DS4SD PHD COURSE - REPRODUCIBLE WORKFLOWS

RMarkdown, Github & Co

Stefan Daume

22. November 2024

SRC 2024 PHD COURSE ‘DATA SCIENCE FOR SUSTAINABLE DEVELOPMENT’

Reproducible Workflows Using R Markdown And GitHub

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

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

22. November 2024

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

```
<p>This is a list:</p>
<ul>
<li>with some <strong>bold</strong>
and</li>
<li>some <em>italic</em> text.</li>
</ul>
<p>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/rmarkdo
{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:

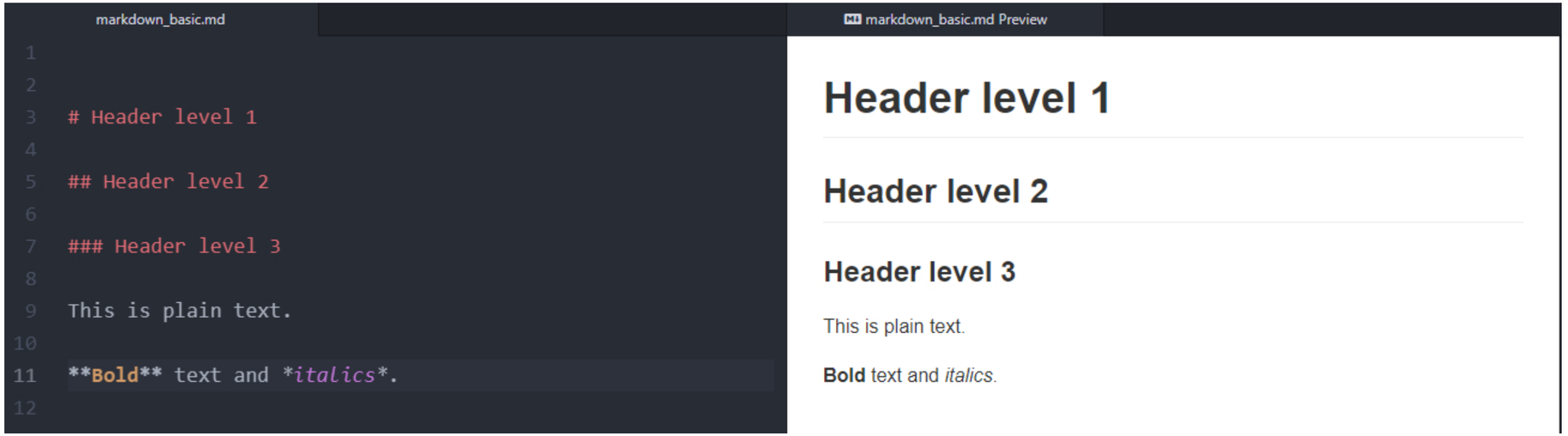
1. **write** content as a Markdown document,
2. **generate** the final document in a suitable output format (commonly HTML, PDF, Word)
3. **publish**

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

markdown_lists_links.md

```
Lists can be **unordered**:

* with each element started
* by an asterisk, potentially
  * even as
  * a nested list

or they can be **ordered**:

1. with each element started
2. by a number
1. ANY number, in fact

Hyperlinks with [custom labels](https://bookdown.org/yihui/rmarkdown/).

Precede with an exclamation mark for images: `![image title](path/to/image)`
```

markdown_lists_links.md Preview

Lists can be **unordered**:

- with each element started
- by an asterisk, potentially
  - even as
  - a nested list

or they can be **ordered**:

1. with each element started
2. by a number
3. ANY number, in fact

Hyperlinks with custom labels.

Precede with an exclamation mark for images: `![image title](path/to/image)`

EVEN TABLES

markdown_tables.md

```
| Column 1      | Column 2       | Column 3       |
| ------------- |:--------------:| --------------:|
| Left-aligned  | Centered       | Right-aligned  |
| is            | Pipes are used |Colons determine|
| the           | to structure   |        the     |
| default.      | the table.     |   alignment.   |
```

markdown_tables.md Preview

Column 1	Column 2	Column 3
Left-aligned	Centered	Right-aligned
is	Pipes are used	Colons determine
the	to structure	the
default.	the table.	alignment.

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 generating an `R Markdown` file in R Studio.

YAML AIN'T MARKUP LANGUAGE!

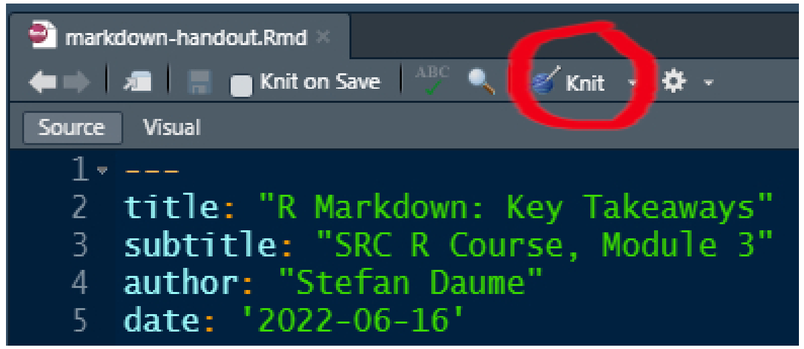
The **YAML header** contains meta-data (e.g. title, date, author(s) etc) as well as information about the output format and style.

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.



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, echo=FALSE}
# here goes your R code
```
````

AN EXAMPLE FROM THE PREVIOUS SESSIONS

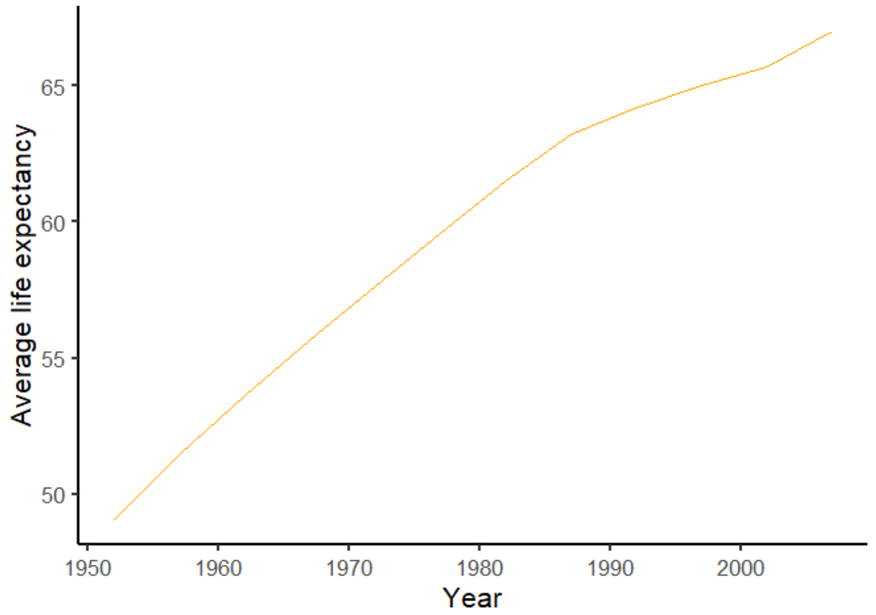
````
```{r life-expectancy, echo=FALSE, fig.cap="A figure caption."}
library(gapminder)

gapminder %>%
    group_by(year) %>%
    summarise(ale = mean(lifeExp)) %>%
    ggplot(aes(x = year, y = ale)) +
    geom_line(color = "orange") +
    labs(x = "Year",
         y = "Average life expectancy") +
    theme_classic(base_size = 16)
```
````

PLOTS IN R MARKDOWN

