Reproducibility and Replicability in Geospatial Data Science

Source | Slides

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Outline

- What is reproducibility and replicability?
- Why do it?
- How do we do it?
- Questions

Learning objectives

- Understand what reproducibility and replicability are
- Know why they are useful
- Be aware of some of the tools that you can use

What is Reproducibility?

- Ability for other people *with a similar level of skill* to reproduce your work.
- Other people
  - colleagues in company,
  - group members in a project,
  - yourself in a year when you want to use your project work for something else,
- Fundamental part of research
- Also is best practice - which will allow others to reproduce your work.

Why do it?

Why do it?

- Fisher also discovered a major error in one piece of software which gave completely incorrect results.
- Highlights the need for:
  - Standards & testing to make sure this doesn’t happen
  - Algorithms used to be published so people can see what is happening
  - Issues when only binary files are available, and not the source code

Fisher, P. F. (1993). Algorithm and implementation uncertainty in viewshed analysis. International Journal of Geographical Information Systems, 7(4), 331–347. https://doi.org/10.1080/02693799308901965

Why do it?

- Riggs & Dean, Colorado State (2007) did a similar investigation on viewshed analysis
- Things have improved since 1993, but there are still differences in different software.

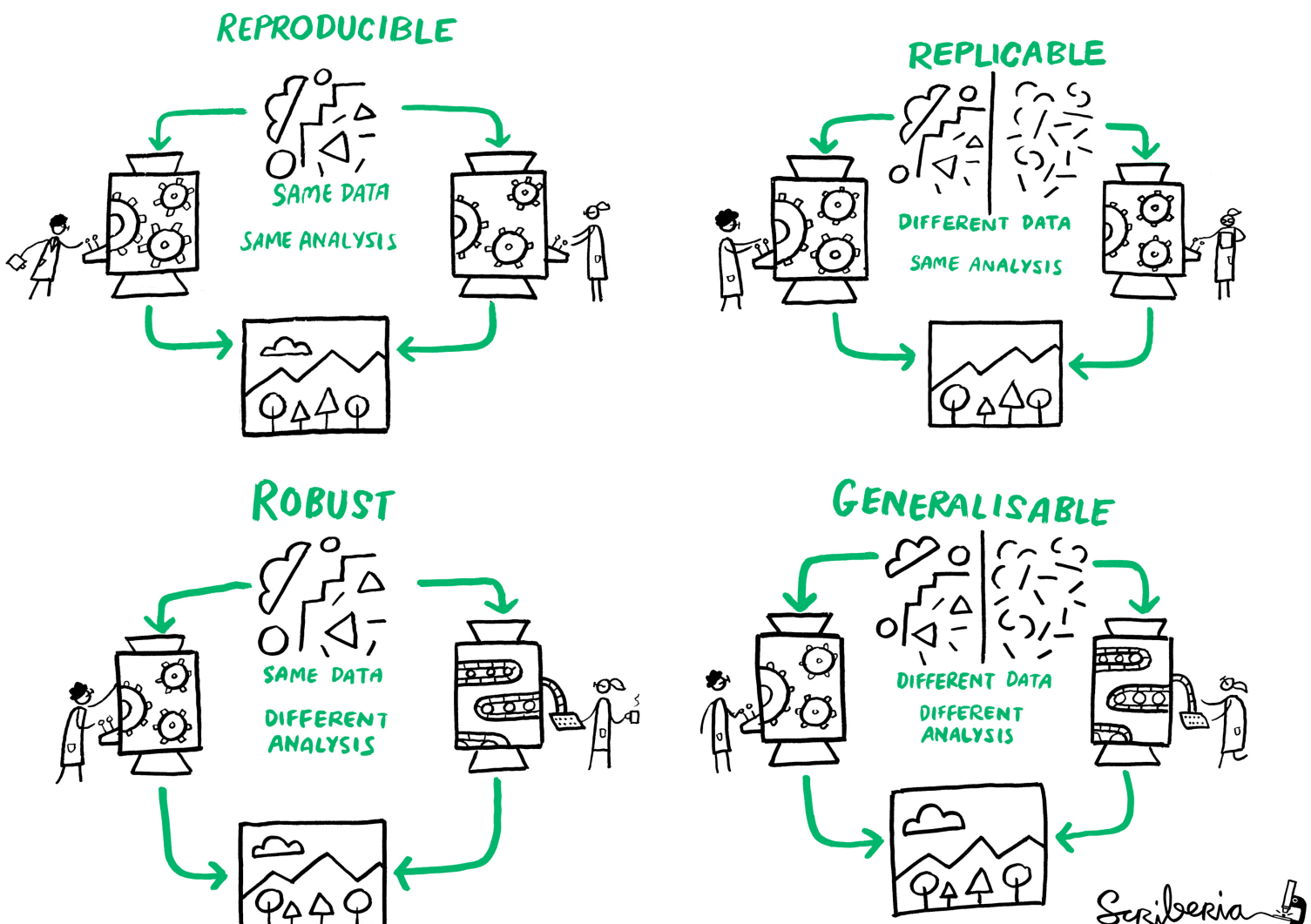
Riggs, P.D. and Dean, D.J. (2007), An Investigation into the Causes of Errors and Inconsistencies in Predicted Viewsheds. Transactions in GIS, 11: 175-196. https://doi.org/10.1111/j.1467-9671.2007.01040.x

Why do it?

- Standards & testing to make sure this doesn’t happen
  - OGC
  - But we probably do need more testing
- Algorithms used to be published so people can see what is happening
  - Publish algorithms in journals
  - Even more important with machine learning - transparency is important
- Issues when only binary files are available, and not the source code
  - Growth in open source software - so you can see (and unpick) what is happening

What is Reproducibility & Replicability?

