Improve your workflow for reproducible science

Mine Çetinkaya-Rundel
University of Edinburgh + Duke University + RStudio

🔗 **bit.ly/repro-workflow**

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The results in Table 1 don’t seem to correspond to those in Figure 2!

61 45 4

94 12 3

20 44

```r
# set.seed
set.seed(20190314)

# generate 8 random numbers between 0 and 99
runif(8, 0, 99) %>% round()
```

more than **70** percent

have tried and **failed** to reproduce
another scientist's experiments

Baker, Monya. "1,500 scientists lift the lid on reproducibility." Nature News 533.7604 (2016): 452.

more than **50** percent

have tried and **failed** to reproduce
their **own** experiments

Baker, Monya. "1,500 scientists lift the lid on reproducibility." Nature News 533.7604 (2016): 452.

Google Scholar yields

1010

results containing the term **reproducibility crisis** just in **2020**

Google Scholar Search, Nov 9, 2020.

setting the stage

Photo by Alexander Dummer on Unsplash].

replicability

same research question

same results

new data

EDITORIAL

The ASA's Statement on *p*-Values: Context, Process, and Purpose

In February 2014, George Cobb, Professor Emeritus of Mathematics and Statistics at Mount Holyoke College, posed these questions to an ASA discussion forum:

> Q: Why do so many colleges and grad schools teach $p = 0.05$?
> A: Because that's still what the scientific community and journal editors use.
> Q: Why do so many people still use $p = 0.05$?
> A: Because that's what they were taught in college or grad school.

Cobb's concerns were a long-overdue recognition of the widespread misuse of statistical methods, often resulting in erroneous scientific conclusions. Misinterpretation and abuse of statistical tests, confidence intervals, and statistical significance are not new. For decades, statisticians have been sounding alarms about these issues, and have been publishing recommendations for how to improve statistical practice. Meanwhile, however, practices continue that combine incomplete descriptions of procedures with misinterpretations of results.

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reproducibility

same research question

same results

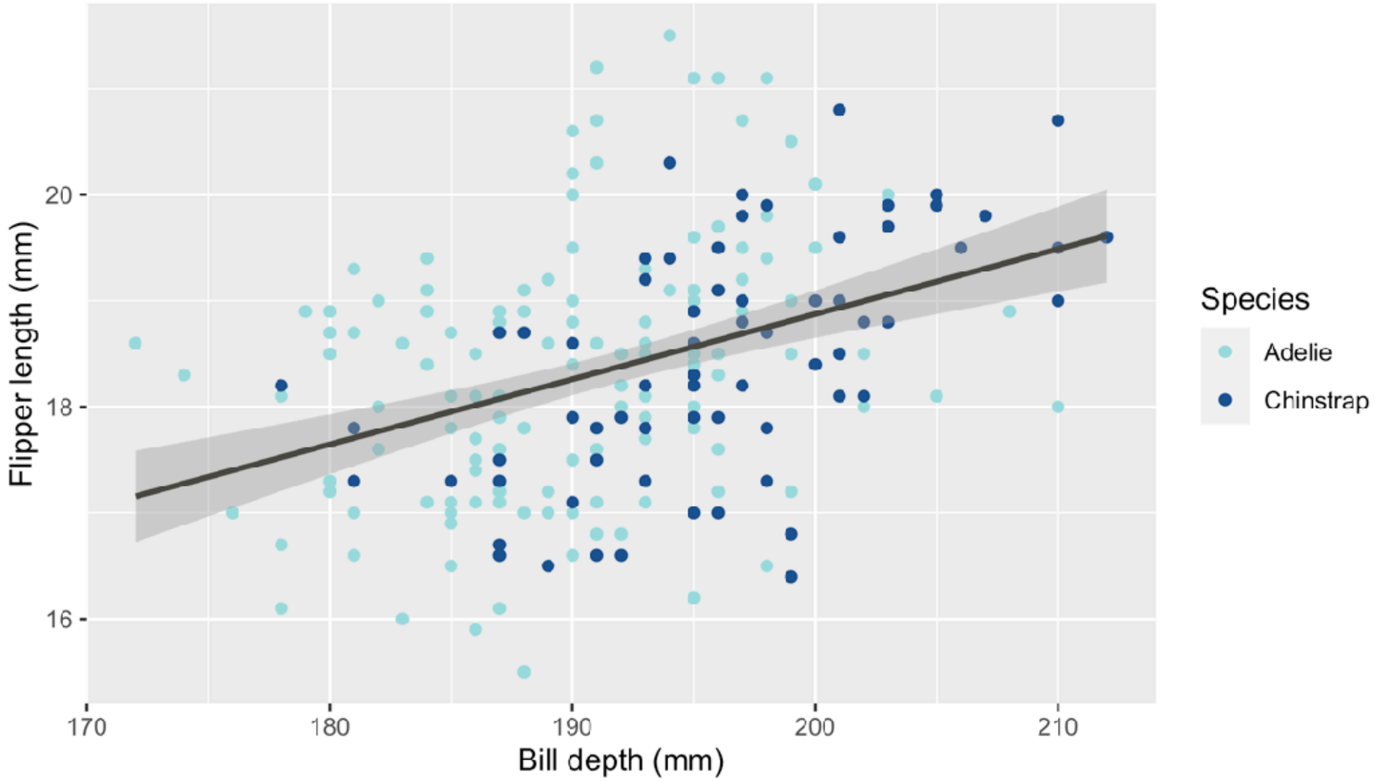
same data

e.g.

Table 1. Regression output for predicting bill depth from flipper length.

term	estimate	std.error	statistic	p.value
(Intercept)	33.6	1.25	27.0	1.39e-86
flipper_length_mm	-0.0820	0.00618	-13.3	1.23e-32

Figure 2. Relationship between bill depth and flipper length.



e.g.

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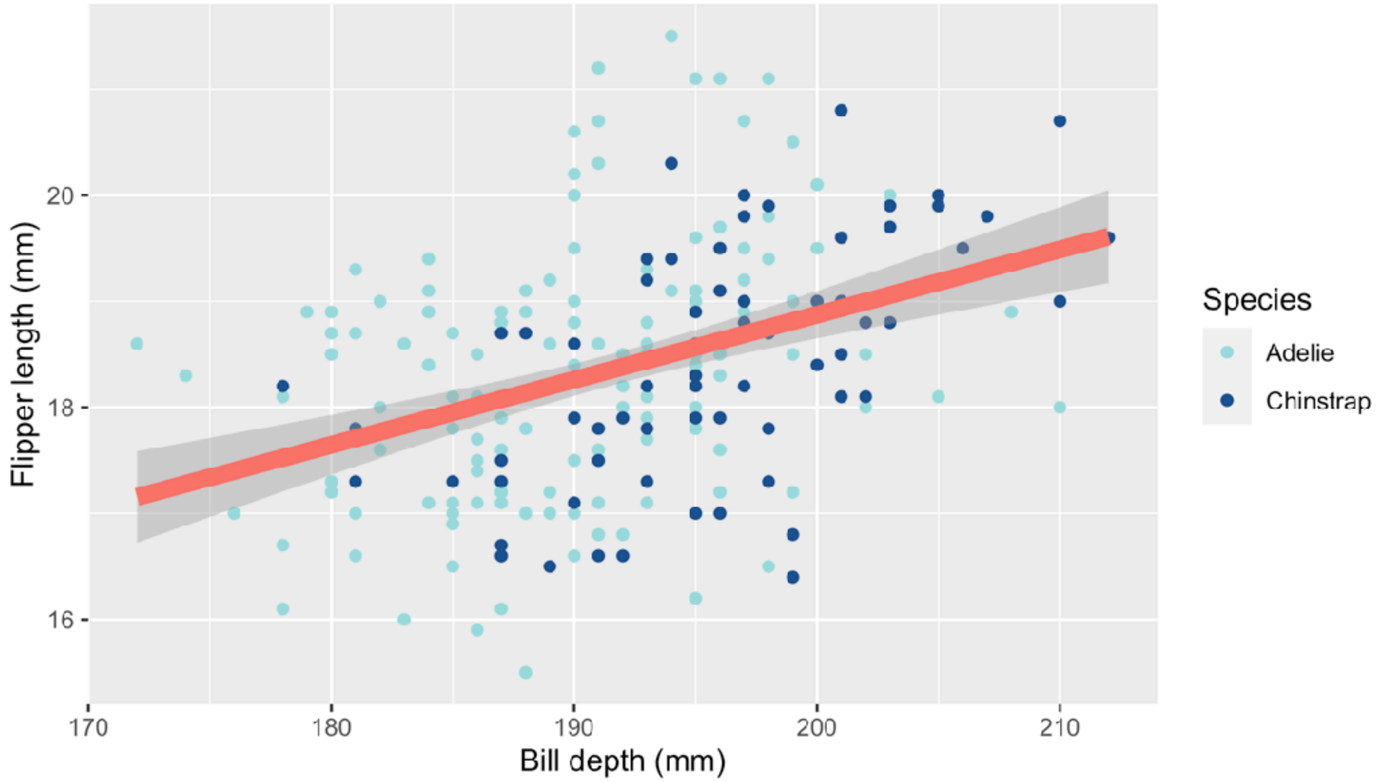

