What they forgot to teach you about R

Scientific workflows: Tools and Tips 

4/20/23

Who am I?

- Ecologist, PhD student for some years and now scientific programmer

What is this lecture series?

Scientific workflows: Tools and Tips 🛠️

📅 Every 3rd Thursday 🕐 4-5 p.m. 📍 Webex

- One topic from the world of scientific workflows
- Topics range from R programming over notetaking, literature management tools and more
- For topic suggestions send me an email
- If you don't want to miss a lecture
  - Check out the lecture website
  - Subscribe to the mailing list
- Slides provided on Github

What they forgot to teach you about R

It's a book by J. Bryan and J. Hesters

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Background

- Reproducibility 
  - Can someone else reproduce my results?
- Reliability 
  - Will my code work in the future?
- Reusability 
  - Can someone else actually use my code?

Basis: Follow **best practices** to write clean, clear and maintainable code.

Chaotic projects and workflows ...

... can make even small changes frustrating and difficult.

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Clean projects and workflows ...

... allow you and others to work productively.

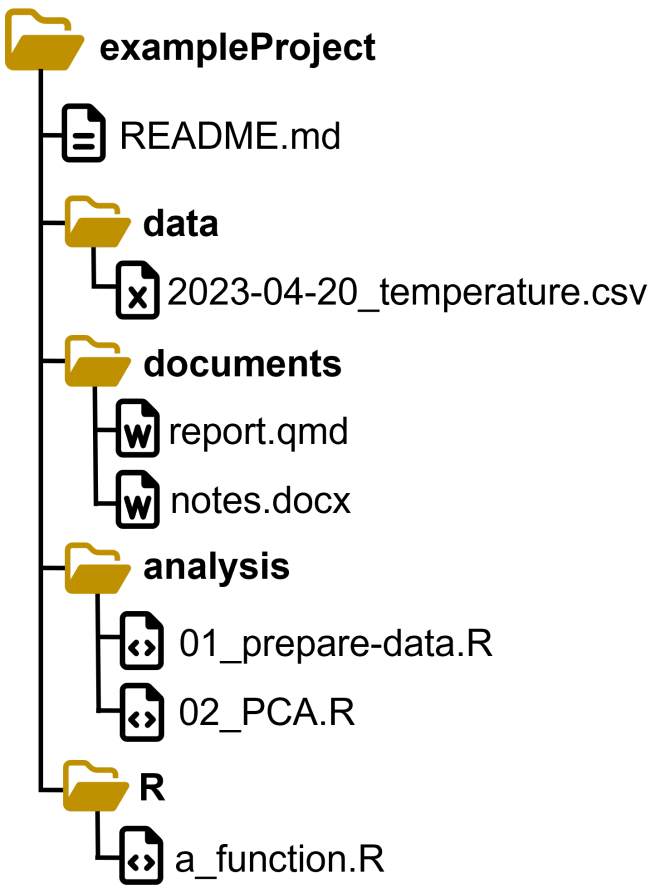
Artwork by Allsion Horst, CC BY 4.0

First things first

Project setup and structure

Keep your files togehter

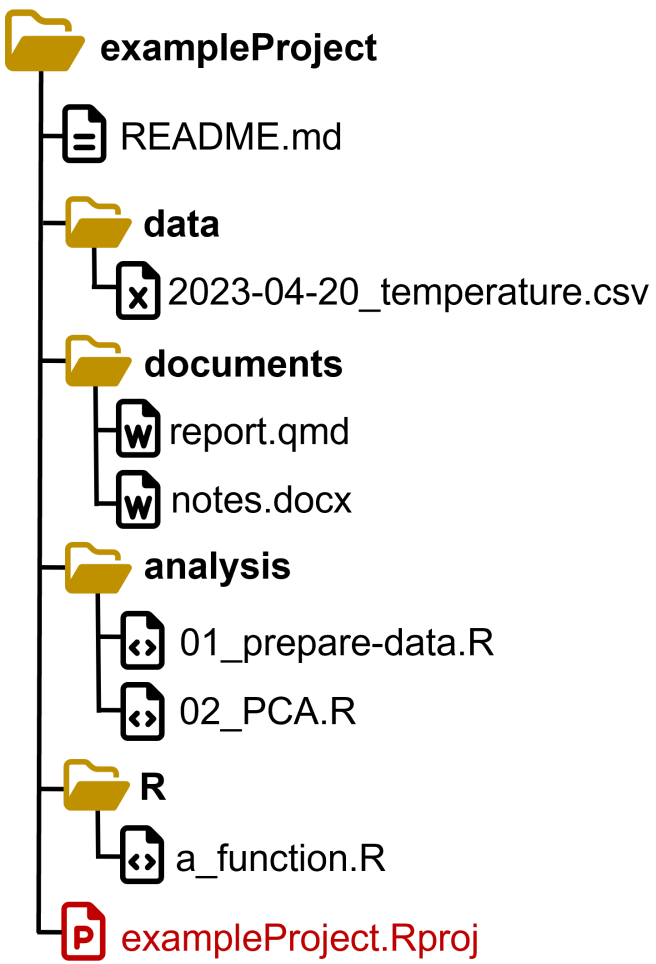
- Everything in one project folder
- Add a README file
  - Explain content of the project, where and how to start, whom to ask questions, …
- Separate folders for `data/`, `documents/`, `analysis/`, `R/` etc.
- Best structure depends on your type of project



Use R Studio projects

Always make your project an R Studio Project (if possible)!