"[…] when the same analysis steps performed on the same dataset […] produce the same answer." (Turing Way)



How do we make our research reproducible? - FAIR:

Findable

- Descriptive metadata and persistent identifier (DOI)

Accessible

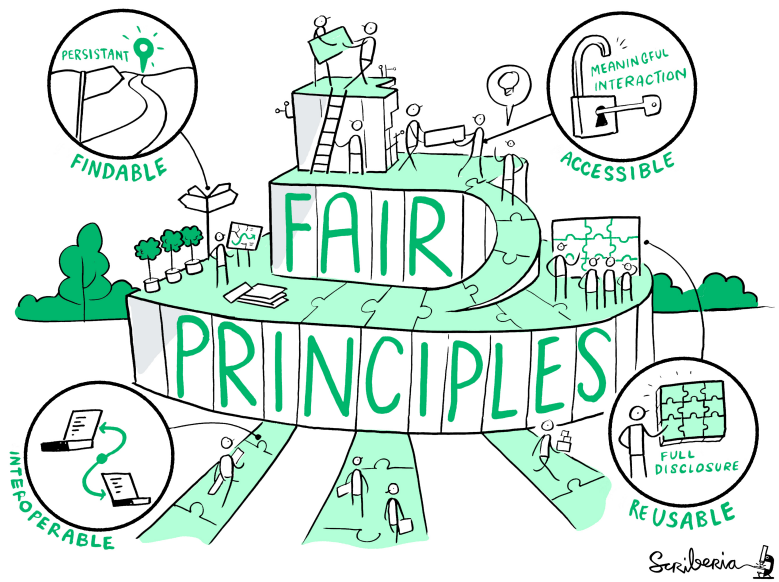
- Code/data could be openly available OR access via authentication and if needed

Interoperable

- Data needs to be integrated with other data and interoperate with applications or workflows (Open formats)

Reusable

- Documentation and license (Open license - e.g. Creative Commons)



Research

- Some journals & conferences ask you to submit code along with your paper
- AGILE - https://reproducible-agile.github.io/
- Anyone (with a similar level of skills) should be able to do reproduce your research and benefit from it.
- One reason for open source tools.
- If you do analysis in ArcGIS Pro, you need ArcGIS Pro to recreate that analysis.
- If you don’t have ArcGIS Pro, what do you do?

It’s not just research

Other work can be useful if it can be reproducible:

- quarterly or annual reports
- repeating work over 200 areas, 50 business units, 365 days,
- coming back to your work 6 months later - “please can you update this with this new data?”

How do we do this?

- Documenting what you did is standard - Methods
- If you can do what you did in a script, then you can also share this
- ArcGIS Pro / QGIS
  - graphical interface, click buttons, etc
- R / Python
  - write out the script

Setup - “environments”

- To replicate a piece of work, you need to know what software they used
- What version
- What libraries / packages
- What version of libraries or packages
- Can record this in text
  - “R 4.3.2, RStudio 2013.12.0, sf library 1.0-16” etc.
- Or in code
  - renv library https://rstudio.github.io/renv/articles/renv.html

Setup - Docker

- Docker gives you a big box to put all this in
- Then you say - I used this Docker environment
- AGILE has a very nice overview

Version Control

- If your project evolves over time, you may need to use version control
- Provides a snapshot of your code at a specific point in time - I used this version of my code
- Version Control (Git) allows you to do this, while still developing your code, and to see the differences (diff).
- GitHub allows you to collaborate with other people on this.

Writing, Presentations

Also works for writing and presentations as well.

- Markdown allows you to write plan text with tags - stars, hashes, etc.
- Can also do analysis in this
- LaTeX is a developved version of Markdown (or Markdown is a simple version of LaTeX)
- RMarkdown allows you to run R code
- Quarto allows you to run other code (Python, R, etc.)
- This presentation is written in Quarto.

Markdown example

Syntax	Output
`*Italic*`	*Italic*
`**Bold**`	**Bold**
`~~strikethrough~~`	~~strikethrough~~
`[Link](url)`	Link
`i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V(\mathbf{r},t) \Psi`	$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V(\mathbf{r},t) \Psi$

Markdown example

- Markdown allows you to write plan text with tags - stars, hashes, etc.

```
---
title: "My document"
format: html
---
. . .
# Introduction

*Hello Quarto!*

```{r}
summary(cars)
```
```

Rendered Output

My document

Introduction

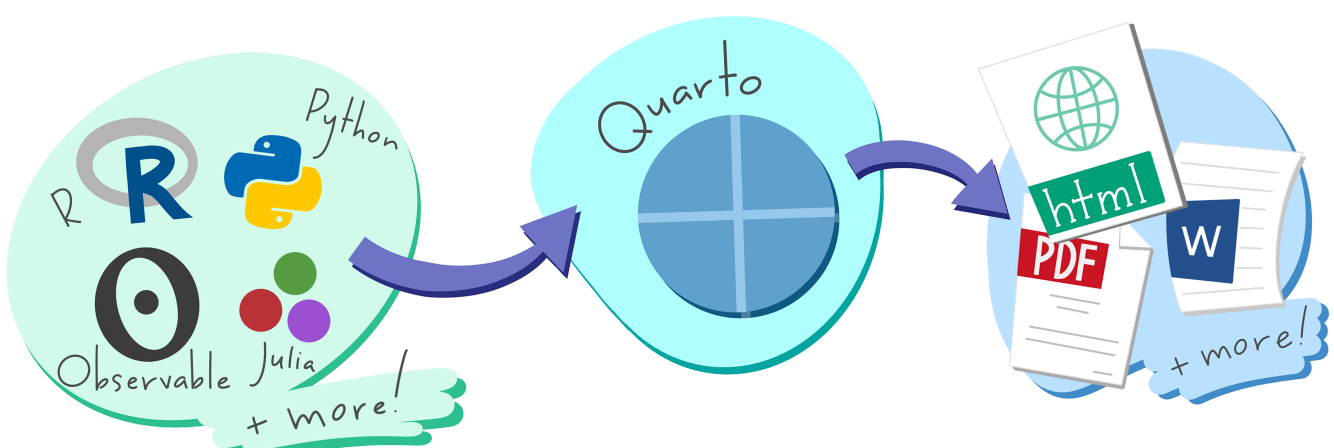
Hello Quarto!

```
summary(cars)
```

```
     speed           dist       
 Min.   : 4.0   Min.   :  2.00  
 1st Qu.:12.0   1st Qu.: 26.00  
 Median :15.0   Median : 36.00  
 Mean   :15.4   Mean   : 42.98  
 3rd Qu.:19.0   3rd Qu.: 56.00  
 Max.   :25.0   Max.   :120.00  
```

