Reproducible computation at scale in R

Will Landau

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Large statistical computation

- Bayesian data analysis
- Bayesian network meta-analysis
- Graph-based multiple comparison procedures
- Subgroup identification
- Predictive modeling
- Deep neural networks
- PK/PD modeling
- Clinical trial simulation
- Target identification

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Common features

1. Heavy use of the R language.
2. Long runtimes.
3. Multiple sub-tasks.
4. Frequent changes to code and data.

https://openclipart.org/detail/275842/sisyphus-overcoming-silhouette

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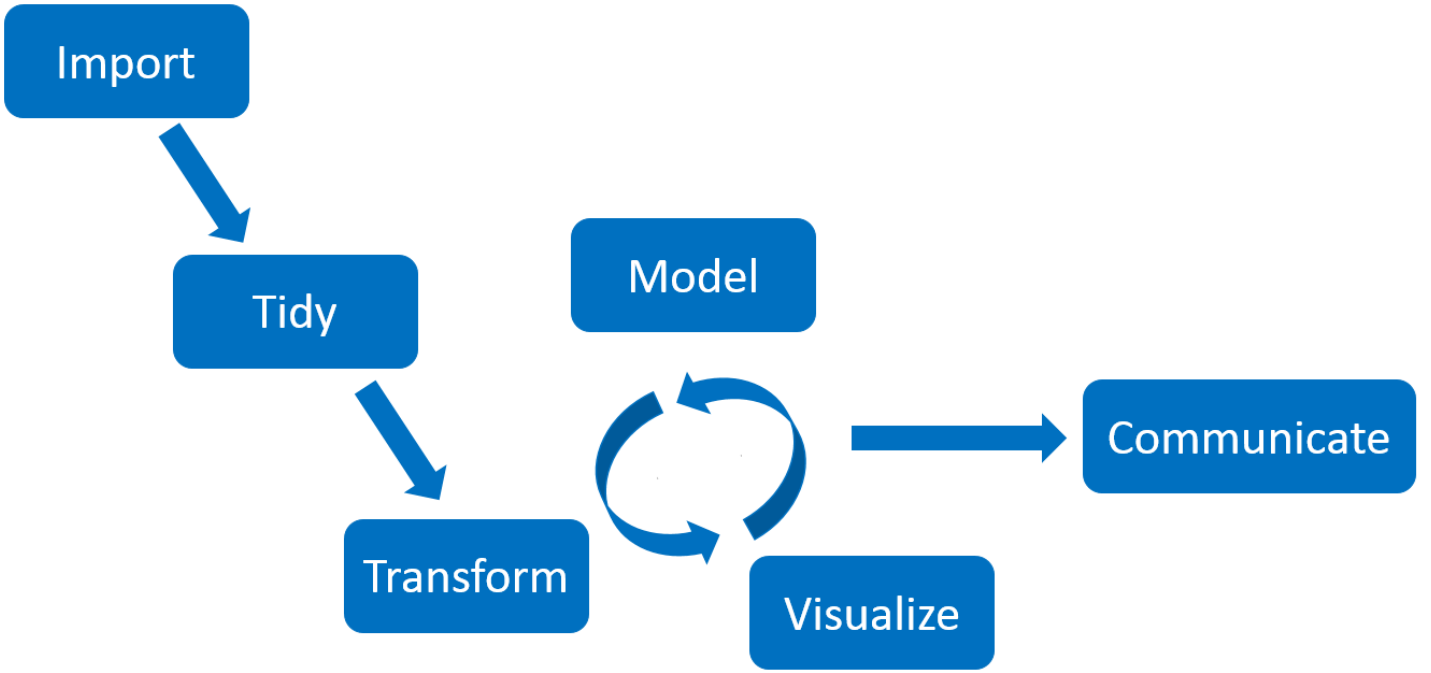
Interconnected tasks