analysis

```r
# fit model
model <- lm(bill_depth_mm ~ flipper_length_mm, data = penguins)

# print model summary
tidy(model)
```

report

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analysis

```
# visualize the relationship
ggplot(penguins) +
  geom_point(
    aes(x = bill_depth_mm, y = flipper_length_mm, color = species)
  ) +
  geom_smooth(
    aes(x = bill_depth_mm, y = flipper_length_mm),
    method = "lm"
  )
```

report

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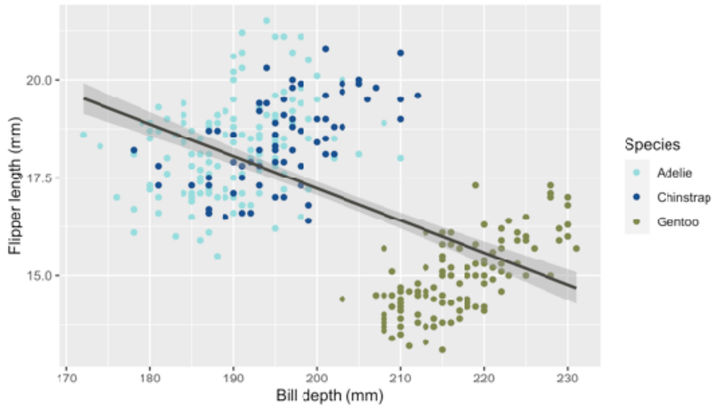

analysis

```r
# filter out Gentoos
penguins_nongentoo <- penguins %>%
  filter(species != "Gentoo")

# visualize the relationship
ggplot(penguins_nongentoo) +
  geom_point(
    aes(x = bill_depth_mm, y = flipper_length_mm, color = species)
  ) +
  geom_smooth(
    aes(x = bill_depth_mm, y = flipper_length_mm),
    method = "lm"
  )
```

report

Table 1. Regression output for predicting bill depth from flipper length.

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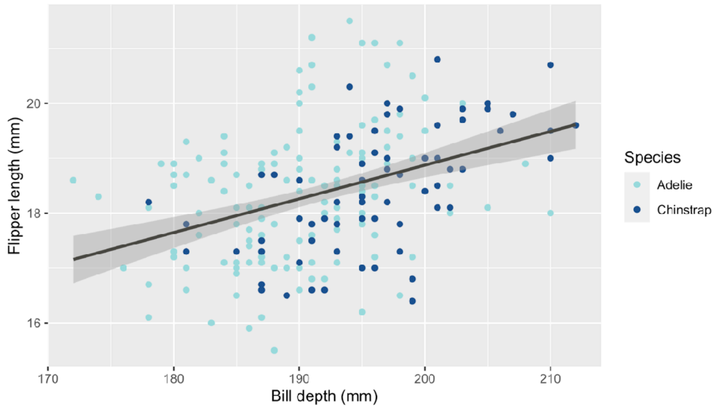

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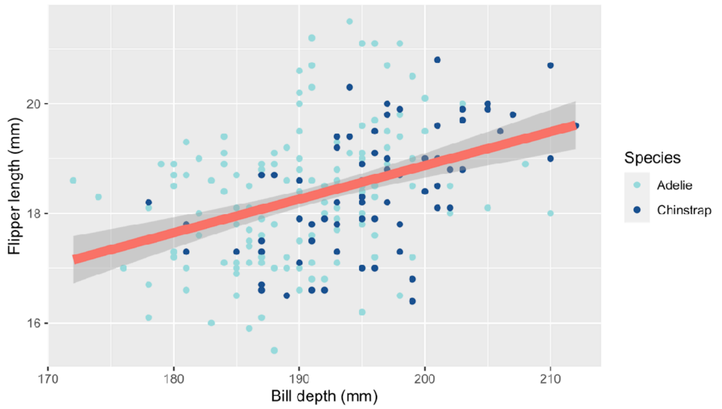
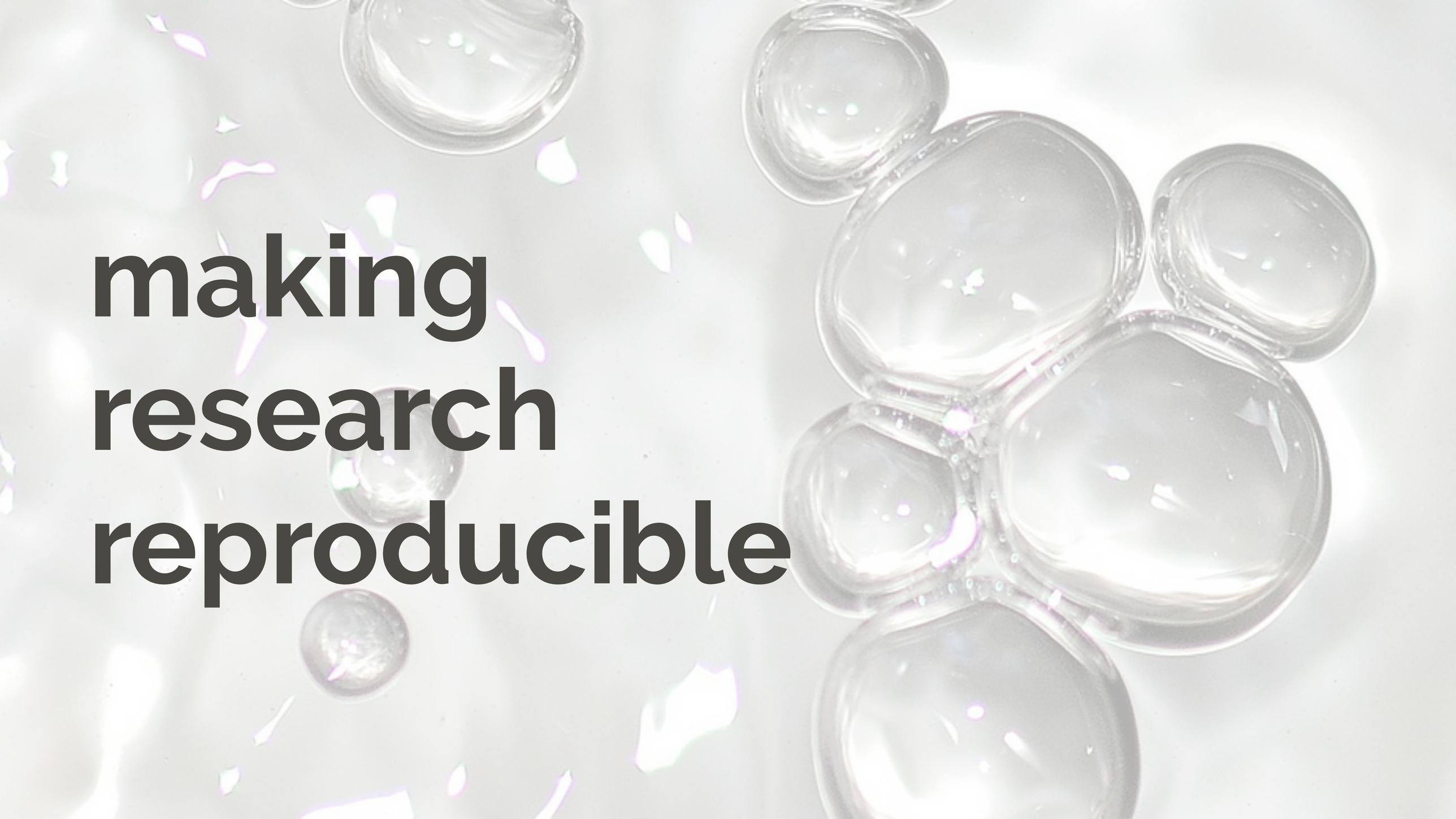