- An R Studio Project is just a normal directory with an `*.Rproj` file
  - double-click this file to open your project in R Studio
- Advantages:
  - Easy to navigate in R Studio
  - Project root is the working directory
  - Open multiple projects in separate R Studio instances



Create an R Studio Project

From scratch:

1. `File -> New Project -> New Directory -> New Project`
2. Enter a directory name (this will be the name of your project)
3. Choose the directory where the project should be initiated
4. `Create Project`

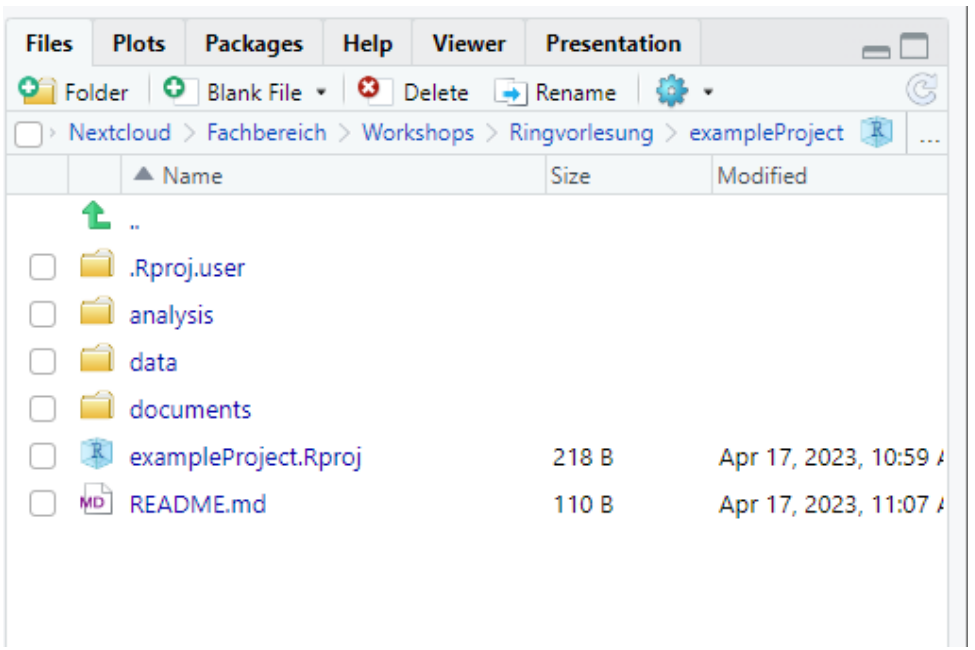
Associate an existing folder with an R Studio Project:

1. `File -> New Project -> Existing Directory`
2. Choose your project folder
3. `Create Project`

Navigate an R Studio Project

You can use the `Files` pane in R Studio to interact with your project folder:

- Navigate and open files
- Create files and folders
- Rename and delete
- …



Set up your project

R Studio offers a lot of settings and options.

So have a  and check out `Tools -> Global Options` and all the other buttons.

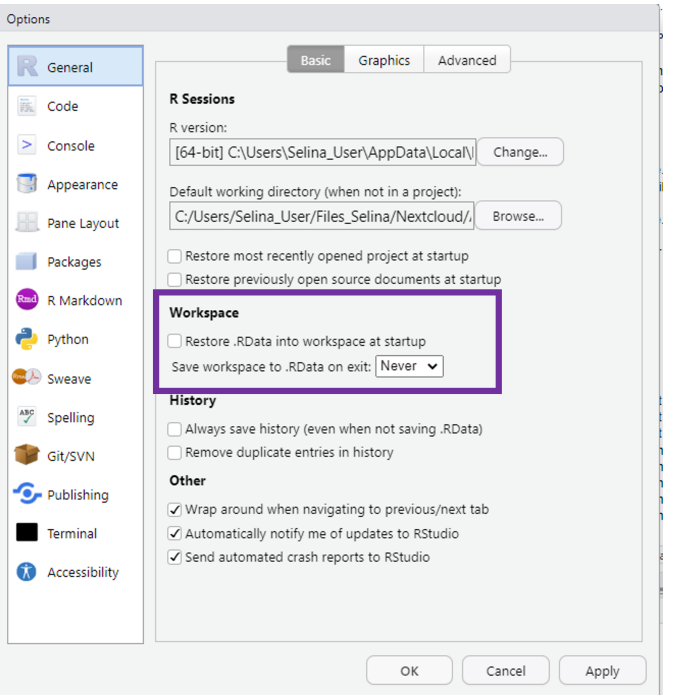
- R Studio cheat sheet that explains all the buttons
- Update R Studio from time to time to get new settings (`Help -> Check for Updates`)

Set up your project

R Studio offers a lot of settings and options.