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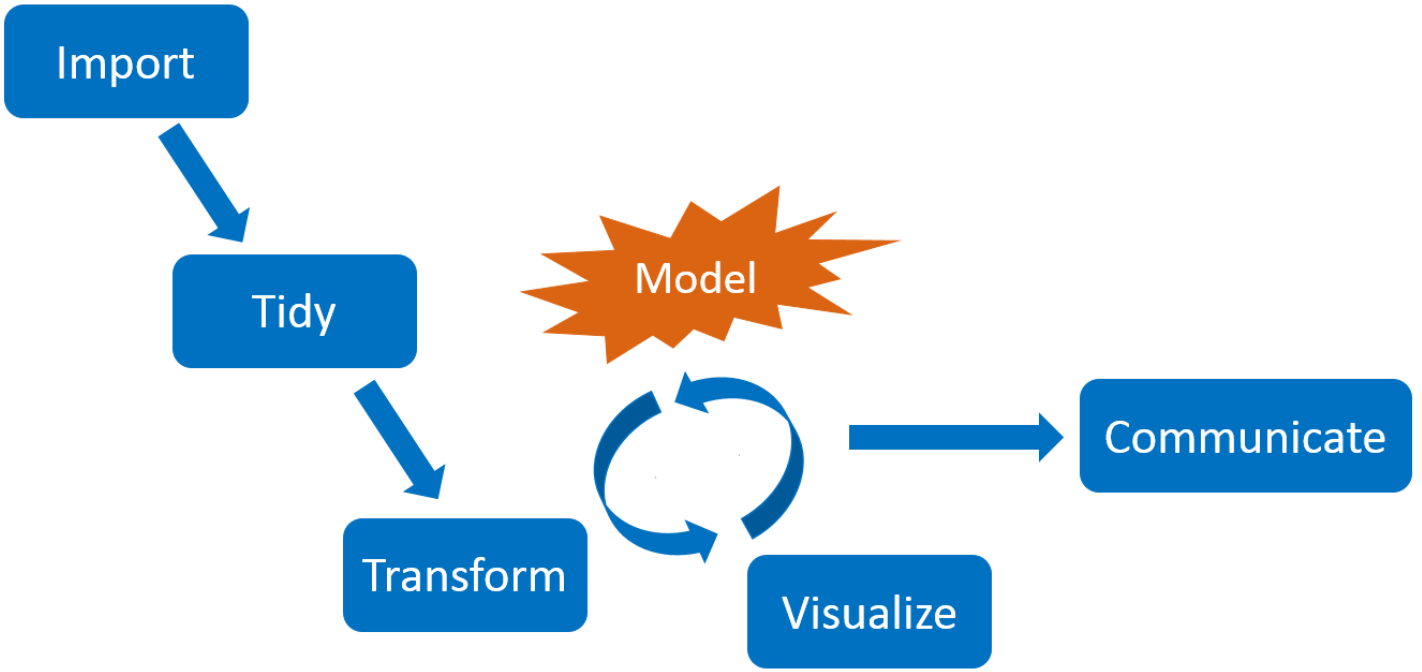
Changes



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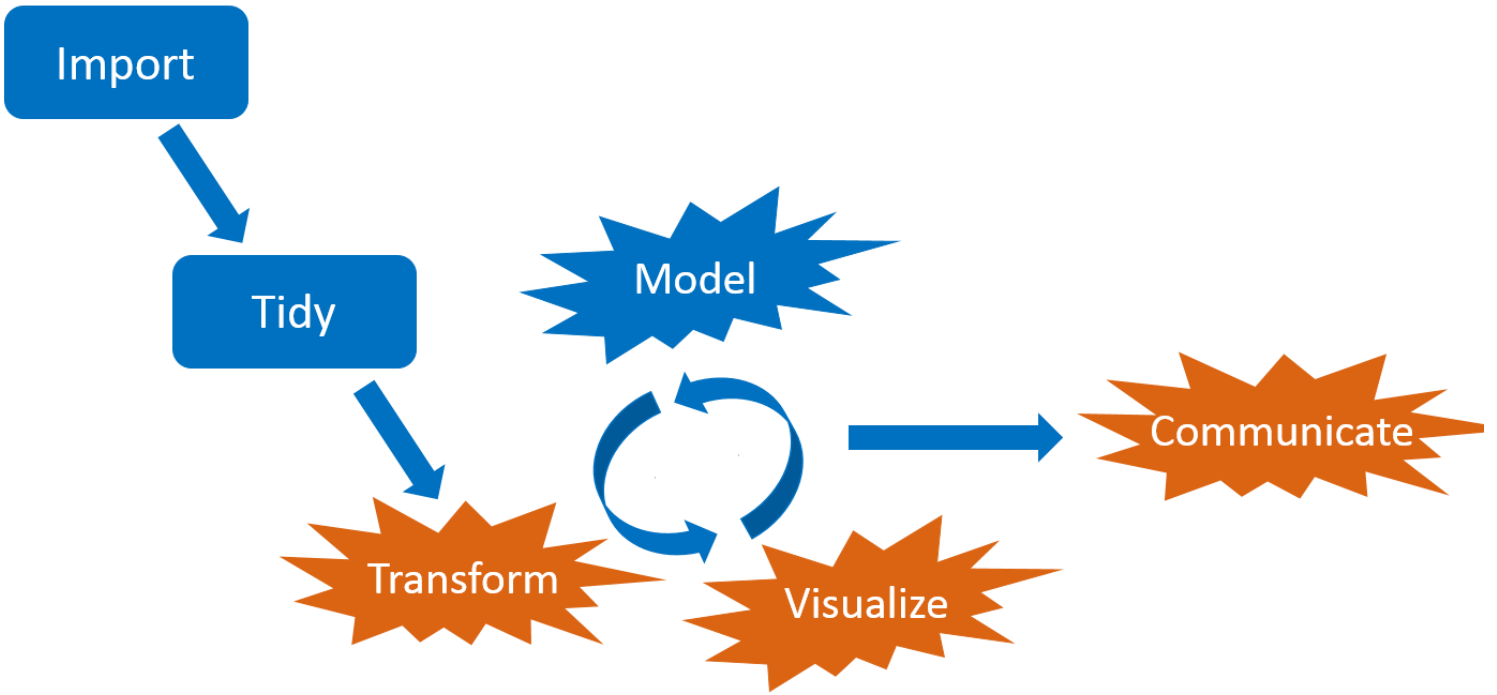
Consequences



