Reproducible Documents with {rmarkdown}

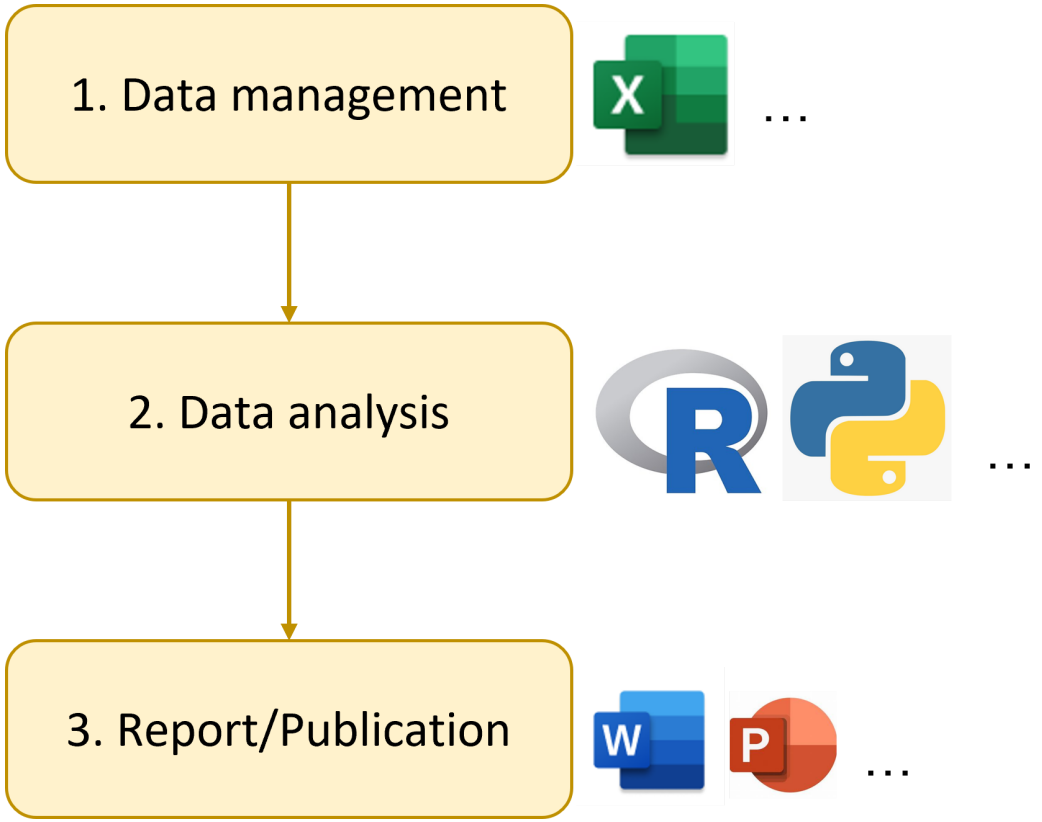
Day 1

Instructor: Selina Baldauf

Freie Universität Berlin - Theoretical Ecology

2022-22-03 (updated: 2022-03-28)

