Reproducible science in R

with `targets`

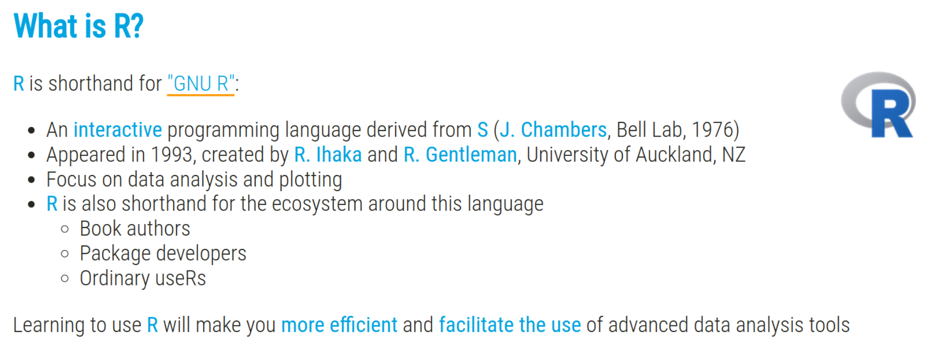
A. Ginolhac | HPC School | 2020-12-16

Introduction to R

Not the scope of this session from the previous sessions

But an introduction to `targets`, a Make-like workflow manager for **R**

- if you are a beginner user, check out this lecture



What is R?

R is shorthand for "GNU R":

- An interactive programming language derived from S (J. Chambers, Bell Lab, 1976)
- Appeared in 1993, created by R. Ihaka and R. Gentleman, University of Auckland, NZ
- Focus on data analysis and plotting
- R is also shorthand for the ecosystem around this language
  - Book authors
  - Package developers
  - Ordinary useRs

Learning to use R will make you more efficient and facilitate the use of advanced data analysis tools

