DS4SD PHD COURSE REPRODUCIBLE WORKFLOWS

RMarkdown, git and Github

Stefan Daume

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SRC 2024 PHD COURSE 'DATA SCIENCE FOR SUSTAINABLE DEVELOPMENT'

Reproducible Workflows Using R Markdown, Git And GitHub

Stefan Daume

Stockholm Resilience Centre, Stockholm University & Beijer Institute of Ecological Economics

@stefandaume
https://scitingly.net/
stefan.daume@su.se

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WHY LEARN R MARKDOWN & GIT/GITHUB?

KEY MOTIVATION

Document your analysis and enable **reproducibility** to follow **Open Science** principles.

Avoid repetitive and error-prone tasks.

(R) MARKDOWN

YOU SHOULD USE R MARKDOWN IF YOU WANT TO ...

- integrate and document your data analysis dynamically, not statically
- concentrate on content rather than formatting
- share one document in many different formats (Markdown, PDF, Word, HTML)
- ensure correct citations and bibliographies
- switch between different citation formats
- ... and much more

MARKDOWN VS MARKUP

Markdown allows us to concentrate on document structure and content. We can then worry about styling and presentation later.

Markdown is a type of **markup language** (like HTML), but it is lightweight and more readable.

SOME TEXT WITH SIMPLE FORMATTING

This is a list:

- with some **bold** and
- some *italic* text.

And a hyperlink for good measure.

MARKUP SAMPLES

HTML

```
This is a list:

with some <strong>bold</strong>
and
some <em>italic</em> text.

And a <a
href="https://bookdown.org/yihui/rmarkdo"
for good measure.</p>
```

LaTeX

```
This is a list:
  \begin{itemize}
  \tightlist
  \item
    with some \textbf{bold} and
  \item
    some \emph{italic} text.
  \end{itemize}

And a
  \href{https://bookdown.org/yihui/rmarkdof{hyperlink} for good
  measure.
```

THE SAME WITH MARKDOWN

Basic Markdown

```
This is a list:

* with some **bold** and

* some *italic* text.

And a [hyperlink] (https://bookdown.org/yihui/rmarkdown/) for good measure.
```

TYPICAL WORKFLOW WITH MARKDOWN:

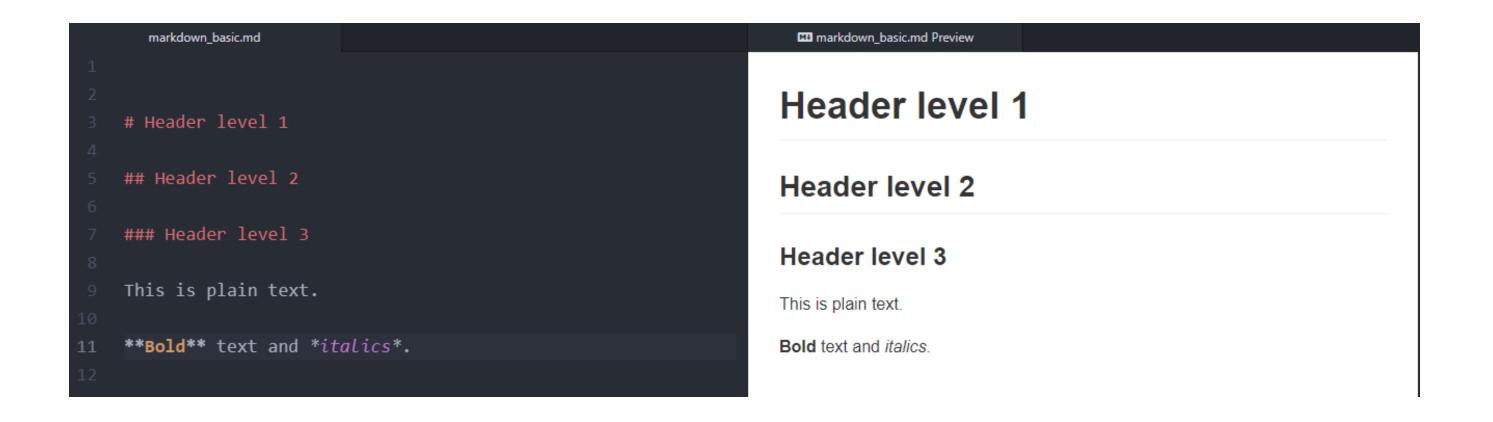
- 1. write content as a Markdown document,
- 2. **generate** the final document in a suitable output format (commonly HTML, PDF, Word)
- 3. publish

ESSENTIAL MARKDOWN SYNTAX

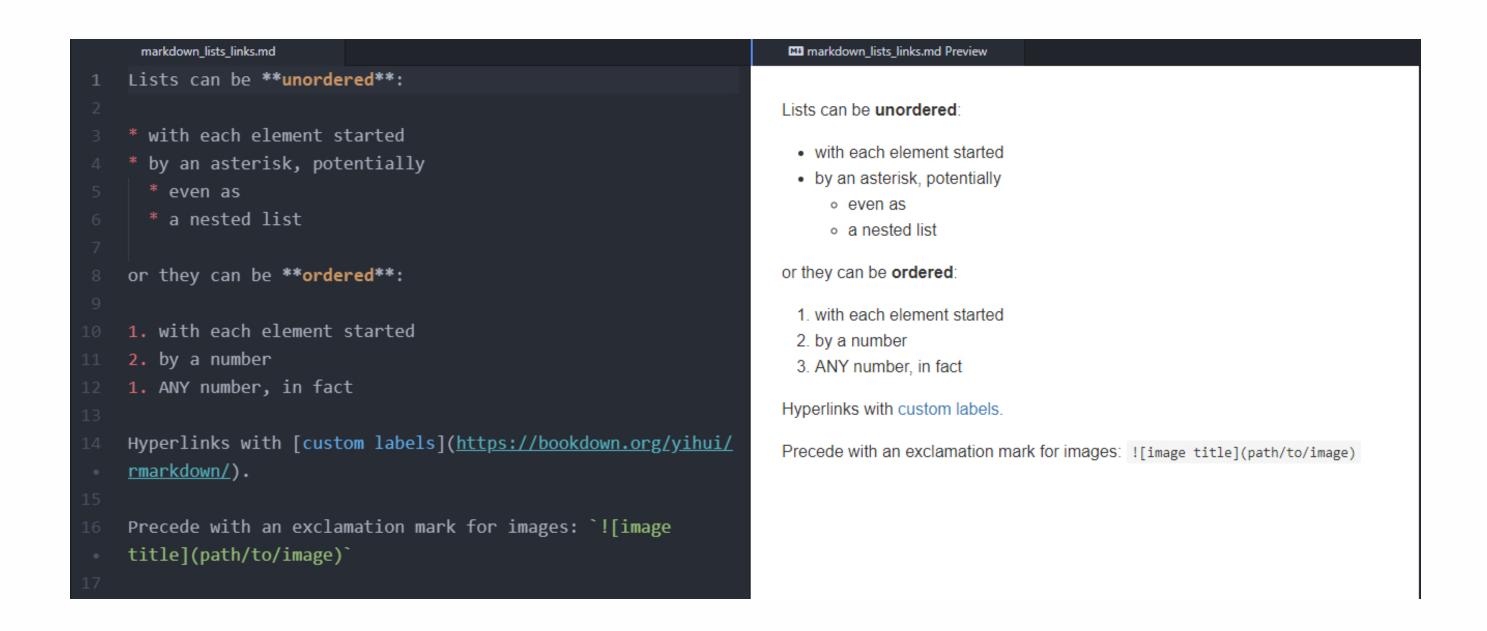
FILE STRUCTURE AND CONVENTIONS

- Markdown files are simple text files and can be created with any text editor.
- Markdown files typically end with the file extension .md

BASIC FORMATTING AND STRUCTURING



LISTS AND LINKS



EVEN TABLES



An overview of core markdown syntax can be found in this R Markdown book chapter and even more options in a condensed form as an R Markdown cheat sheet.

'R MARKDOWN' VS 'MARKDOWN'

- Purpose: dynamically weave together text, data and analysis workflows.
- This is accomplished with the knitr package, an R package conveniently integrated into the R Studio UI.