Most important setting:

- Never save or restore your workspace as `.Rdata` -> You always want to start working with a clean slate



Other nice settings:

- Code display settings (`Code -> Display`), e.g. highlight colors or rainbow parentheses

Name your files properly

Your collaborators and your future self will love you for this.

Principles [1]

File names should be

1. Machine readable
2. Human readable
3. Working with default file ordering

1 From this talk by J. Bryan

1. Machine readable file names

Names should allow for easy **searching**, **grouping** and **extracting information** from file names (if needed).

- No whitespace & special characters
- Separate metadata to work with regular expressions (e.g. `_` to separate metadata and `-` to make it readable)

Bad examples ❌


`2023-04-20 temperature göttingen.csv`


`2023-04-20 rainfall göttingen.csv`

Good examples ✅


`2023-04-20_temperature_goettingen.csv`


`2023-04-20_rainfall_goettingen.csv`

2. Human readable file names

Which file names would you like to read at 4 a.m. in the morning?

- File names should reveal the file content
- Use separators to make it readable

Bad examples ❌


`01preparedataforanalysis.R`


`01firstscript.R`

Good examples ✔


`01_prepare-data-for-analysis.R`


`01_lm-temperature-trend.R`

3. Default ordering

If you order your files by name, the ordering should make sense:

- (Almost) always put something numeric first
  - Left-padded numbers (`01`, `02`, ...)
  - Dates in `YYYY-MM-DD` format

Chronological order


`2023-04-20_temperature_goettingen.csv`

`2023-04-21_temperature_goettingen.csv`

Logical order


`01_prepare-data.R`

`02_lm-temperature-trend.R`

`helper01_load-data.R`

Let's start coding

Follow coding guidelines

> "It's harder to read code than to write it."
> — Joel Spolsky

- Try to write code that others (i.e. future you) can understand
- Follow standard style guides for readable and maintainable code
  - I recommend tidyverse styleguide

Standard code structure

1. General comment with purpose of the script, author, …
2. `library()` calls on top
3. Set default variables and global options
4. Source additional code
5. Write the actual code, starting with loading all data files

```
# This code replicates figure 2 from the
# Baldauf et al. 2022 Journal of Ecology pa
# Authors: Selina Baldauf, Jane Doe, Jon Do

library(tidyverse)
library(vegan)

# set defaults
input_file <- "data/results.csv"

# source files
source("R/my_cool_function.R")

# read input
input_data <- read_csv(input_file)
```

Mark sections

- Use comments to break up your file into sections

```
# Load data ------------------------------------------------------------

input_data <- read_csv(input_file)

# Plot data ------------------------------------------------------------

ggplot(input_data, aes(x = x, y = y)) +
  geom_point()
```

- Insert a section label with `Ctrl/Cmd + Shift`
- Navigate sections in the file outline

Split your workflow

- Don't put all analysis into one long file
  - Write multiple files that can be called sequentially
    - Store results as `.Rdata` if you don't want always run the script
  - Write functions that can be called in other scripts
- Use the `source()` function to source these files
- Have main workflow files that manage your workflow

Split your workflow

01_prepare-data.R

```r
# Purpose: Calculate daily mean temperature and store in data/
# Authors: Selina Baldauf
library(data.table)

# read raw data
temperatures <- data.table::fread("data/huge_temperature_dataset.csv")

# calculate daily mean temperature
temperature_mean <- temperatures[, mean := mean(temperature), by = c("city", "date")]

# save as .Rdata file
save(temperature_mean, file = "data/temperature_mean.Rdata")
```

02_linear-model-analysis.R

```r
# Purpose: Conduct linear model analysis of daily mean temperature in cities
# Authors: Selina Baldauf

load(file = "data/temperature_mean.Rdata")

# linear model
temp_lm <- lm(temperature ~ date, data = temperature_mean)
```

Split your workflow

R/helper01_prepare-data.R

```
# Purpose: Function to read and prepare data for analysis
# Authors: Selina Baldauf
prepare_data <- function(path) {
  the_data <- readr::read_csv(file = path)
  the_data <- the_data %>%
    group_by(city) %>%
    summarize(temperature = mean(temperature))
}
```

analysis/01_linear-model-analysis.R

```
# Purpose: Conduct linear model analysis of daily mean temperature in cities
# Authors: Selina Baldauf

input_file <- "data/huge_temperature_dataset.csv"

source("R/helper01_prepare-data.R")

# read and prepare the data
temperature <- prepare_data(path = input_file)
```

Use save paths

To read and write files, you need to tell R where to find them.

Common workflow: set **working directory** with `setwd()`, then read files from there. But to this Jenny Bryan said:

> If the first line of your R script is
> `setwd("C:\Users\jenny\path\that\only\I\have")`
> I will come into your office and SET YOUR COMPUTER ON FIRE 🔥.