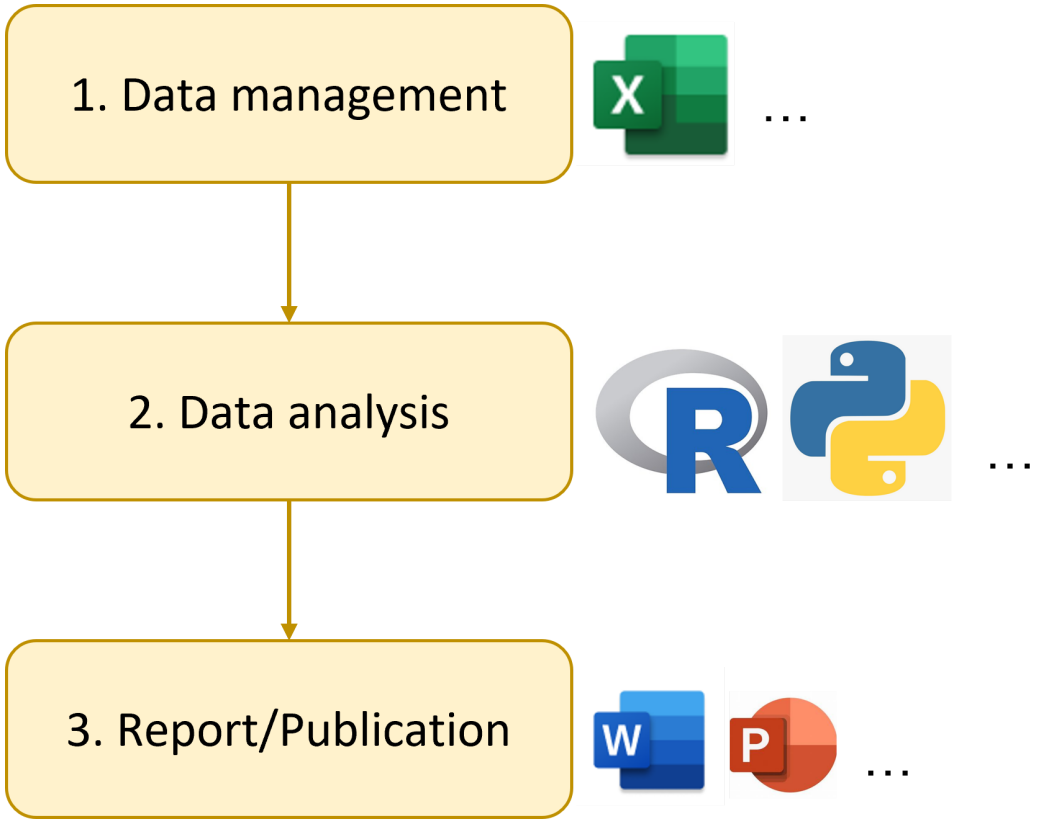
A standard workflow



Hard to answer questions:

- How did you produced this figure? What analysis is behind it?
- What data did you use for this table? Did you leave any data points out?
- Were does this value come from?
- I found an error in the raw data. Can you repeat the analysis?

A standard workflow



Main problem with this workflow: **error prone** and **non-reproducible**

If you have to repeat the analysis

- Redo all figures and tables
- Update document and presentation manually
  - Manual copy pasting of values is very error prone
- Annoying and you probably have to repeat this several times

Solution: A workflow using `{rmarkdown}`

Basic idea: Have everything (code, text, metadata) in one place. Let `{rmarkdown}` do the magic:

- Run code and add output to the document
- Return a nice document of the desired output format

Motivation for using `{rmarkdown}`

- Reproducibility
  - Easy to redo analysis
  - Easy to verify and check
  - No more copy pasting
  - Continuous workflow that is independent of the person that wrote the workflow (no clicking involved)
- Documentation/Text, Code & Output in one place
- Use R pipeline to produce documents
  - Create an automatic workflow
- Fun

Example use cases

Any type of document, especially if it contains something produced by code

- Data analysis reports
  - For yourself
  - For your supervisors
  - ...
- Publication + Publication of analysis
  - E.g. also good for publishing code
- Presentations
- Websites
- Books
- ...

The `rmarkdown` universe

- Many packages that provide additional functionality
  - Additional output formats
  - Templates
  - Formatting tools
  - Printing tools
  - ...

Just some examples:

There are many more ...