About Quarto

- Quarto is a new, open-source, scientific and technical publishing system
- Combine text and code to produce formatted documents
- Publish reproducible and dynamic presentations, dashboards, websites, blogs, and books in HTML, PDF, MS Word, etc.
- Multi-language support for R, Python, Julia, and more
- Quarto extends RMarkdown and shares similarities with Juypter Notebooks.



Artwork from “Hello, Quarto” keynote by Julia Lowndes and Mine Çetinkaya-Rundel, presented at RStudio Conference 2022. Illustrated by Allison Horst.

Formats

- **Documents**: HTML, PDF, MS Word, Open Office, ePub
- **Presentations**: Revealjs, PowerPoint,
- **Wikis**: MediaWiki, JiraWiki, …
- Many templates exist for academic documents: quarto-journals
- And much more: Jupyter, RTF, InDesign, …

Short Paper

Alice Anonymous[a,1,*], Bob Security[b,2], Cat Memes[b,3], Derek Zoolander

[a]*Some Institute of Technology, Street Address, City, Postal Code,*
[b]*Another University, Street Address, City, Postal Code,*

Abstract

This is the abstract.

It consists of two paragraphs.

Keywords: keyword1, keyword2

Please make sure that your manuscript follows the guidelines in the Guide for Authors of the relevant journal. It is not necessary to typeset your manuscript in exactly the same way as an article, unless you are submitting to a camera-ready copy (CRC) journal.

For detailed instructions regarding the elsevier article class, see https://www.elsevier.com/authors/policies-and-guidelines/latex-instructions

1. Bibliography styles

Here are two sample references: Feynman and Vernon Jr. [1963; 1].

By default, natbib will be used with the `authoryear` style, set in `classoption` variable in YAML. You can sets extra options with `natbiboptions` variable in YAML header. Example

`natbiboptions: longnamesfirst,angle,semicolon`

There are various more specific bibliography styles available at https://support.stmdocs.in/wiki/index.php?title=Model-wise_bibliographic_style_files. To use one of these, add it in the header using, for example, `biblio-style: model1-num-names`.

1.1. Using CSL

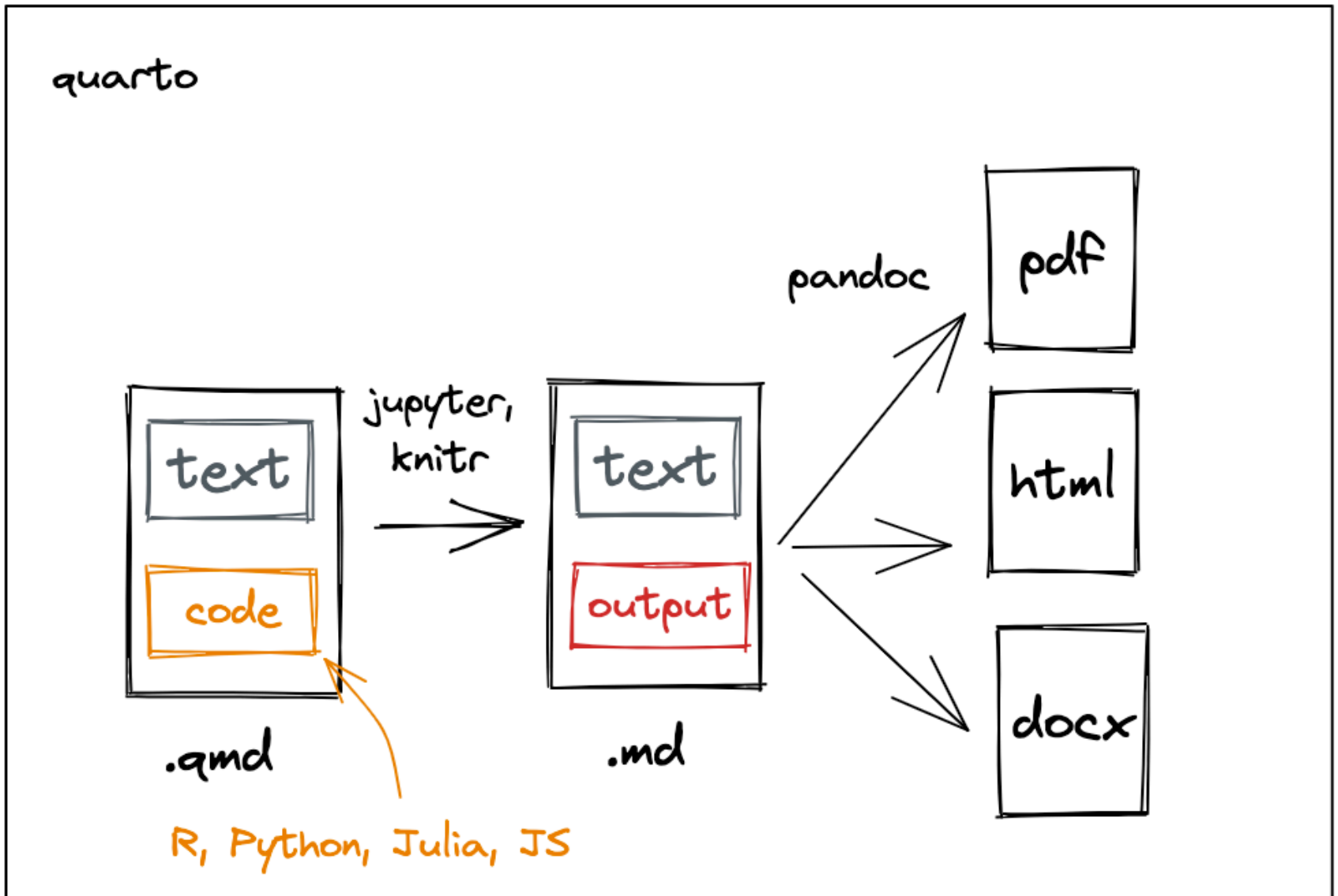
If `cite-method` is set to `citeproc` in `elsevier_article()`, then pandoc is used for citations instead of `natbib`. In this case, the `csl` option is used to format the references. By default, this template will provide an appropriate style, but alternative `csl` files are available from https://www.zotero.org/styles?q=elsevier. These can be downloaded and stored locally, or the url can be used as in the example header.

