>, Justin Kitzes<sup>4</sup>, Lex Nederbragt<sup>5</sup>, Tracy K. Teal<sup>6</sup>

- 1) Software Carpentry Foundation / [gvwilson@software-carpentry.org](mailto:gvwilson@software-carpentry.org)  
2) University of British Columbia / [jenny@stat.ubc.ca](mailto:jenny@stat.ubc.ca)  
3) Duke University / [karen.cranston@duke.edu](mailto:karen.cranston@duke.edu)  
4) University of California, Berkeley / [jkitzes@berkeley.edu](mailto:jkitzes@berkeley.edu)  
5) University of Oslo / [lex.nederbragt@ibv.uio.no](mailto:lex.nederbragt@ibv.uio.no)  
6) Data Carpentry / [titeal@datacarpentry.org](mailto:titeal@datacarpentry.org)

A PDF of this paper can be found at <http://arxiv.org/abs/1609.00037>. We would appreciate feedback of all kinds; please email comments to the authors.

### Abstract

We present a set of computing tools and techniques that every researcher can and should consider adopting. These recommendations synthesize inspiration from our own work, from the experiences of the thousands of people who have taken part in Software Carpentry and Data Carpentry workshops over the past six years, and from a variety of other guides. Our recommendations are aimed specifically at people who are new to research computing.

### Author Summary

Computers are now essential in all branches of science, but most researchers are never taught the equivalent of basic

- [Good Enough Practices for Scientific Computing](#) gives the following recommendations for project organization:
  - Each project in its own directory, which is named after the project
  - Text documents associated with the project in the doc directory
  - Raw data and metadata in the data directory (raw-data)
  - Files generated during cleanup and analysis in a results directory

Wilson., et al, 2017

- [Good Enough Practices for Scientific Computing](#) gives the following recommendations for project organization:
  - Project's scripts and programs in the src directory
  - Programs brought in from elsewhere or compiled locally in the bin directory
  - Name all files to reflect their content or function

Wilson., et al, 2017

- Additional files to include:
  - [README file](#), to communicate important information about your project
  - [LICENSE file](#), so that others are free to use, change, and distribute the software
  - [CITATION.cff file](#), to let others know how you would like them to cite your work
- Student version of the PowerPoint has more resources to explore