DIFFERENCES TO BASIC MARKDOWN

- R Markdown files use the file extension . Rmd instead of .md.
- R Markdown files must start with a so-called YAML header section.
- R Markdown files are still text files but R Studio should be used to work with those files efficiently.

YAML - YET ANOTHER MARKUP LANGUAGE?

The YAML header must be placed at the beginning of a document and is enclosed by three dashes ---.

```
---
title: "Untitled"
output: html_document
date: '2024-11-22'
---
```

Above is the default YAML header when creating a new R Markdown file in R Studio.

YAML AIN'T MARKUP LANGUAGE!

The YAML header contains meta-data (e.g. title, date, author(s) etc) as well as information about the output format and style.

A YAML header with more options might look like this:

```
title: "R Course SRC"
subtitle: "Module 3"
date: "`r Sys.Date()`"
author: 'Stefan Daume'
output:
  html_document:
    toc: yes
bibliography: references.bib
link-citations: yes
---
```

EXERCISE

- 1. Create a default 'R Markdown' document in R Studio.
- 2. "knit" the document to HTML and view the result.
- 3. Use the **Knit** button to select different output formats and check the YAML header afterwards.

```
markdown-handout.Rmd ×

Image: Knit on Save ABC Knit 

Source Visual

1 ---

2 title: "R Markdown: Key Takeaways"

3 subtitle: "SRC R Course, Module 3"

4 author: "Stefan Daume"

5 date: '2022-06-16'
```

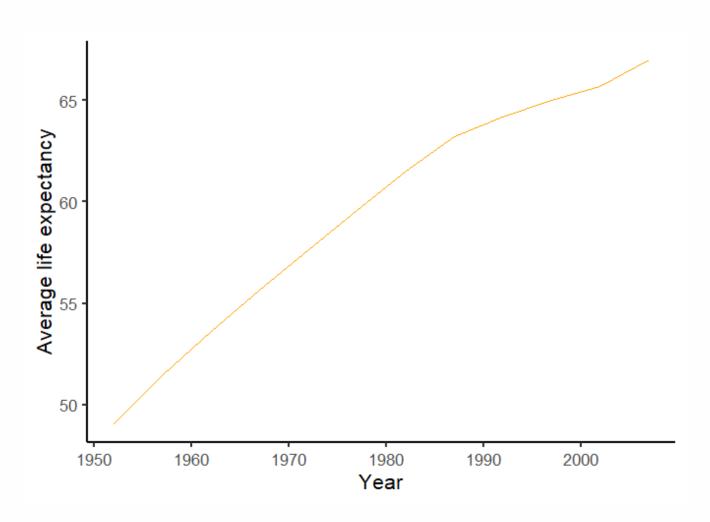
R MARKDOWN: DATA-DRIVEN DOCUMENTS

- R Markdown allows to integrate your analysis as R code into the document
- The analysis (i.e. the R code) is executed and the results updated when you **knit** the document.
- Text and code are interspersed.
- Code sections are included in code chunks like this.

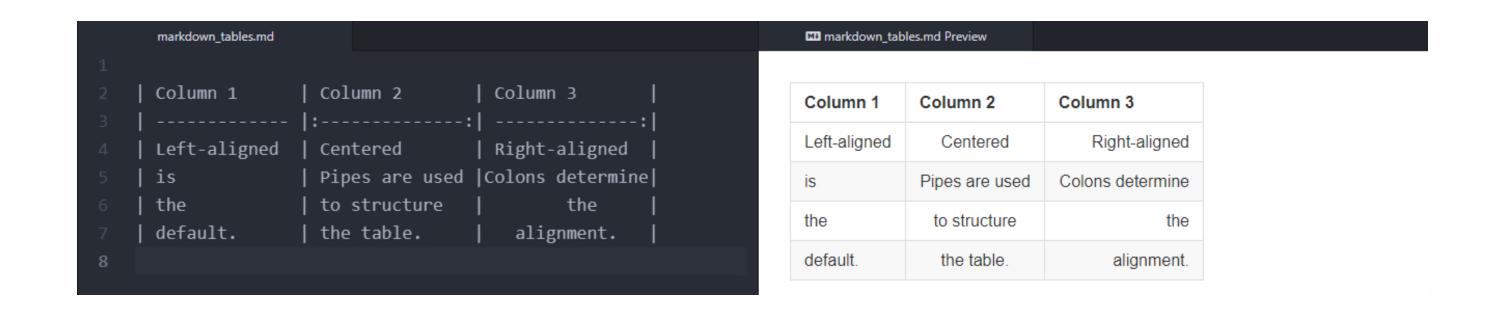
```
```{r some-explanatory-label, eval=TRUE, echo=FALSE}
here goes your R code
```
```

AN EXAMPLE FROM THE PREVIOUS SESSIONS

PLOTS IN R MARKDOWN



REMEMBER THE MARKDOWN TABLE FORMAT?



DYNAMIC TABLES WITH R MARKDOWN

This code ...

... creates this table:

| continent | avrg_le | avrg_gdp |
|-----------|----------|-----------|
| Africa | 54.80604 | 3089.033 |
| Americas | 73.60812 | 11003.032 |
| Asia | 70.72848 | 12473.027 |
| Europe | 77.64860 | 25054.482 |
| Oceania | 80.71950 | 29810.188 |

CUSTOMIZING kable TABLES

This code ...

... creates this table:

| continent | avrg_le | avrg_gdp |
|-----------|---------|----------|
| Africa | 54.8 | 3089.03 |
| Americas | 73.6 | 11003.03 |
| Asia | 70.7 | 12473.03 |
| Europe | 77.6 | 25054.48 |
| Oceania | 80.7 | 29810.19 |

MORE EXPRESSIVE TABLES WITH kableExtra OR gt

The kableExtra and gt packages offer even more options:

- data-driven colouring
- interactive tables
- grouped headers
- tables with (interactive) sparklines
- and more ...

kableExtra EXAMPLE

Table caption: Dynamic formatting with the the help of kableExtra. This example shows Gapminder data summarised by continent for the year 2007.

| Continent | Mean life expectancy | Mean GDI |
|-----------|----------------------|----------|
| | | |

| Africa | 54.8 | 3089.03 |
|----------|------|----------|
| Americas | 73.6 | 11003.03 |
| Asia | 70.7 | 12473.03 |
| Europe | 77.6 | 25054.48 |
| Oceania | 80.7 | 29810.19 |

gt EXAMPLE

Table caption: Dynamic formatting with the the help of the gt package. This example shows Gapminder data summarised by continent for the year 2007.

| Continent | Mean life expectancy | Mean GDP |
|-----------|----------------------|-----------|
| Africa | 54.8 | 3,089.03 |
| Americas | 73.6 | 11,003.03 |
| Asia | 70.7 | 12,473.03 |
| Europe | 77.6 | 25,054.48 |
| Oceania | 80.7 | 29,810.19 |

CENTRAL 'SETUP' CODE SECTION

```
\``\{r setup, include=FALSE}
knitr::opts_chunk$set(echo = FALSE)

library(readr)
library(dplyr)
library(ggplot2)
library(gapminder)

year_of_interest <- 2007
\```</pre>
```

Simplify library import and prepare datasets for reference in the whole document.

HANDLING CITATIONS

CITATIONS AND BIBLIOGRAPHIES

One of the most useful and powerful features for researchers using R Markdown.

REQUIRES A BIBTEX DATABASE

A **BibTeX** database is simply a text file with the extension .bib and entries such as:

```
@misc{XieAllaire_et_2022,
   author = {Xie, Yihui and Allaire, J. J. and Grolemund, Garrett},
   title = {{R Markdown: The Definitive Guide}},
   url = {https://bookdown.org/yihui/rmarkdown/},
   urldate = {2022-06-07},
   year = {2022}
```

No need to write those. Export from your reference manager or journal pages.

INCLUDE CITATIONS

Point to the .bib file in the YAML header.

```
title: "R Course SRC"
subtitle: "Module 3"
date: "2024-11-21"
author: 'Stefan Daume'
output:
  html_document:
    toc: yes
bibliography: references.bib
link-citations: yes
---
```

And then include citations in the text with the format [@CitationKey], which in the previously shown example was [@XieAllaire_et_2022], which is a reference to (Xie, Allaire, and Grolemund 2022).