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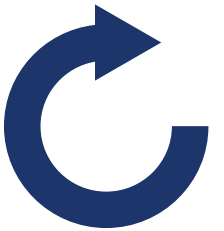
Pipeline tools and workflow managers

Scale up the work you need.

Skip the work you don't.



See evidence of reproducibility.

- Tons exist already: github.com/pditommaso/awesome-pipeline.
- Most are language-agnostic or designed for Python or the shell.

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What distinguishes `targets`?

- Fundamentally designed for R.
- Supports a clean, modular, function-oriented programming style.
- Abstracts files as R objects and automatically manages data.
- Surpasses the permanent limitations of its predecessor, `drake`: https://wlandau.github.io/targets/articles/need.html

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What about `drake`?

- `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.
  1. Stronger guardrails by design.
  2. A friendlier, lighter, more transparent data management system.
  3. Show which *functions* are up to date.
  4. More flexible dynamic branching, including compatibility with `dplyr::group_by()`.
  5. Improved parallel efficiency.
  6. Designed for custom user-side metaprogramming and target archetypes: https://wlandau.github.io/tarchetypes/.
- The statement of need describes the details: https://wlandau.github.io/targets/articles/need.html.

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Guardrails in `targets`

- The only way to use `targets` is the correct way.
- Main guardrails:
  1. Always run in a fresh R process (unless you deliberately configure `targets` for debugging).
  2. Require a `_targets.R` configuration file in the project root.
  3. Require the `_targets/` data store to always be in the project root.

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drake's cache

```
.drake/
├── config/
├── data/
├──── 17bfcef645301416.rds
├──── 21935c86f12692e2.rds
├──── 37caf5df2892cfc4.rds
├──── ...
├── drake/
├── keys/
├──── memoize/
├──── meta/
├──── objects/
├──── ...
└── scratch/
```

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The data store in `targets`

```
_targets/
├── meta/
├────── meta
├────── progress
├── objects/
├────── target_name_1
├────── target_name_2
├────── target_name_3
└────── ...
```