The basic workflow

1. Create an `.Rmd` document
2. Write text and R code in the document
3. Render the document to a defined output format using `rmarkdown`

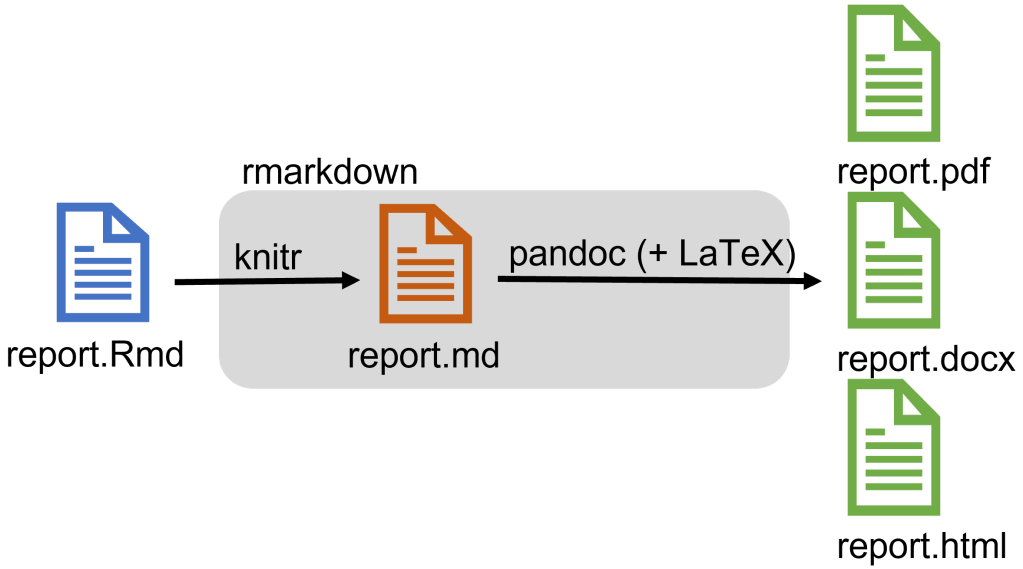


Figure adapted from BES Guides to better science: Reproducible code

Basic workflow in practice

Step 1: Create a new `.Rmd` document

- **Empty**: Create a new file in your project and save it with file ending `.Rmd`
- **From a template**:

  Rmarkdown itself comes with some templates

  - `File` -> `New File` -> `Rmarkdown...`

  Additional packages come with additional packages

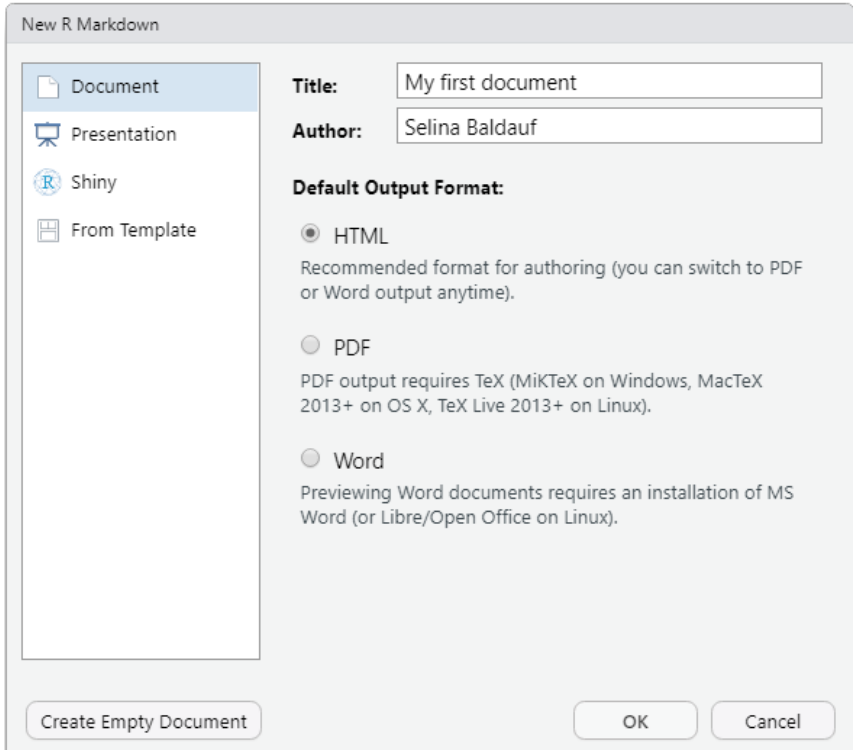
  - `{rticles}` for article templates
  - `{xaringan}` for presentations ...