```
```{r life-expectancy, echo=FALSE}
library(gapminder)

gapminder %>%
    group_by(year) %>%
    summarise(ale = mean(lifeExp)) %>%
    ggplot(aes(x = year, y = ale)) +
    geom_line(color = "orange") +
    labs(x = "Year",
         y = "Average life expectancy")
+
    theme_classic(base_size = 16)
```
```



REMEMBER THE MARKDOWN TABLE FORMAT?

markdown_tables.md

```
| Column 1      | Column 2       | Column 3       |
| ------------- |:--------------:| --------------:|
| Left-aligned  | Centered       | Right-aligned  |
| is            | Pipes are used |Colons determine|
| the           | to structure   |        the     |
| default.      | the table.     |   alignment.   |
```

markdown_tables.md Preview

Column 1	Column 2	Column 3
Left-aligned	Centered	Right-aligned
is	Pipes are used	Colons determine
the	to structure	the
default.	the table.	alignment.

DYNAMIC TABLES WITH R MARKDOWN

This code …

````
```{r}
# summarize gapminder data by
continent
gapminder_latest <- gapminder %>%
  filter(year == year_of_interest)
%>%
  group_by(continent) %>%
  summarise(avrg_le =
mean(lifeExp),
            avrg_gdp =
mean(gdpPercap))

# print the results as a table
gapminder_latest %>%
  knitr::kable()
```
````

… 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 …

````
```{r}
# summarize gapminder data by
continent
gapminder_latest <- gapminder %>%
  filter(year == year_of_interest)
%>%
  group_by(continent) %>%
  summarise(avrg_le =
mean(lifeExp),
            avrg_gdp =
mean(gdpPercap))

# print the results as a table
gapminder_latest %>%
  knitr::kable(digits = c(0,1,2))
```
````

… 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 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

`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
```
````

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.