*Corresponding author
Email addresses: `alice@example.com` (Alice Anonymous), `bob@example.com` (Bob Security), `cat@example.com` (Cat Memes), `derek@example.com` (Derek Zoolander)
[1]This is the first author footnote.
[2]Another author footnote, this is a very long footnote and it should be a really long footnote. But this footnote is not yet sufficiently long enough to make two lines of footnote text.
[3]Yet another author footnote.

Preprint submitted to Elsevier *July 20, 2022*

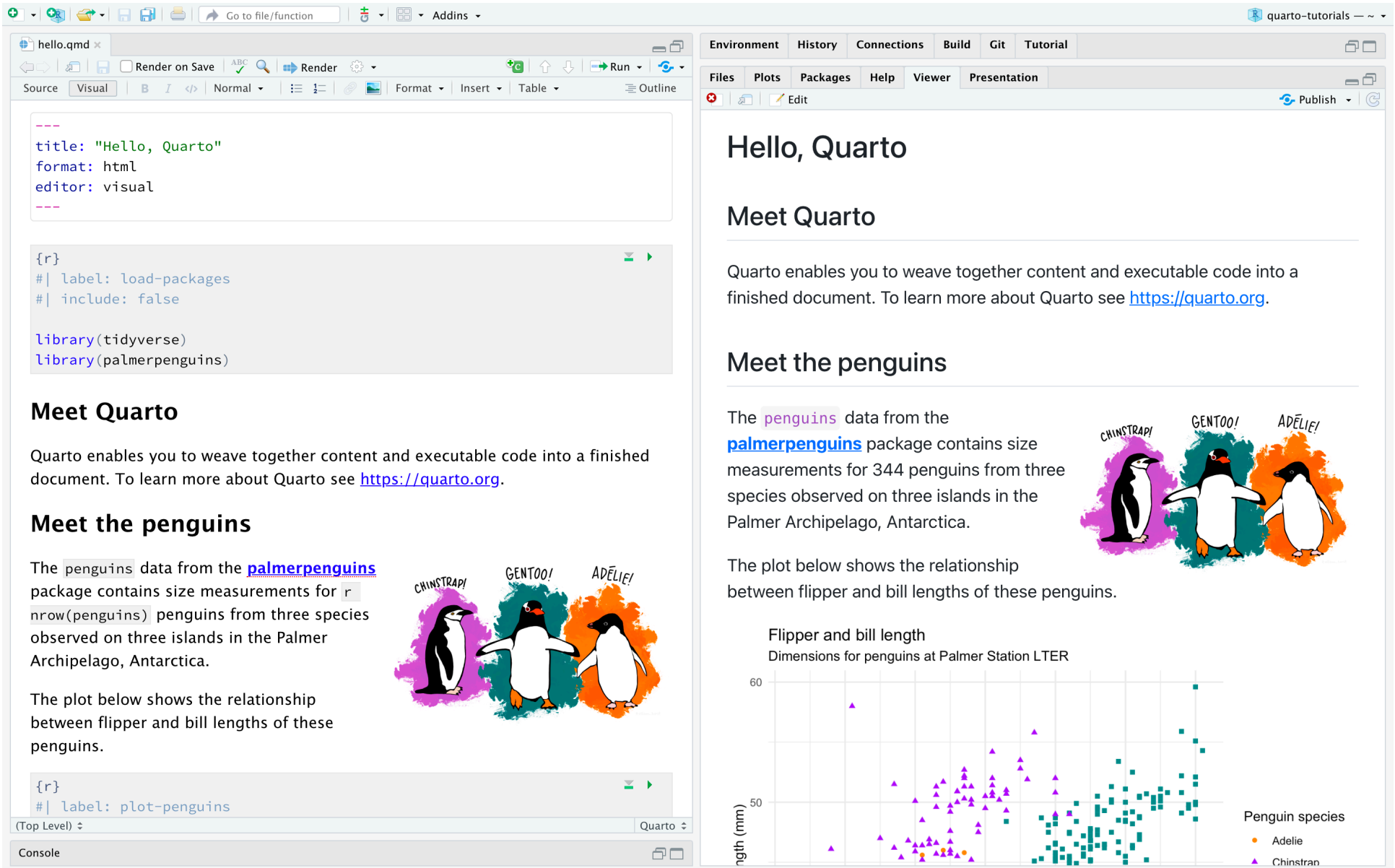
taken from quarto-journals

How does Quarto work?