- if you are an advanced user, interested in programming, check out this lecture

Evaluation in programming

`tidyeval`

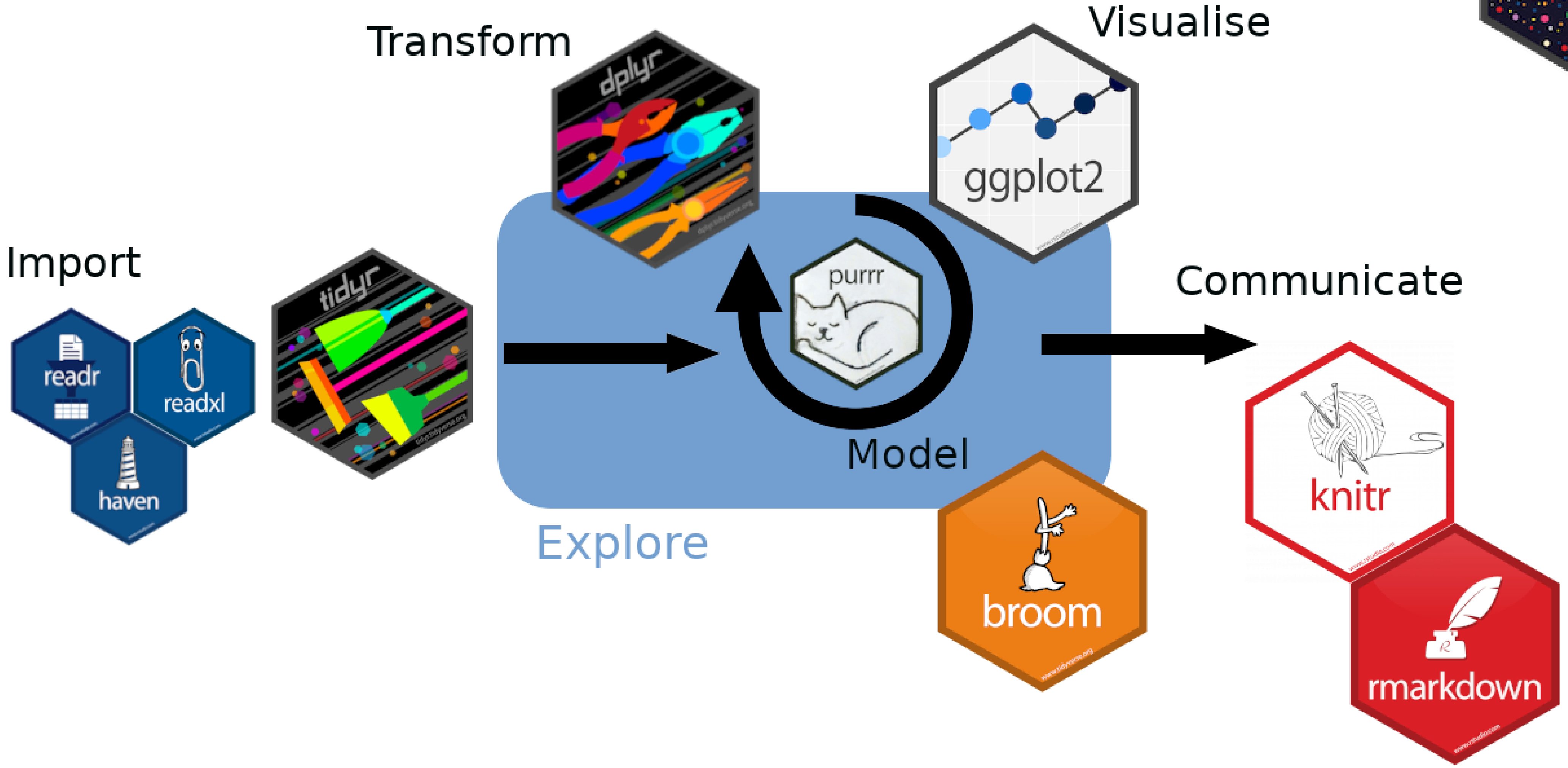
A. Ginolhac | rworkshop | 2020-11-30

About this lecture

Learning objectives

- Why a workflow manager is saving you time and stress
- Understand how it is implemented in `targets`
  - folder structure
  - define your `targets`
  - connect `targets` to create the dependencies
  - check dependencies with `visnetwork`
  - embrace dynamic branching
  - run only what needs to be executed
  - bundle dependencies in a Rmarkdown document with `tar_render()`
  - increase reproducibility with the package manager `renv`
- Practice on a dataset, running > 100 linear models in the `tidyverse` framework

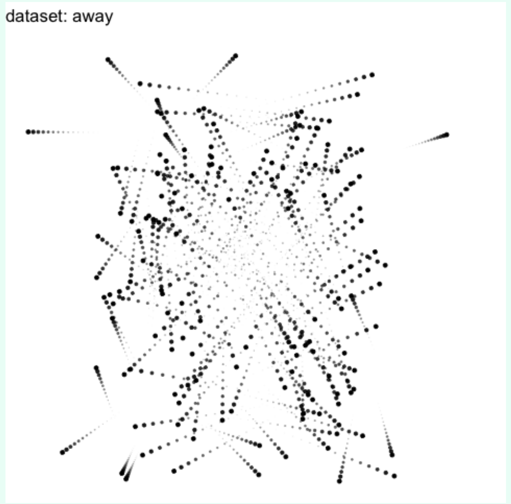
Tidyverse set of packages



Practical sessions

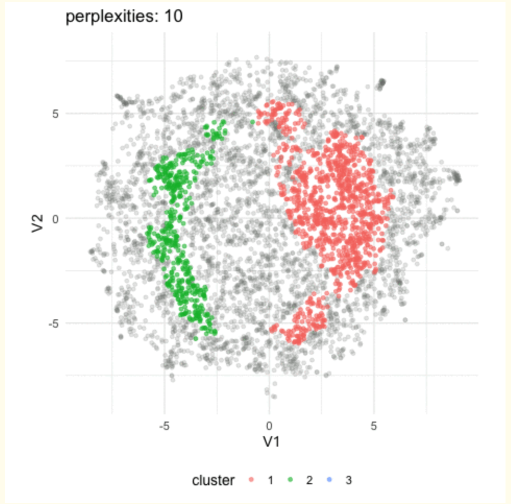
For beginners

- dataSaurus



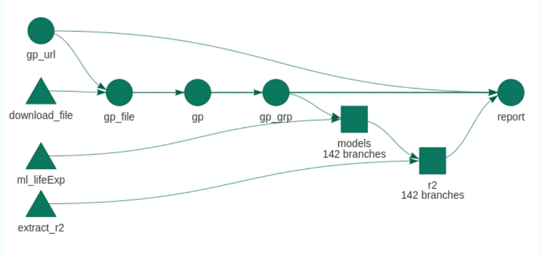
For intermediates

- exercises and `furrr`



For targets

- targets



If you wonder about drake

- drake, is the most used workflow manager for R. 1,300 ★ on Github

Rationale for rewriting from scratch

- drake is still an excellent choice for pipeline management, but it has permanent user-side limitations.
- targets was created to overcome these limitations and create a smoother user experience.
- Stronger guardrails by design.
- A friendlier, lighter, more transparent data management system.
- Show which functions are up to date.
- More flexible dynamic branching.
- Improved parallel efficiency.
- Designed for custom user-side metaprogramming (`tarchetypes`/`stantargets`).