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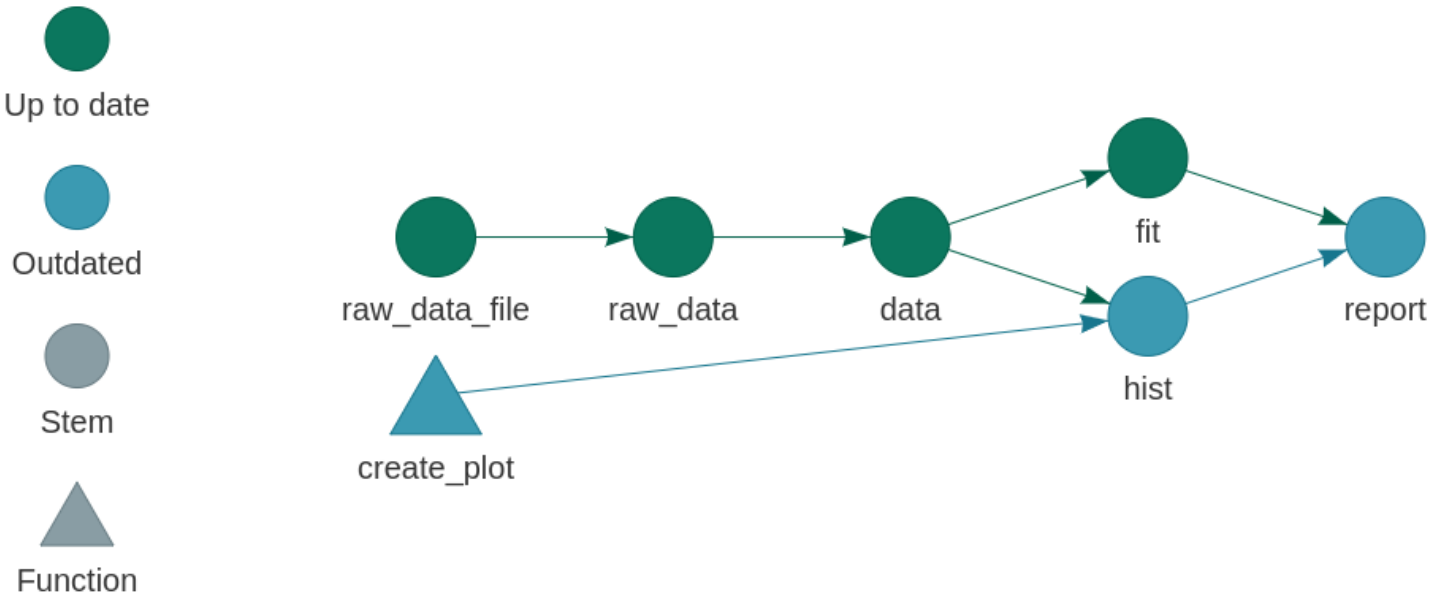
Show which functions are out of date



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Dynamic branching with `dplyr`

```
library(dplyr)
library(targets)
data.frame(
  x = seq_len(6),
  id = rep(letters[seq_len(3)], each = 2)
) %>%
  group_by(id) %>%
  tar_group()
#> # A tibble: 6 x 3
#> # Groups:   id [3]
#>       x id    tar_group
#>   <int> <chr>     <int>
#> 1     1 a             1
#> 2     2 a             1
#> 3     3 b             2
#> 4     4 b             2
#> 5     5 c             3
#> 6     6 c             3
```

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Define a target with groups.

```
tar_target(
  data,
  data.frame(
    x = seq_len(6),
    id = rep(letters[seq_len(3)], each = 2)
  ) %>%
    group_by(id) %>%
    tar_group(),
  iteration = "group"
)
```

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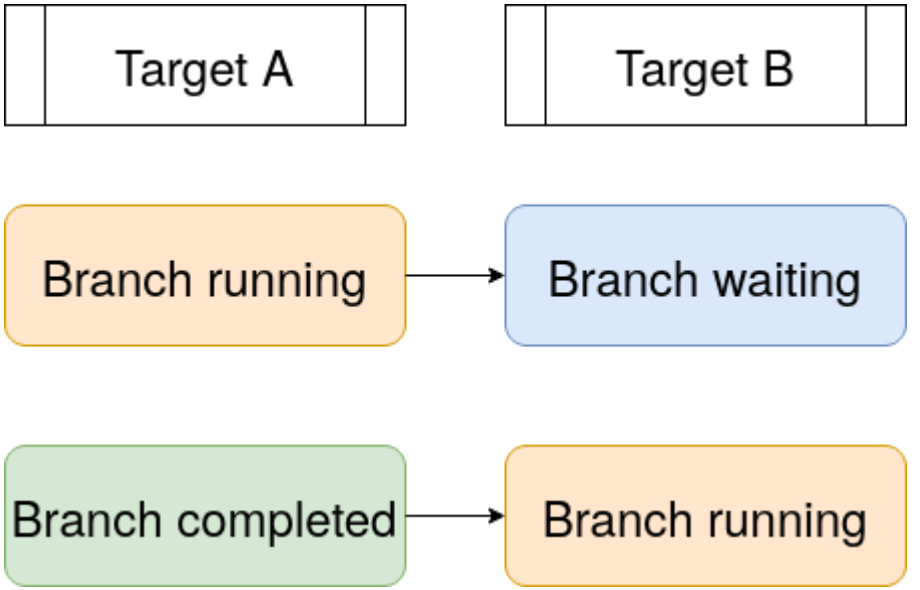
Parallel efficient dynamic branching



