

MONASH BUSINESS SCHOOL

Efficient reproducible workflows with R

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Outline

- 1 quarto
- 2 renv
- 3 targets

Research tools



Outline

- 1 quarto
- 2 renv
- 3 targets

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 #|

```
#| 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

Add a custom format

From the CLI: quarto add quarto-monash/memo

New folder/files added

Add a custom format

From the CLI: quarto add quarto-monash/memo

New folder/files added

Update YAML

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

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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.
 - 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

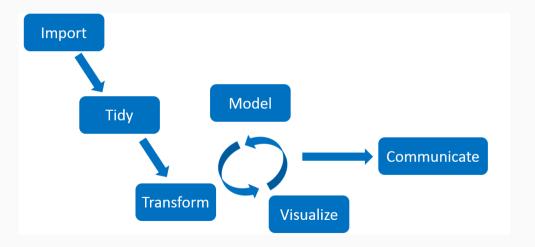
- 1 quarto
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targets: reproducible computation at scale

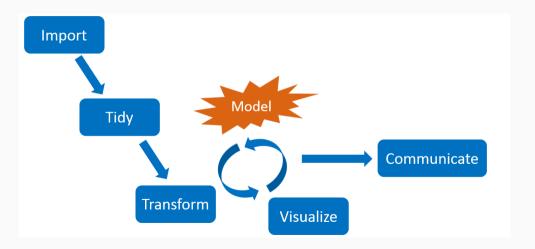


- Supports a clean, modular, function-oriented programming style.
- Learns how your pipeline fits together.
- Runs only the necessary computation.
- Abstracts files as R objects.
- Similar to Makefiles, but with R functions.

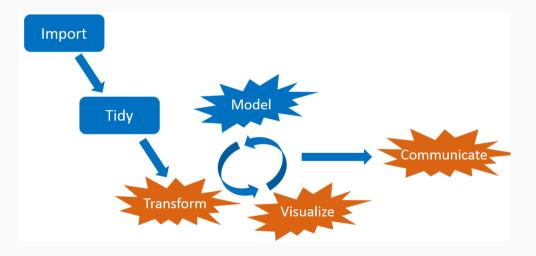
Interconnected tasks



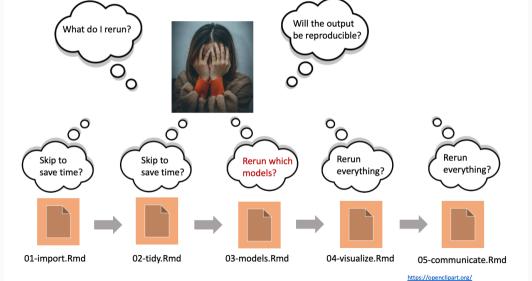
Interconnected tasks



Interconnected tasks

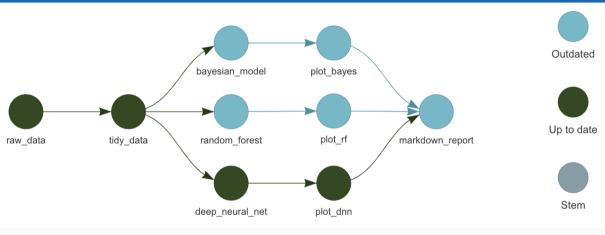


Dilemma: short runtimes or reproducible results?



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)</pre>
```

Typical project structure

no_targets.R

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my_data <- read_csv("data/my_data.csv")
my_model <- model_function(my_data)</pre>
```

_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)
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")
)
```

- 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

```
#| label: fig-chunklabel
#| fig-caption: My figure
mtcars |>
    ggplot(aes(x = mpg, y = wt)) +
    geom_point()
```

Chunk options

Chunk with regular R code

```
"\fr\"
# | label: fig-chunklabel
# | fig-caption: My figure
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



JOURNAL OF THE OPERATIONAL RESEARCH SOCIETY



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

robjhyndman.com/postdoc