INCLUDE A BIBLIOGRAPHY

By default a bibliography is added to the end of the generated (i.e., knitred) document.

After presenting all results we have now reached the end of the document. Here should follow the bibliography.

References

Add the header # References at the end of your document, knit and the complete bibliography is added to the output document.

SWITCH CITATION AND BIBLIOGRAPHY STYLES DYNAMICALLY

Specify citation style in the YAML header.

```
title: "R Course SRC"
subtitle: "Module 3"
date: "2024-11-21"
author: 'Stefan Daume'
output:
  html_document:
    toc: yes
bibliography: references.bib
link-citations: yes
csl: ecology-and-society.csl
---
```

The Citation Style Database database contains thousands of journal citation styles.

Download the relevant one, reference in the YAML header and the output document will

have the required citation style.

EASY SHARING AND ONLINE PUBLISHING

- 1. knit your R Markdown document to HTML
- 2. push the HTML to Github (next part of this module)
- 3. enable sharing of **Github Pages**

This is how this presentation works (and the others before).

"CONTINUOUS ANALYSIS" AS THE ULTIMATE GOAL

KEY RESOURCES

- R Markdown
 - R Markdown: The Definitive Guide (Xie, Allaire, and Grolemund 2022)
 - R Markdown Cookbook (Xie, Dervieux, and Riederer 2024)
 - Cheatsheet: Dynamic documents with rmarkdown cheatsheet

GIT & GITHUB

YOU NEED GIT AND GITHUB IF ... (NON-EXHAUSTIVE LIST)

- ... you have files like this, but realise that this is not efficient
 - my_paper_draft_2021_05_16.docx
 - my_paper_draft_2021_05_18.docx
 - my_paper_draft_2021_05_19.docx
 - my_paper_draft_2021_05_19_v1.docx
 - my_paper_draft_2021_05_19_v2.docx
 - my_paper_draft_2021_05_19_v3_with_comments.docx
- ... you are not creating regular backups of your work
- ... you want to collaborate with others
- ... you want to maintain projects rather than a single file (Google Doc)
- ... you want to be able to easily revert back to previous versions of your work

FOCUS OF THIS SESSION

git & GitHub are extremely versatile, feature-rich tools that enable collaboration on complex software projects.

FOCUS OF THIS SESSION

We will only scratch the surface and focus on basic recipes and elements, namely:

- understanding the basic idea behind git
- use GitHub as a repository/backup for your work
- integrate git/GitHub into your workflow with R Studio
- share and collaborate with others

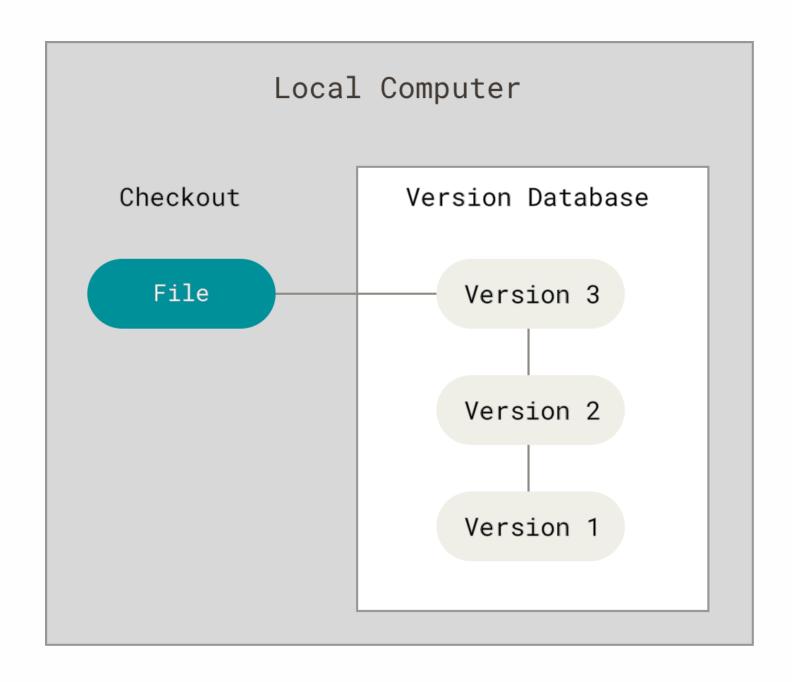
KEY RESOURCES

- Git/Github:
 - Happy Git and GitHub for the useR (Bryan 2021)
 - "Excuse me, do you have a moment to talk about version control?"
 (Bryan 2017)
 - Advanced git use: Pro Git book (Chacon and Straub 2014)
 - How to write a great commit message

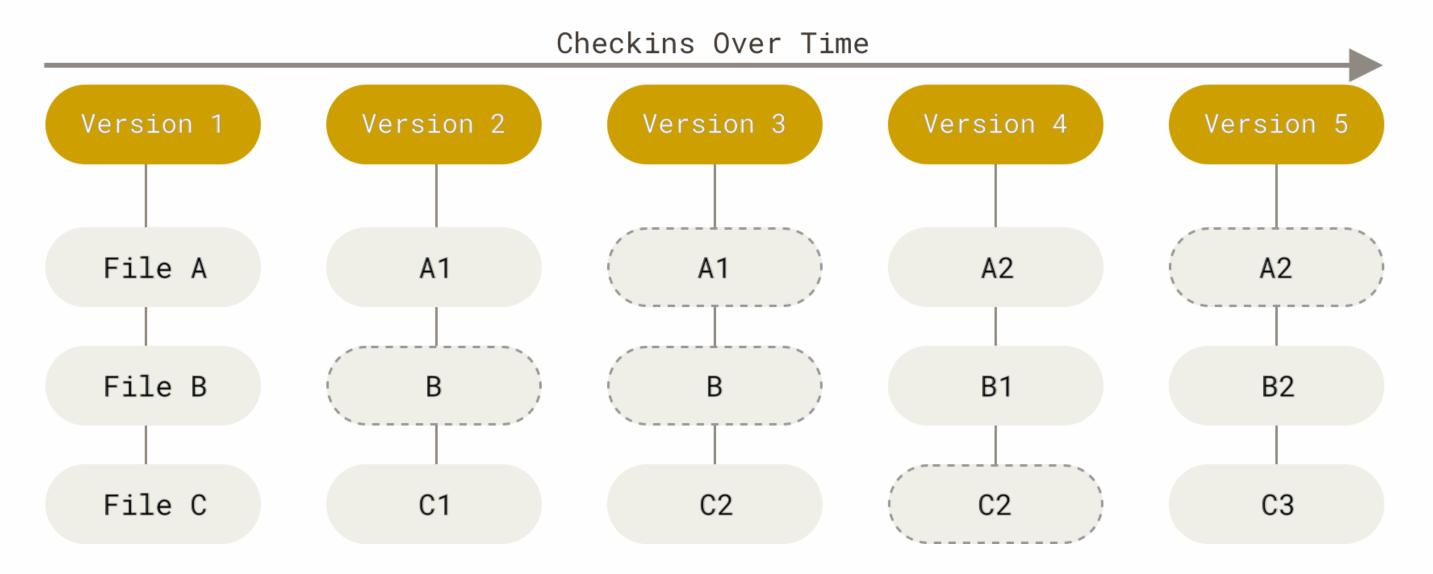
GIT HISTORY

- Linux development, started 2005
- a version management system, i.e. tracks changes in project resources
- git takes snapshots of a managed project (image)
- distributed version control system (that means you always have a complete copy of your version history on your local computer)