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Metaprogramming

- `tar_target_raw()` avoids non-standard evaluation and supports third-party metaprogramming.
- The following are equivalent ways to define a target.

```
# For most users:
tar_target(data, simulate_data(), pattern = map(index))

# For developers who metaprogram reusable pipeline archetypes:
tar_target_raw(
  "data",
  quote(simulate_data()),
  pattern = quote(map(index))
)
```

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Target archetypes

- The `tarchetypes` package has helpers for commonly used targets: https://wlandau.github.io/tarchetypes/

Function	Target archetype
`tar_render()`	Render a dependency-aware R Markdown report.
`tar_knit()`	Run a dependency-aware `knitr` report.
`tar_change()`	Always run a target when a custom object changes.
`tar_force()`	Always run a target when a custom condition is true.
`tar_suppress()`	Never run a target when a custom condition is true.
`tar_plan()`	Simplified `drake`-like syntax for `targets` pipelines.

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Example targets workflow

- Find the model that best predicts which customers will cancel their telecom subscriptions.
- IBM Watson Telco Customer Churn dataset.
- Workflow principles generalize to the other fields, such as the life sciences.

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❌ Move away from numbered imperative scripts.

```
run_everything.R
R/
├── 01-data.R
├── 02-munge.R
├── 03-model.R
├── 04-results.R
└── 05-plot.R
data/
└── customer_churn.csv
```

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 Embrace **functions.**

> - Everything that exists is an object.
> - Everything that happens is a function call.
>
> John Chambers

```
add_things <- function(argument1, argument2) {
  argument1 + argument2
}

add_things(1, 2)
#> [1] 3

add_things(c(3, 4), c(5, 6))
#> [1]  8 10
```

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Functions for customer churn

```
split_data <- function(churn_file) {
  read_csv(churn_file, col_types = cols()) %>%
    initial_split(prop = 0.3)
}

prepare_recipe <- function(churn_data) {
  churn_data %>%
    training() %>%
    recipe(Churn ~ .) %>%
    step_rm(customerID) %>%
    step_naomit(all_outcomes(), all_predictors()) %>%
    step_discretize(tenure, options = list(cuts = 6)) %>%
    step_log(TotalCharges) %>%
    step_mutate(Churn = ifelse(Churn == "Yes", 1, 0)) %>%
    step_dummy(all_nominal(), -all_outcomes()) %>%
    step_center(all_predictors(), -all_outcomes()) %>%
    step_scale(all_predictors(), -all_outcomes()) %>%
    prep()
}
```

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Functions for customer churn

```
define_model <- function(churn_recipe, units1, units2, act1, act2, ac
  # ...
}

train_model <- function(churn_recipe, units1, units2, act1, act2, act
  # ...
}

test_accuracy <- function(churn_data, churn_recipe, churn_model) {
  # ...
}

test_model <- function(churn_data, churn_recipe, units1, units2, acti
  # ...
}

retrain_run <- function(churn_run, churn_recipe) {
  # ...
}
```

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Typical project structure

- There are many variations on this theme.

```
_targets.R # Required top-level configuration file.
R/
└── functions.R
data/
└── customer_churn.csv
```

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Build up your workflow as a pipeline of targets.

```
# _targets.R
library(targets)
source("R/functions.R")
tar_option_set(packages = c("keras", "tidyverse", "rsample", "recipes
tar_pipeline(
  tar_target(churn_file, "data/customer_churn.csv", format = "file"),
  tar_target(churn_data, split_data(churn_file)),
  tar_target(churn_recipe, prepare_recipe(churn_data))
)
```

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The pipeline is a collection of skippable *targets*.

```
tar_manifest(fields = c("name", "command"))
#> # A tibble: 3 x 2
#>   name         command
#>   <chr>        <chr>
#> 1 churn_recipe "prepare_recipe(churn_data)"
#> 2 churn_data   "split_data(churn_file)"
#> 3 churn_file   "\"data/customer_churn.csv\""
```