Basic workflow in practice

Step 1: Create a new `.Rmd` document

`File` -> `New File` -> `Rmarkdown...`

- Select template on left
- Add title and author metadata
  - Can also be left blank and done later
- Select output format
- Click `OK`

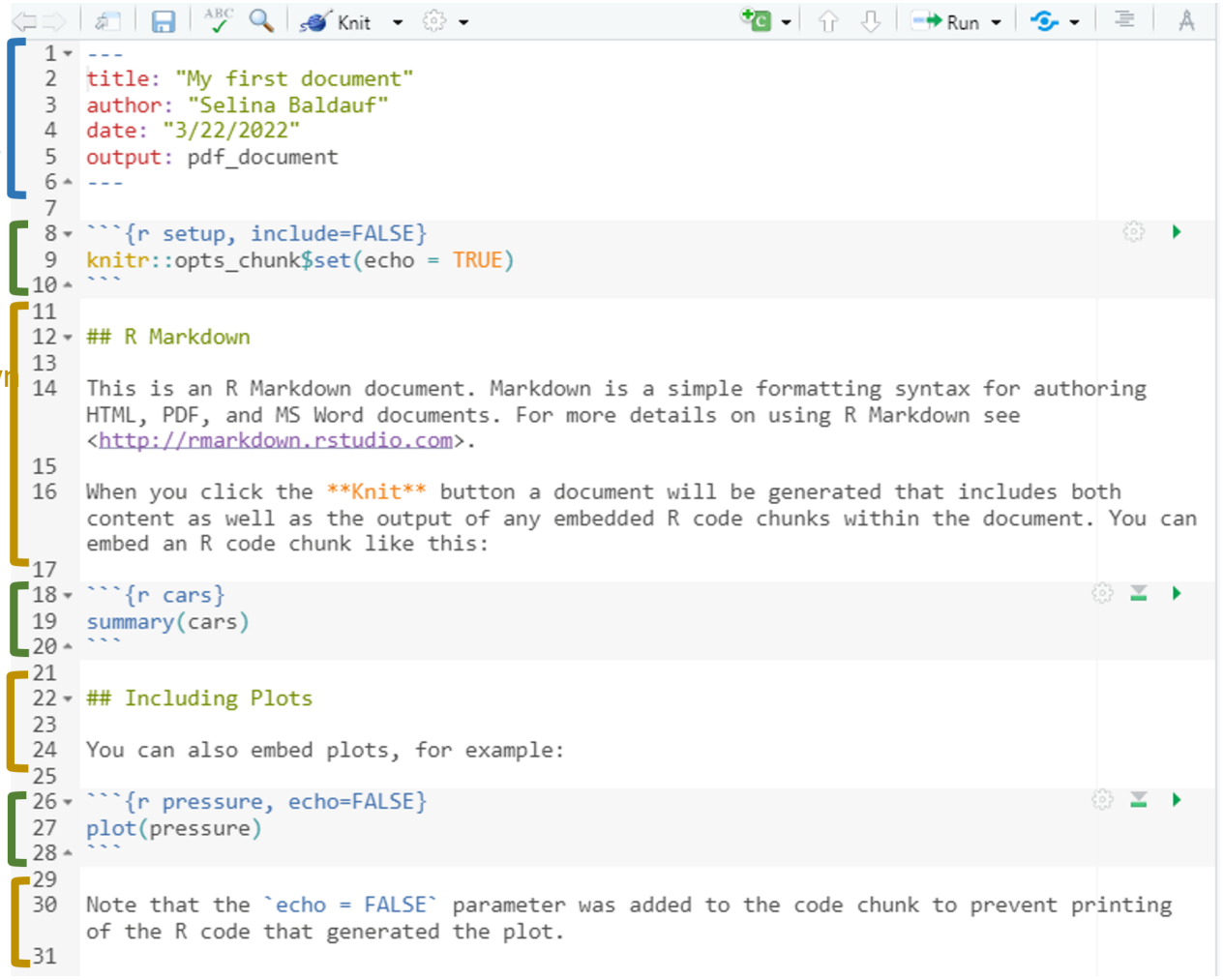


Structure of an `rmarkdown` document

YAML header with **metadata**

R code in **code chunks**

Text in Markdown syntax



Basic workflow in practice

Step 2: Write your document

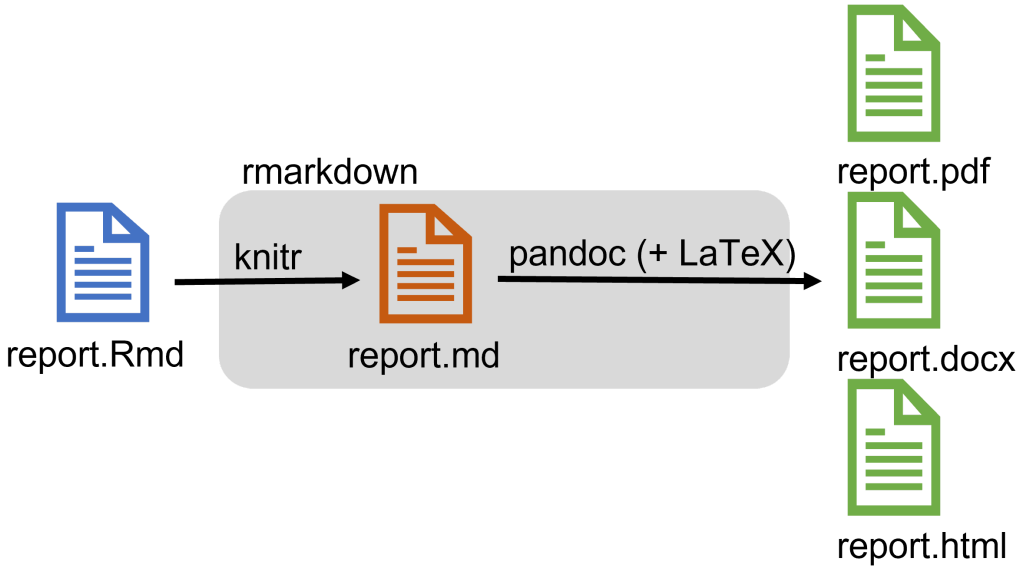
- Metadata
- Text
- R code

Basic workflow in practice

Step 3: Render/Knit the document to the desired output format

A multipstep process that is coordinated by the `rmarkdown` package

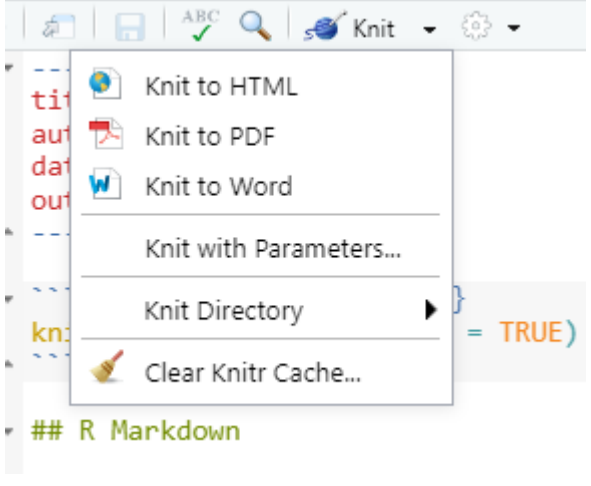
- `{knitr}` (an R package) runs the code and adds the output to the text
- `knitr` creates a `.md` document
- Pandoc (+ LaTeX) converts the markdown document to the desired output format
- Document is knitted in a new R session
    - This makes sure that the document is reproducible and that it does not depend on the current environment



Basic workflow in practice

Step 3: Render/Knit the document to the desired output format

- Click the `Knit` Button
- Use the keyboard shortcut `Ctrl/Cmd + Shift + K`
- For more options, click the little arrow next to the `Knit` button



→ Iterate through steps 2 and 3 until finished

I recommend to knit often, otherwise it can become a pain to debug.

