MONASH University

MONASH BUSINESS SCHOOL

Efficient reproducible workflows with R

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Outline

1. quarto
2. renv
3. targets

Research tools

Outline

Reproducibility

Not reproducible:

- Data edited in a spreadsheet
- Click and point analysis
- Copy and paste graphs and tables
- Tables typed by hand

Reproducible

- All data edits scripted
- All analysis scripted
- Graphs and tables automatically pulled in to the thesis
- Tables generated with scripts

Quarto

- Next generation of Rmarkdown.
- Supports R, Python, Javascript and Julia chunks.
- Separates style from content
- Format complex equations
- Automatic numbering and bibliography
- Many output formats, and many options for customizing format.
- Download and help: quarto.org

Code chunks

Chunk options use the hash-pipe `#|`

````
```{r}
#| label: fig-chunklabel
#| fig-caption: My figure
#| fig-width: 6
#| fig-height: 4
mtcars |>
  ggplot(aes(x = mpg, y = wt)) +
  geom_point()
```
````

Reference the figure using `@fig-chunklabel`.

Some chunk options

- `label`: name of chunk. Useful for cross-references
- `eval`: whether to evaluate the code chunk
- `echo`: whether to display the code chunk
- `output`: whether to show chunk output
- `results: 'asis'` includes the output without markup
- `message`: whether to display messages
- `warning`: whether to display warnings
- `error: true`: continue even if code returns an error.
- `fig-cap`: caption for the figure
- `fig-width`, `fig-height`: width and height of the figure
- `cache`: whether to cache the code chunk
- `dependson`: cache dependencies

Extensions and templates

- Quarto extensions modify and extend functionality.
- They are stored locally, in the `_extensions` folder alongside the qmd document.
- See https://quarto.org/docs/extensions/ for a list.
- Templates are extensions used to define new output formats.
- Journal templates at https://quarto.org/docs/extensions/listing-journals.html
- Monash templates at https://github.com/quarto-monash

quarto on the command line

- `quarto render` to render a quarto or Rmarkdown document.
- `quarto preview` to preview a quarto or Rmarkdown document.
- `quarto add <gh-org>/<gh-repo>` to add an extension from a github repository.
- `quarto update <gh-org>/<gh-repo>` to update an extension
- `quarto remove <gh-org>/<gh-repo>` to remove an extension
- `quarto list extensions installed`
- `quarto use template <gh-org>/<gh-repo>` to use existing repo as starter template.

Add a custom format

From the CLI: `quarto add quarto-monash/memo`

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New folder/files added

```
├── _extensions
│   └── quarto-monash
│       └── memo
│           └── ...
```

Add a custom format

From the CLI: `quarto add quarto-monash/memo`

New folder/files added

```
├── _extensions
│   └── quarto-monash
│       └── memo
│           └── ...
```

Update YAML

```
---
title: "My new file using the Monash memo format"
format: memo-pdf
---
```

Outline

Reproducible environments

- To ensure that your code runs the same way on different machines and at different times, you need the computing environment to be the same.
  1. Operating system
  2. System components
  3. R version
  4. R packages
- Solutions for 1–4: Docker, Singularity, `containerit`, `rang`
- Solutions for 4: `packrat`, `checkpoint`, `renv`

Reproducible environments

- Creates project-specific R environments.
- Uses a package cache so you are not repeatedly installing the same packages in multiple projects.
- Does not ensure R itself, system dependencies or the OS are the same.
- Not a replacement for Docker or Apptainer.

Reproducible environments

- Can use packages from CRAN, Bioconductor, GitHub, Gitlab, Bitbucket, etc.
- `renv::init()` to initialize a new project.
- `renv::snapshot()` to save state of project to `renv.lock`.
- `renv::restore()` to restore project as saved in `renv.lock`.

renv package

- `renv::install()` can install from CRAN, Bioconductor, GitHub, Gitlab, Bitbucket, etc.
- renv uses a package cache so you are not repeatedly installing the same packages in multiple projects.
- `renv::update()` gets latest versions of all dependencies from wherever they were installed from.
- `renv::deactivate(clean = TRUE)` will remove the renv environment.