VERSION CONTROL



VERSIONS AS SNAPSHOTS

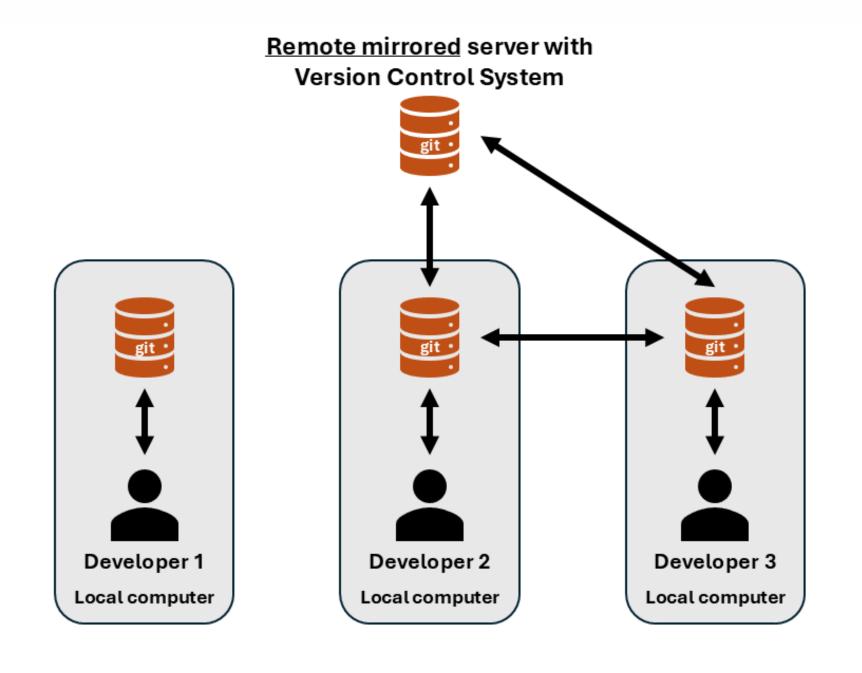


Versions as snapshots diagram, in Pro Git by Scott Chacon and Ben Straub, licensed under CC BY-NC-SA 3.0