Why?

This is **100% not reproducible**: Your computer at exactly this time is (probably) the only one in the world that has this working directory

Avoid `setwd()` if it is possible in any way!

Avoid `setwd()`

Use R Studio projects

- Project root is automatically the working directory
- Give your project to a friend at it will work on their machine as well

Instead of

```
# my unique path from hell with Windows delimiters, white space and special characters
setwd("C:\Users\Selina's PC\My Projects\Göttingen Temperatures\temperatures")

read_csv("data/2023-04-20_temperature_goettingen.csv")
```

You just need

```
read_csv("data/2023-04-20_temperature_goettingen.csv")
```

Avoid `setwd()`

Use the `{here}` package for reproducible paths

- Define the location of your scripts relative to a project root
- `here` will automatically determine the project root based on this
  - `here` will also recognize an `.Rproj` file as a project root
- Build your paths with the `here()` function relative to the project root

```
# Check where my here project root is
here::dr_here()

# set a path relative to the project root and read file
readr::read_csv(here::here("data/2023-04-20_temperature_goettingen.csv"))
```

Write beautiful code

Artwork by Allsion Horst, CC BY 4.0

- Every programming language has one/many styleguides
  - For R: tidyverse style guide
- Style guides define
  - File names and code organization
  - Syntax standards (naming convention, spacing, …)
  - …

Coding style - Object names

- Variables and function names should only have lowercase letters, numbers, and _
- Use snake_case for longer variable names
- Try to use concise but meaningful names

```
# Good
day_one
day_1

# Bad
DayOne
dayone
first_day_of_the_month
dm1
```

Coding style - Object names

- Variables and function names should only have lowercase letters, numbers, and _
- Use snake_case for longer variable names
- Try to use concise but meaningful names
- Avoid re-using names of common functions and variables

```
# Bad
T <- data.frame(temperature = 1:10)
c <- 10
data_frame <- data.frame(temperature = 1:10)
sum <- function(x) mean(x)
```

Coding style - Spacing

- Always put spaces after a comma

```
# Good
x[, 1]

# Bad
x[ , 1]
x[,1]
x[ ,1]
```

Coding style - Spacing

- Always put spaces after a comma
- No spaces around parentheses for normal function calls

```
# Good
mean(x, na.rm = TRUE)

# Bad
mean (x, na.rm = TRUE)
mean ( x, na.rm = TRUE )
```

Coding style - Spacing

- Always put spaces after a comma
- No spaces around parentheses for normal function calls
- Spaces before and after `()` in `if` or `for`

```
# Good
if (debug) {
  show(x)
}

# Bad
if(debug){
  show(x)
}
```

Coding style - Spacing

- Always put spaces after a comma
- No spaces around parentheses for normal function calls
- Spaces before and after `()` in `if` or `for`
- Spaces around most operators (`<-`, `==`, `+`, etc.)

```
# Good
height <- (feet * 12) + inches
mean(x, na.rm = TRUE)

# Bad
height<-feet*12+inches
mean(x, na.rm=TRUE)
```

Coding style - Spacing

- Always put spaces after a comma
- No spaces around parentheses for normal function calls
- Spaces before and after `()` in `if` or `for`
- Spaces around most operators (`<-`, `==`, `+`, etc.)
- Spaces before pipes (`%>%`, `|>`) followed by new line

```
# Good
iris %>%
  group_by(Species) %>%
  summarize_if(is.numeric, mean) %>%
  ungroup()

# Bad
iris %>% group_by(Species) %>% summarize_all(mean) %>% ungroup()
```

Coding style - Spacing

- Always put spaces after a comma
- No spaces around parentheses for normal function calls
- Spaces before and after `()` in `if` or `for`
- Spaces around most operators (`<-`, `==`, `+`, etc.)
- Spaces before pipes (`%>%`, `|>`) followed by new line
- Spaces before in ggplot `+` followed by new line

```
# Good
ggplot(aes(x = Sepal.Width, y = Sepal.Length, color = Species)) +
  geom_point()

# Bad
ggplot(aes(x = Sepal.Width, y = Sepal.Length, color = Species))+geom_point()
```

Coding style - Line width

Try to limit your line width to 80 characters.