```yaml
---
title: "R Course SRC"
subtitle: "Module 3"
date: "2024-11-19"
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., `knitr`ed) 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.

```yaml
---
title: "R Course SRC"
subtitle: "Module 3"
date: "2024-11-19"
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).

“CONTINOUS ANALYSIS” AS THE ULTIMATE GOAL

KEY RESOURCES

- R Markdown
  - R Markdown: The Definitive Guide (Xie, Allaire, and Grolemund 2022)
  - 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

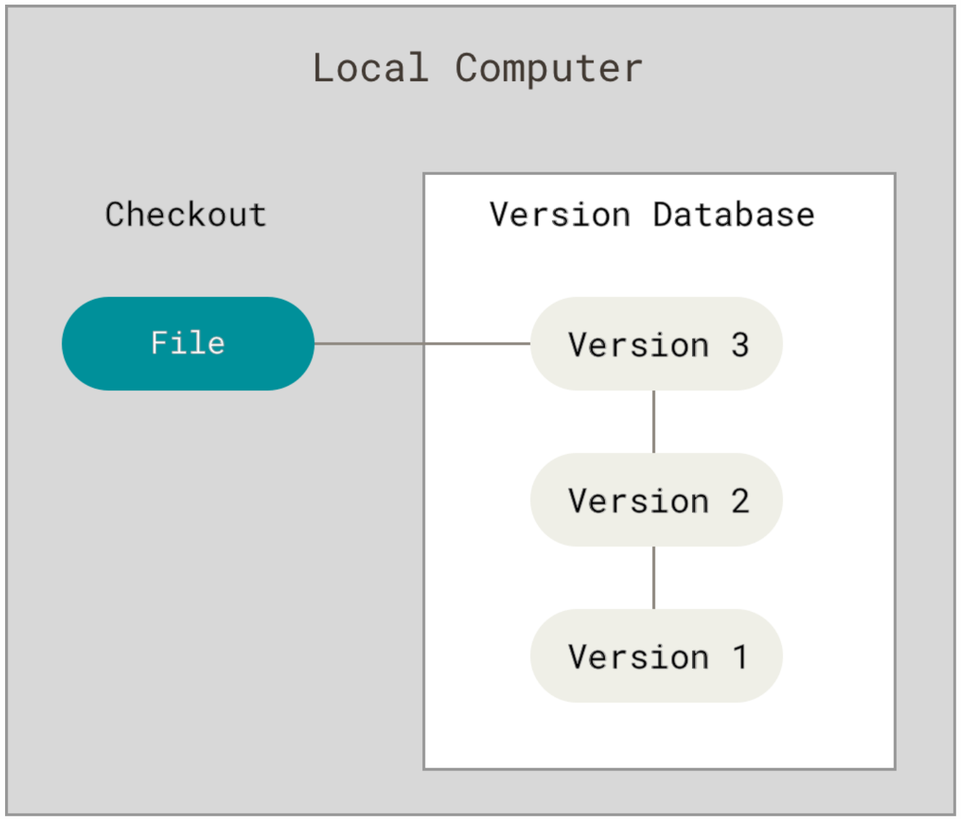
KEY RESOURCES

- 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