Outline

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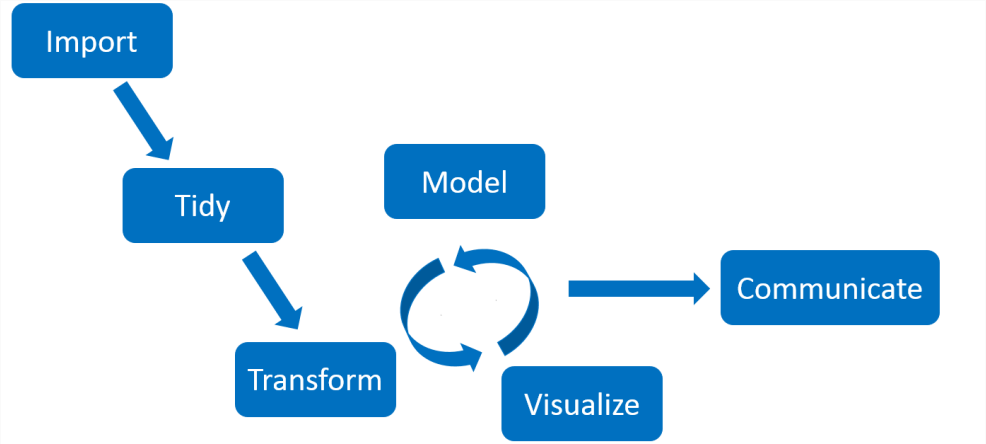
targets: reproducible computation at scale

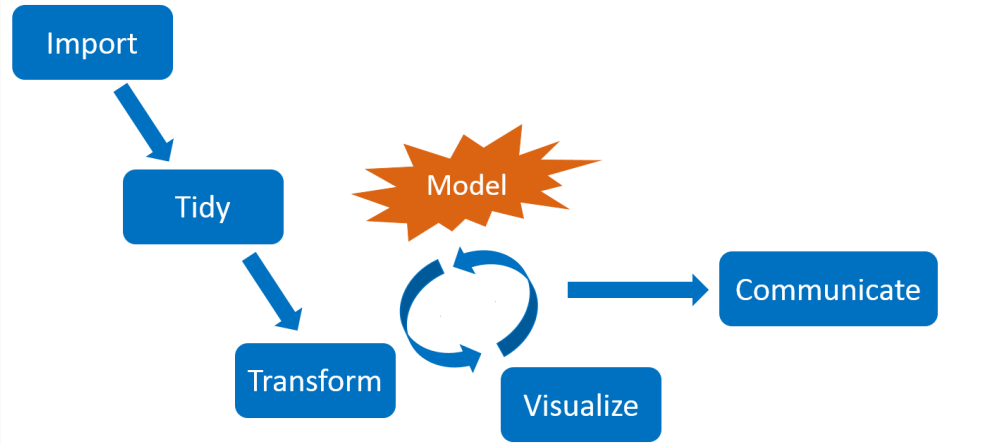
- Supports a clean, modular, function-oriented programming style.
- Learns how your pipeline fits together.
- Runs only the necessary computation.
- Abstracts files as R objects.
- Similar to Makefiles, but with R functions.