- You don't want to scroll to the right to read all code
- 80 characters can be displayed on most displays and programs
- Split your code into multiple lines if it is too long

```
# Bad
iris %>%
  group_by(Species) %>%
  summarise(Sepal.Length = mean(Sepal.Length), Sepal.Width = mean(Sepal.Width), Species =

# Good
iris %>%
  group_by(Species) %>%
  summarise(
    Sepal.Length = mean(Sepal.Length),
    Sepal.Width = mean(Sepal.Width),
    Species = n_distinct(Species)
  )
```

Coding style

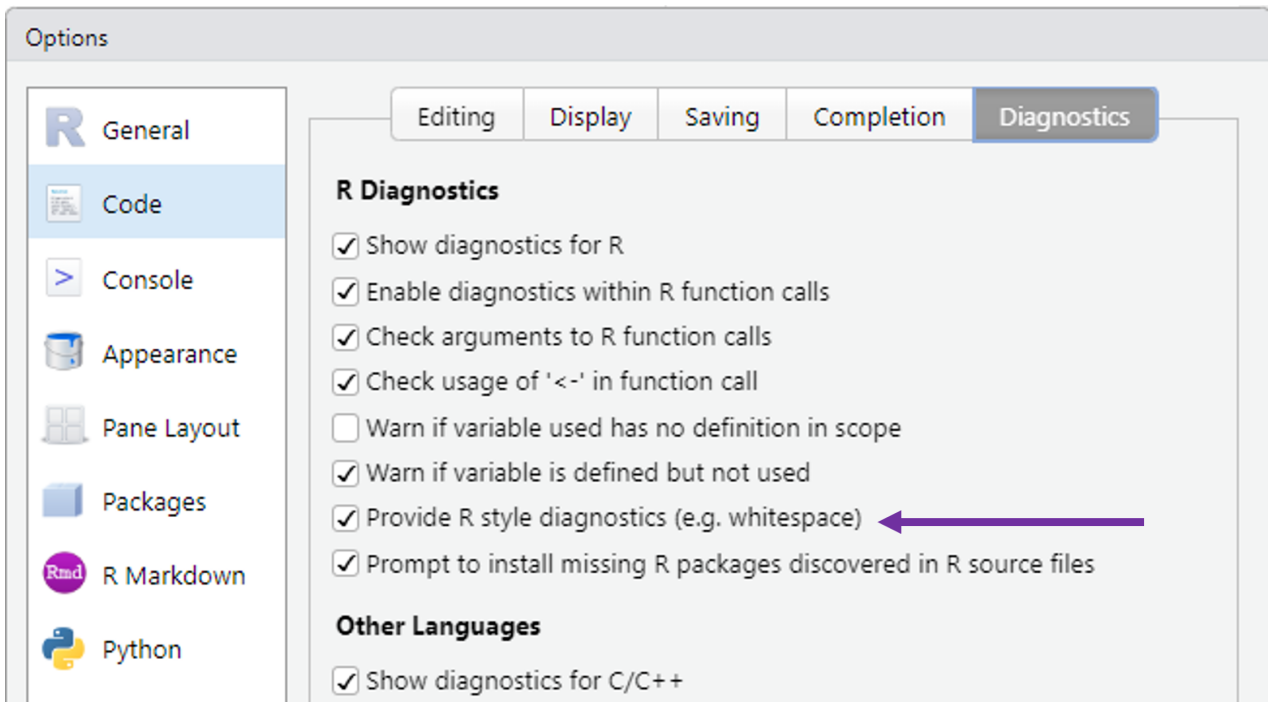
Do I really have to remember all of this?

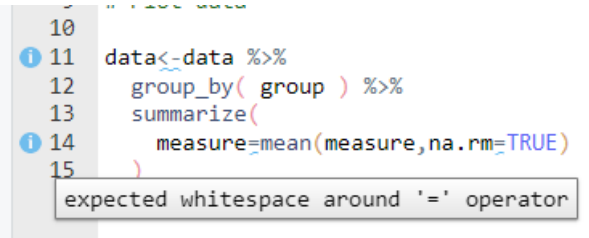
Luckily, no! R and R Studio provide some nice helpers