making
research
reproducible

make

raw data

code & documentation to reproduce the analysis

specifications of your computational environment

available and accessible

Peng, Roger. "The reproducibility crisis in science: A statistical counterattack." Significance 12.3 (2015): 30-32.
Gentleman, Robert, and Duncan Temple Lang. "Statistical analyses and reproducible research." Journal of Computational and Graphical Statistics 16.1 (2007): 1-23.

“The most important tool is the **mindset**, when starting, that the end product will be reproducible.”

– Keith Baggerly

nobody,
not even yourself,
can recreate any part
of your analysis

push button
reproducibility
in published work

“There’s **no one-size-fits-all solution** for computational reproducibility.”

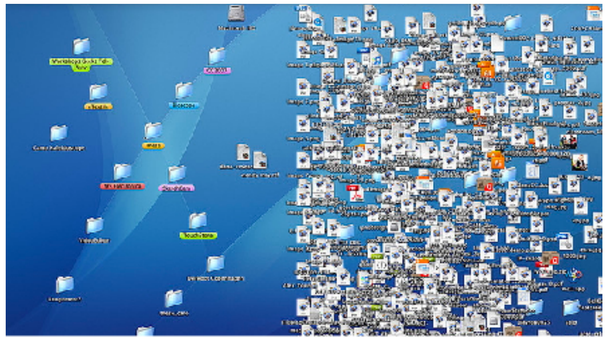
Perkel, Jeffrey M. "A toolkit for data transparency takes shape." Nature 560 (2018): 513-515.

8 principles

but the following might help…

organize your project

level of organization



simpler analysis

- raw-data
- processed-data
- manuscript
  - manuscript.Rmd

more complex analysis

- raw-data
- processed-data
- scripts
- figures
- manuscript
  - manuscript.Rmd

stick with the conventions of your peers

write READMEs liberally

raw-data

├ README.md

├ airlines.csv

├ airports.csv

├ flights.csv

├ planes.csv

├ weather.csv

processed-data

scripts

figures

manuscript

README

This folder contains the raw data
for the project.
All datasets were downloaded from
openflights.org/data.html
on 2019-04-01.

- airlines: Airline names
- airports: Airports metadata
- flights: Flight data
- planes: Plane metadata
- weather: Hourly weather data

keep data tidy & machine readable

Student	Exam Grade		
Name	1	2	Major
Barney Donaldson	89	76	Data Science, Public Policy
Clay Whelan	67	83	Public Policy
Simran Bass	82	90	Statistics
Chante Munro	45	72	Political Science, Statistics
Gabrielle Cherry	32	79	.
Kush Piper	98	sick	Statistics
Faizan Ratliff	82	75	Data Science
Torin Ruiz	70	80	Sociology, Statistics
Reiss Richardson	missed exam	34	Neuroscience
Ajwa Cochran	50	65	Data Science

record code + document non-code steps + write tests

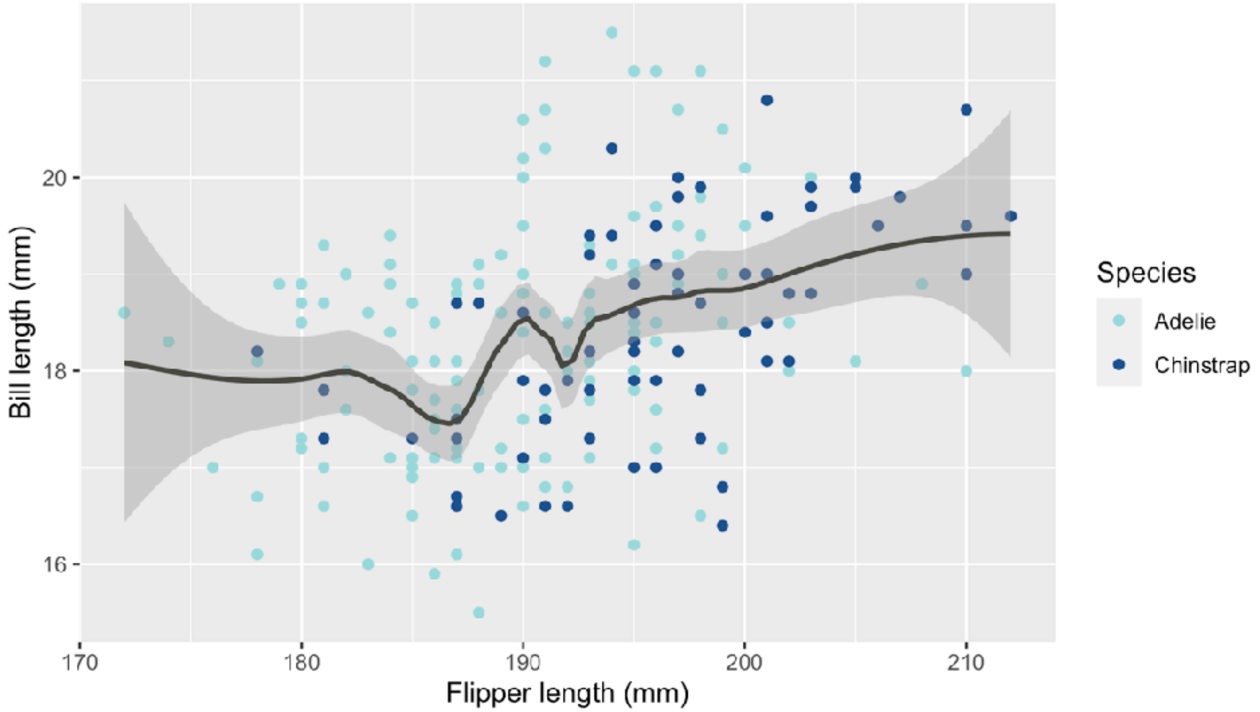
name	exam_1	exam_2	first_major	second_major	participation
Barney Donaldson	89	76	Data Science	Public Policy	ok
Clay Whelan	67	83	Public Policy	NA	ok
Simran Bass	82	90	Statistics	NA	ok
Chante Munro	45	72	Political Science	Statistics	Low
Gabrielle Cherry	32	79	NA	NA	ok
Kush Piper	98	NA	Statistics	NA	ok
Faizan Ratliff	82	75	Data Science	NA	ok
Torin Ruiz	70	80	Sociology	Statistics	ok
Reiss Richardson	NA	34	Neuroscience	NA	low
Ajwa Cochran	50	65	Data Science	NA	low