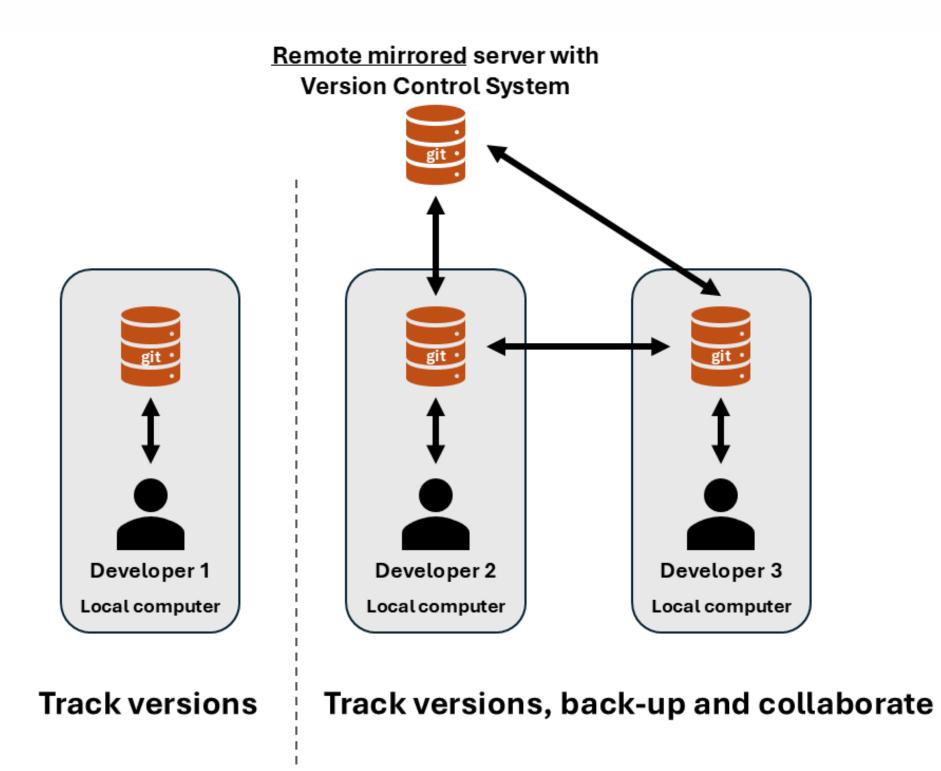
CENTRALIZED VERSION CONTROL

Examples: CVS, Subversion

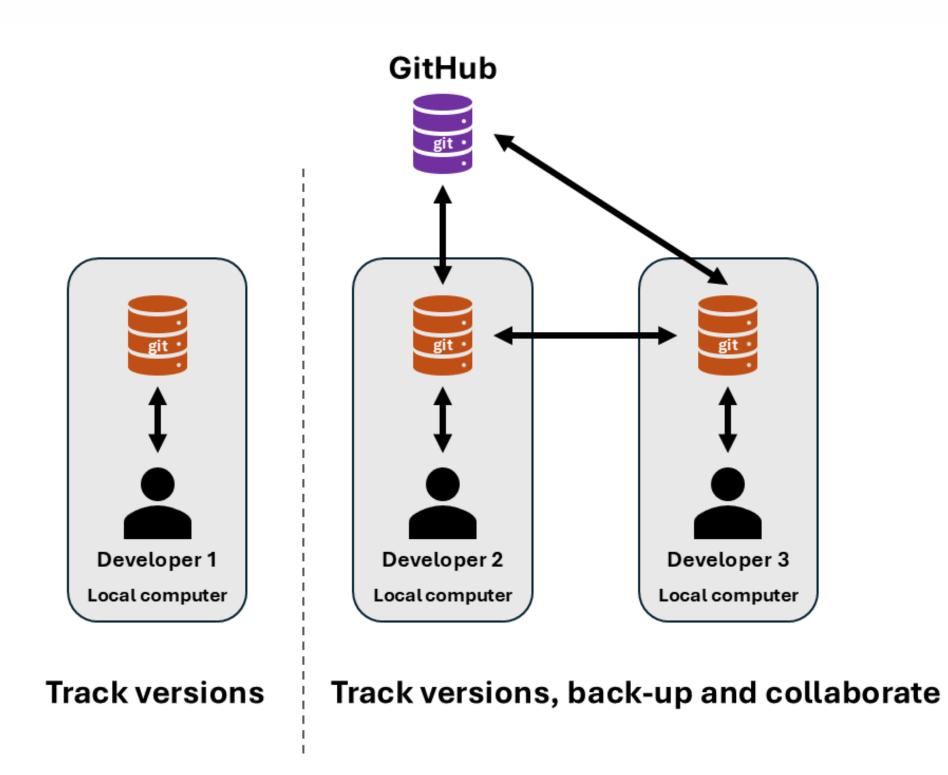
DISTRIBUTED VERSION CONTROL



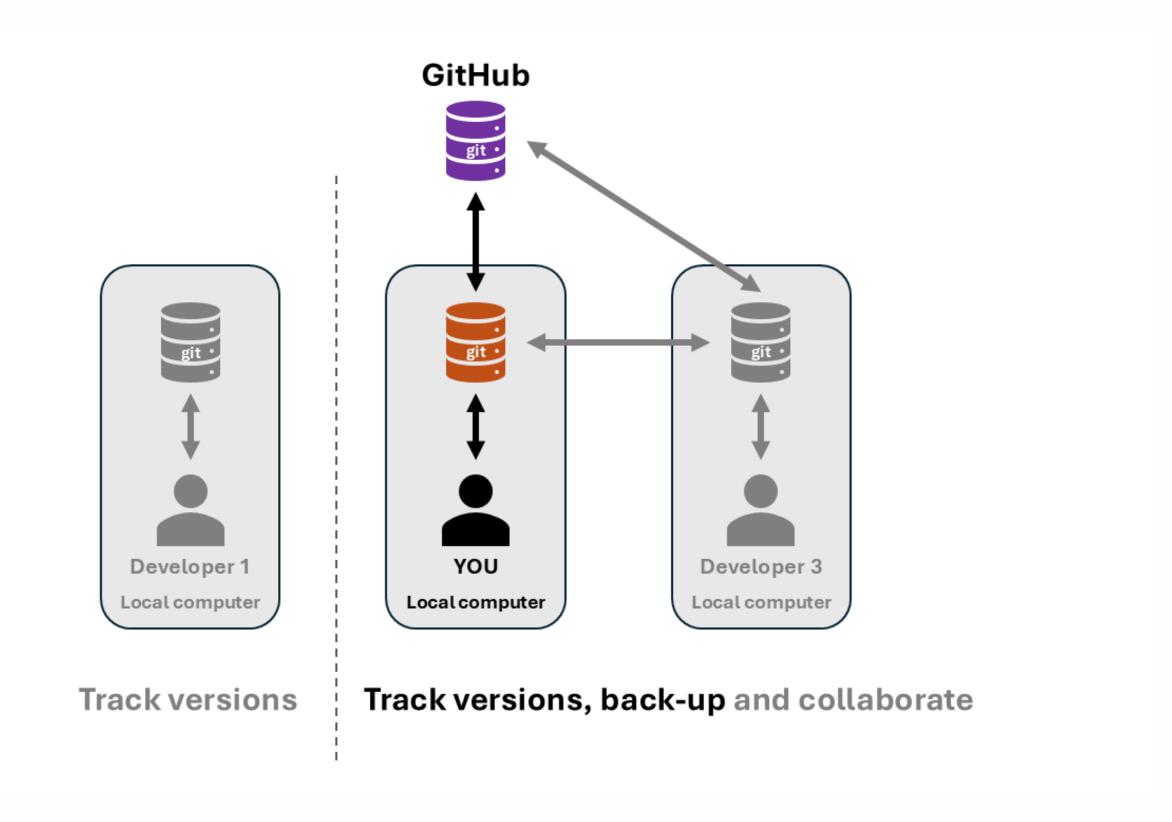
DISTRIBUTED VERSION CONTROL



GITHUB AS A HOSTED GIT REPO



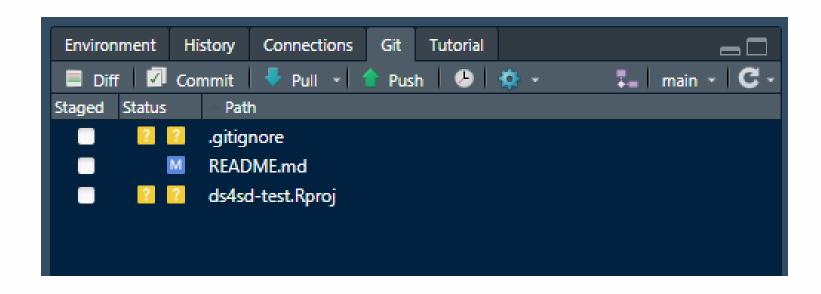
FOCUS FOR TODAY



A SIMPLE GIT/GITHUB USAGE SCENARIO

- create a project and enable versioning with git
- connect it with a remote copy (for sharing and backup)
- do work locally and track (commit) versions of your files
- push your changes (sync to the remote copy on GitHub)
- pull other's changes (sync from the remote copy on GitHub)

INTEGRATED INTO R STUDIO



KEY CONCEPTS

- repo
- cloning
- staging
- commit
- diff
- push
- pull
- branch (advanced)
- merge (advanced)
- remote origin

SETTING GIT/GITHUB UP WITH R STUDIO

DO THIS ONCE:

- sign up for a Github account
- install git locally (see (Bryan 2021))
- create a Personal Access Token (PAT)
 - either via Github (https://github.com/settings/tokens)
 - or via R with: usethis::create_github_token()
 - and then store it with gitcreds::gitcreds_set()

INSTALLING AND CONFIGURING GIT

Select the installer for your OS: https://git-scm.com/

On the command line set:

```
$ git config --global user.name "JohnDoe"
$ git config --global user.email johndoe@example.com
```

Use the same username/email you use for your GitHub account!

Check your settings:

```
$ git config --list
```

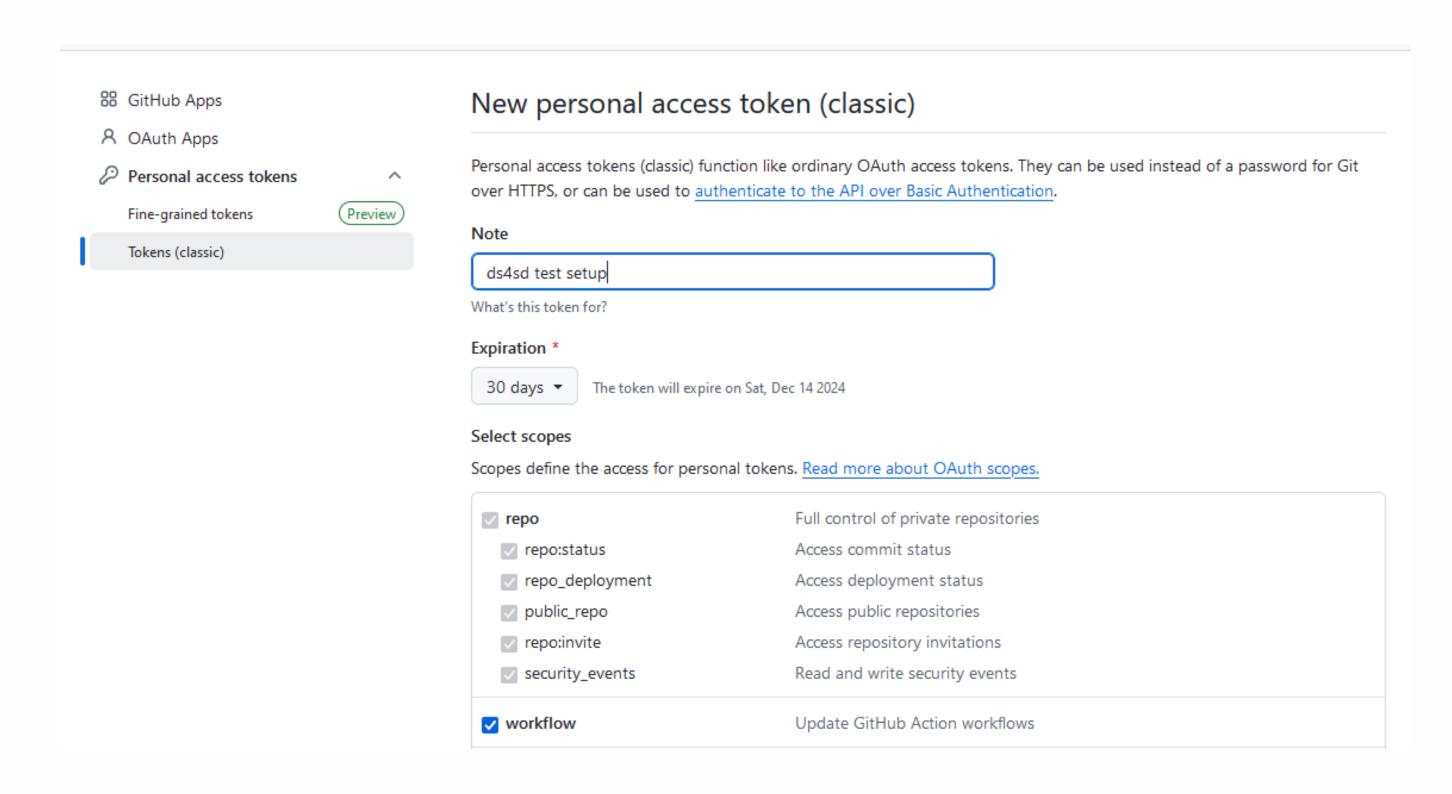
CREATE A PAT (PERSONAL ACCESS TOKEN)

You can go to GitHub directly or trigger it from the command line:

usethis::create_github_token()