Coding style helpers - R Studio

R Studio has style diagnostics that tells you where something is wrong

- `Tools -> Gloabl Options -> Code -> Diagnostics`

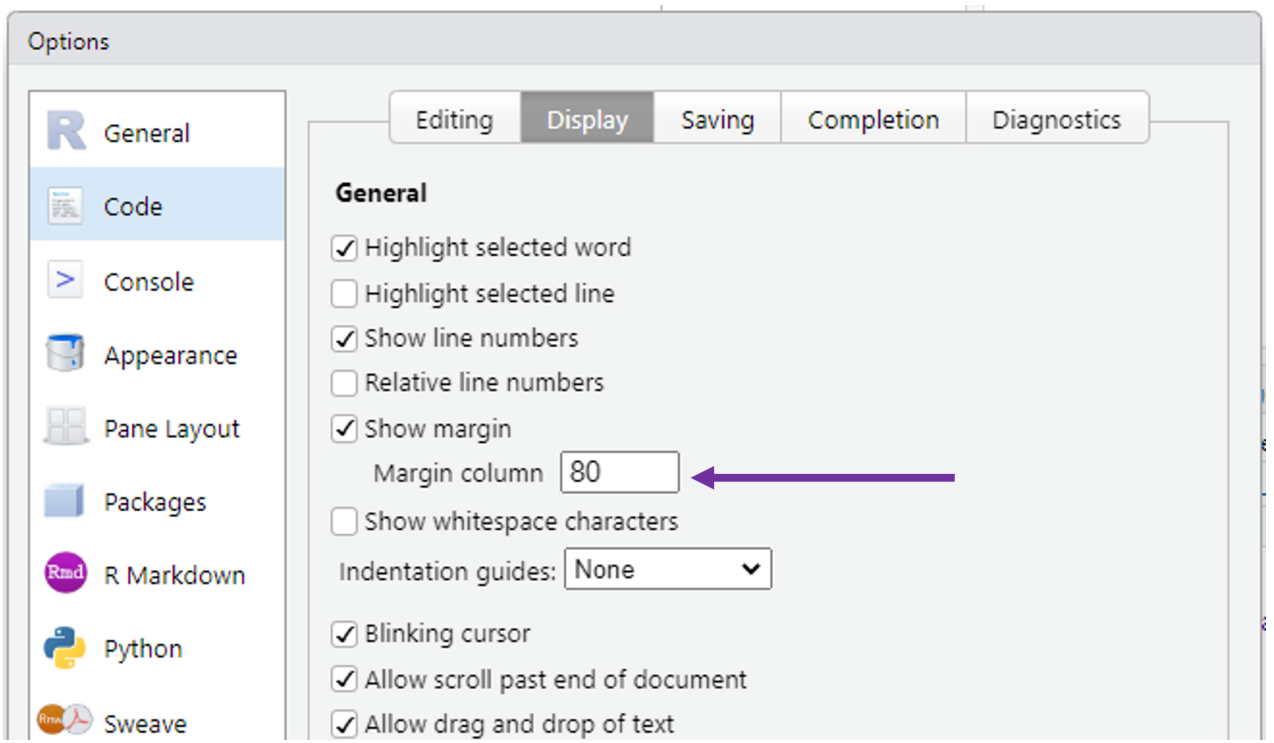


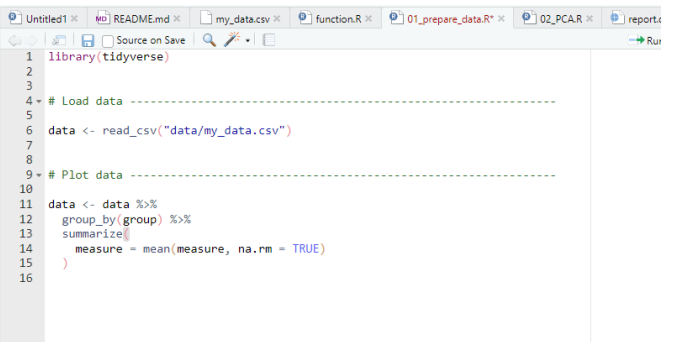


Coding style helpers - R Studio

You can show a margin line to help you keep 80 characters line width

- `Tools -> Gloabl Options -> Code -> Display`



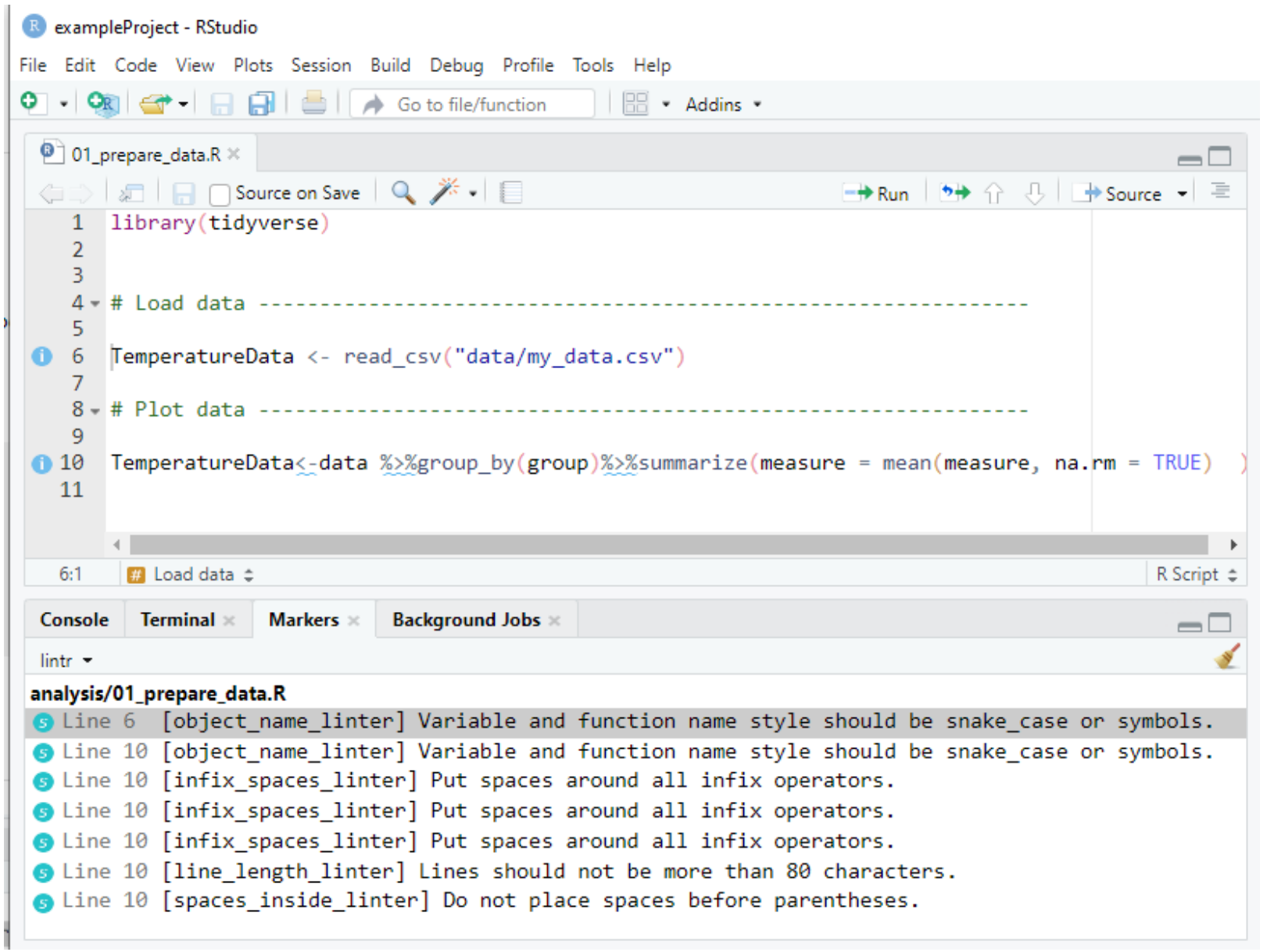


Coding style helpers - {lintr}