Low participation

Broman, Karl W., and Kara H. Woo. "Data organization in spreadsheets." The American Statistician 72.1 (2018): 2-10.

comment your code

```r
# use loess smoothing
ggplot(penguins_nongentoo) +
  geom_point(
    aes(x = flipper_length_mm, y = bill_depth_mm, color = species)
  ) +
  geom_smooth(
    aes(x = flipper_length_mm, y = bill_depth_mm),
    method = "loess", span = 0.375
  )
```



use literate programming

tab1-fig2.Rmd

Knit | Run

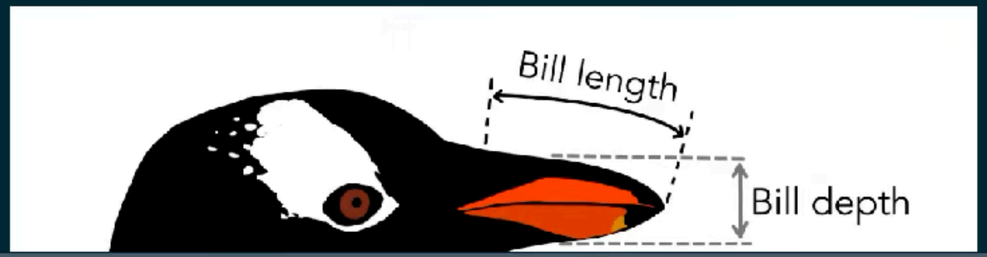
Normal | Format | Insert | Table

```yaml
---
title: "Table 1 matches Figure 2!"
author: "Mine Çetinkaya-Rundel"
date: "`r Sys.Date()`"
output:
  bookdown::html_document2:
    fig_caption: yes
bibliography: references.bib
---
```

```{r chunk-options, include=FALSE}
knitr::opts_chunk$set(echo = FALSE, message = FALSE)
```

```{r setup}
library(broom)          # for tidy model output
library(glue)           # for gluing strings to data
library(knitr)          # for kable
library(palmerpenguins) # for data
library(tidyverse)      # for data wrangling and visualisation
```

In this report we evaluate the relationship between relationship between bill depth and flipper length of penguins. The data come from @gorman2014.



Exploratory data analysis | R Markdown

improve-repro-workflow-reproducibilitea-2020 - RStudio

tab1-fig2.Rmd

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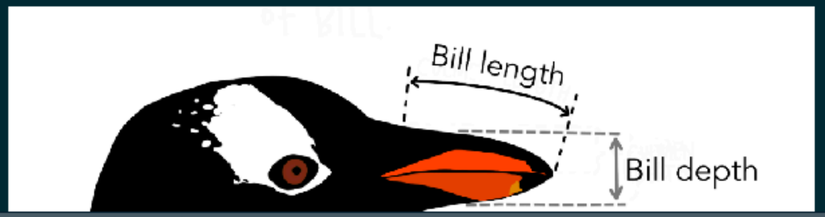
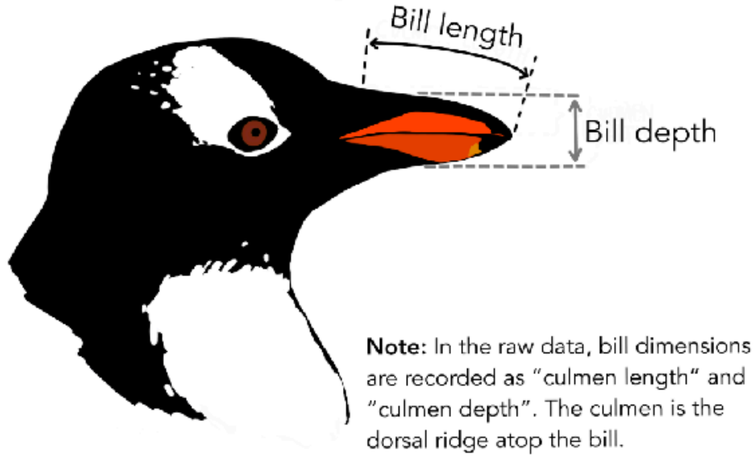


Table 1 matches Figure 2!

Mine Çetinkaya-Rundel

2020-11-10

In this report we evaluate the relationship between relationship between bill depth and flipper length of penguins. The data come from Gorman, Williams, and Fraser (2014).



Note: In the raw data, bill dimensions are recorded as "culmen length" and "culmen depth". The culmen is the dorsal ridge atop the bill.

The original dataset has 3 species (Adelie, Gentoo, and Chinstrap), but we will only work with Adelie and Chinstrap species.

1 Exploratory data analysis

Table 1.1 shows some summary statistics.

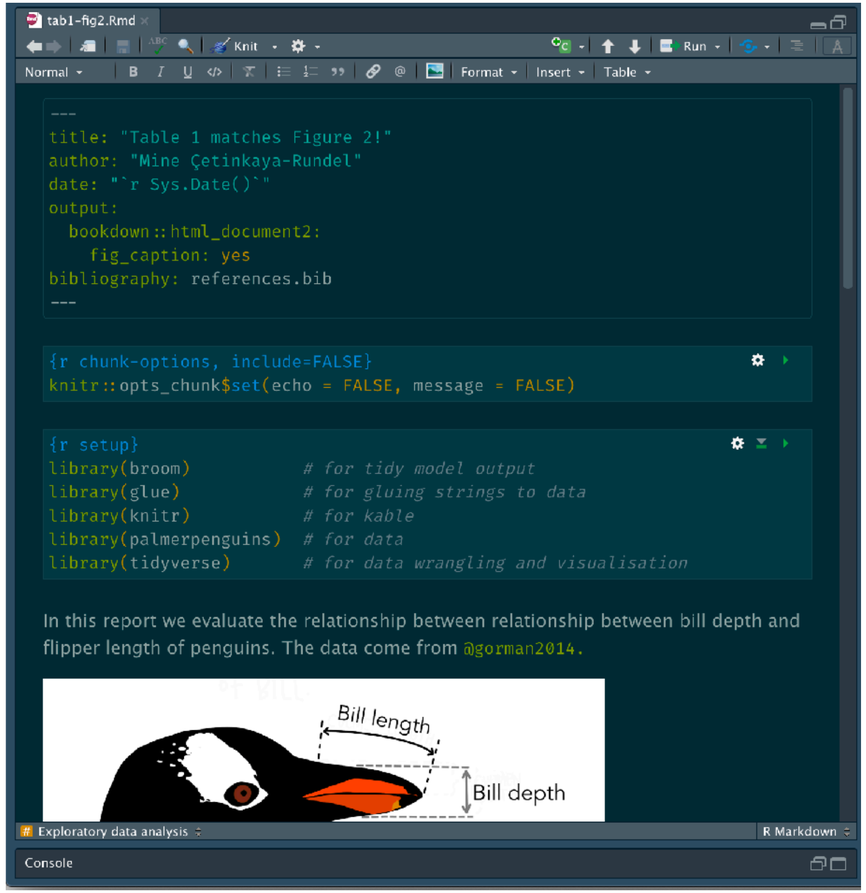
Table 1.1: Summary statistics

demo
rmarkdown

more resources...