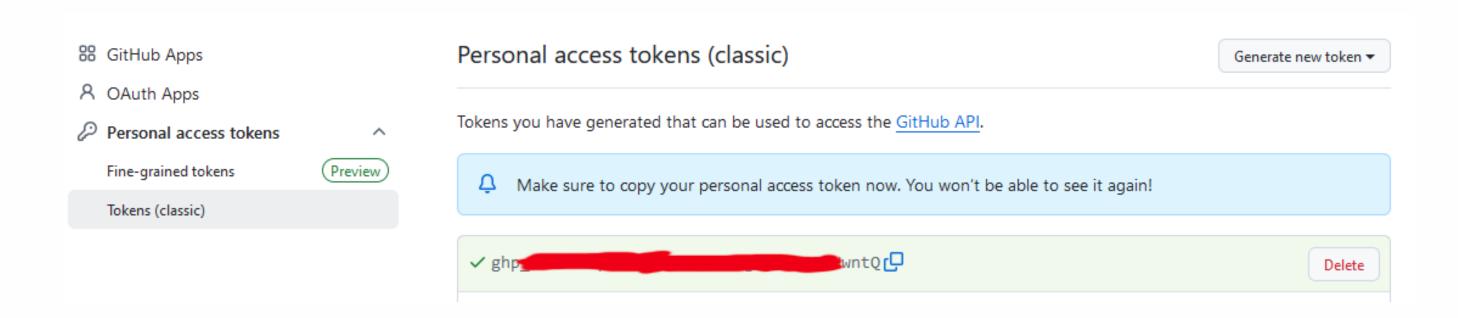
CREATE A PAT (PERSONAL ACCESS TOKEN)

Configure and create PAT:



CREATE A PAT (PERSONAL ACCESS TOKEN)

Than copy it:



STORE THE PAT FOR LOCAL USE

Set the credentials from the command line in R Studio:

```
gitcreds::gitcreds_set()
```

Follow instructions and finally provide the PAT:

- -> Adding new credentials...
- -> Removing credentials from cache...
- -> Done.

ALTERNATIVE TO PATS

You can also configure **SSH** keys to connect to GitHub.

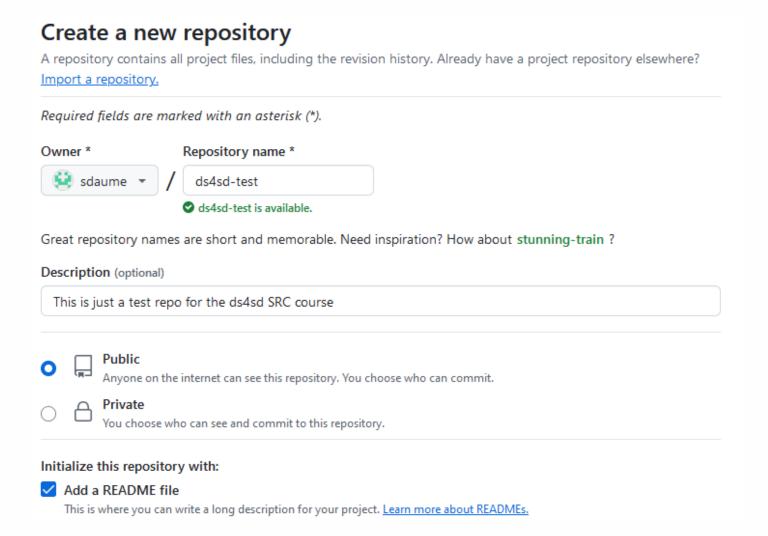
Consult Set up keys for SSH (Bryan 2021) to explore this option.

DO THIS FOR EVERY NEW PROJECT:

- create a Github repo first (follow the New project, Github first workflow in (Bryan 2021))
 - Why? Its easiest! You have everything in place to create remote backups!
- say yes to creating a README
- copy the HTTPS link of your new repo
- then create an R Studio project with the option from "Version control"
 > git"

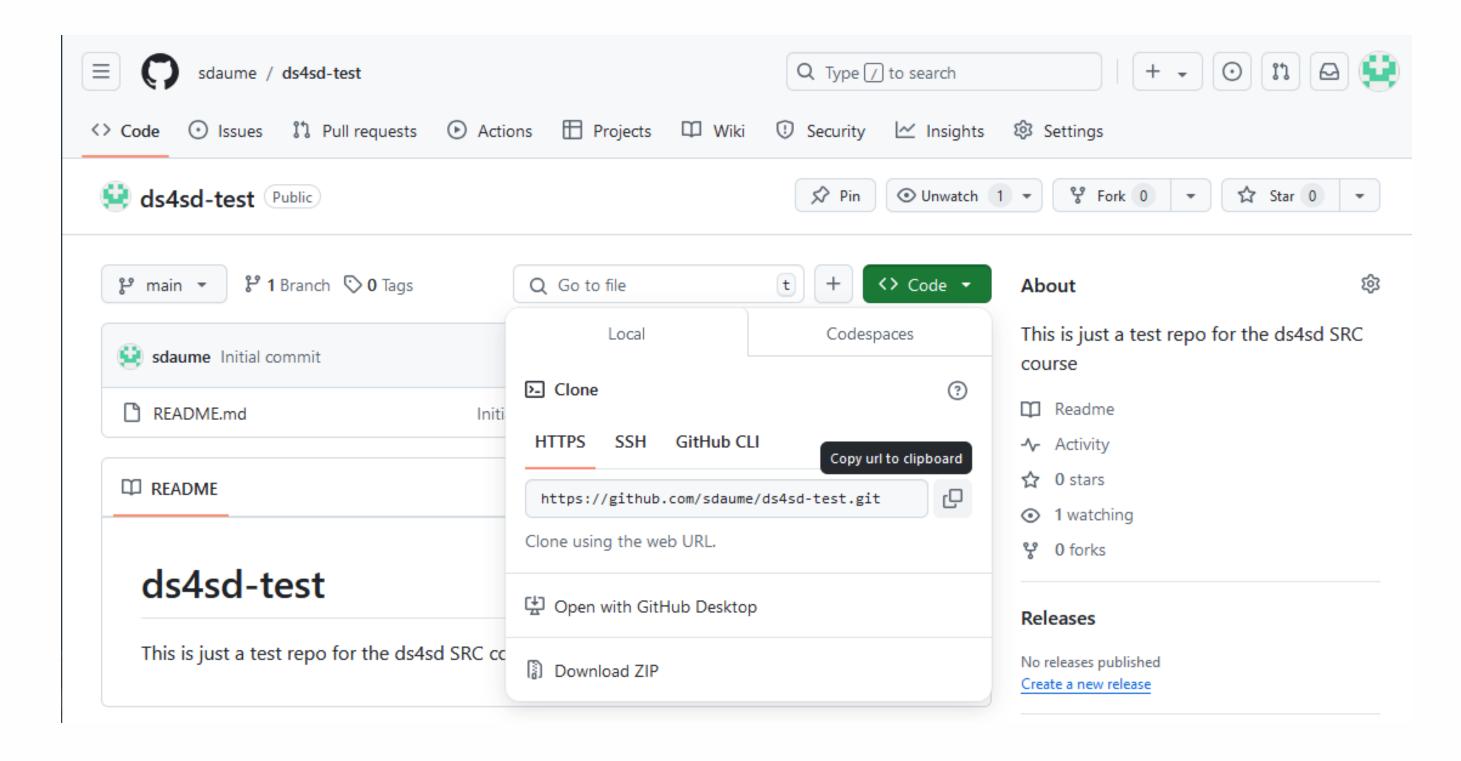
CREATE A NEW GITHUB REPO

- In your GitHub profile go to Repositories, and press "New".
- Provide the repo information and press "Create Repository".



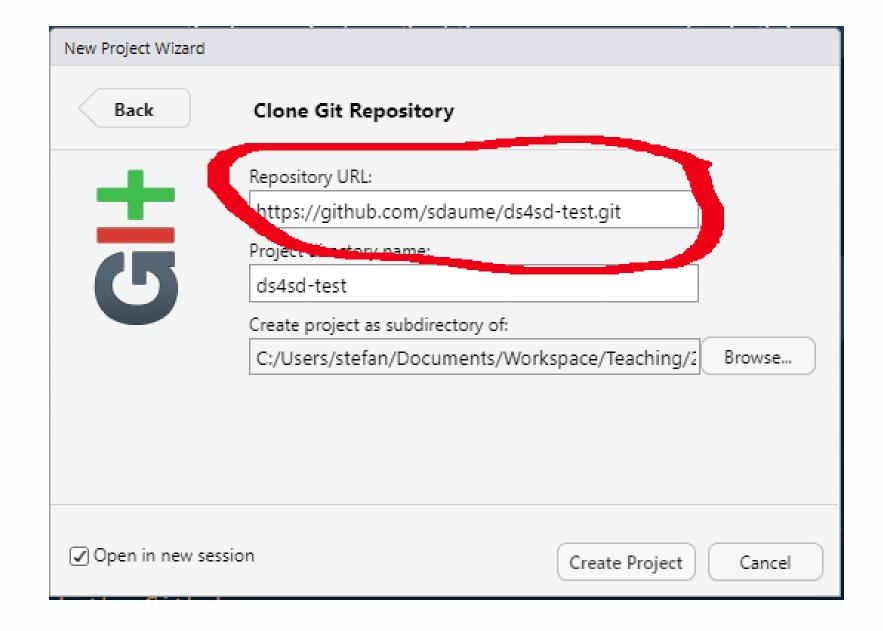
COPY THE REPO URL

- Go to Repositories and select the new repo.
- Copy the HTTPS repo URL.