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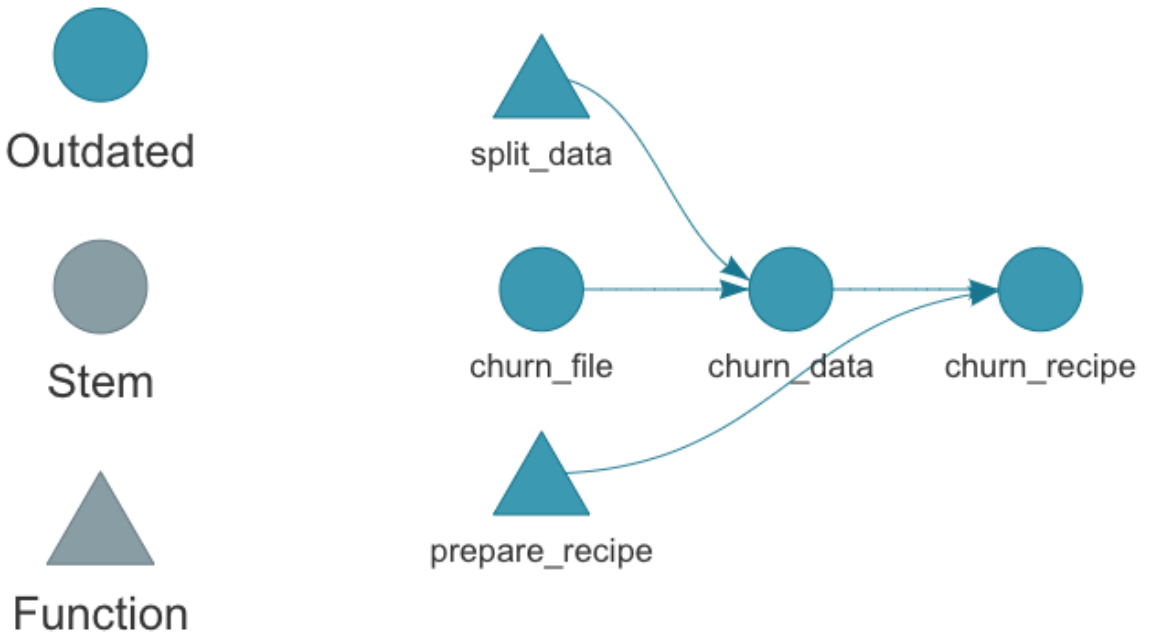
targets understands code and data dependencies.

```
tar_visnetwork()
```



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Build your first targets.

```
tar_make()
```

```
#> ● run target churn_file
#> ● run target churn_data
#> ● run target churn_recipe
```

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Check the targets for problems

- `tar_load()` and `tar_read()` get targets from the `_targets/` data store.

```
ncol(training(tar_read(churn_data)))
#> [1] 21

tar_load(churn_recipe)
ncol(juice(churn_recipe))
#> [1] 36
```

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Build up the pipeline *gradually*.

1. Add a couple targets.
2. Run the pipeline with `tar_make()`.
3. Inspect the new targets with `tar_load()` and `tar_read()`.
4. Repeat often. Not very time-consuming because `tar_make()` skips up-to-date targets.

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Add some models.

```
# _targets.R
library(targets)
source("R/functions.R")
tar_option_set(packages = c("keras", "tidyverse", "rsample", "recipes
tar_pipeline(
  tar_target(churn_file, "data/customer_churn.csv", format = "file"),
  tar_target(churn_data, split_data(churn_file)),
  tar_target(churn_recipe, prepare_recipe(churn_data)),
  tar_target(run_relu, test_model(act1 = "relu", churn_data, churn_re
  tar_target(run_sigmoid, test_model(act1 = "sigmoid", churn_data, ch
)
```

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Previous work is still up to date.

```
tar_outdated()
```

```
#> [1] "run_relu"    "run_sigmoid"
```