- Learn more about **R Markdown**:
  - Documentation: rmarkdown.rstudio.com
  - Book: bookdown.org/yihui/rmarkdown
  - Book: bookdown.org/yihui/rmarkdown-cookbook
- Learn more about the **visual editor**:
  - Documentation: rstudio.github.io/visual-markdown-editing
  - Blog post: blog.rstudio.com/2020/09/30/rstudio-v1-4-preview-visual-markdown-editing
  - Blog post: blog.rstudio.com/2020/11/09/rstudio-1-4-preview-citations

use version control



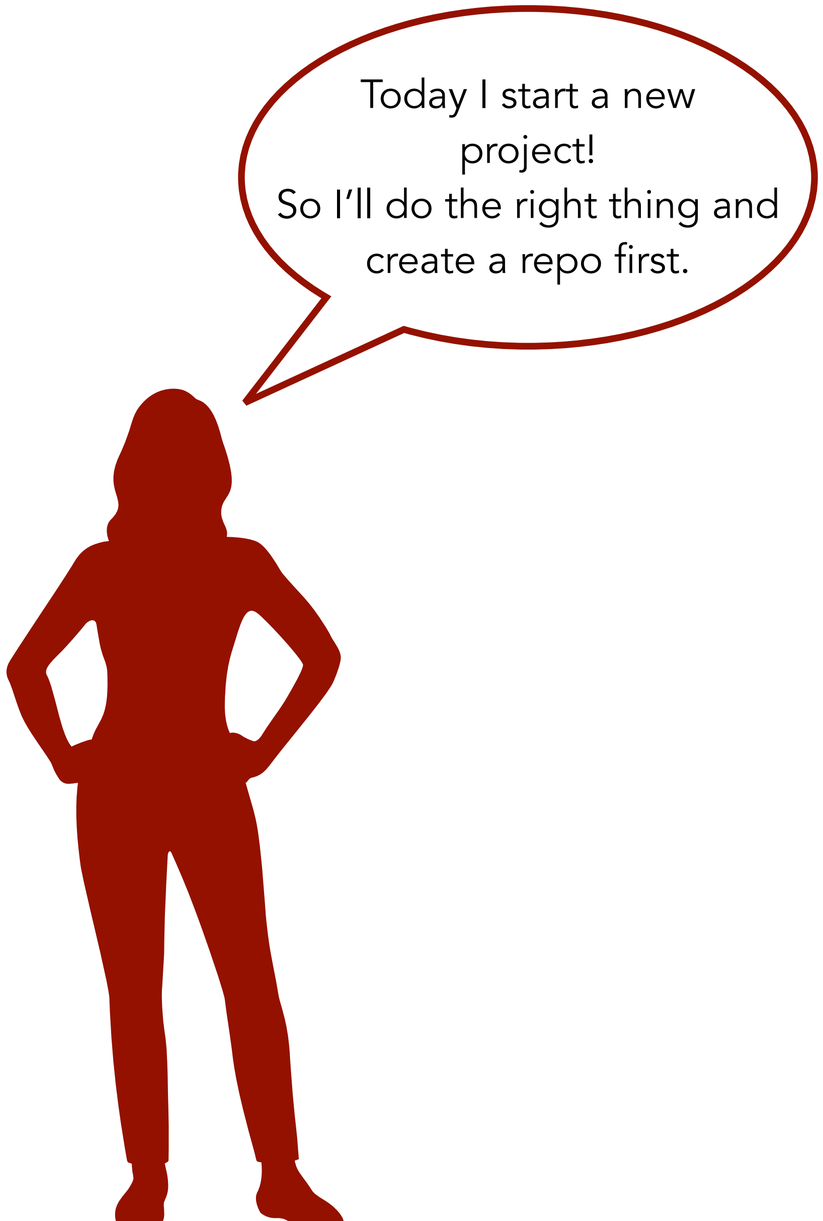
changes tracked by

hosted on

2 Git workflows

- GitHub first
- Local first

GitHub first