Not on CRAN yet

```r
library(remotes)
# Landau is not using 'master'
install_github("wlandau/targets@main")
install_github("wlandau/tarchetypes@main")
```

- Debugging! with workspaces (wishing this exists in `snakemake`)

Source: targets slides W. Landau. NY Meetup hackR

Folder structure

```
├── .git/
├── run.R
├── _targets.R
├── _targets/
├── Repro.Rproj
├── R
│   ├── functions.R
│   └── utils.R
├── run.R*
├── renv/
├── renv.lock
└── report.Rmd
```

- with `renv`
- `_targets.R` is the only mandatory file
- use a R sub-folder for functions, gets closer to a R package
- a `run.R` file for custom building in RStudio
- `chmod +x run.R` in the Terminal for execution rights
- Rmd file allows to gather results in a report
- in a RStudio project
- version tracked with `git`

Main file _targets.R

```r
# Beginning of _targets.R
library(targets)
source("R/functions.R")
options(tidyverse.quiet = TRUE)
tar_option_set(
  packages = c("dplyr")
)
# Pipeline description
tar_pipeline(
  tar_target(a, 1:3),
  tar_target(b, a + 1,
             pattern = map(a))
)
```

- add `library(tarchetypes)` for extra-utilities
- optional helpers like silencing `tidyverse` loading
- declare packages that will be loaded by default
- each `target` can have their own additional lib calls (avoid loading for nothing)
- using bar names of targets, create the dependencies
- `pattern = map()` creates dynamic branching

Guardrails

- all targets are fresh R processes
- `_targets.R` must be at the project root

Formats, Patterns, Iterations

Formats

- `"rds"`: default
- `"qs"`: faster binary objects (see `qs::qsave()`)
- `"fst"`: amazing speed for `data.frame`, (see `fst::write_fst()`)
- `"fst_dt"`: same for `data.table` objects
- `"fst_tbl"`: same for `tibbles` objects
- `"keras"`
- `"torch"`
- `"url"`: automatic Last-Modified time stamp check
- `"file"`: automatic hashing check
- `"aws_rds/aws_file"`: for AWS S3 cloud

Patterns

- `map()`: iterate over one or more targets in sequence.
- `cross()`: iterate over combinations of slices of targets.
- `head()`: restrict branching to the first few elements.
- `tail()`: restrict branching to the last few elements.
- `sample()`: restrict branching to a random subset of elements.

Iterations

- `"vector"`: using `vctrs`
- `"list"`: less strict than `vctrs::vec_c()`
- `"group"`:handy for `dplyr::group_by()` tibble

and `tar_target` reference page

Source: W. Landau, NYhackr

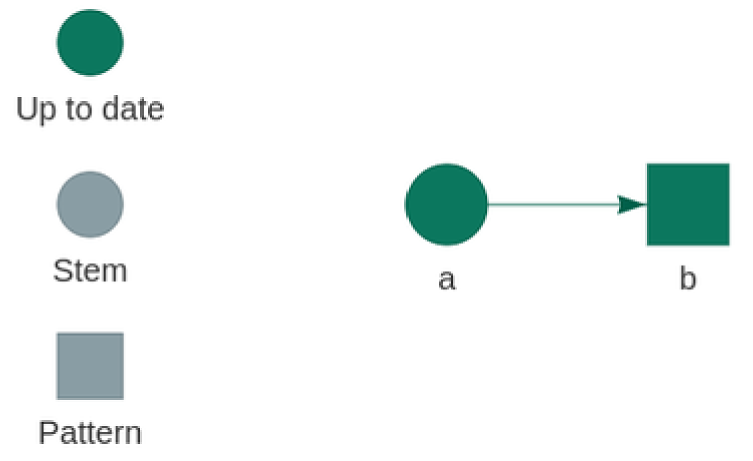
Toy example

```r
library(targets)
tar_pipeline(
  tar_target(a, 1:3),
  tar_target(b, a + 1,
             pattern = map(a))
)
# graph dependency BEFORE tar_make()
tar_visnetwork()
# run the pipeline
tar_make()
#> ● run target a
#> ● run branch b_0a91b2ed
#> ● run branch b_847c5ae2
#> ● run branch b_1619f1a0

# read a target content
tar_read(b_0a91b2ed)
#> [1] 2
```

re-run with `tar_make()`: all skipped

```r
tar_make()
#> ✓ skip target a
#> ✓ skip branch b_0a91b2ed
#> ✓ skip branch b_847c5ae2
#> ✓ skip branch b_1619f1a0
#> ✓ Already up to date.
tar_read(b_0a91b2ed)
#> [1] 2
# graph dependency AFTER tar_make()
tar_visnetwork()
```