taken from What is Quarto - A Quick Intro FAQ

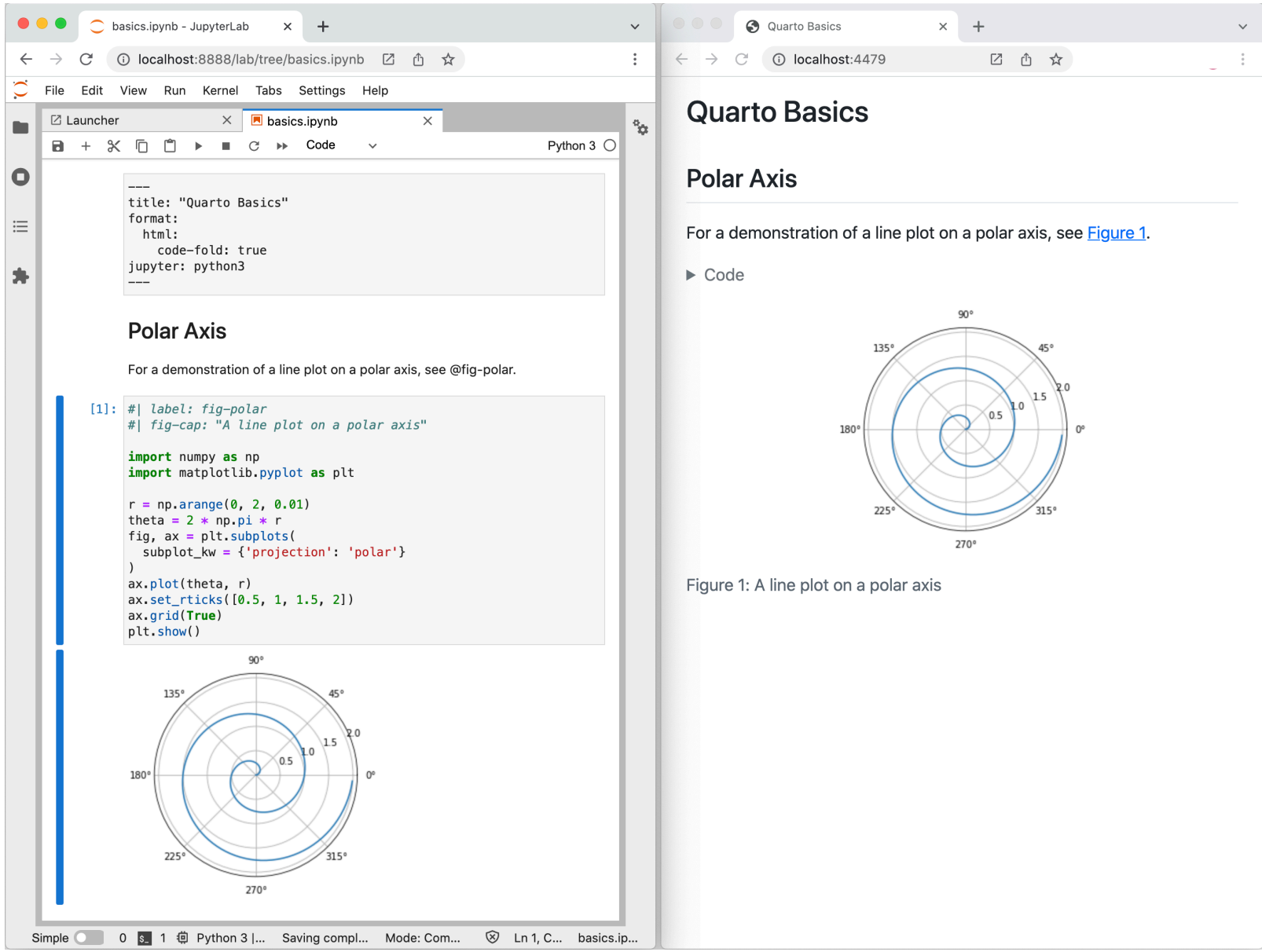
.qmd


Go to file/function
Addins
quarto-tutorials — ~
hello.qmd
Render on Save
Render
Run
Source
Visual
Normal
Format
Insert
Table
Outline
---
title: "Hello, Quarto"
format: html
editor: visual

{r}
#| label: load-packages
#| include: false
library(tidyverse)
library(palmerpenguins)
Meet Quarto
Quarto enables you to weave together content and executable code into a finished document. To learn more about Quarto see https://quarto.org.
Meet the penguins
The penguins data from the palmerpenguins package contains size measurements for r nrow(penguins) penguins from three species observed on three islands in the Palmer Archipelago, Antarctica.
The plot below shows the relationship between flipper and bill lengths of these penguins.
CHINSTRAP!
GENTOO!
ADĒLIE!
{r}
#| label: plot-penguins
(Top Level)
Quarto
Console
Environment
History
Connections
Build
Git
Tutorial
Files
Plots
Packages
Help
Viewer
Presentation
Edit
Publish
Hello, Quarto
Meet Quarto
Quarto enables you to weave together content and executable code into a finished document. To learn more about Quarto see https://quarto.org.
Meet the penguins
The penguins data from the palmerpenguins package contains size measurements for 344 penguins from three species observed on three islands in the Palmer Archipelago, Antarctica.
The plot below shows the relationship between flipper and bill lengths of these penguins.
Flipper and bill length
Dimensions for penguins at Palmer Station LTER
60
50
Penguin species
Adelie
Chinstrap