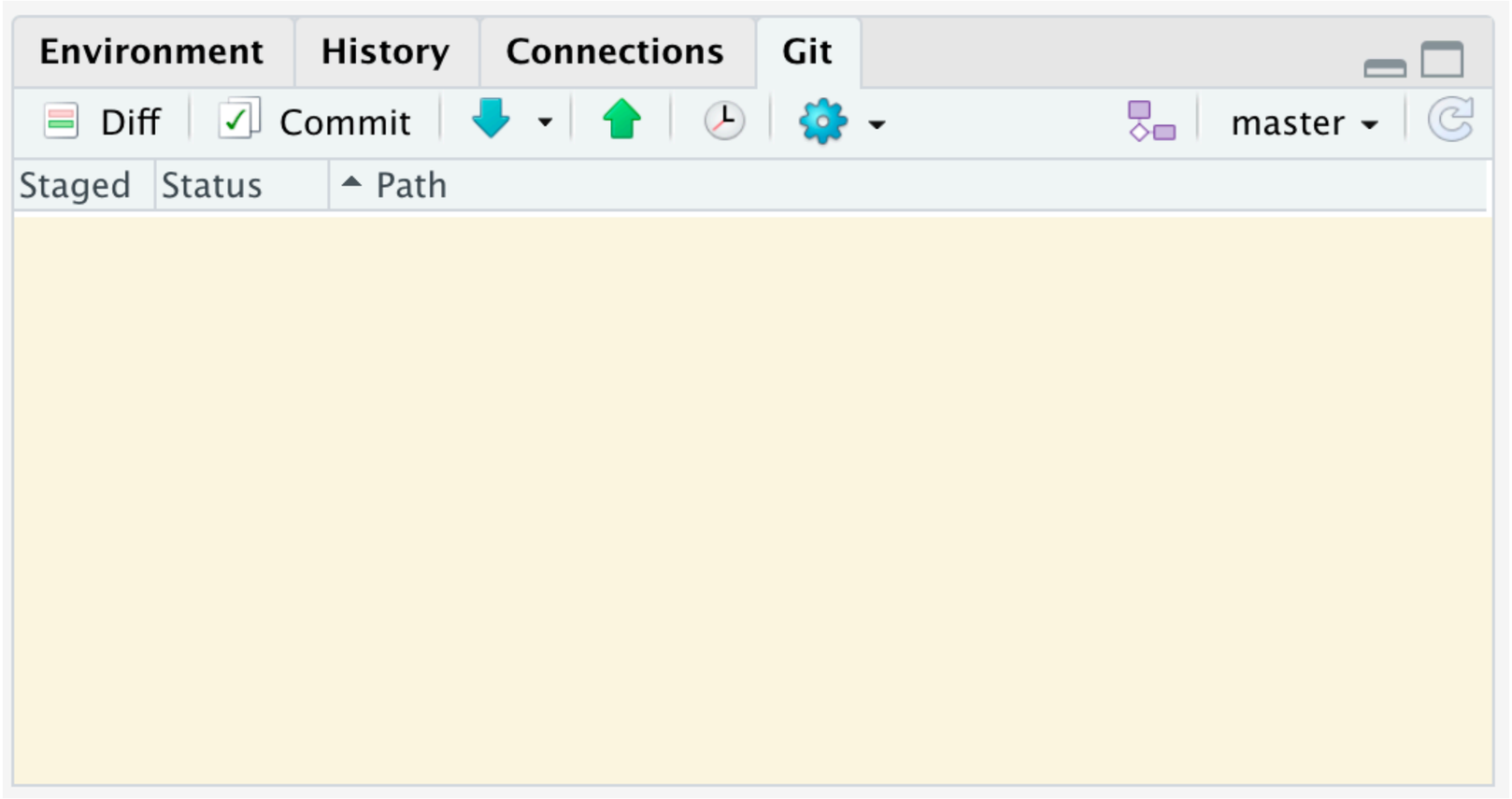


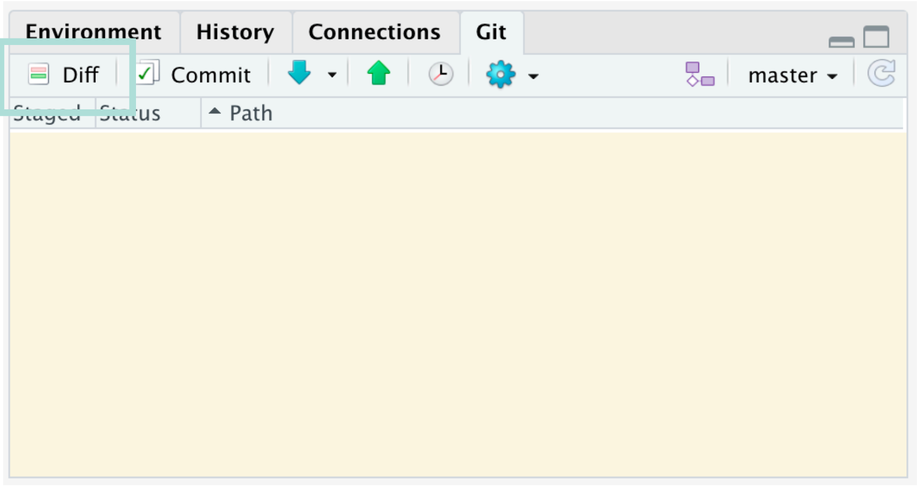
- Step 1: Create a new repo on GitHub
- Step 2: Copy the repo URL
- Step 3: Clone it using RStudio
- Step 4: Make changes locally
- Step 6: Commit and push to GitHub
- Step 7: Confirm your changes have propagated to GitHub

Local first

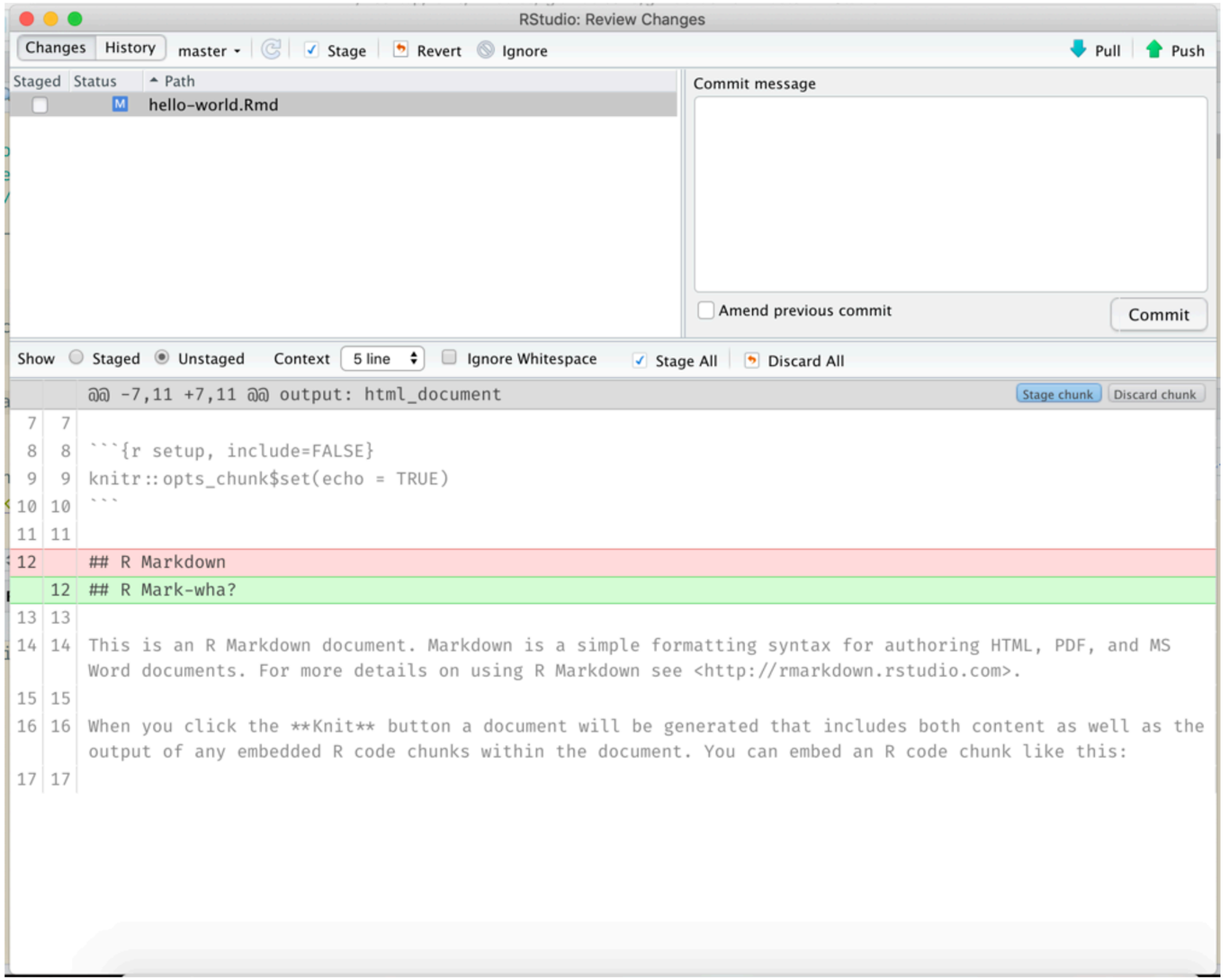
- Step 1: Create an RStudio Project from existing directory (if an `.Rproj` file doesn't already exist)
- Step 2: `usethis::use_git()` and follow instructions
- Step 3: `usethis::use_github()` and follow instructions