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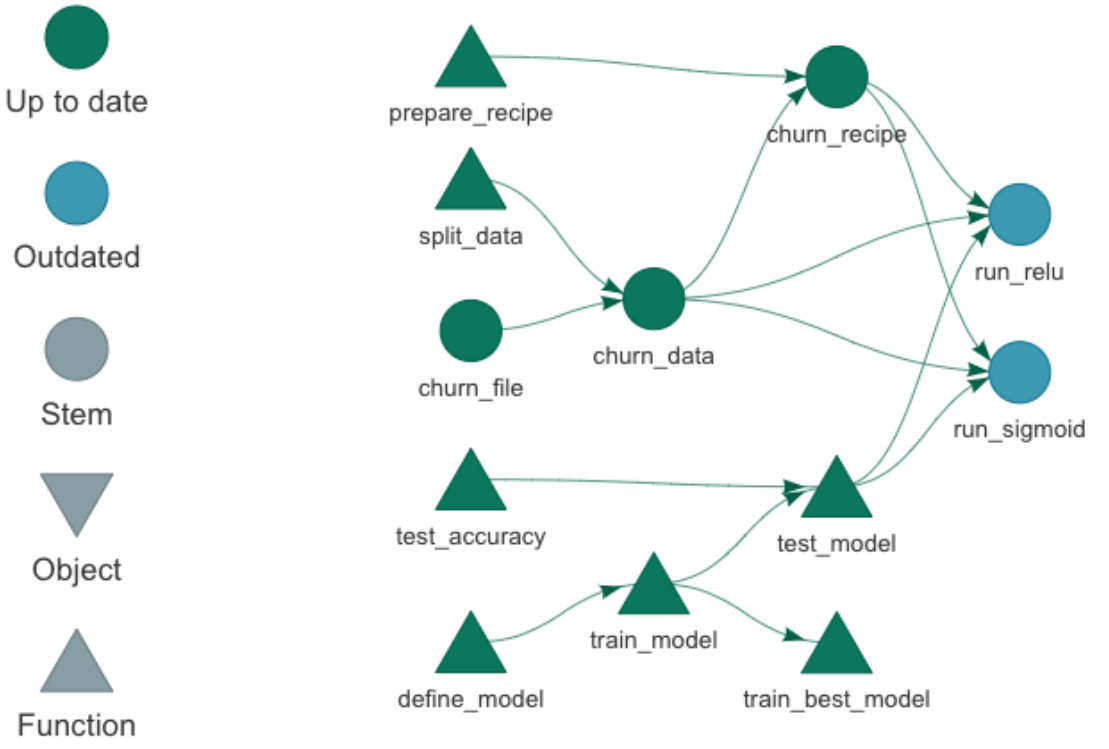
Previous work is still up to date.

```
tar_visnetwork()
```



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Up-to-date targets are skipped.

```
tar_make()
```

```
#> ✓ skip target churn_file
#> ✓ skip target churn_data
#> ✓ skip target churn_recipe
#> ● run target run_relu
#> ● run target run_sigmoid
```

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Inspect the newest targets.

```
tar_read(run_relu)
#> # A tibble: 1 x 6
#>   accuracy units1 units2 act1  act2  act3
#>      <dbl>  <dbl>  <dbl> <chr> <chr> <chr>
#> 1    0.799     16     16 relu  relu  sigmoid

tar_read(run_sigmoid)
#> # A tibble: 1 x 6
#>   accuracy units1 units2 act1    act2  act3
#>      <dbl>  <dbl>  <dbl> <chr>   <chr> <chr>
#> 1    0.799     16     16 sigmoid relu  sigmoid
```

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Find the best model

```
# _targets.R
library(targets)
source("R/functions.R")
tar_option_set(packages = c("keras", "tidyverse", "rsample", "recipes
tar_pipeline(
  ...,
  tar_target(run_relu, test_model(act1 = "relu", churn_data, churn_re
  tar_target(run_sigmoid, test_model(act1 = "sigmoid", churn_data, ch
  tar_target(
    best_run,
    bind_rows(run_relu, run_sigmoid) %>%
      top_n(1, accuracy) %>%
      head(1)
  ),
  tar_target(
    best_model,
    retrain_run(best_run, churn_recipe),
    format = "keras"
  )
)
```

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Find the best model

```
tar_make()
```

```
#> ✓ skip target churn_file
#> ✓ skip target churn_data
#> ✓ skip target churn_recipe
#> ✓ skip target run_relu
#> ✓ skip target run_sigmoid
#> ● run target best_run
#> ● run target best_model
```

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Find the best model

```
tar_read(best_model)
#> Model
#> Model: "sequential_2"
#> _________________________________________________________________
#> Layer (type)                 Output Shape              
#> =================================================================
#> dense_6 (Dense)              (None, 16)                
#> _________________________________________________________________
#> dropout_4 (Dropout)          (None, 16)                
#> _________________________________________________________________
#> dense_7 (Dense)              (None, 16)                
#> _________________________________________________________________
#> dropout_5 (Dropout)          (None, 16)                
#> _________________________________________________________________
#> dense_8 (Dense)              (None, 1)                 
#> =================================================================
#> Total params: 865
#> Trainable params: 865
#> Non-trainable params: 0
#> _________________________________________________________________
```

