

Hit your reproducibility {targets}

UK Gov Data Science Festival, 2020-09-30



Reproducevangelism

		Data	
		Same	Different
Analysis	Same	Reproducible	Replicable
	Different	Robust	Generalisable

From The Turing Way by The Alan Turing Institute



Reproducible Analytical Pipelines

Can I recreate what you did:

- from scratch?
- on a different machine?
- in the future?
- without you present?

R has many reproducibility tools, like:

- RStudio Projects to keep everything together
- R Markdown for reproducible docs
- packages for reusable functions
- {here} for relative filepaths
- {renv} for dependency management

Today's focus:

- 1. Make workflows reproducible
- 2. Try {targets}

1. Make workflows reproducible

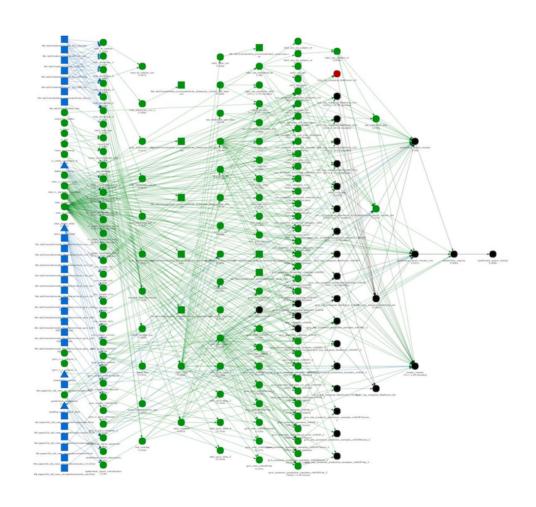
What about your analytical workflow itself?

How do you keep track of function, file and object relationships?

What if:

- you haven't recorded the steps?
- the interdependencies become complex?
- some steps are computationally intensive?
- something changes?

You can't remember this



Let a workflow manager handle it

- Dagobah Simple DAG-based job scheduler in Python.
- Dagr A scala based DSL and framework for writing and executing bioinformatics pipelines as Directed Acyclic GRaphs.
- Dagster Python-based API for defining DAGs that interfaces with popular workflow managers for building data applications.
- DataJoint an open-source relational framework for scientific data pipelines.
- Dask Dask is a flexible parallel computing library for analytics.
- Dockerflow Workflow runner that uses Dataflow to run a series of tasks in Docker.
- Doit Task management & automation tool.
- Drake Robust DSL akin to Make, implemented in Clojure.
- Drake R package Reproducibility and high-performance computing with an easy R-focused interface. Unrelated to Factual's Drake.
- Dray An engine for managing the execution of container-based workflows.
- eHive System for creating and running pipelines on a distributed compute resource.
- Fission Workflows A fast, lightweight workflow engine for serverless/FaaS functions.
- Flex Language agnostic framework for building flexible data science pipelines (Python/Shell/Gnuplot).
- Flowr Robust and efficient workflows using a simple language agnostic approach (R package).



2. Try {targets}



{targets} by Will Landau

From the manual:

...learns how your pipeline fits together, skips costly runtime for tasks that are already up to date, runs only the necessary computation, supports implicit parallel computing, abstracts files as R objects, shows tangible evidence that the results match the underlying code and data.

Plus excellent docs:

- the site and source
- the {targets} R package user manual
- minimal example (can be run in RStudio Cloud)
- targetsketch: a Shiny app for learning {targets}
 and setup new projects

More available from the {targets} README.

Supersedes {drake} by Will Landau



...major user-side limitations regarding data management, collaboration, and parallel efficiency

At its simplest:

- 1. Write a pipeline script
- 2. Execute the script
- 3. Change stuff
- 4. Go to 2



Contrived, simple demo

The goal: a {targets} pipeline that creates a chart and table for an R Markdown file and renders it.

Then change something and re-run the pipeline.

Generate _targets.R in working directory

```
tar_script()
```

You can view the file for this example online

Set up functions and options in _targets.R

```
tar_option_set(
  packages = c(
    "targets", "tarchetypes", "knitr",
    "dplyr", "ggplot2", "rphylopic",
  )
)
```

```
b_plot <- function(data, image) {
   ggplot(data, aes(id, temp)) +
      geom_boxplot() +
      labs(title = "Weasel temperatures") +
      add_phylopic(image)
}</pre>
```

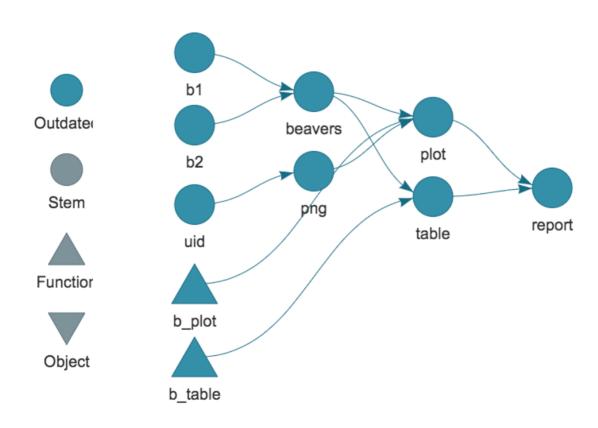
Set up pipeline in _targets.R

```
targets <- list(</pre>
  tar_target(b1, mutate(beaver1, id = "A")),
  tar_target(b2, mutate(beaver2, id = "B")),
  tar target(beavers, bind rows(b1, b2)),
  tar target(uid, "be8670c2-a5bd-4b44-88e8-92f8b0c7f4
  tar_target(png, image_data(uid, size = "512")[[1]])
  tar_target(plot, b_plot(beavers, png)),
  tar_target(table, b_table(beavers)),
  tarchetypes::tar_render(report, "beavers-report.Rmd
tar_pipeline(targets)
```