The lintr package analyses your code files or entire project and tells you what to fix.

```
# install the package before you can use it
install.packages("lintr")
# lint specific file
lintr::lint(filename = "analysis/01_prepare_data.R")
# lint a directory (by default the whole project)
lintr::lint_dir()
```

Coding style helpers - {lintr}

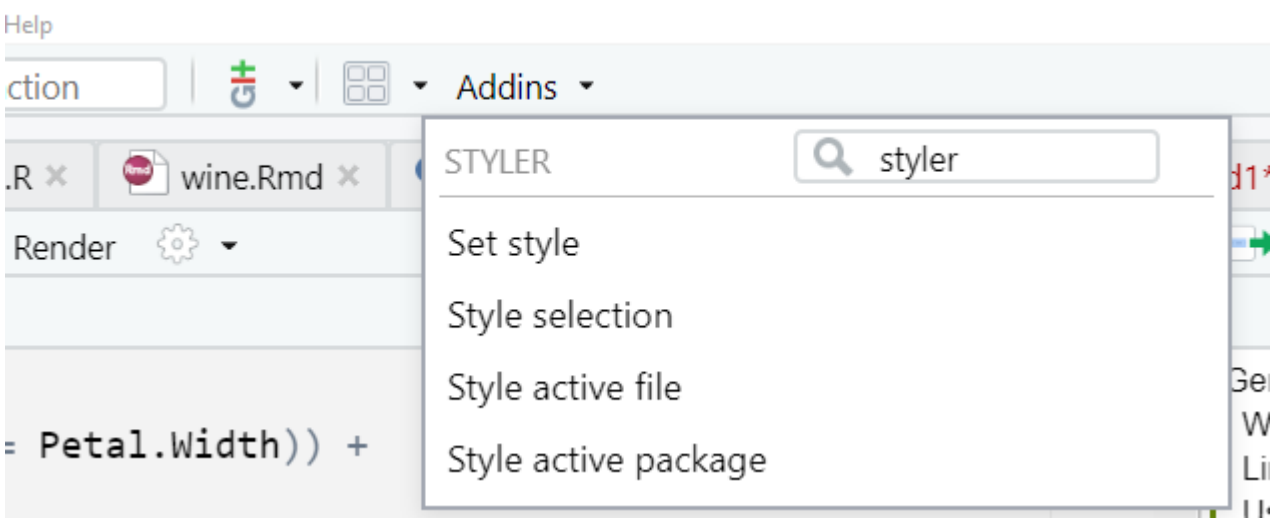


Coding style helpers - {styler}

The styler package package automatically styles your files and projects according to the tidyverse style guide.