The text body

The text body

- Text body in Markdown syntax
- Markdown is simple markup language to create formatted text
- Rmarkdown uses pandoc's markdown syntax
    - Find a full documentation here

The text body

The basics

- Bold: `**text**` becomes **text**
- Italic: `*text*` becomes *text*
- Subscript: `H~3~PO~4~` becomes H_3PO_4
- Superscript: `Cu^2+^` becomes Cu^{2+}

The text body

Code blocks

- Inline code: becomes `code`
- Code blocks: fenced of with 3 backticks

````
```
code
```
````

becomes

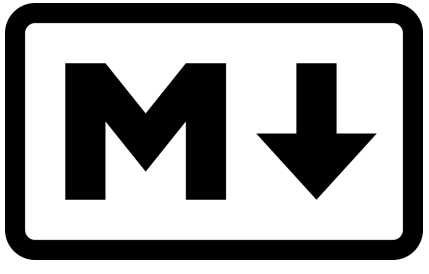
```
code
```

The text body

- Links: `[text](link)`
  - `[RStudio](https://www.rstudio.com)` becomes RStudio

The text body

- Include image (from file/web): `![Alt text/Figure caption](some/image)`
  - `![Markdown logo](https://upload.wikimedia.org/wikipedia/commons/thumb/4/48/Markdown-mark.svg/1200px-Markdown-mark.svg.png)` becomes



Markdown logo

- Footnote: `^[a footnote]`
  - Markdown logo by Dustin Curtis`^[available on [Wikimedia](https://en.wikipedia.org/wiki/Markdown#/media/File:Markdown-mark.svg)]` becomes
  - Markdown logo by Dustin Curtis[1]

[1] available on Wikimedia

The text body

Headers

```
# First level header

## Second level header

### Third level header
```

The text body

Itemized lists

```
- item 1
  - another item
- item 2
- item 3
```

becomes

- item 1
  - another item
- item 2
- item 3

Numbered lists

```
1. item 1
2. item 2
3. item 3
```

The text body

Math expressions can be written in in LaTeX syntax

- Inline (enclosed with `$`)

`$f(k) = {n \choose k} p^{k} (1-p)^{n-k}$` returns $f(k) = \binom{n}{k} p^k (1-p)^{n-k}$

- As a separate block (enclosed with `$$`)

$$f(k) = \binom{n}{k} p^k (1-p)^{n-k}$$

The text body

You don't need to remember all of this. Here is a quick reference for the most important things.

Always use spaces around markdown objects so that they can be rendered correctly, e.g.

```
## My section

This is an ordered list:

1. item 1
2. item 2
```

instead of

```
## My section
This is an ordered list:
1. item 1
2. item 2
```

The text body

Let's look at an example together

Can you identify the formatting elements in this document?

Now you

Task 1: Create some markdown text

Find the task description here

The R code

The R code

R code can be included in **code chunks** as **inline code**

- R code can be displayed or hidden in output document
  - Inline code is hidden
- Code chunks can contain any type of R code
- R code is (by default) executed and output is included in document
  - Text output
  - Figures
  - Prepare future data analysis
  - ...

The R code

Code chunks starts and ends with 3 backticks

````
```{r}
# code goes here
```
````

Example

````
```{r}
mean(1:3)
```
````

looks like this:

```
mean(1:3)
```

```
## [1] 2
```

The R code

Inline code starts and ends with 1 backtick

```
## `r `
```

Example

```
The mean of the values 1, 2 and 3 is `r mean(1:3)`
```

looks like this:

The mean of the values 1, 2 and 3 is 2.