Toy example

Add one element to a, ➔ one more b branch

```
tar_pipeline(
  tar_target(a, 1:4),
  tar_target(b, a + 1,
             pattern = map(a))
)
tar_make()
#> ● run target a
#> ✓ skip branch b_0a91b2ed
#> ✓ skip branch b_847c5ae2
#> ✓ skip branch b_1619f1a0
#> ● run branch b_9401bbb6
```

change b ➔ all branches re-run

```
tar_pipeline(
  tar_target(a, 1:4),
  tar_target(b, a + 2,
             pattern = map(a))
)
tar_make()
#> ✓ skip target a
#> ● run branch b_0a91b2ed
#> ● run branch b_847c5ae2
#> ● run branch b_1619f1a0
#> ● run branch b_9401bbb6
tar_read(b_0a91b2ed)
#> [1] 3
```

Toy parallelism, using `future`

`future` by Henrik Bengtsson is available. Only one worker

```
library(future)
plan(multisession)
tar_pipeline(
  tar_target(a, 1:3),
  tar_target(b, {
    # fake a long process
    Sys.sleep(5)
    a + 1
  },
  pattern = map(a))
)
system.time(tar_make_future(workers = 1L))
#> ● run target a
#> ● run branch b_0a91b2ed
#> ● run branch b_847c5ae2
#> ● run branch b_1619f1a0
#>    user  system elapsed
#>   2.156   0.284  20.807
```

with 3 workers

```
library(future)
plan(multisession)
tar_pipeline(
  tar_target(a, 1:3),
  tar_target(b, {
    # fake a long process
    Sys.sleep(5)
    a + 1
  },
  pattern = map(a))
)
system.time(tar_make_future(workers = 3L))
#> ● run target a
#> ● run branch b_0a91b2ed
#> ● run branch b_847c5ae2
#> ● run branch b_1619f1a0
#>    user  system elapsed
#>   2.126   0.164  12.920
```

Still overhead, but individual target can be parallelised (`deployment` / `resources` args)

Deploy only heavy computation **remotely** possible with `clustermq`. TBD

Custom Build in RStudio

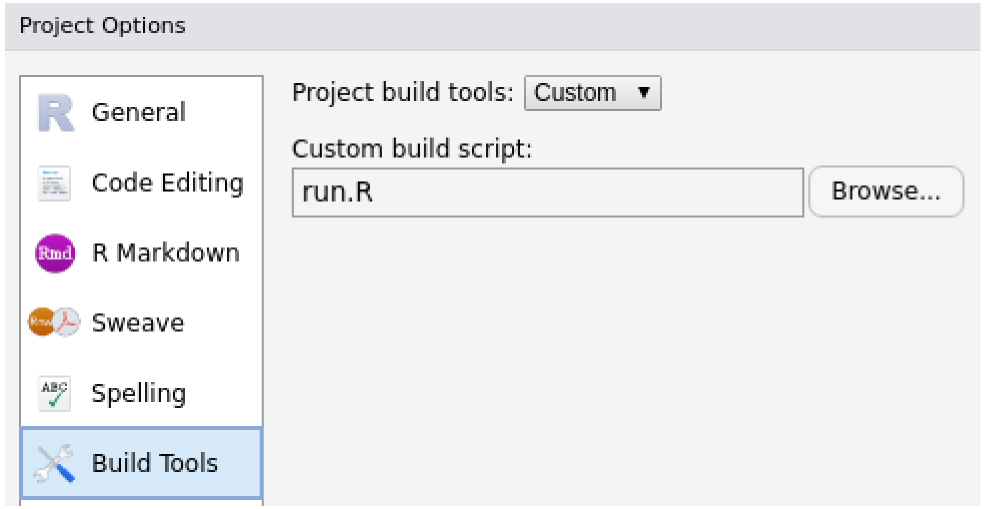
`run.R` is essentially a call to `tar_make()` as seen below:

```
#!/usr/bin/env Rscript

targets::tar_make()
```