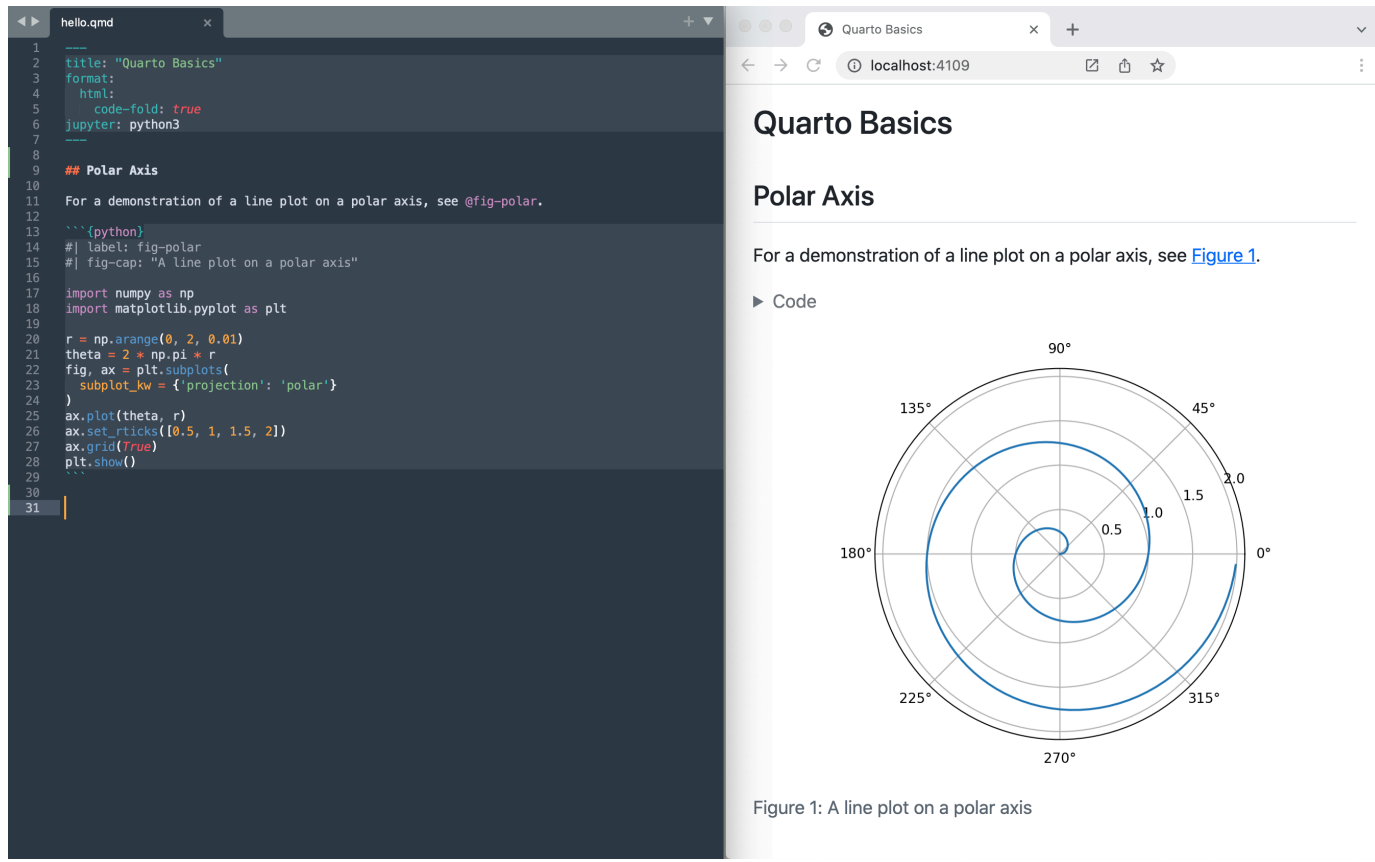
qmd file

.ipynb



jupyter notebook

Tools




```
$ quarto render hello.qmd --to doxc
```

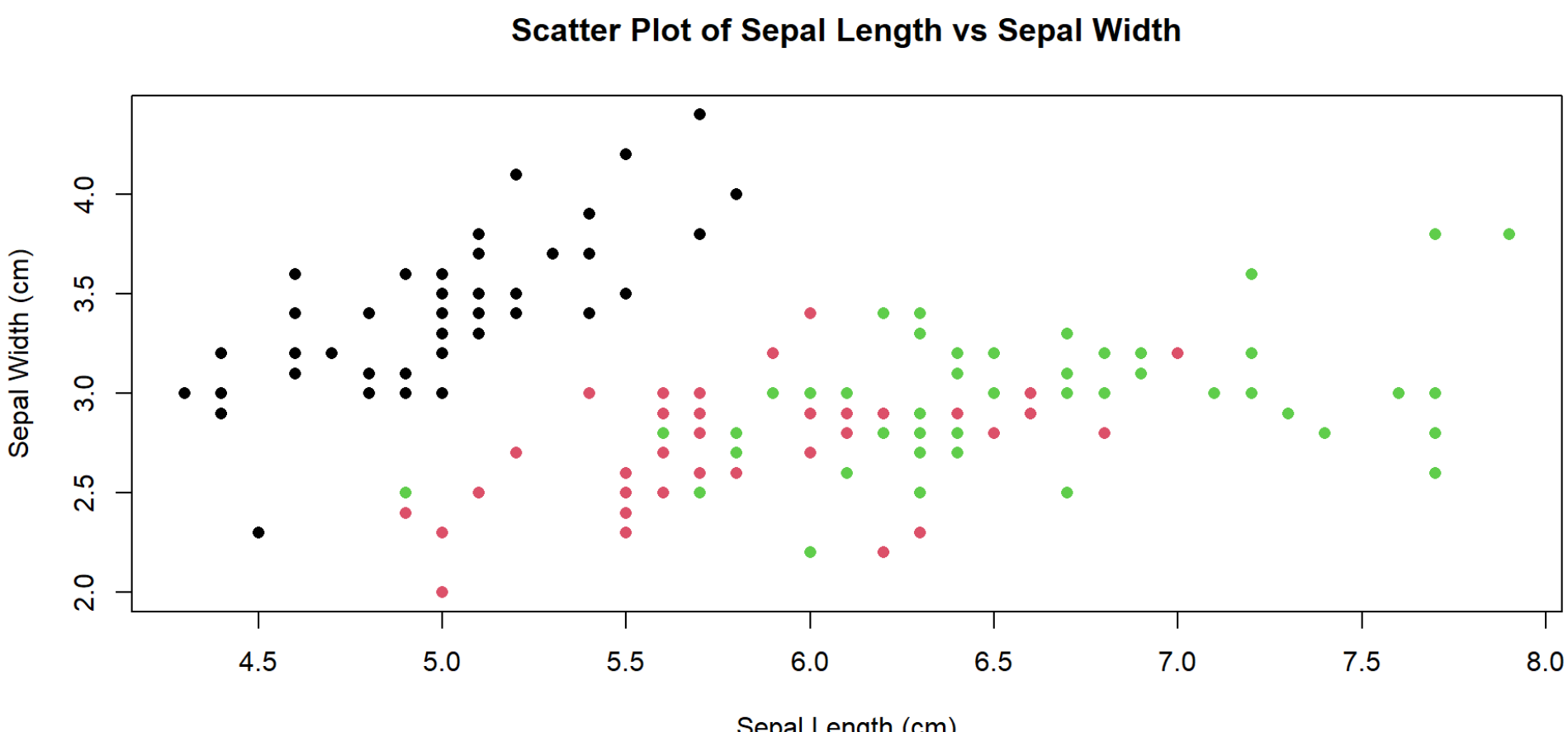
Markdown text

Syntax	Output
`*Italic*`	*Italic*
`**Bold**`	**Bold**
`~~strikethrough~~`	~~strikethrough~~
`[Link](url)`	Link
`i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V(\mathbf{r},t) \Psi`	$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V(\mathbf{r},t) \Psi$

Code chunks

```r
data(iris)

plot(iris$Sepal.Length, iris$Sepal.Width,
     main = "Scatter Plot of Sepal Length vs Sepal Width",
     xlab = "Sepal Length (cm)",
     ylab = "Sepal Width (cm)",
     pch = 16, col = iris$Species)
```



Code chunks

```{r}
#| label: "iris-plot"
#| echo: TRUE
#| fig-format: svg
#| cache: TRUEs

data(iris)

plot(iris$Sepal.Length, iris$Sepal.Width,
     main = "Scatter Plot of Sepal Length vs Sepal Width",
     xlab = "Sepal Length (cm)",
     ylab = "Sepal Width (cm)",
     pch = 16, col = iris$Species)

```

defaults to *knitr* engine (you can override the engine with `engine: jupyter`)

```{python}
#| label: fig-polar
#| fig-cap: "A line plot on a polar axis"

import numpy as np
import matplotlib.pyplot as plt

r = np.arange(0, 2, 0.01)
theta = 2 * np.pi * r
fig, ax = plt.subplots(
  subplot_kw = {'projection': 'polar'}
)
ax.plot(theta, r)
ax.set_rticks([0.5, 1, 1.5, 2])
ax.grid(True)
plt.show()
```