The R code

Insert a code chunk

- Insert a code chunk by going to `Code` -> `Insert chunk`
- Use the keyboard shortcut `Ctrl + Alt + I` / `Cmd + Option + I`
- Inline chunks have to be typed

The R code

Chunk names

- Code chunks can have names (but they don't have to)
- Names are added inside the code chunk

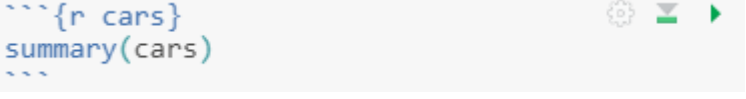
````
```{r calculate-mean}
mean(1:3)
```
````

- Easier to debug
- Code chunks appear in document outline

The R code

Run code chunk

- Code chunks are evaluated by `knitr` when rendering the document
- Code chunks can also be run like normal R code
- Run Code chunk by clicking on the green arrow next to the chunk



Chunk options

- Code chunks options give you fine control over the behavior of a chunk
- Chunk options are separated by commas

````
```{r calculate-mean, warning=TRUE, message=TRUE}
mean(1:3)
```
````

- Chunk options have a `name` and a `value`
    - Chunk options have default values
- Different document outputs support different chunk options

Chunk options

Some important general options

- `message`: `TRUE`, `FALSE`, Show message in output?
- `warning`: `TRUE`, `FALSE`, Show warning in output?
- `eval`: `TRUE`, `FALSE`, Evaluate the chunk?
- `echo`: `TRUE`, `FALSE`, Show source code in output?
- `include`: `TRUE`, `FALSE`, Include anything from the chunk in the output?
    - Runs the code but does not show any output or source code

Chunk options

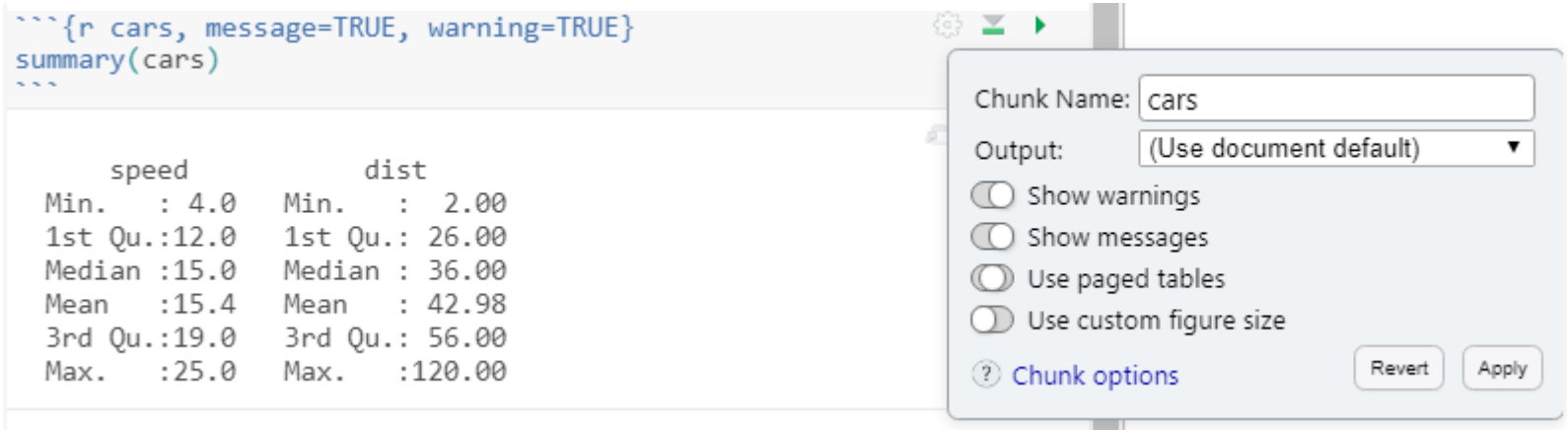
Some important figure related options

- `fig.width` and `fig.height`: Size of graphical device in inches (i.e. size of the plots)
- `out.width` and `out.height`: Scale output of R plots, e.g. to scale images `out.width = "80%"`
- `fig.align`: Plot alignment, one of `"left"`, `"center"`, `"right"`
- `fig.cap`: A figure caption as a string

````
```{r important-figure, fig.cap="This is a nice plot.", fig.width=4, fig.height=4}
plot(1:10, 1:10)
```
````