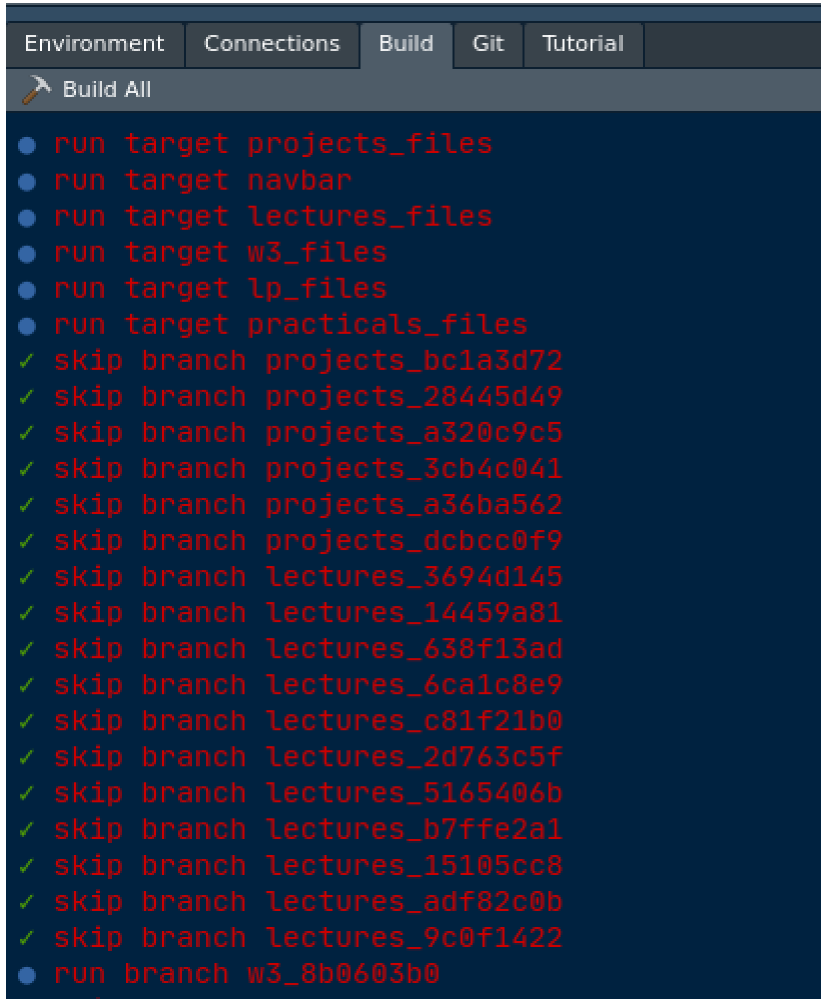
- `chmod +x run.R` in the Terminal for execution rights

Then specified in RStudio project building option:



Project build tools: Custom
Custom build script: run.R

Example (also nice to use the keyboard shortcut)



```
● run target projects_files
● run target navbar
● run target lectures_files
● run target w3_files
● run target lp_files
● run target practicals_files
✓ skip branch projects_bc1a3d72
✓ skip branch projects_28445d49
✓ skip branch projects_a320c9c5
✓ skip branch projects_3cb4c041
✓ skip branch projects_a36ba562
✓ skip branch projects_dcbcc0f9
✓ skip branch lectures_3694d145
✓ skip branch lectures_14459a81
✓ skip branch lectures_638f13ad
✓ skip branch lectures_6ca1c8e9
✓ skip branch lectures_c81f21b0
✓ skip branch lectures_2d763c5f
✓ skip branch lectures_5165406b
✓ skip branch lectures_b7ffe2a1
✓ skip branch lectures_15105cc8
✓ skip branch lectures_adf82c0b
✓ skip branch lectures_9c0f1422
● run branch w3_8b0603b0
```