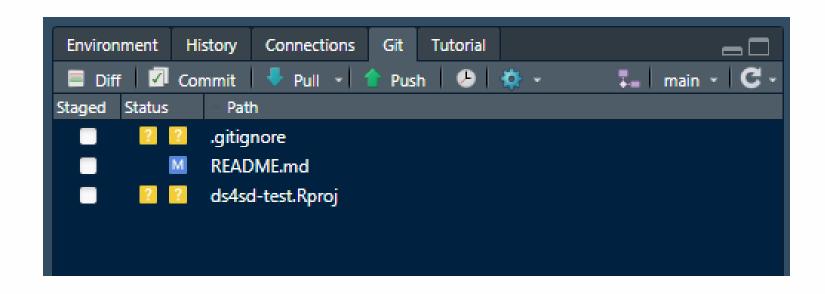


CREATE AN R STUDIO PROJECT WITH THE REPO

Create a new project via File > New Project > Version Control > Git



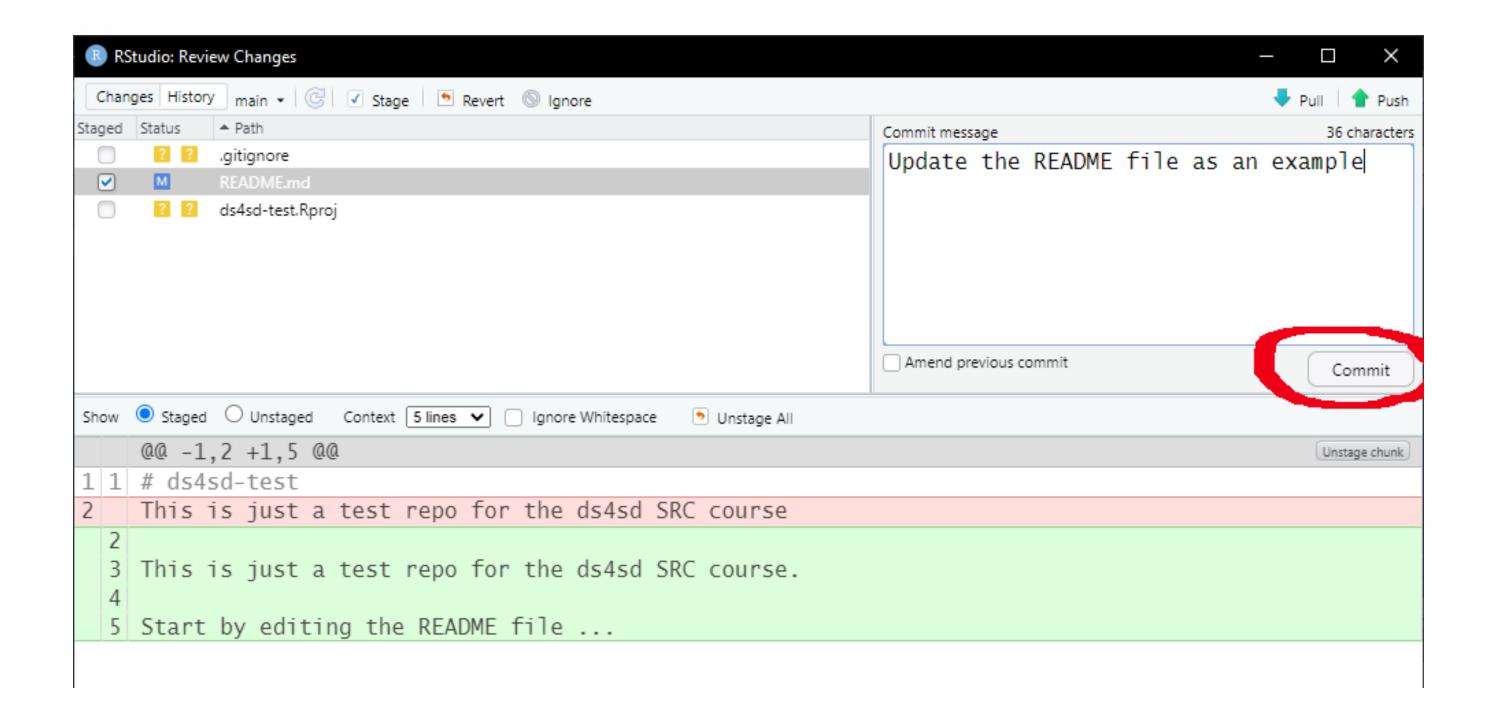
NEW PROJECT TRACKED WITH GIT



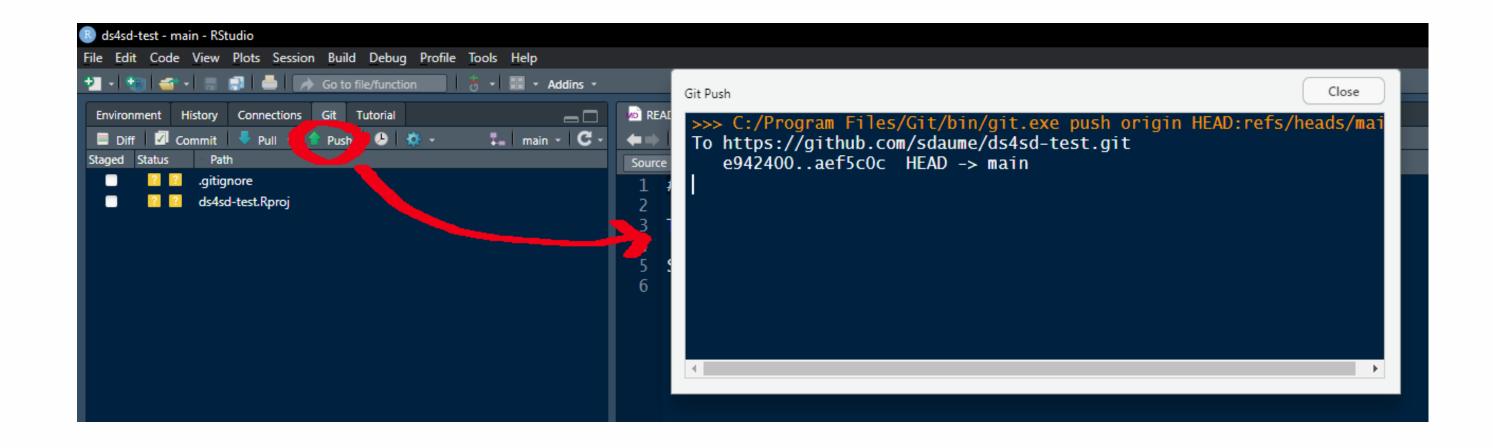
WHEN YOUR NEW PROJECT IS SET UP

- make a change to the README.md (a useful project description)
- commit the changes of the README file
- and push to the remote Github repo
- check the Github repo