Chunk options

- See here for a comprehensive list of all chunk options
- Some chunk options can be set by clicking on the gear icon next to the chunk



The setup chunk

- Set default chunk options in the beginning of the document
- Default options can be overwritten in individual chunks
- Default chunk options can be set via `knitr` in an R code chunk:

````
```{r setup, inlcude=FALSE}
knitr::opts_chunk$set(
  echo = TRUE,
  warning = FALSE
  )
```
````

Other language engines

You can also run code chunks of other languages:

```
names(knitr::knit_engines$get())
```

```
##  [1] "awk"        "bash"       "coffee"     "gawk"       "groovy"     "haskell"    "lein"
##  [8] "mysql"      "node"       "octave"     "perl"       "psql"       "Rscript"    "ruby"
## [15] "sas"        "scala"      "sed"        "sh"         "stata"      "zsh"        "asis"
## [22] "asy"        "block"      "block2"     "bslib"      "c"          "cat"        "cc"
## [29] "comment"    "css"        "dot"        "embed"      "fortran"    "fortran95"  "go"
## [36] "highlight"  "js"         "julia"      "python"     "R"          "Rcpp"       "sass"
## [43] "scss"       "sql"        "stan"       "targets"    "tikz"       "verbatim"
```

See here if you are interested

Metadata with the YAML header

YAML (/ˈjæməl/) header

- YAML is a data-serialization language
- Goes between `---` on top
- Used for
    - Meta data
    - Document output formats and their options
- Is used by Pandoc, `rmarkdown` and `knitr`

YAML (/ˈjæməl/) header

Example

```
---
title: "My first document"
author: "Selina Baldauf"
date: "3/22/2022"
output:
  html_document:
    toc: true
    toc_float: true
bibliography: references.bib
---
```

- YAML Syntax: Indentation is important
  - Two spaces or a tab for lists
  - Values follow a `:`
- Translation:
  - `TRUE`, `FALSE`, `NULL` become `true`, `false`, `null`
  - Strings can be quoted but don't have to (if they don't contain special characters)
- Can also contain inline code to be evaluated

YAML (/ˈjæməl/) header

Metadata

```
---
title: "My first document"
subtitle: "Whatever subtitle makes sense"
author: "Selina Baldauf"
date: "`r Sys.Date()`"
---
```

- Inline R code can print the current date at knitting time

YAML (/ˈjæməl/) header

Document outputs

- `html_document`
- `pdf_document`
- `word_document`
- `beamer_presentation`
- `powerpoint_presentation`
- …

To use the default version of an output format add

```
output: html_document
```

or

```
output:
  html_document: default
```

YAML (/ˈjæməl/) header

Document output options

- Every output format has options than can be specified in the YAML header
  - Some options are shared between formats
  - Some options are specific to formats
- Have a look at `?rmarkdown::pdf_document`, `?rmarkdown::html_document`, etc. to see all options and their default values
- Use the rmarkdown cheat sheet as reference for the most important options

YAML (/ˈjæməl/) header

Document output options

```
output:
  html_document:
    toc: true
    toc_depth: 2
    number_sections: true
    fig_caption: true
    highlight: "espresso"
```

- `toc`: Show table of contents?
- `toc_depth`: Lowest header level for table of contents
- `number_sections`: Should sections be numbered?
- `fig_caption`: Render figure captions?
- `highlight`: Which style to use for syntax highlighting?
  - Some options: `"kate"`, `"tango"`, `"zenburn"`

YAML (/ˈjæməl/) header

Document parmeters

```
params:
  species: "setosa"
```

Document parameter values can be use in R code (inline or code chunks) with `params$param_name`

````
```{r iris-figure, fig.width=4, fig.height=4}
to_plot <- subset(iris, Species == params$species)
plot(Sepal.Length, to_plot, data = to_plot)
```
````