A more realistic example

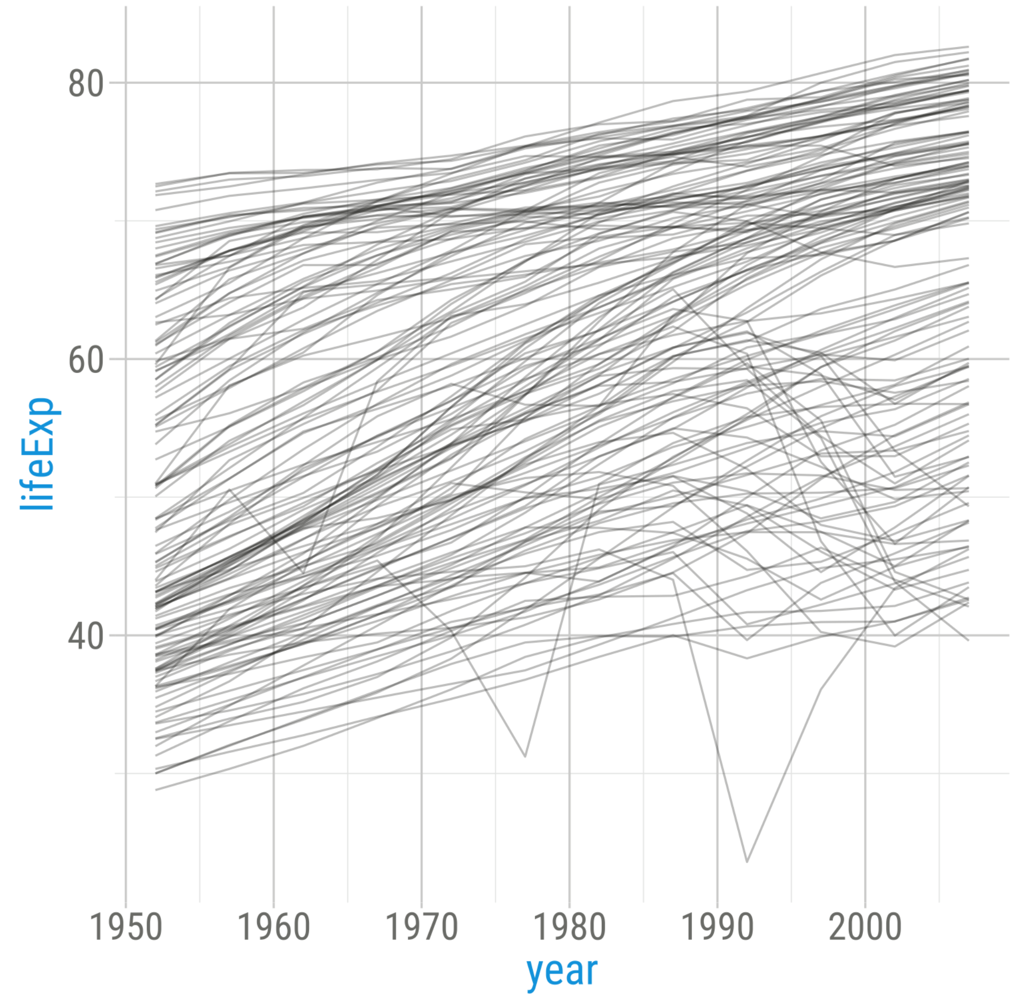
Linear modelling on the `gapminder` dataset

142 countries, 12 yearly observations of 3 parameters

country	continent	year	lifeExp	pop	gdpPercap
Afghanistan	Asia	1952	28.8	8425333	779
Afghanistan	Asia	1957	30.3	9240934	821
Afghanistan	Asia	1962	32	10267083	853

…

country	continent	year	lifeExp	pop	gdpPercap
Zimbabwe	Africa	1997	46.8	11404948	792
Zimbabwe	Africa	2002	40	11926563	672
Zimbabwe	Africa	2007	43.5	12311143	470