Wilson., et al, 2017



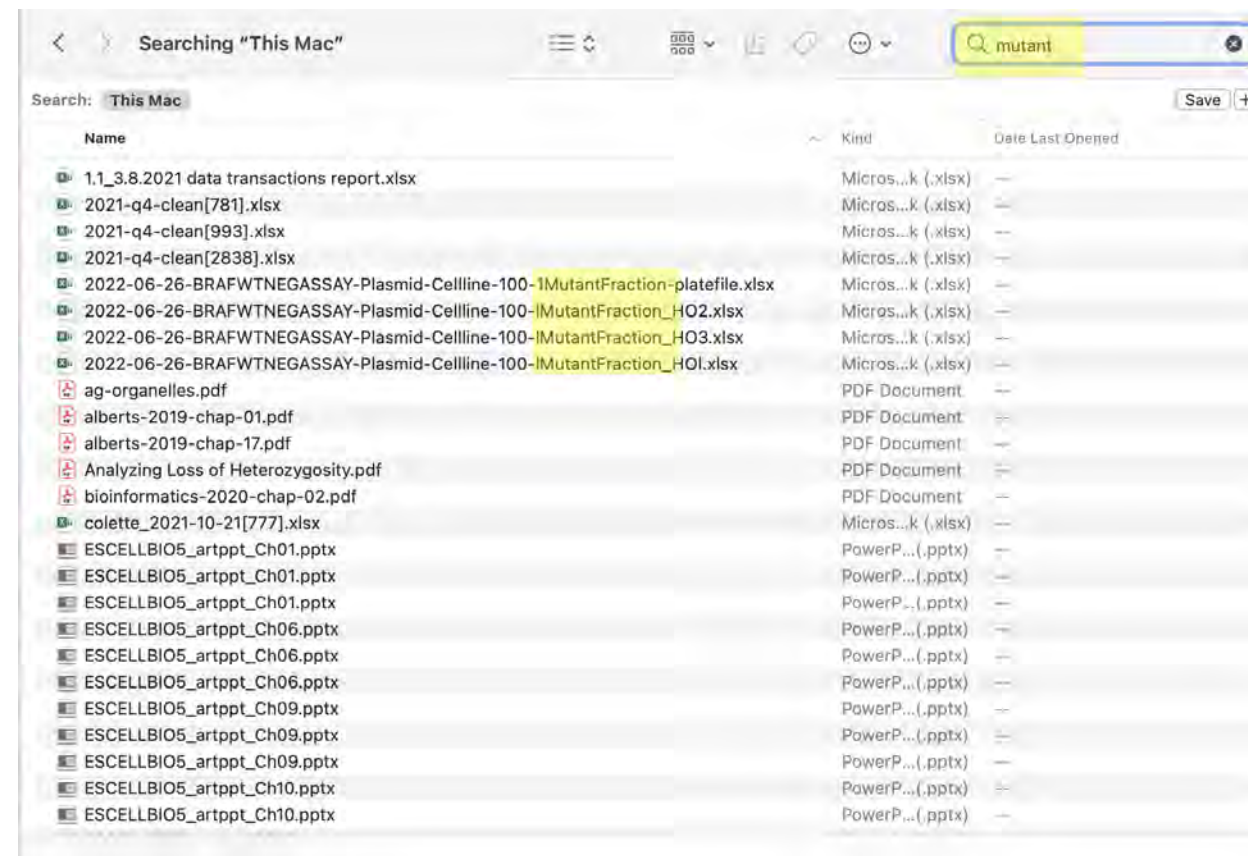
1. Machine readable
2. Human readable
3. Plays well with default ordering



Wilson., et al, 2017

# Naming Files: Why This is Important

- Globbing: using wildcard characters to request or evaluate sets of files with the same partial names or sets of character
- Regular expression friendly
- “Findability”
- Global name changes



- **Machine-readable**

- No spaces, unsupported punctuation, accented characters, or case-sensitive file names
- Deliberate use of delimiters (i.e. for splitting file names)
- Consistently use the same delimiters: data-analyses-fig1.R as an example

- **Human-readable**

- Name contains brief description of content: i.e. anova-analyses-control.R

- With **chronological ordering**, file name starts with date:
  - 2022-02-26-BRAFWTNEGASSAY-FFPEDNA-CRC-1-41-AO2.csv
  - 2022-02-26-BRAFWTNEGASSAY-FFPEDNA-CRC-1-41-AO3.csv
  - 2022-02-26-BRAFWTNEGASSAY-FFPEDNA-CRC-1-41-AO4.csv

Consider using [ISO 8601 date standard](#)

- With **logical ordering**, the filename starts with a number or keyword/number combo.
  - 01-marshall-data.r *see code directory*
  - 02-pre-dea-filtering.r *see code directory*
  - 03-explore-dea-limma-voom.r
  - 04-exploe-dea-results.r helper
  - 01-load-counts.rmd
  - helper02-load-exp-des.r
  - helper03-extract-and-tidy.r

- As illustrated on the previous slide, left-pad your numbers to facilitate sorting. If you do not do this, your data sorts like this...which is really sad
  - 01-marshall-data.r *see code directory*
  - 04-exploe-dea-results.r
  - 2-explore-dea-limma-voom.r
  - 3-helper-extract-and-tidy.r
  - helper01-load-counts.rmd

Adapted from <https://datacarpentry.org/rr-organization1/01-file-naming/index.html>. For more tips on file naming, check: [The Dos and Don'ts of File Naming](#).