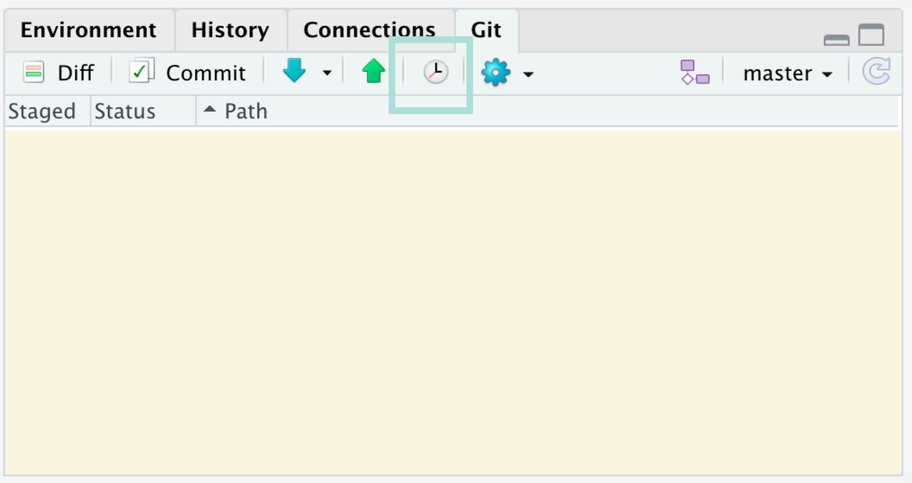
demo
git & github


Environment
History
Connections
Git
Diff
Commit
master
Staged
Status
Path

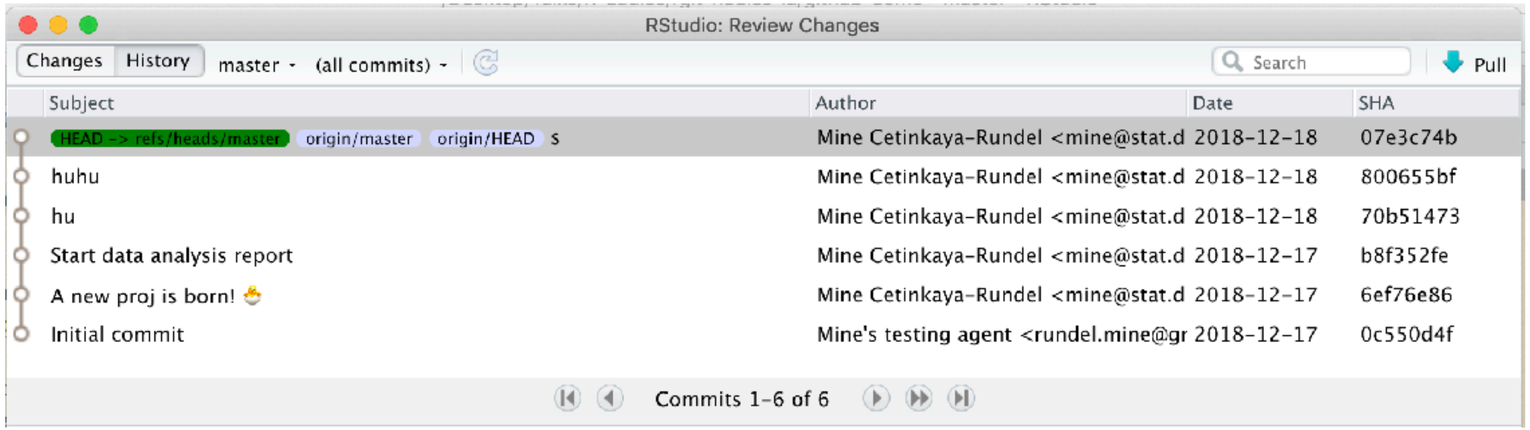


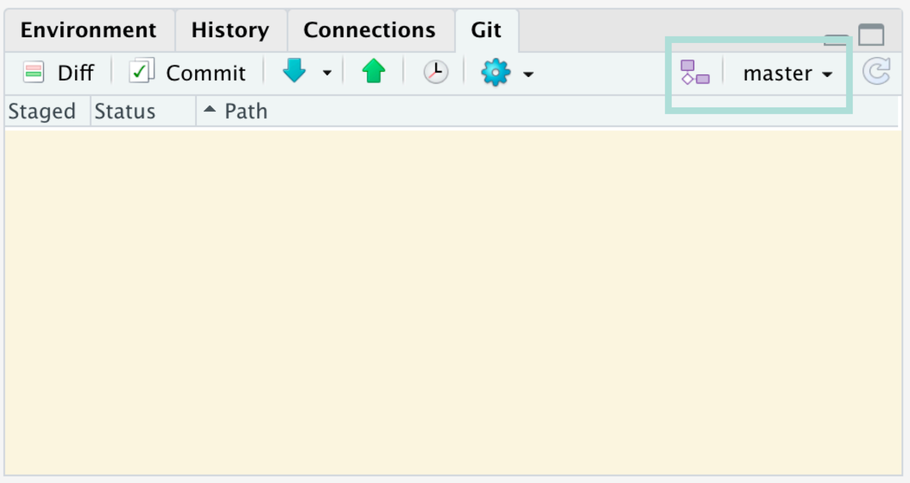
- View options
- Staging and committing all changes in a document at once
- Staging and committing various changes within a document one by one
- Commit messages
- Amending a previous commit
- Pushing



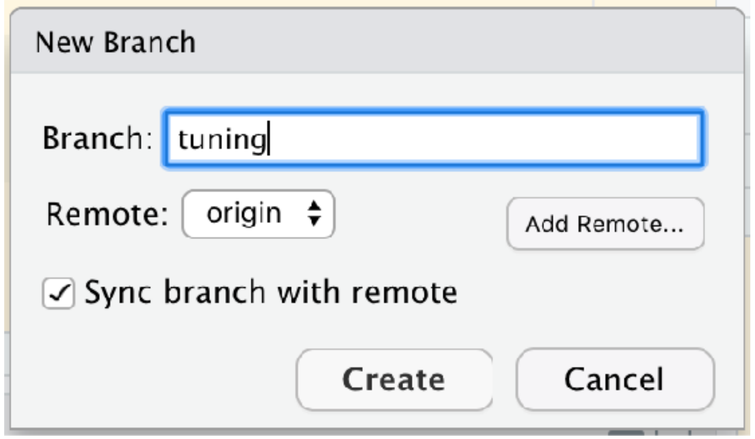


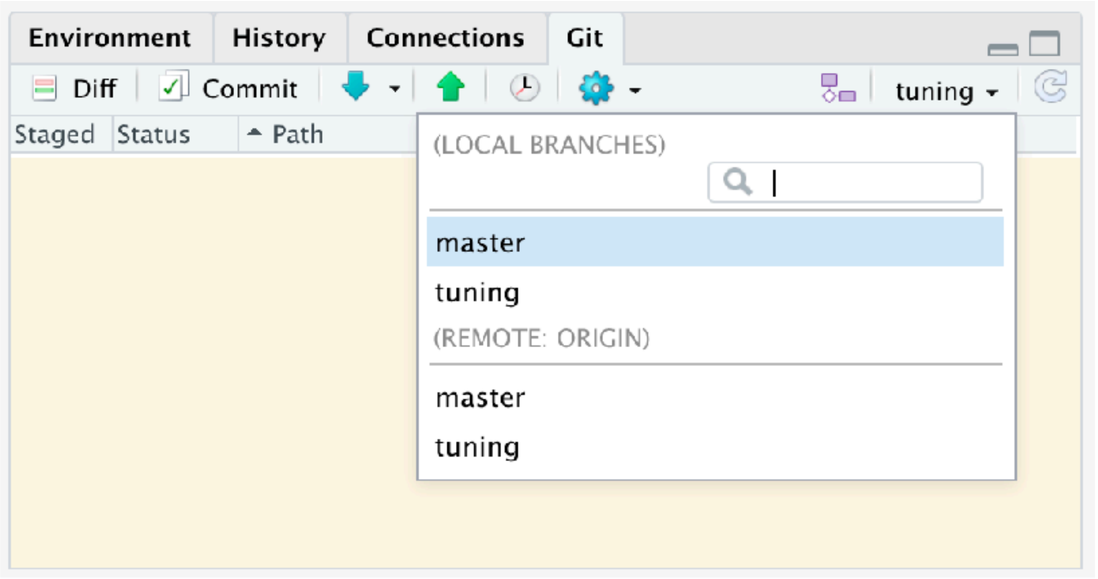
- History of commits
- What is HEAD?
- Filtering history of commits by File or Directory





- Branching
- Switching between branches





demo
pull requests

more resources...