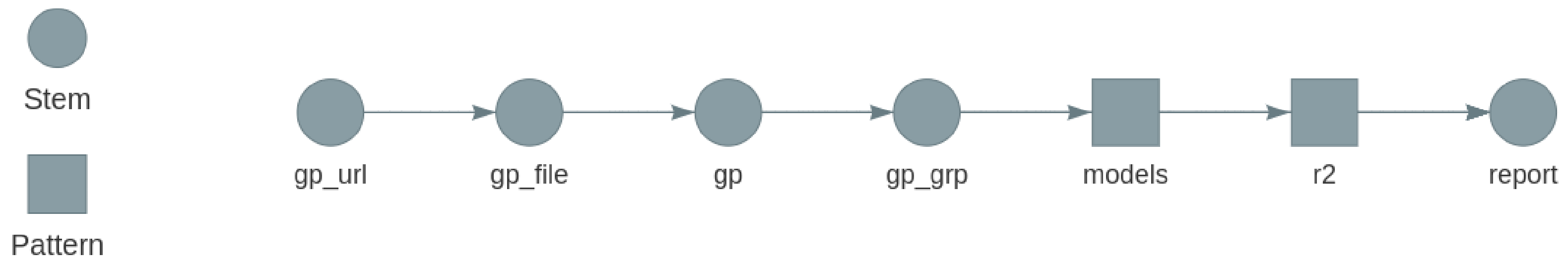


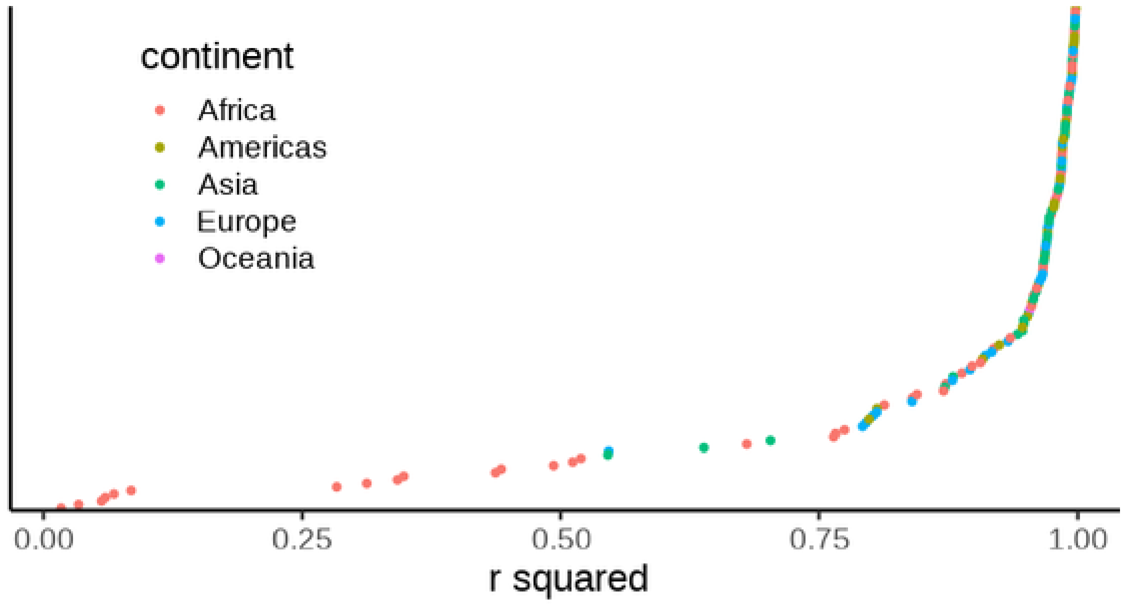
Now practical

session

Aim: life expectancy explained by time for each country

- `gapminder` as `tsv` URL (Jenny Bryan)
- download the file
- read `tsv` as `tibble`
- group by `country`
- run 142 linear models
- extract 142 r^2
- bundle results in a `Rmarkdown`
- snake plots the r^2





dependency graph from `tar_glimpse()`

Step1: set-up and data URL

Set-up

- Create an RStudio project
- install `tidyverse`, `fst`, `rmarkdown`, `visNetwork`
- install `targets`, `tarchetypes` (slide 6)
- `run.R` and custom build (slide 13)
- Create an empty file `R/functions.R`
- Create a `_targets.R` file with (copy icon on top right corner)

```r
library(targets)
library(tarchetypes)
source("R/functions.R")
options(tidyverse.quiet = TRUE)
# necessary packages to load in isolated R ses
tar_option_set(packages = c("tidyverse", "fst"
# Define the pipeline
tar_pipeline(
  tar_url(gp_url, "https://raw.githubuserconte
)
```

- Build
- check that the target is correct:

```r
tar_read(gp_url)
#> [1] "https://raw.githubusercontent.com/jenn
```

Step 2: download and load the file

- `download.file()` does not return anything.
- we need a filename, so create a wrapper `download_file()`
  - format is `file`, tsv will be tracked
- load the file with `readr::read_tsv()`
  - format is `tibble` via `fst` super fast
- run the pipeline
  - `gp_url` should be skipped
  - `tar_read(gp)` should return a `tibble`

lines for `R/functions.R`

```
#' wrap download.file to return the filename
download_file <- function(url, out) {
  download.file(url, out, quiet = TRUE)
  out
}
```

lines for `_targets.R`

```
tar_file(gp_file, download_file(gp_url, "gapmi
tar_fst_tbl(gp, read_tsv(gp_file, col_types = 
```

Step 3: Group by country

- `dplyr::group_by()` by continent and country
  - pipe to `tar_group()` which create extra column
  - specify `iteration = "group"`

```
tar_fst_tbl(gp_grp,
            group_by(gp, continent, country) %
              tar_group(),
            # tell downstream targets about th
            iteration = "group")
```

- don't forget the **comma** between targets.
- run the Build

Step 4: run the models

- add a function to wrap `lm`
- add the target `models`
  - pattern is map over the countries
  - specify `iteration = "list"`

lines for `R/functions.R`

```r
#' linear model on country, lifeExp explained
#' so we get meaningful intercept
ml_lifeExp <- function(.data) {
  gp <- mutate(.data, year1950 = year - 1950)
  lm(lifeExp ~ year1950, data = gp)
}
```

lines for `_targets.R`

```r
tar_target(models,
           ml_lifeExp(gp_grp),
           pattern = map(gp_grp),
           # lm is complex, combine in a list
           iteration = "list")
```

- run `tar_visnetwork(labels = "branches")`, 142 expected
- run the Build, should see 142 branches