- Configuration for exercises
- Introduction to [Reproducible Publications with RStudio](#)
- R for [Reproducible Scientific Analysis](#)



- Reproducible [Research Data and Project Management in R](#)
- Using [Projects in Rstudio](#)
- email me for a copy:  
[douglas.joubert@nih.gov](mailto:douglas.joubert@nih.gov)

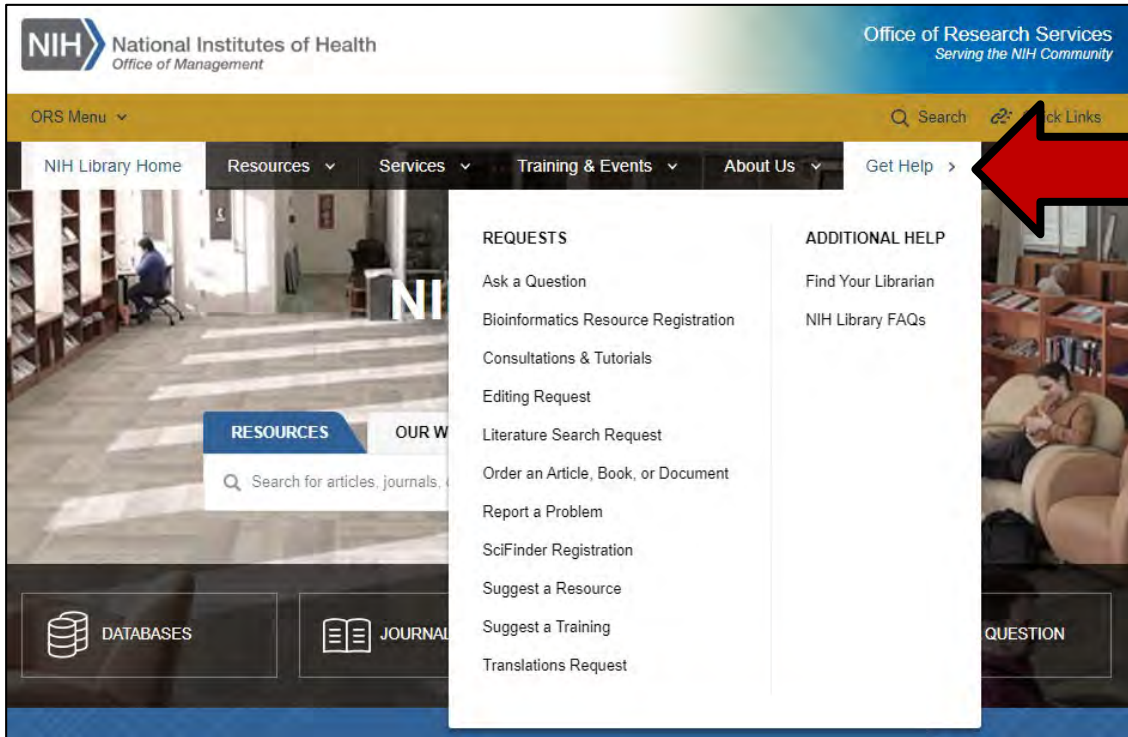






- Classes on a variety of data-related topics, including:
  - Data management
  - Data visualization
  - Data analysis
  - R and RStudio
- Computers which offers a suite of tools for data analysis, processing, and visualization

# Contact Us for Ongoing Support



**Doug Joubert**

Bioinformatics Support Program

301-827-3829

douglas.joubert@nih.gov

**NIH Library Help Desk**

(301) 496-1080

- **Ask a Question:** <https://www.nihlibrary.nih.gov/get-help/ask-question>
- **Request a Tutorial:** <https://www.nihlibrary.nih.gov/get-help/consultations-tutorials>
- **Sign up for Additional Classes:** <https://www.nihlibrary.nih.gov/training/calendar>



National Institutes of Health  
*Office of Management*