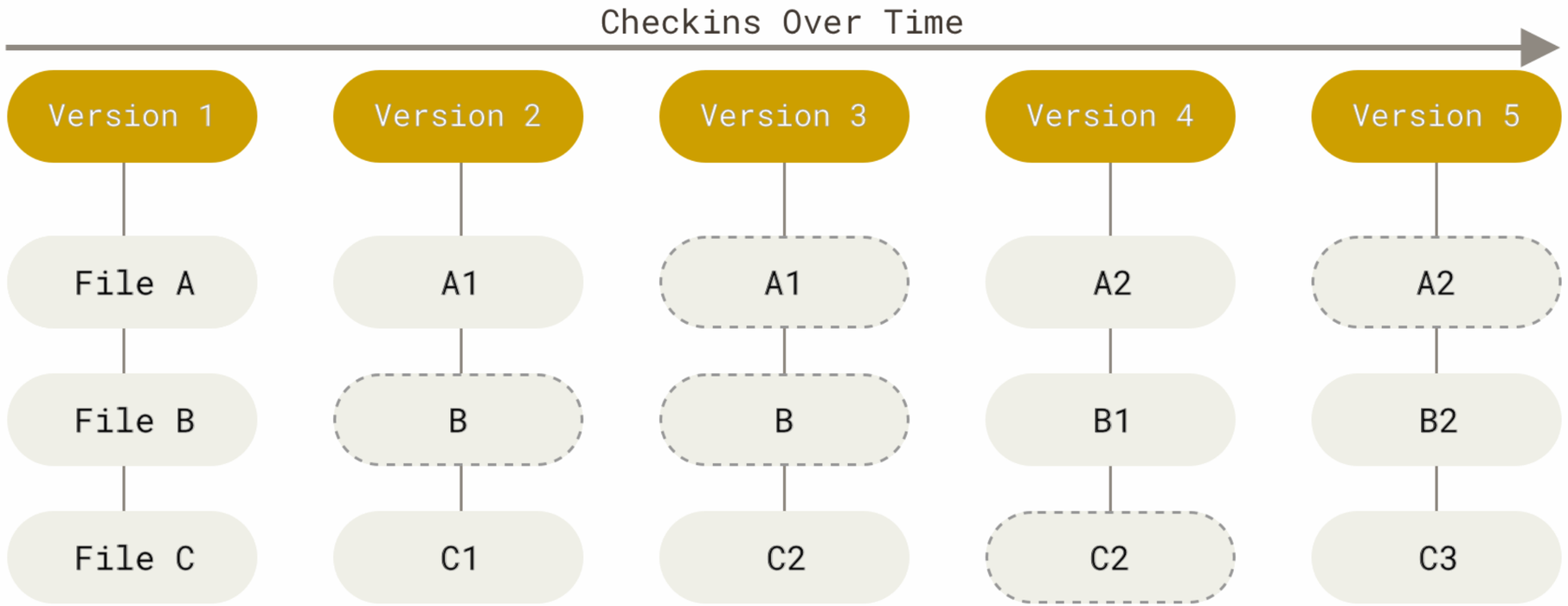
- Linux development, started 2005
- a version management system, i.e. tracks changes in project resources
- git takes snapshots of a managed project (image)
- distributed version control system (that means you always have a complete copy of your version history on your local computer)

VERSION CONTROL



Local version control diagram, in Pro Git by Scott Chacon and Ben Straub, licensed under CC BY-NC-SA 3.0

VERSIONS AS SNAPSHOTS

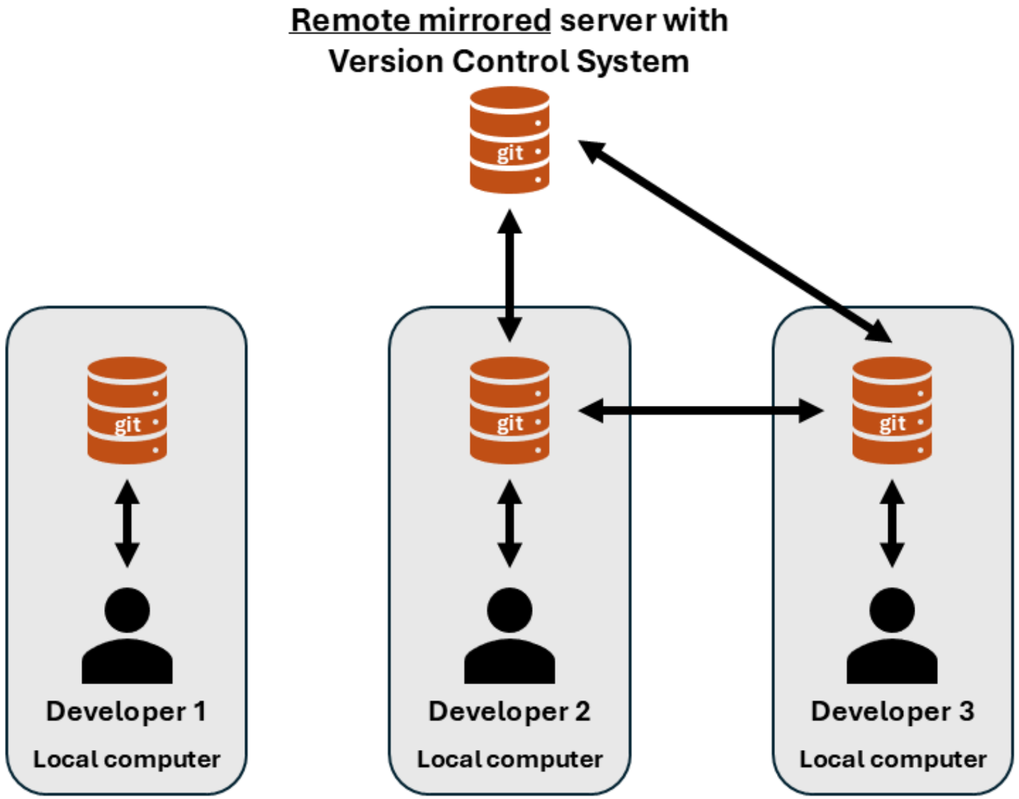


Versions as snapshots diagram, in Pro Git by Scott Chacon and Ben Straub, licensed under CC BY-NC-SA 3.0

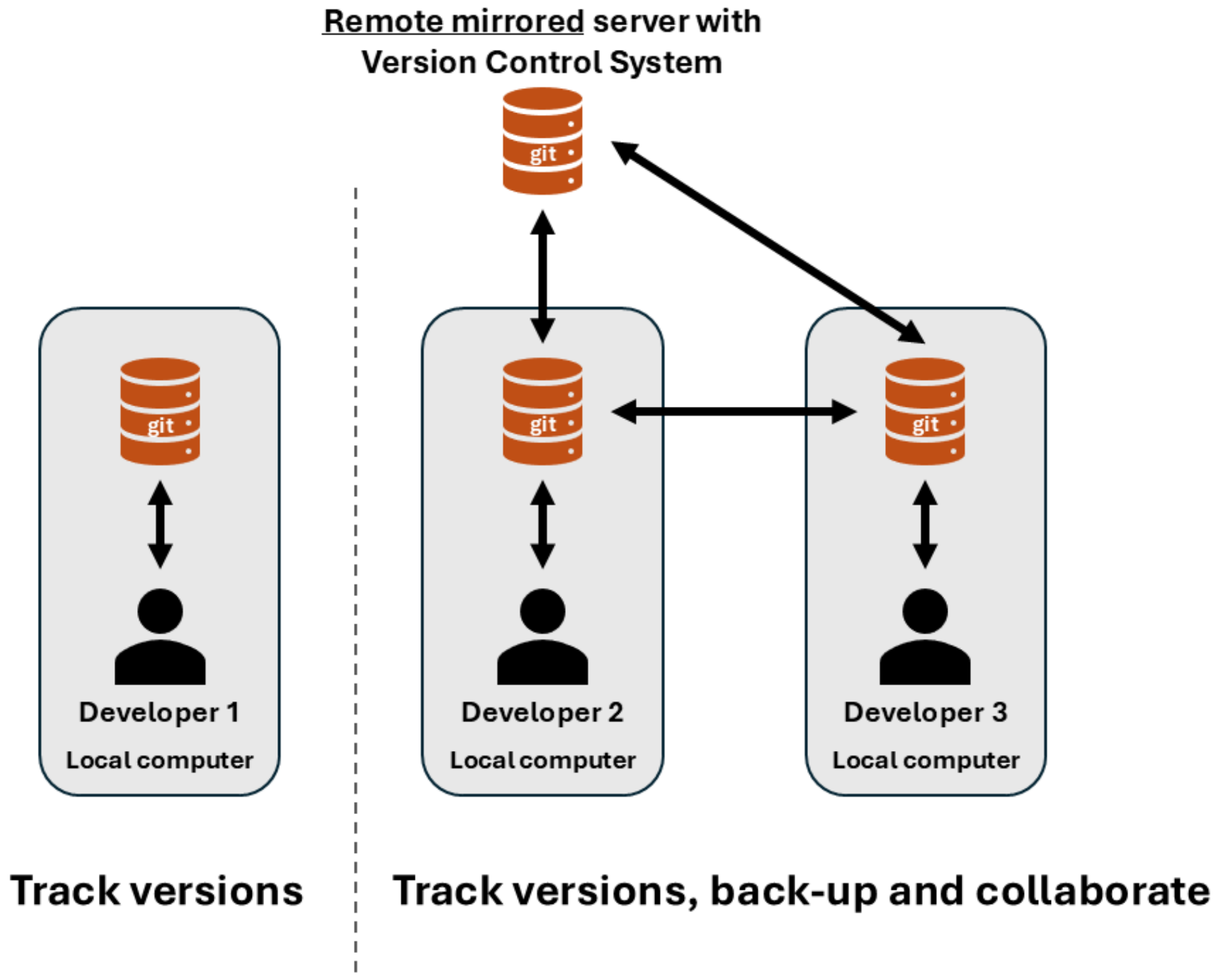