Some images from https://wlandau.github.io/targets-tutorial

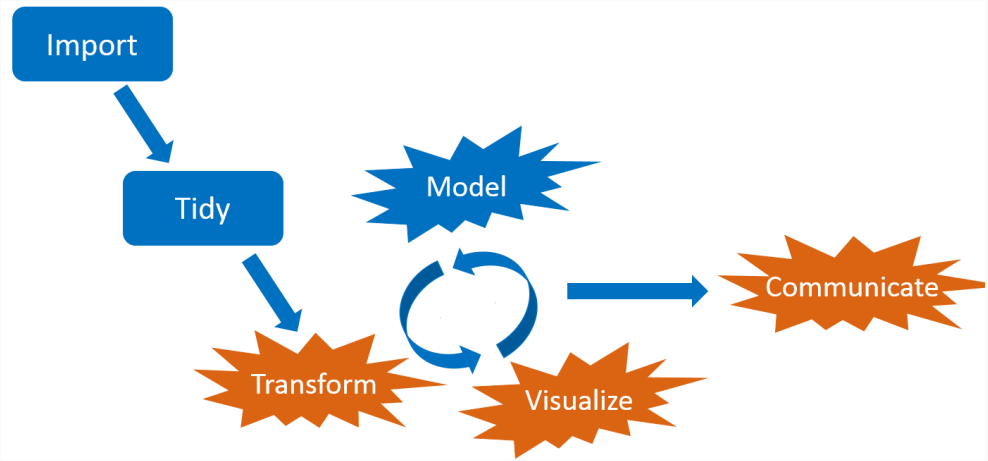
Interconnected tasks



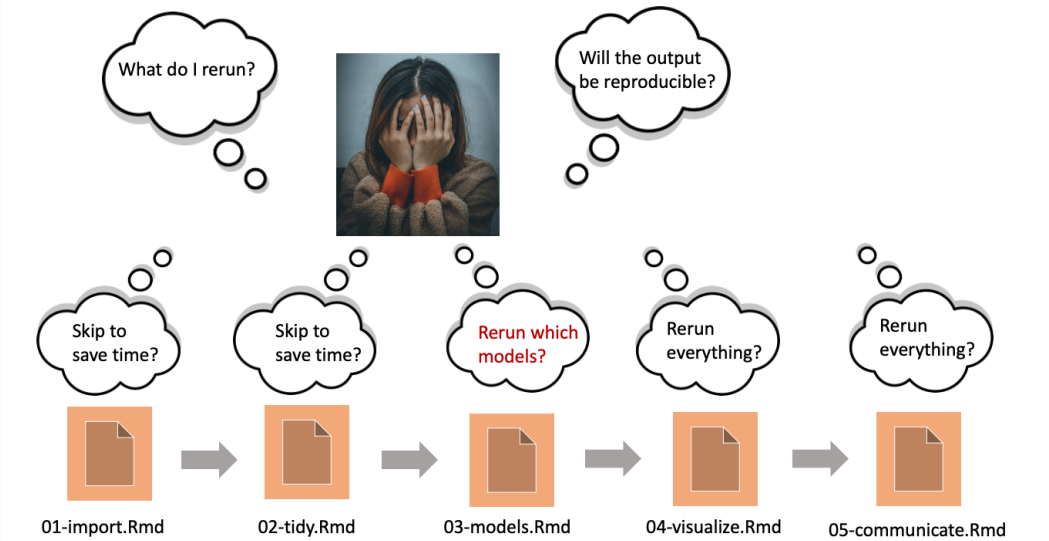
Interconnected tasks



Interconnected tasks

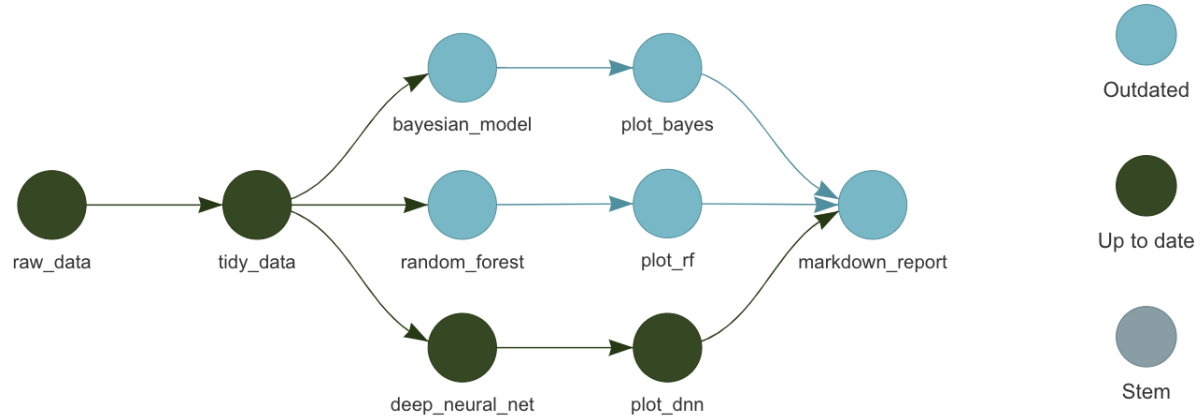


Dilemma: short runtimes or reproducible results?



https://openclipart.org/
https://unsplash.com/photos/_sh9vkVbVgo

Let a pipeline tool do the work



- Save time while ensuring computational reproducibility.
- Automatically skip tasks that are already up to date.

Typical project structure

no_targets.R

```
library(tidyverse)
library(fable)
source("R/functions.R")
my_data <- read_csv("data/my_data.csv")
my_model <- model_function(my_data)
```

Typical project structure

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library(tidyverse)
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```

_targets.R

```
library(targets)
tar_option_set(packages = c("tidyverse", "fable"))
tar_source() # source all files in R folder
list(
  tar_target(my_file, "data/my_data.csv", format = "file"),
  tar_target(my_data, read_csv(my_file)),
  tar_target(my_model, model_function(my_data))
)
```

Generate `_targets.R` in working directory

```
library(targets)
tar_script()
```

Useful targets commands

- `tar_make()` to run the pipeline.
- `tar_make(starts_with("fig"))` to run only targets starting with “fig”.
- `tar_read(object)` to read a target.
- `tar_load(object)` to load a target.
- `tar_load_everything()` to load all targets.
- `tar_manifest()` to list all targets
- `tar_visnetwork()` to visualize the pipeline.
- `tar_destroy()` to remove all targets.
- `tar_outdated()` to list outdated targets.

Random numbers