- Learn more about using **Git and GitHub with R**:
  - Book: happygitwithr.com
- Learn more about **Git setup**:
  - Documentation: usethis.r-lib.org/articles/articles/usethis-setup.html

7

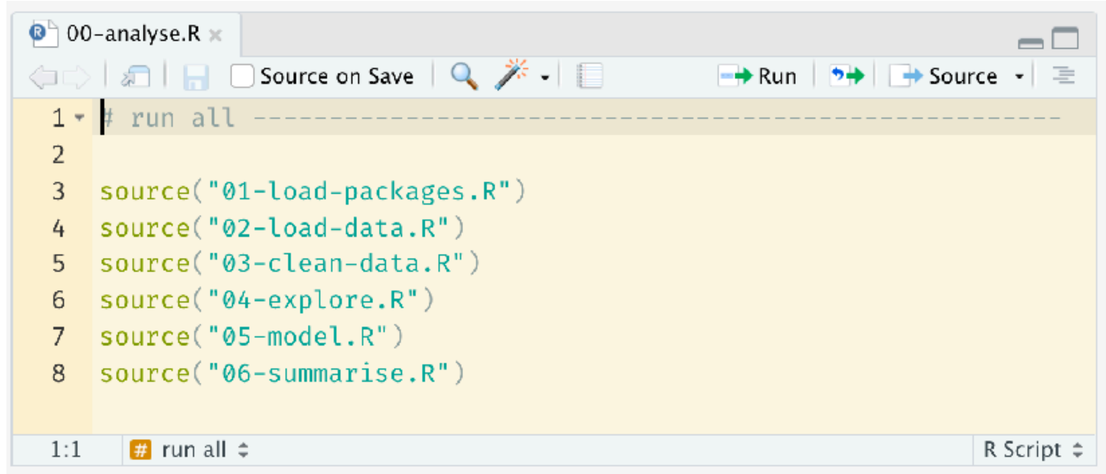
automate your process

raw-data

processed-data

scripts

- 00-analyse.R
- 01-load-packages.R
- 02-load-data.R
- 03-clean-data.R
- 04-explore.R
- 05-model.R
- 06-summarise.R



figures

manuscript

minimal make A minimal tutorial on make

I would argue that the most important tool for reproducible research is not Sweave or knitr but *GNU make*.

Consider, for example, all of the files associated with a manuscript. In the simplest case, I would have an R script for each figure plus a LaTeX file for the main text. And then a BibTeX file for the references.

Compiling the final PDF is a bit of work:

- Run each R script through R to produce the relevant figure.
- Run latex and then bibtex and then latex a couple of more times.

And the R scripts need to be run before latex is, and only if they've changed.

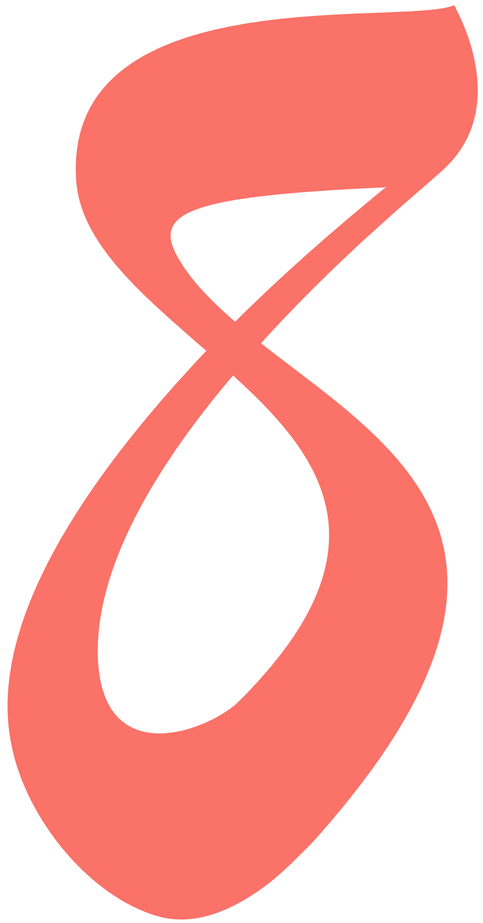
A simple example

GNU make makes this easy. In your directory for the manuscript, you create a text file called `Makefile` that looks something like the following (here using pdflatex).

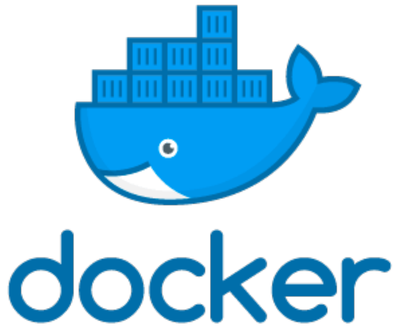
```
mypaper.pdf: mypaper.bib mypaper.tex Figs/fig1.pdf Figs/fig2.pdf
    pdflatex mypaper
    bibtex mypaper
    pdflatex mypaper
    pdflatex mypaper

Figs/fig1.pdf: R/fig1.R
    cd R;R CMD BATCH fig1.R

Figs/fig2.pdf: R/fig2.R
    cd R;R CMD BATCH fig2.R
```

Each batch of lines indicates a file to be created (the *target*), the files it depends on (the *prerequisites*), and then a set of commands needed to construct the target from the dependent files. Note that the lines with the commands *must* start with a **tab** character (**not spaces**).

Broman, Karl "Minimal Make", kbroman.org/minimal_make.



share computing environment


docker

binder

R Studio

1 **organize** your project

2 write **READMEs** liberally

3 keep data **tidy & machine readable**

4 **comment** your code

5 use **literate programming**

6 use **version control**

7 **automate** your process

8 share computing **environment**

Greg Wilson, Jennifer Bryan, Karen Cranston,
Justin Kitzes, Lex Nederbragt, Tracy K. Teal
“Good enough practices in scientific computing."
PLoS computational biology 13.6 (2017): e1005510.

PLOS | COMPUTATIONAL BIOLOGY

PERSPECTIVE

Good enough practices in scientific computing

Greg Wilson[1☯*], Jennifer Bryan[2☯], Karen Cranston[3☯], Justin Kitzes[4☯], Lex Nederbragt[5☯], Tracy K. Teal[6☯]

1 Software Carpentry Foundation, Austin, Texas, United States of America, 2 RStudio and Department of Statistics, University of British Columbia, Vancouver, British Columbia, Canada, 3 Department of Biology, Duke University, Durham, North Carolina, United States of America, 4 Energy and Resources Group, University of California, Berkeley, Berkeley, California, United States of America, 5 Centre for Ecological and Evolutionary Synthesis, University of Oslo, Oslo, Norway, 6 Data Carpentry, Davis, California, United States of America

☯ These authors contributed equally to this work.
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Author summary

Computers are now essential in all branches of science, but most researchers are never taught the equivalent of basic lab skills for research computing. As a result, data can get lost, analyses can take much longer than necessary, and researchers are limited in how effectively they can work with software and data. Computing workflows need to follow the same practices as lab projects and notebooks, with organized data, documented steps, and the project structured for reproducibility, but researchers new to computing often don't know where to start. This paper presents a set of good computing practices that every researcher can adopt, regardless of their current level of computational skill. These practices, which encompass data management, programming, collaborating with colleagues, organizing projects, tracking work, and writing manuscripts, are drawn from a wide variety of published sources from our daily lives and from our work with volunteer organizations that have delivered workshops to over 11,000 people since 2010.

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Overview

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 6 years, and from a variety of other guides. Our recommendations are aimed specifically at people who are new to research computing.

Introduction

Three years ago, a group of researchers involved in Software Carpentry and Data Carpentry wrote a paper called "Best Practices for Scientific Computing" [1]. That paper provided recommendations for people who were already doing significant amounts of computation in their research. However, as computing has become an essential part of science for all researchers, there is a larger group of people new to scientific computing, and the question then becomes, "where to start?"

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