CENTRALIZED VERSION CONTROL

Examples: CVS, Subversion

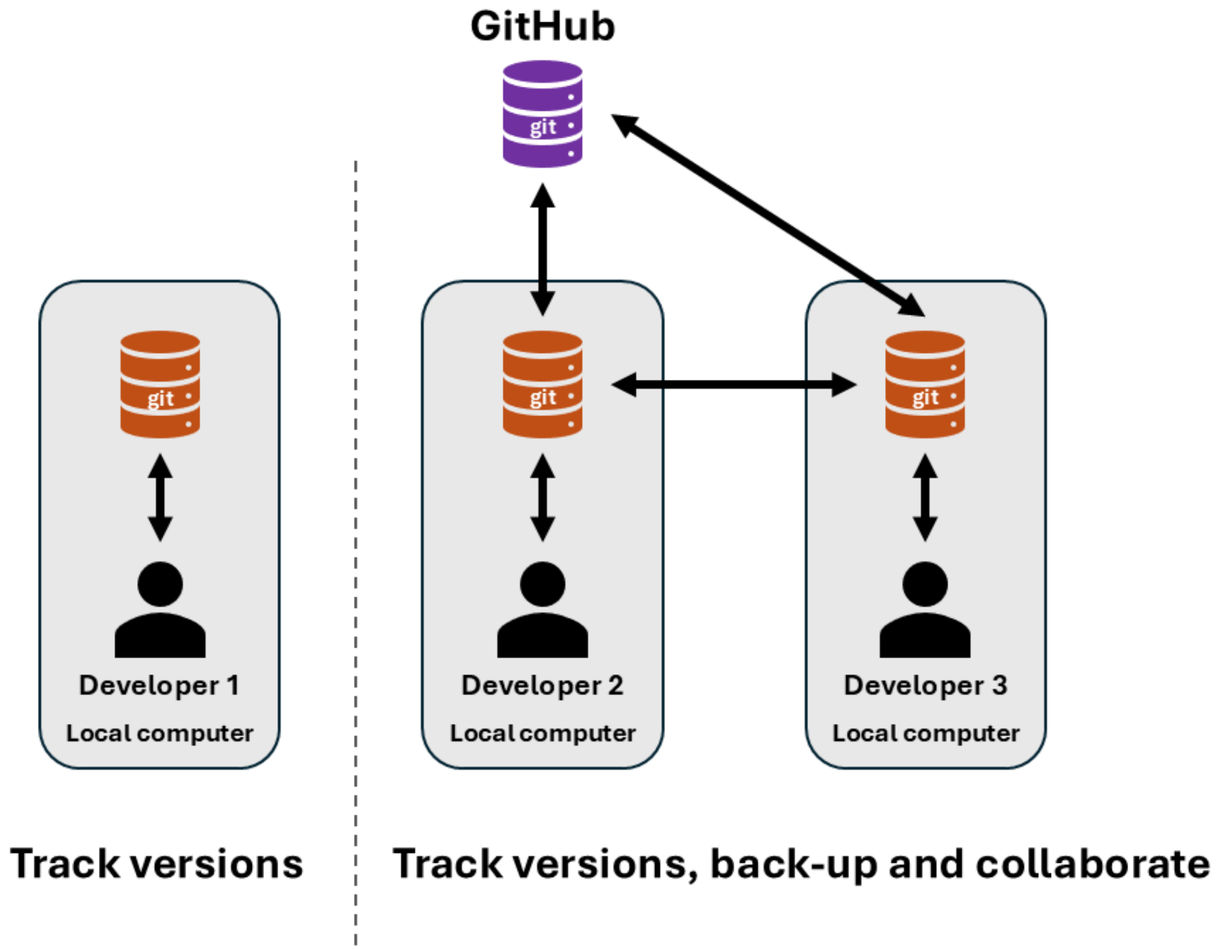
DISTRIBUTED VERSION CONTROL



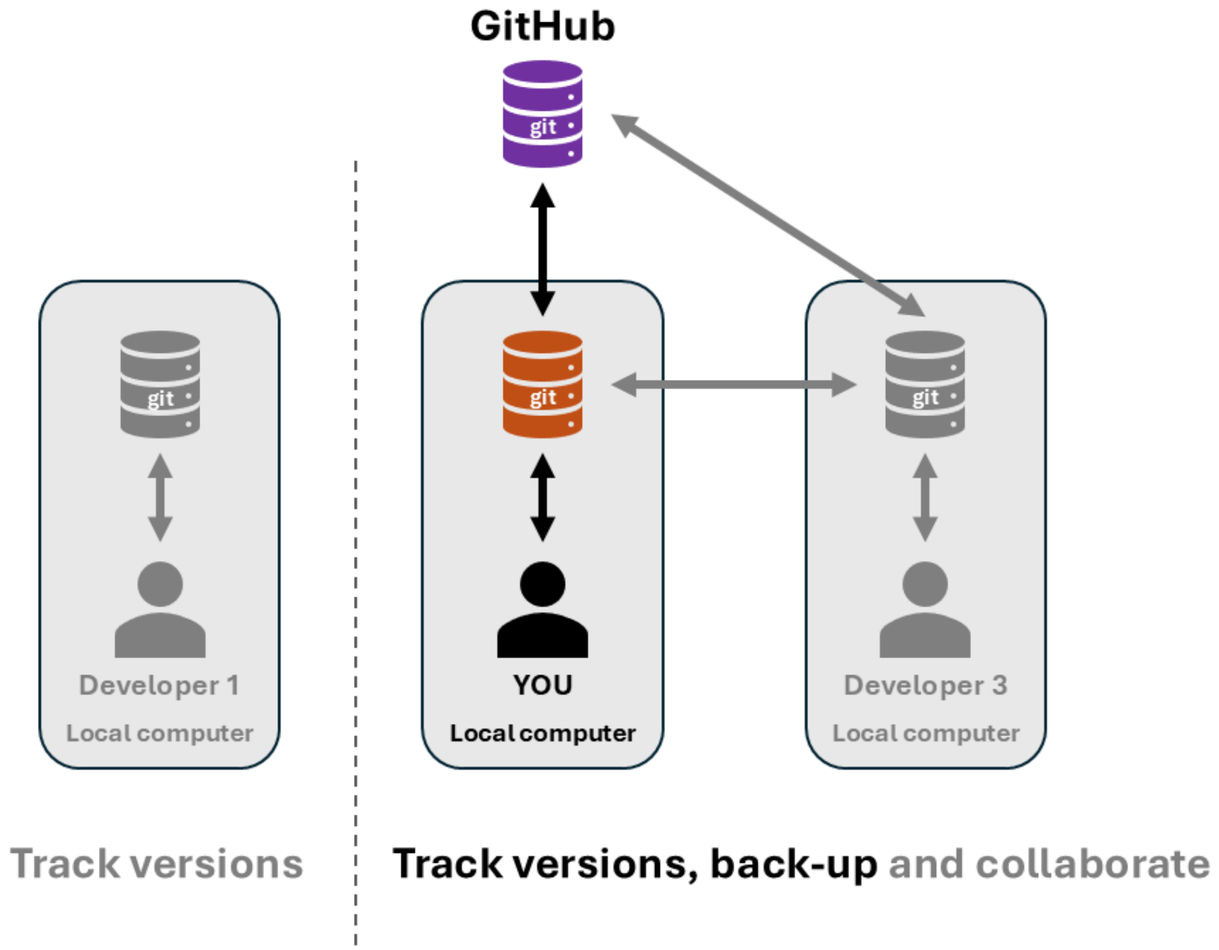
DISTRIBUTED VERSION CONTROL



GITHUB AS A HOSTED GIT REPO



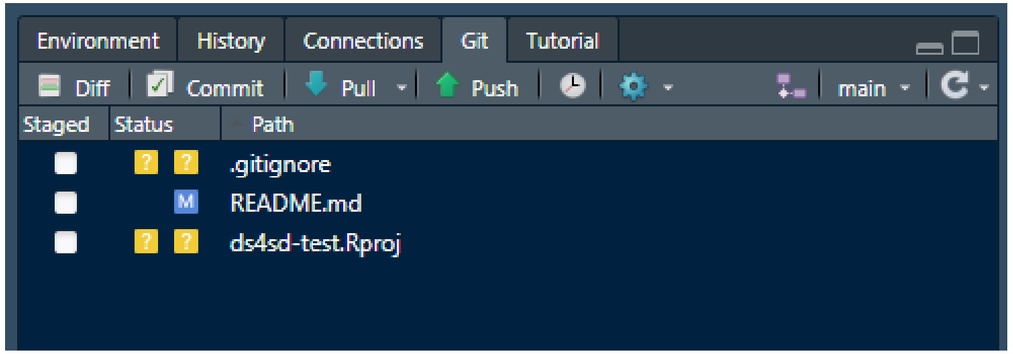
FOCUS FOR TODAY



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 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:

- install git locally (see (Bryan 2021))
- sign up for a Github account
- create a personal access token
  - 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 "John Doe"
$ git config --global user.email johndoe@example.com
```