COMMIT CHANGES



PUSH CHANGES TO REMOTE GITHUB REPO

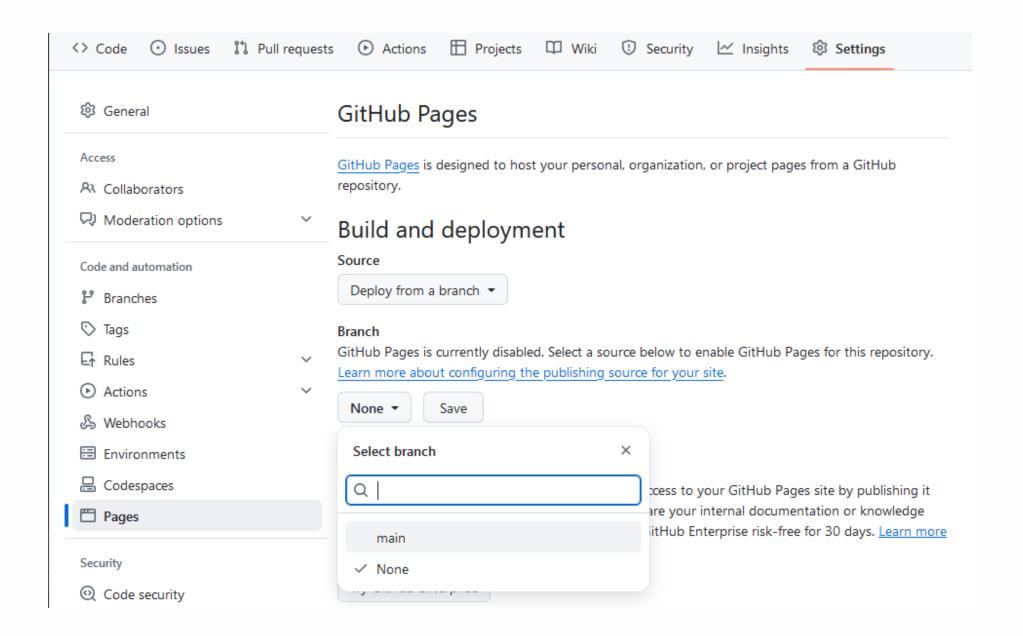


PUBLISH YOUR CONTENT

Repo content can be hosted online via GitHub pages.

ENABLE GITHUB PAGES FOR A REPO

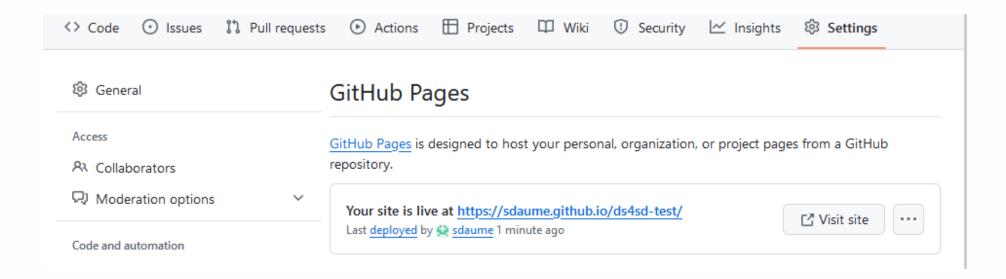
Go to Settings > Pages and select Branch > main



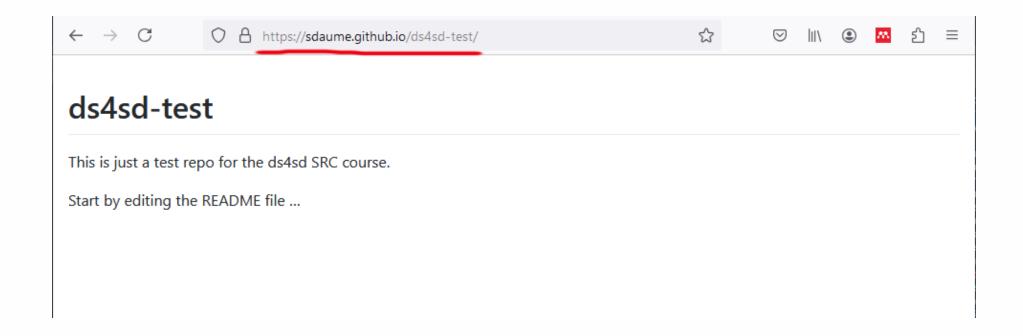
ONE GITHUB PAGE PER REPO

Once enabled a site becomes available with the format:

https://[GITHUB_USER].github.io/[REPO_NAME]/



DEPLOYED GITHUB PAGE



By default either the README is served or the content of a file called *index.html*, if it is available.

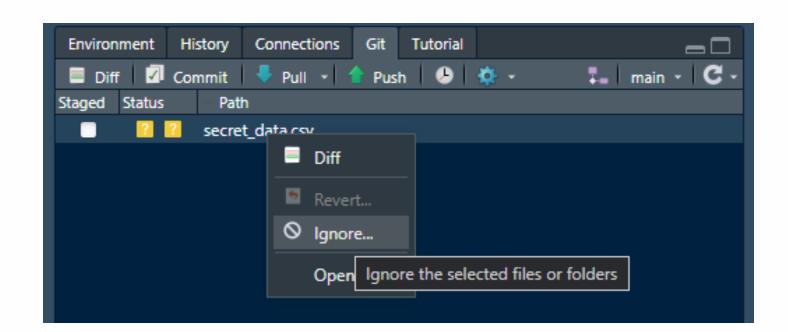
Alternatively, provide the filename in the URL, e.g., https://sdaume.github.io/ds4sd-test/default.html

USEFUL TO KNOW FOR COMMITS

NOT TRACKING RESOURCES

.gitignore allows to exclude resources from being tracked.

You may have sensitive files (e.g., pass keys, private data) that should not end up in a public repo.



HOW TO WRITE A GREAT COMMIT COMMENT

Most important:

Keep things atomic!

Document consistently:

- Keep the subject line short.
- Use the imperative mood in the subject line (Because a commit message should always complete the following line: "If applied, this commit will [YOUR_SUBJECT_LINE].")
- Use the body to explain what and why vs. how (Because "the how" can be obtained from the *diff*. The commit message should provide the context for "the how".)

EXERCISES

EXERCISE 1: SETUP GIT/GITHUB WITH R STUDIO

- Create a new repo on GitHub and
- Clone it as a new project in R Studio
- Edit the default README in your new R Studio project
- Commit the changes
- Push the changes to GitHub

EXERCISE 2: CREATE AN R MARKDOWN DOCUMENT WITH DIFFERENT OUTPUT FORMATS

- In your new project create an R Markdown file
- Edit the file and insert
 - a simple plot with your own or Gapminder data
 - citation to references exported from your reference manager
- knit to the default output format (HTML)
- Try different output formats: PDF, Word

EXERCISE 3: PUBLISH AN R MARKDOWN DOCUMENT VIA GITHUB

- Use your earlier R Markdown document
- knit to HTML, push to GitHub and publish the document
- Extra: Try to create a presentation as output

REFERENCES

Bryan, Jennifer. 2017. "Excuse me, do you have a moment to talk about version control?" *PeerJ Preprints* 5:e3159v2 (August). https://doi.org/10.7287/PEERJ.PREPRINTS.3159V2.

——. 2021. "Happy Git and GitHub for the useR." https://happygitwithr.com/.

Chacon, Scott, and Ben Straub. 2014. *Pro Git*. Apress. https://doi.org/10.1007/978-1-4842-0076-6.

Xie, Yihui, J. J. Allaire, and Garrett Grolemund. 2022. "R Markdown: The Definitive Guide." https://bookdown.org/yihui/rmarkdown/.

Xie, Yihui, Christophe Dervieux, and Emily Riederer. 2024. *R Markdown Cookbook*. https://bookdown.org/yihui/rmarkdown-cookbook/.

COLOPHON

SRC 2024 PhD course 'Data Science for Sustainable Development' — Reproducible Workflows using R Markdown and GitHub by Stefan Daume

Presented on 22. November 2024.

PRESENTATION DETAILS

Author/Affiliation: Stefan Daume, Stockholm Resilience Centre, Stockholm University

Presentation URL: https://sdaume.github.io/ds4sd-2024-modules/workflows/slides/

Presentation Source: https://github.com/sdaume/ds4sd-2024-modules

Presentation PDF: https://github.com/sdaume/ds4sd-2024-modules/workflows/slides/2024-ds4sd-workflows.pdf

CREDITS & LICENSES

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