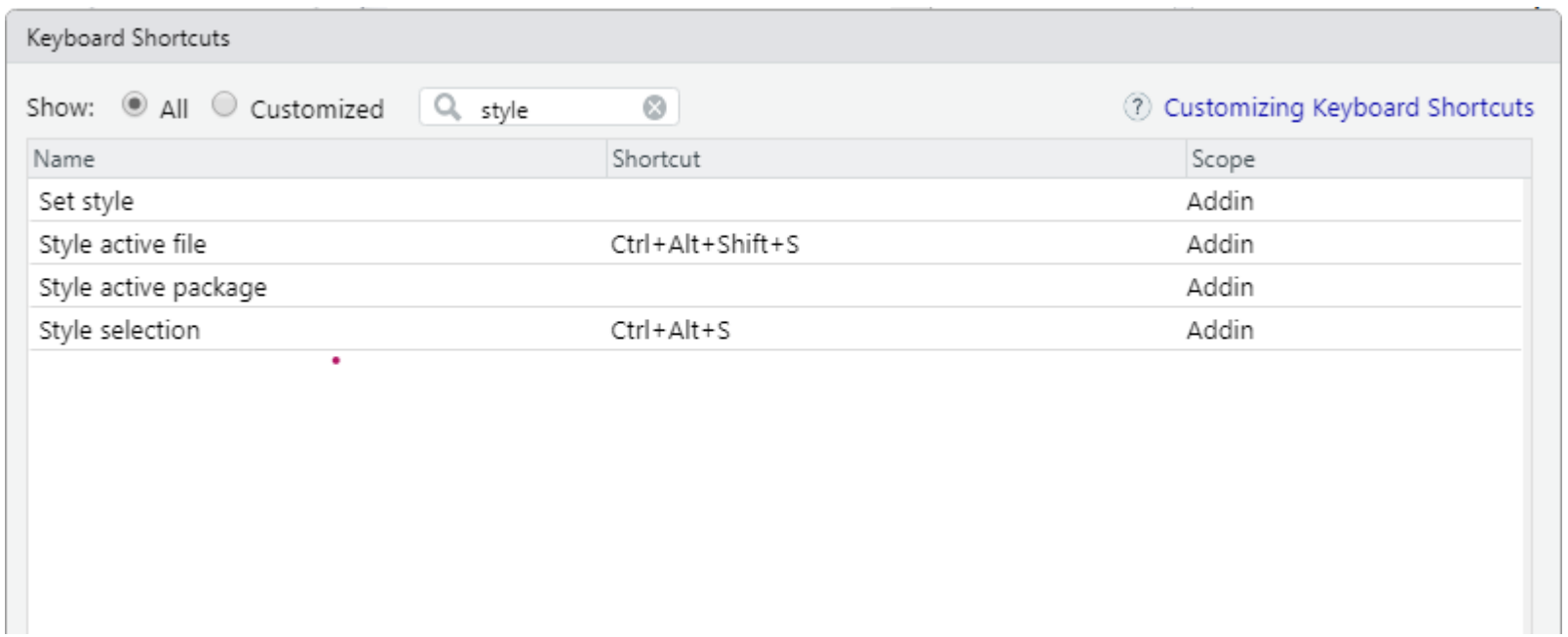
```
# install from CRAN
install.packages("styler")
```

- Use the R Studio `Addins` for styler:



Coding style helpers - {styler}

- Pro-Tip: Add a custom keyboard short cut to style your files
  - `Tools -> Modify Keyboard Shortcuts`



Manage dependencies with {renv}

Idea: Have a **project-local environment** with all packages needed by the project

- Keep log of the packages and versions you use
- Restore the local project library on other machines

Why this is useful?

- Code will still work even if packages upgrade
- Collaborators can recreate your local project library with one function
- Explicit dependency file states all dependencies

Check out the renv website for more information

Manage dependencies with {renv}

```
# Get started
install.packages("renv")
```

Very simple to use and integrate into your project workflow:

```
# Step 1: initialize a project level R library
renv::init()
# Step 2: save the current status of your library to a lock file
renv::snapshot()
# Step 3: restore state of your project from renv.lock
renv::restore()
```

- Your collaborators only need to install the `renv` package, then they can also call `renv::restore()`
- When you create an R Studio project there is a check mark to initialize with `renv`

Summary

Take aways

There are a lot of things that require minimal effort and that you can start to implement into your workflow NOW

1. Use R Studio projects -> Avoid `setwd()`!
2. Keep your projects clean

- Sort your files into folders
- Give your files meaningful names

3. Use `styler` to style your code automatically
4. Use `lintr` and let R analyse your project
5. Consider `renv` for project local environments

Clean projects and workflows...

... increase

- Reproducibility
- Reliability
- Reusability

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Outlook

Of course there is much more:

- Version control with Git
- Using R packages to build a research compendium
- Docker containers for full reproducibility
- ...

But this is for another time

Next lecture

Package your research in an R 

A research compendium is a **collection of all the digital parts of your research projects** (data, code, documents). R packages have a similar structure and therefore can be used to publish a fully reproducible version of your project.

Paper: Packaging data analytical work reproducibly using R (and friends) by Ben Marwick

 11th May  4-5 p.m.  Webex

- For topic suggestions and/or feedback send me an email
- Subscribe to the mailing list

Thank you for your attention :)

Questions?

References

- What they forgot to teach you about R book by Jenny Bryan and Jim Hester
- Blogpost by Jenny Bryan on good project-oriented workflows
- R best practice blogpost by Krista L. DeStasio
- Book about coding style for R: The tidyverse style guide
- The Turing way book General concepts and things to think about regarding reproducible research
- renv package website
- styler package website
- lintr package website