View targets

```
tar_manifest(fields = "command")
```

tar_visnetwork()

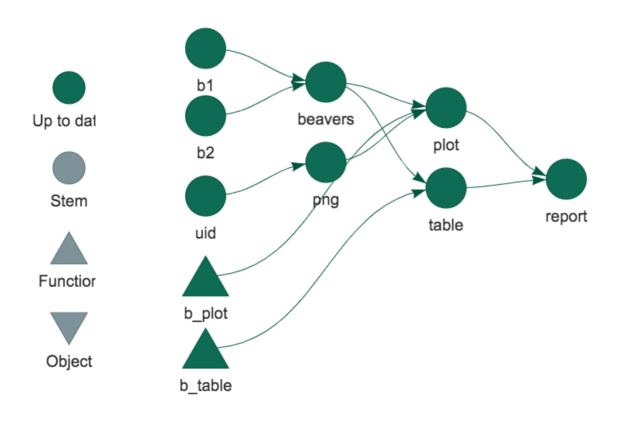


Execute the pipeline

```
tar_make()
```

- run target uid
- run target b1
- run target b2
- run target png
- run target beavers
- run target plot
- run target table
- run target report

tar_visnetwork()



Whoops...

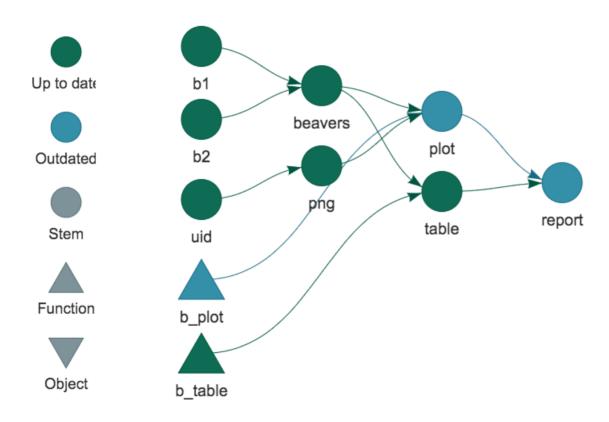
- -labs(title = "Weasel temperatures")
- + labs(title = "Beaver temperatures")

Check what has become outdated as a result

```
tar_outdated()

[1] "report" "plot"
```

tar_visnetwork()



Only outdated targets are re-run

```
tar_make()

√ skip target uid

√ skip target b1

√ skip target b2

√ skip target png

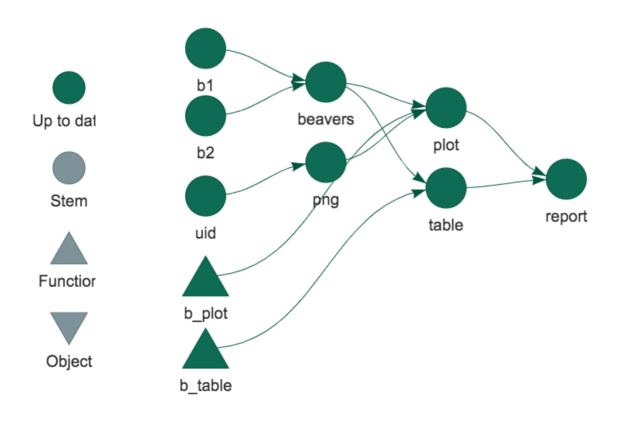
√ skip target beavers

run target plot

√ skip target table

• run target report
```

tar_visnetwork()



The final product

R's built-in beavers dataset

Matt Dray

23 September 2020

About

From the ?beavers help page:

Reynolds (1994) describes a small part of a study of the long-term temperature dynamics of beaver Castor canadensis in north-central Wisconsin. Body temperature was measured by telemetry every 10 minutes for four females, but data from a one period of less than a day for each of two animals is used there.

Data

What does the distribution of body temperatures look like?

To recap:

- 1. tar_script() creates _targets.R
- 2. Add tar_targets()
- 3. Check tar_manifest()
- 4. tar_visnetwork() to visualise
- 5. Execute with tar_make()
- 6. Change stuff, check tar_outdated()
- 7. Go to 4



Hit your reproducibility {targets}

- Maki workflow reproducible
- Try {targets}

Revisit materials:

- these slides
- source code
- blog post
- {drake} version of this talk and a blog post

Image sources:

- RAP hex logo
- {targets} hex logo
- {drake} hex logo
- {drake} hairball by Frederik Aust
- Castor canadensis from PhyloPic