- Each target runs with its own seed based on its name and the global seed from `tar_option_set(seed = ???)`
- So running only some targets, or running them in a different order, will not change the results.

Folder structure

```
├── .git/
├── .Rprofile
├── .Renviron
├── renv/
├── index.Rmd
├── _targets/
├── _targets.R
├── _targets.yaml
├── R/
├──── functions_data.R
├──── functions_analysis.R
├──── functions_visualization.R
├── data/
└──── input_data.csv
```

`_targets.R` with quarto

```
library(targets)
library(tarchetypes)                                                    ①
tar_source() # source all files in R folder
tar_option_set(packages = c("tidyverse", "fable"))
list(
  tar_target(my_file, "data/my_data.csv", format = "file"),
  tar_target(my_data, read_csv(my_file)),
  tar_target(my_model, model_function(my_data)),
  tar_quarto(report, "file.qmd", extra_files = "references.bib")        ②
  )
```

① Load `tarchetypes` package for quarto support.

② Add a quarto target.

Replace quarto chunks with `tar_read()` or `tar_load()`.

Chunk options

Chunk with regular R code

````
```{r}
#| label: fig-chunklabel
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mtcars |>
  ggplot(aes(x = mpg, y = wt)) +
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```
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mtcars |>
  ggplot(aes(x = mpg, y = wt)) +
  geom_point()
```
````

Chunk with targets

````
```{r}
#| label: fig-chunklabel
#| fig-caption: My figure
tar_read(my_plot)
```
````

Example paper

Hyndman RJ, Rostami-Tabar B (2024) Forecasting interrupted time series, *Journal of the Operational Research Society*, in press.

bahmanrostamitabar/
forecasting_interrupted_time_series

Slides and links

robjhyndman.com/pku2025