Step 5: extract r^2 from models

- add a function to extract r^2
- add the target `r2`
  - pattern is map over the models
  - specify `iteration = "vector"`

lines for `R/functions.R`

```
#' extract r.square from lm object
extract_r2 <- function(model) {
  summary(model)$r.squared
}
```

lines for `_targets.R`

```
  tar_target(r2,
             extract_r2(models),
             pattern = map(models),
             # now vector is enough
             iteration = "vector")
```

- run `tar_visnetwork(labels = "branches")`, 142 expected
- run the Build, should see 142 branches for r2

Step 6: add the report

- edit the `report.Rmd`
- add the special target `tar_render()`

lines for `report.Rmd`

```
---
title: "gapminder report"
author: "your name"
date: "2020-12-16"
output: html_document
---

## Gapminder Data

we used the URL `r targets::tar_read(gp_url)`
```

lines for `_targets.R`

```
tar_render(report, "report.Rmd")
```

- run `tar_visnetwork(labels = "branches")`
- run the Build

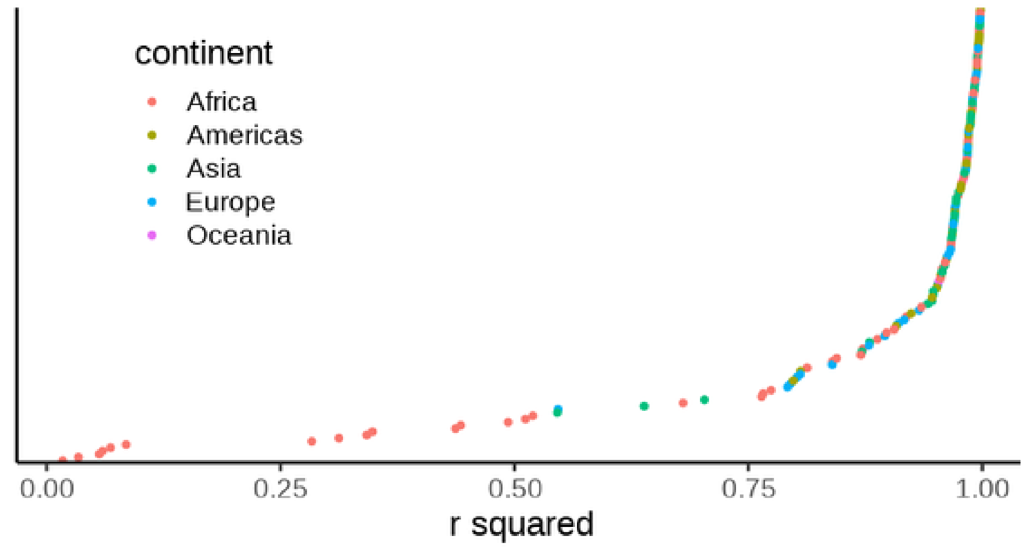
Step 7: more code to the report

Combine gapminder and r^2 by `tar_group`

```
tar_read(gp_grp) %>%
  group_by(continent, country, tar_group) %>%
  tidyr::nest() %>%
  ungroup() %>%
  inner_join(tibble(rsq = tar_read(r2),
                    tar_group = seq_len(length(
gp_r2
#> Joining, by = "tar_group"
#> # A tibble: 142 x 5
#>    country     continent tar_group data
#>    <chr>       <chr>         <int> <list>
#>  1 Afghanistan Asia             78 <tibble
#>  2 Albania     Europe          111 <tibble
#>  3 Algeria     Africa            1 <tibble
#>  4 Angola      Africa            2 <tibble
#>  5 Argentina   Americas         53 <tibble
```

Snake plot

```
gp_r2 %>%
  ggplot(aes(x = rsq, y = forcats::fct_reorder(
  geom_point(aes(colour = continent)) +
  labs(y = NULL,
       x = "r squared") +
  theme_classic(18) +
  theme(legend.position = c(0.2, 0.7),
        axis.text.y = element_blank(),
        axis.ticks.y = element_blank())
```



Before we stop

You learned to:

- apprehend `targets`
- discover the advantages of workflow managers
- Makefile-like approach and project design

Acknowledgments 🙏 👏

- William Landau obviously
- Eric Koncina early adopter of `targets`
- Hadley Wickham
- Henrik Bengtsson
- Xie Yihui and Garrick Aden-Buie for `xarigan`/`xaringanExtra`
- Jennifer Bryan

Further reading

- `targets` manual by William Landau
- `targets` reference by William Landau
- `tarchetypes` reference by William Landau
- NY Open Statistical Meeup, Dec 2020, targets presentation by William Landau

Thank you for your attention!

4-days Rworkshop in May 2021

- Elixir-LU event
- 6th - 11th May