Check your settings:

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

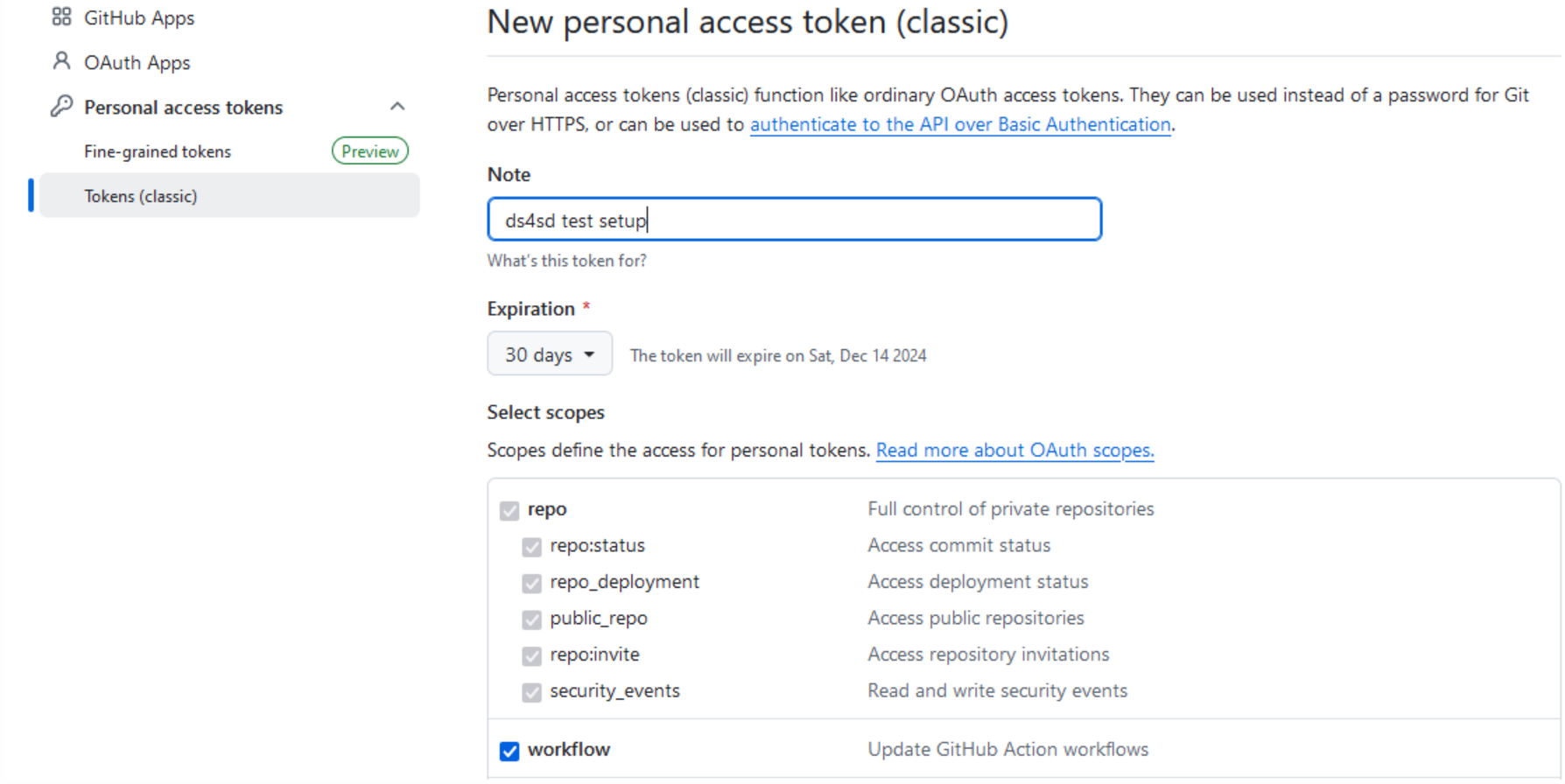
CREATE A PAT (PERSONAL ACCESS TOKEN)

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:



STORE THE PAT FOR LOCAL USE

Set the credentials from the command line:

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

Follow instructions and finally provide the PAT:

```
? Enter new password or token: ghp_xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx
-> Adding new credentials...
-> Removing credentials from cache...
-> Done.
```

ALTERNATIVE TO PATS

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

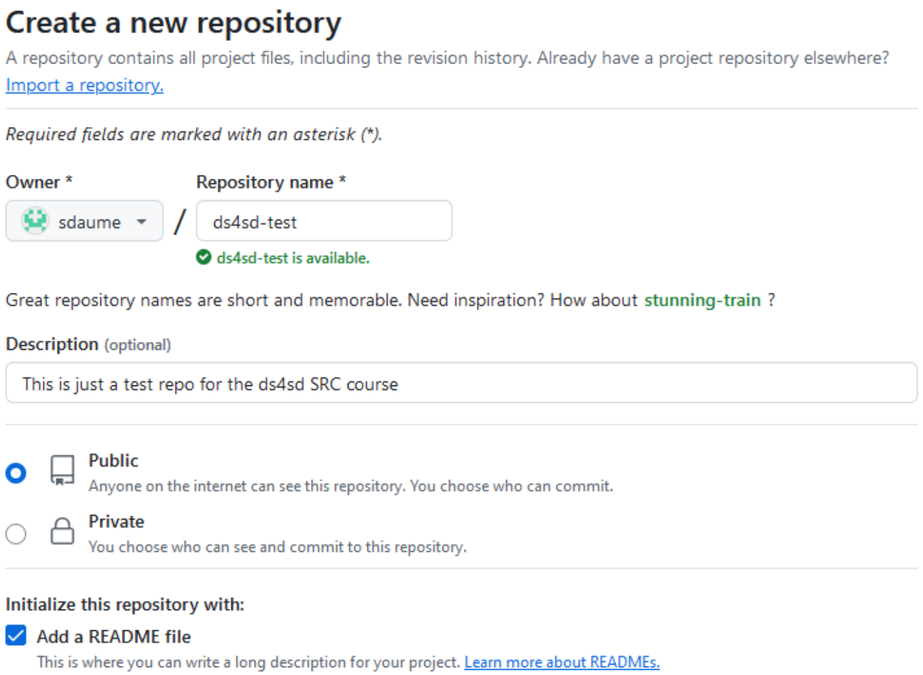
Consult **Set up keys for SSH** (Bryan 2021) to explore this option.