defaults to *jupyter* engine

You can use Python and R code together using the `reticulate` package

Quarto Showcase

Fragments

Fade in

Fade out

Highlight red

Slide up while fading in

Tab | Set

Hello…

Quarto Showcase

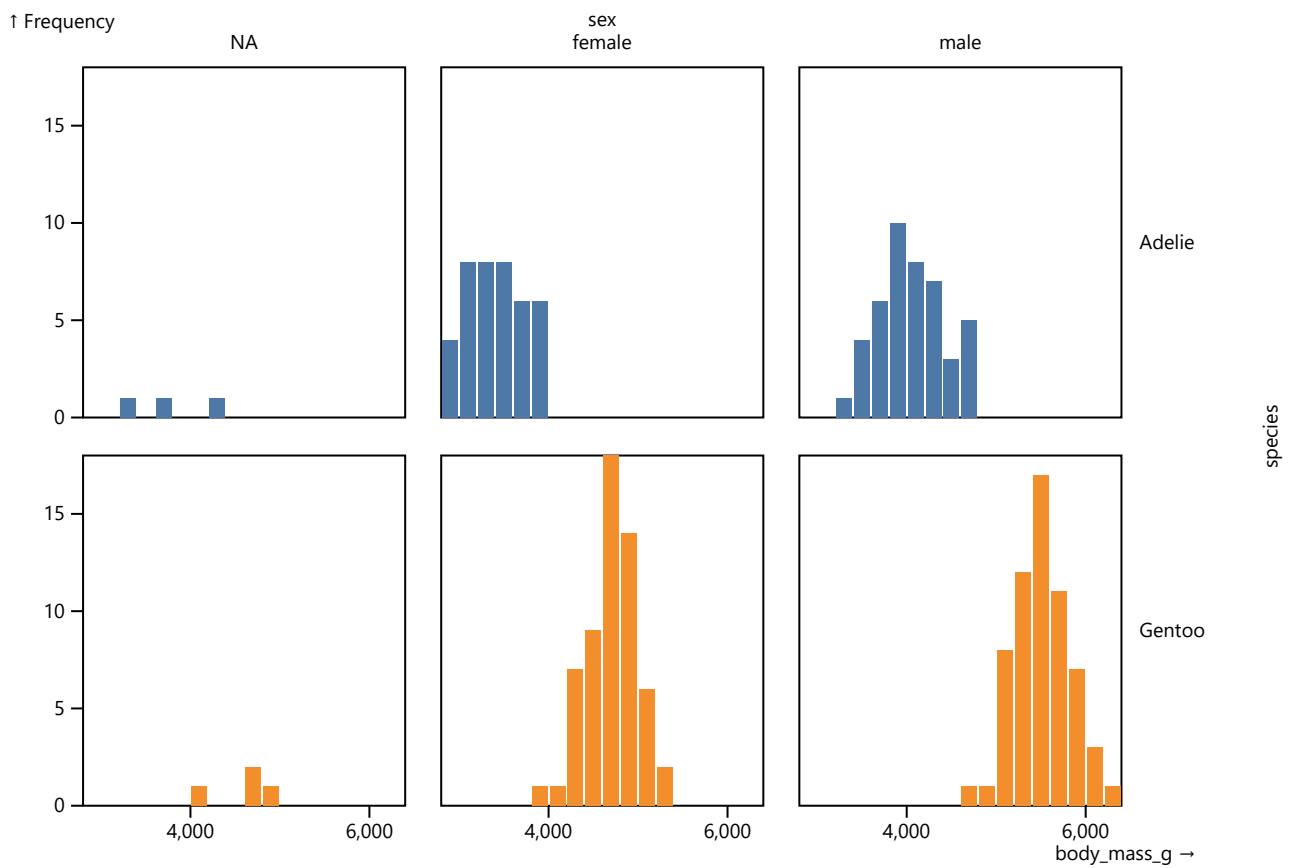
Bill length (min):

35

Islands:

- [x] Torgersen
- [x] Biscoe
- [ ] Dream

Plot | Data



When to use Quarto?

Strengths & Weaknesses of Quarto *for slides*

Strengths 💪

- Consistency in Output
  - Focus on content
- Support for (Explicit) Version Control (e.g. git)
- Great for Code (in Slides)
- Automation / Generated Contents
- Interactivity

Weaknesses 😥

- Harder to do fine layouting
  - No WYSIWYG
- New Syntax to learn
- Software Maturity

Key Benefit: (Explicit) Version Control 🔃

- Going back through time
- Great for collaboration
- Allow sharing and adaptation
  - Just like this presentation
- Allows automation

Practice what you preach!

By setting up your teaching materials in a reproducible manner, you demonstrate the value of reproducibility directly

- Useful for others
- Useful for future you when you teach this course again

Reproducible training materials are beneficial to us!

- *I used some slides from a workshop I took part in on reproducible materials, which we developed:*

Nick Bearman

GitHub

Unai Fischer Abaigar

GitHub

Jan Simson

GitHub

Images: Scriberia with The Turing Way community (License: CC BY 4.0)

Slides: Slides are publicly available at github.com/jansim/dra-reproducible-materials

Software: Reproducible slides build with Quarto and deployed to GitHub Pages using GitHub Actions (details in the Quarto docs)

Source: Source code is available at github.com/jansim/dra-reproducible-materials

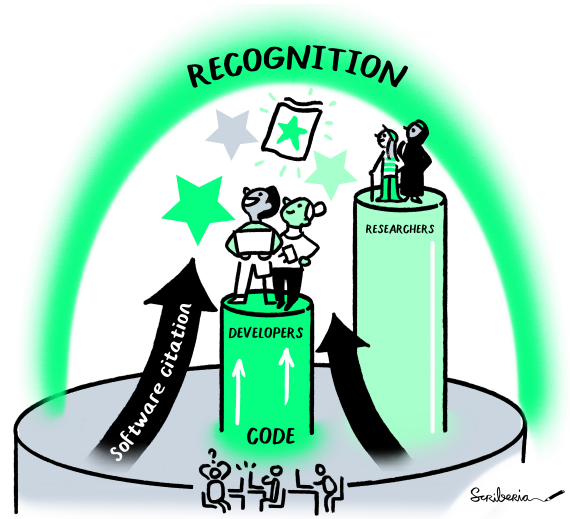
DOI: DOI 10.5281/zenodo.10652988 (generated using GitHub + Zenodo, see GitHub docs)

License: Creative Commons Attribution 4.0 International (CC BY 4.0)

Contact: We welcome any feedback via email or GitHub issues. Thank you!

Reproducible training materials are beneficial to us!

- *We used the Reproducible and FAIR Teaching Materials slides from the Aug 2023 Train the Trainer programme*
- **Thank you** very much to Esther Plomp and Lennart Wittkuhn 🙏 whose Quarto slides we used and developed!



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GitHub
Mastodon

Additional Resources

- The Turing Way handbook to reproducible, ethical and collaborative data science
- Richard McElreath (2020). Science as amateur software development. YouTube
- Quarto
  - Quarto Documentation
  - Quarto for Academics by Mine Çetinkaya-Rundel
- Version Control
  - Version Control Book
  - https://github.com/git-guides

Questions ?

Thank you! 🙏

Nick Bearman

GitHub

🖼️ **Images:** Scriberia with The Turing Way community (License: CC BY 4.0)

💻 **Slides:** Slides are publicly available at github.com/jansim/dra-reproducible-materials

📦 **Software:** Reproducible slides build with Quarto and deployed to GitHub Pages using GitHub Actions (details in the Quarto docs)

Source: Source code is available at Github.com/nickbearman/reproducibility-replicability-gds-penn

💬 **Contact:** We welcome any feedback via email or GitHub issues. Thank you!