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”

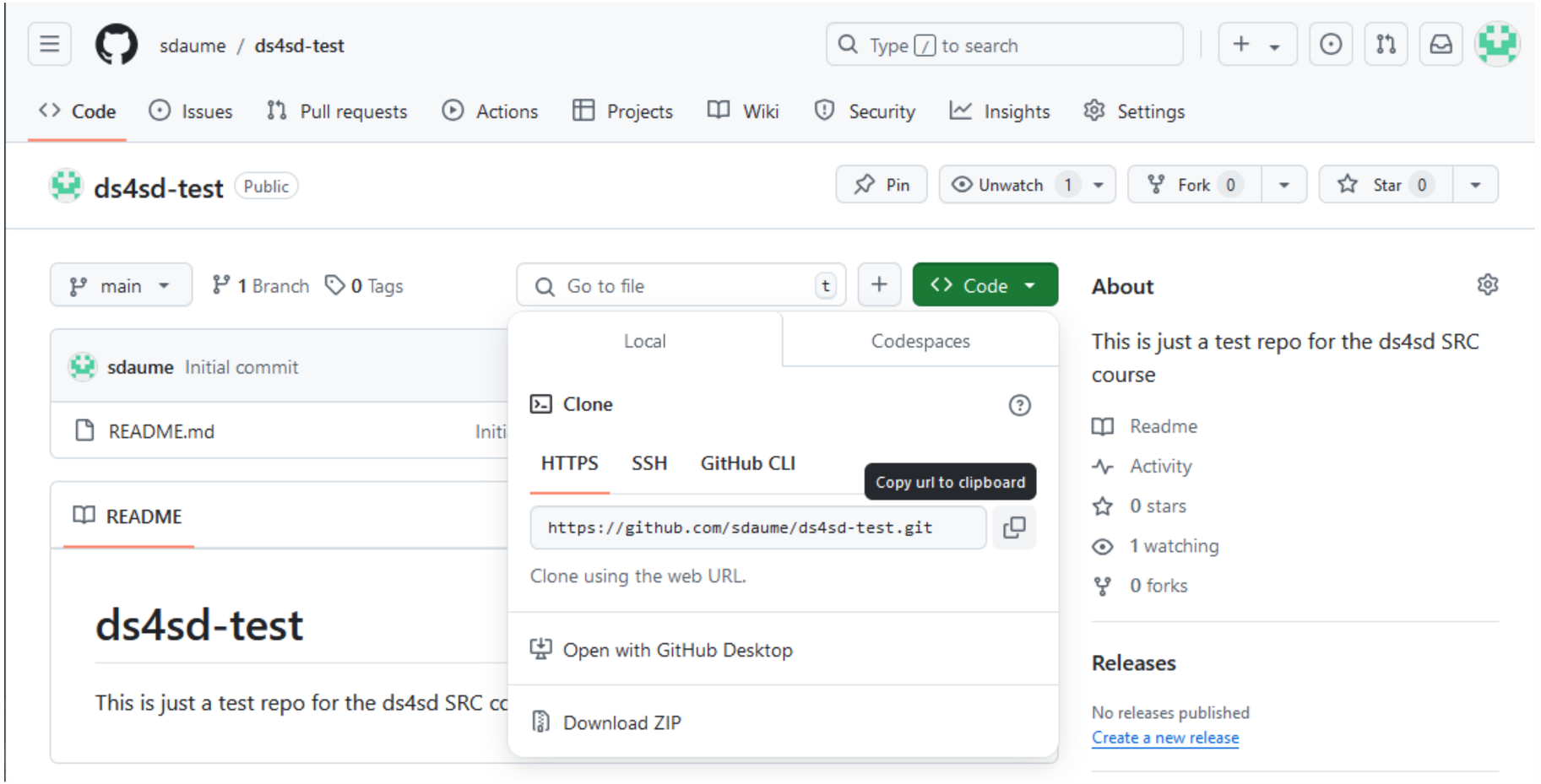
CREATE A NEW GITHUB REPO

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



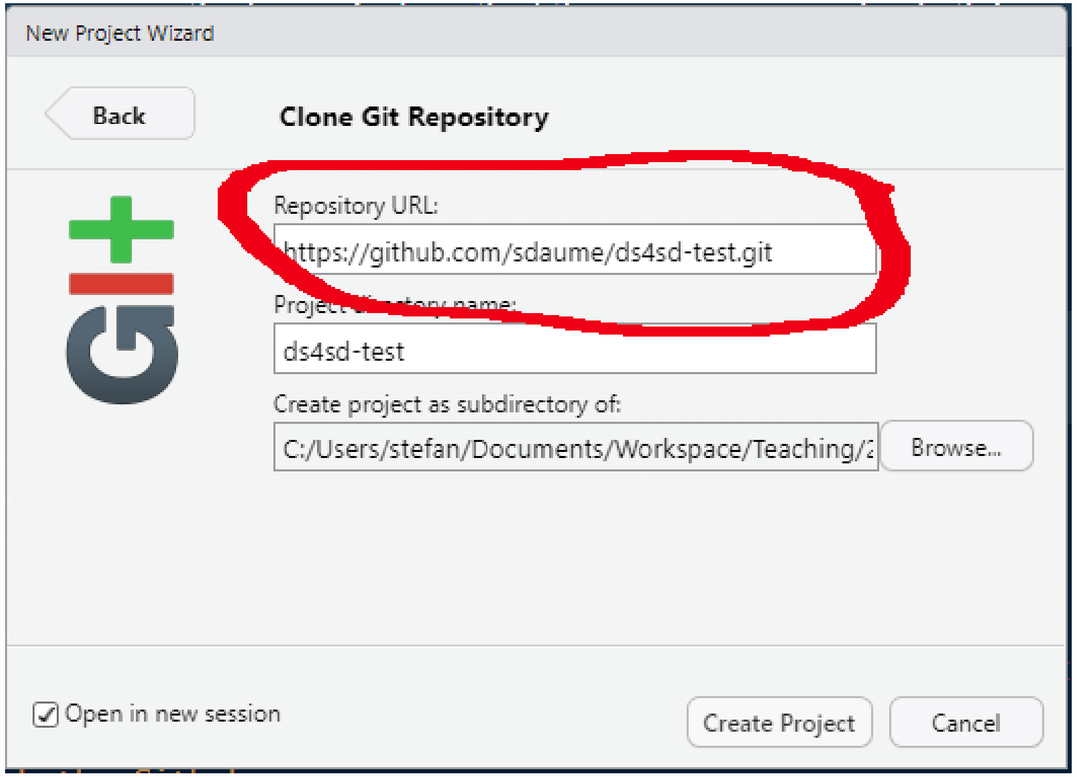
COPY THE REPO URL

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

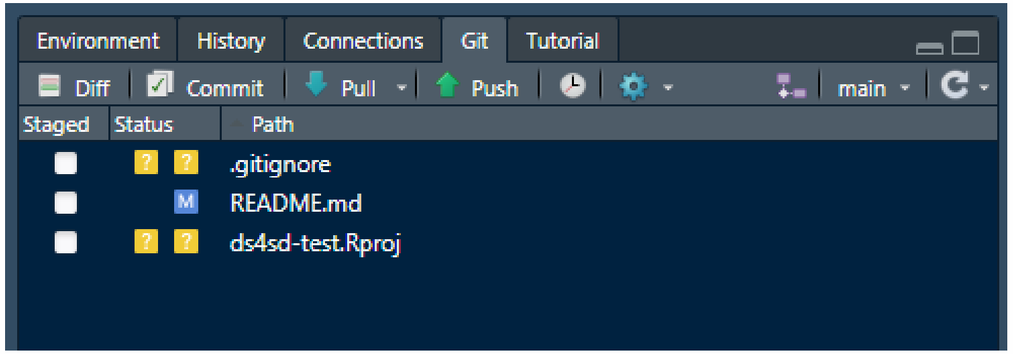


CREATE AN R STUDIO PROJECT WITH THE REPO

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



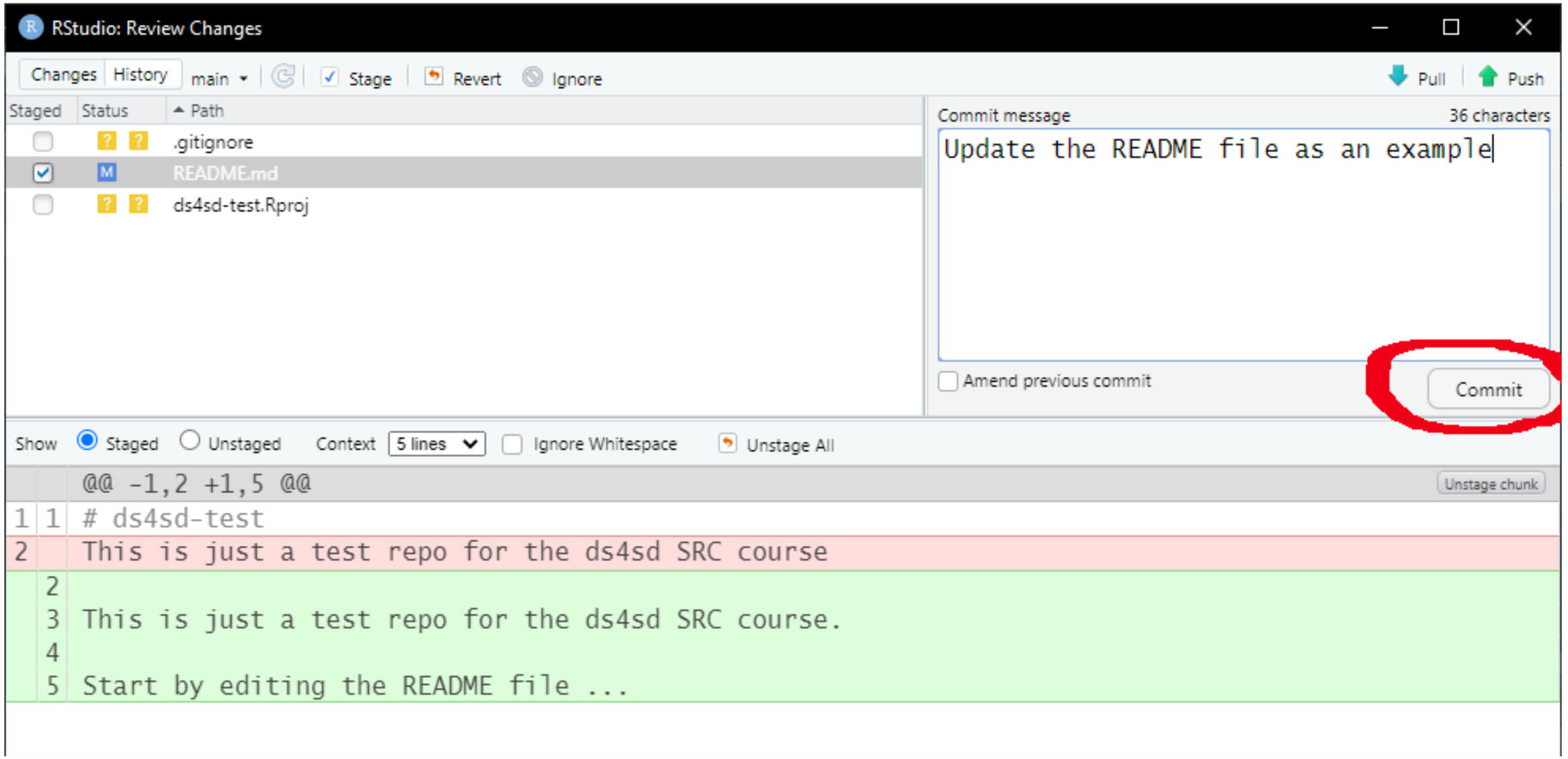
NEW PROJECT TRACKED WITH GIT



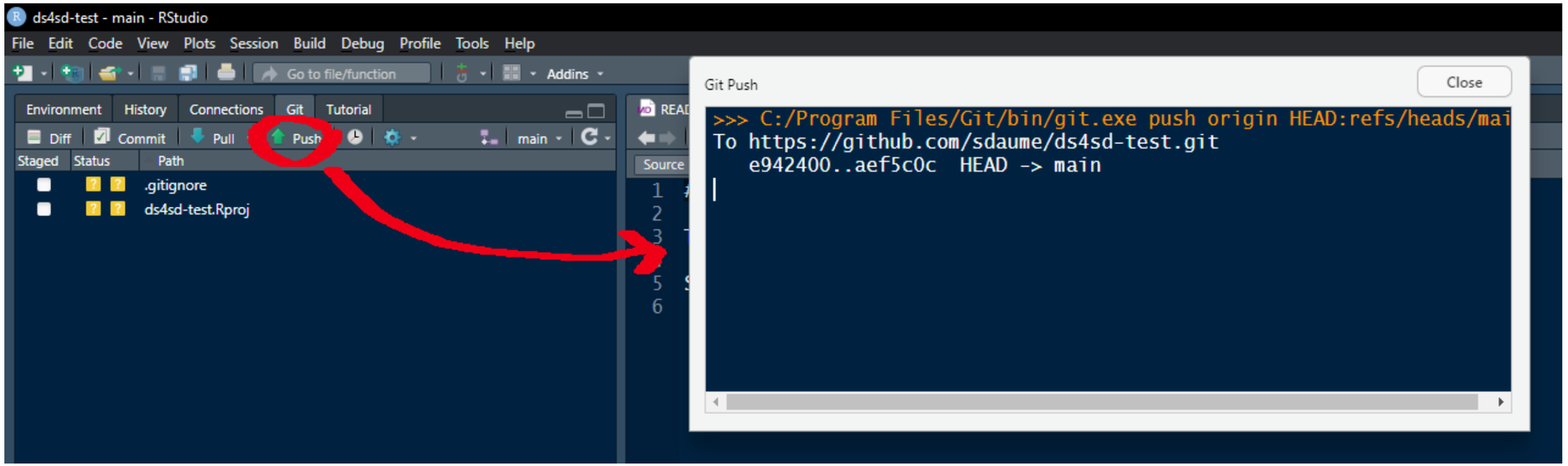
WHEN YOUR NEW PROJECT IS SET UP

- 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

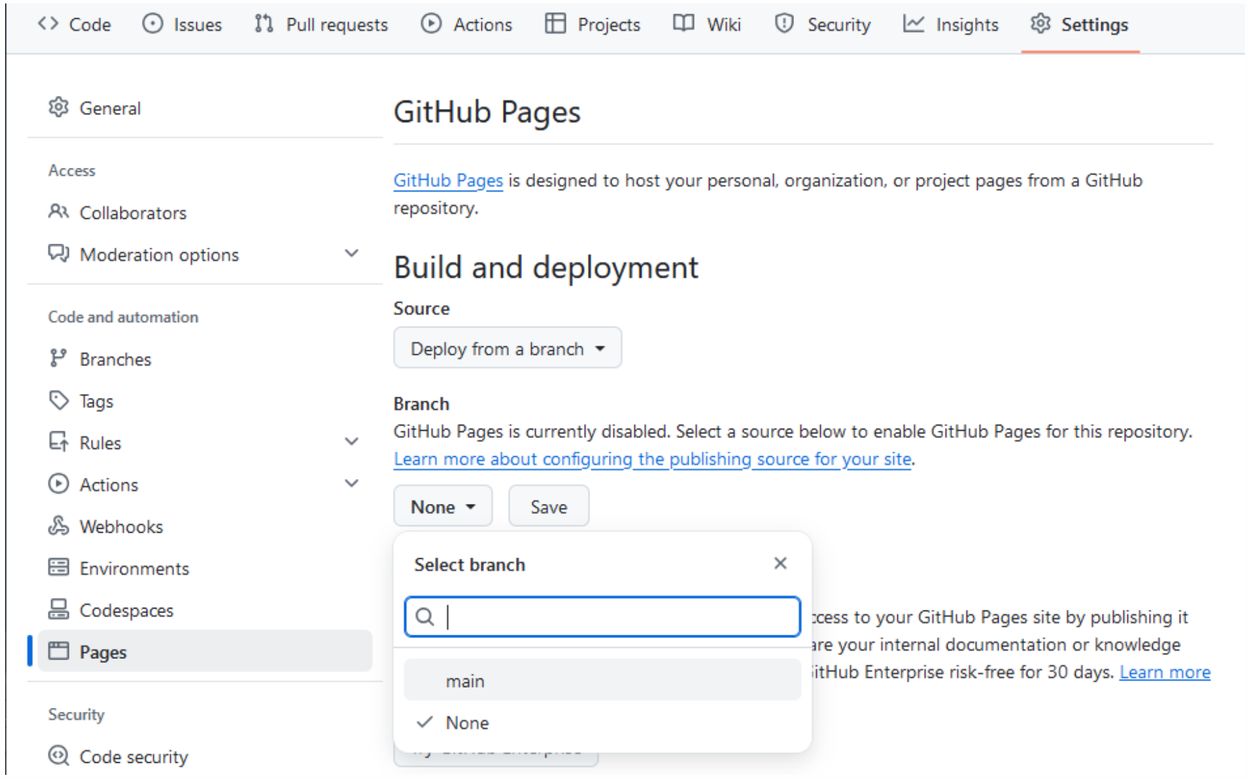


PUBLISH YOUR CONTENT

Repo content can be hosted online via GitHub pages.

ENABLE GITHUB PAGES FOR A REPO

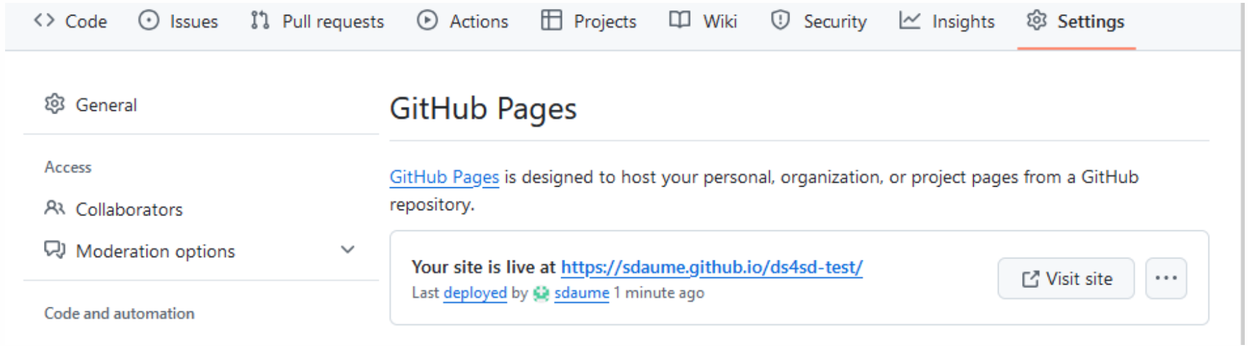
Go to *Settings* > *Pages* and select *Branch* > *main*



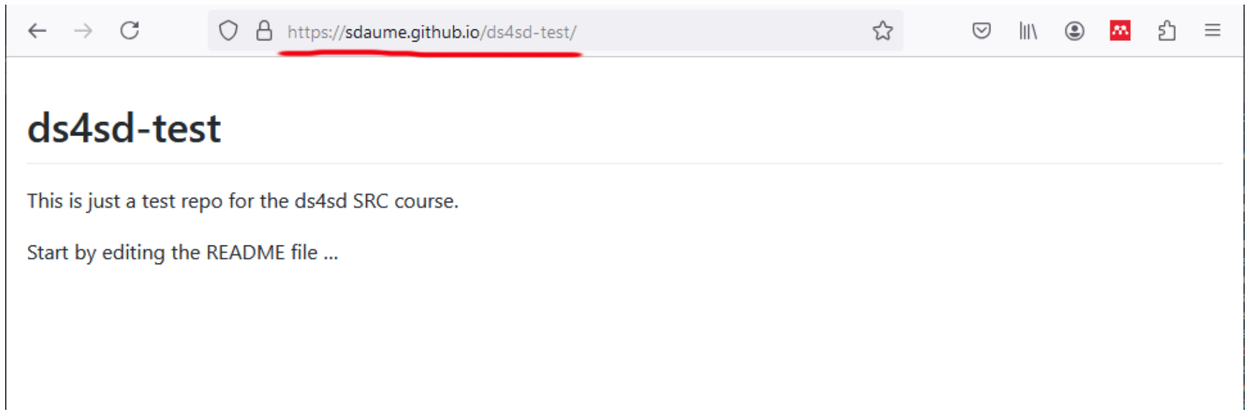
ONE GITHUB PAGE PER REPO

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/.

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
This presentation is delivered with the help of several free and open source tools and libraries. It utilises the reveal.js presentation framework and has been created using RMarkdown, knitr, RStudio and Pandoc. highlight.js provides syntax highlighting for code sections. MathJax supports the rendering of mathematical notations. PDF and JPG copies of this presentation were generated with DeckTape. Please note the respective licenses of these tools and libraries.

If not noted and attributed otherwise, the contents (text, charts, images) of this presentation are **Copyright © 2024 of the Author** and provided under a *CC BY 4.0* public domain license.