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Try another model.

```
# _targets.R
library(targets)
source("R/functions.R")
tar_option_set(packages = c("keras", "tidyverse", "rsample", "recipes
tar_pipeline(
  ...,
  tar_target(run_relu, test_model(act1 = "relu", churn_data, churn_re
  tar_target(run_sigmoid, test_model(act1 = "sigmoid", churn_data, ch
  tar_target(run_softmax, test_model(act1 = "softmax", churn_data, ch
  tar_target(
    best_run,
    bind_rows(run_relu, run_sigmoid, run_softmax) %>%
      top_n(1, accuracy) %>%
      head(1)
  ),
  ...
)
```

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What gets done stays done.

```
tar_outdated()
```

```
#> [1] "run_softmax" "best_run"    "best_model"
```

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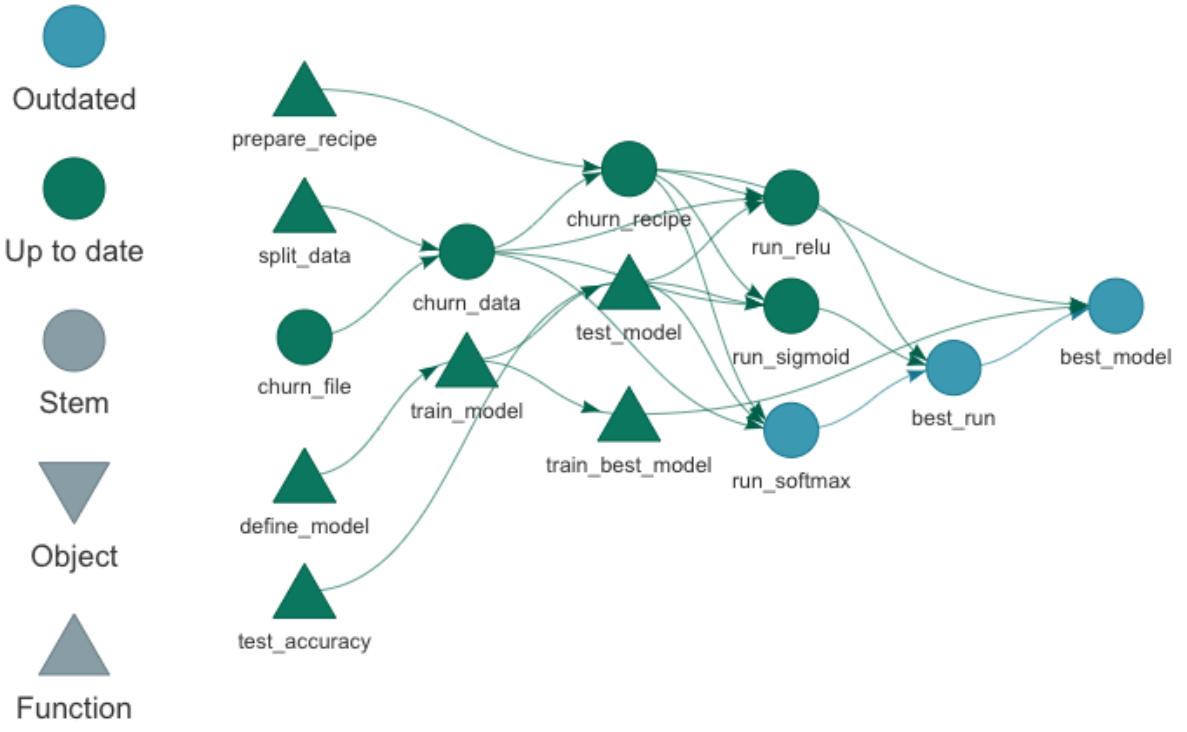
What gets done stays done.

```
tar_visnetwork()
```



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New best model?

- Only if the new run beats the old runs, which would invalidate target `best_run`.
- Otherwise, `drake` does not bother to retrain the best model.

```
tar_make()
#> ✓ skip target churn_file
#> ✓ skip target churn_data
#> ✓ skip target churn_recipe
#> ✓ skip target run_relu
#> ✓ skip target run_sigmoid
#> ● run target run_softmax
#> ● run target best_run
#> ✓ skip target best_model
```

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What if we need to change a function?

```
define_model <- function(churn_recipe, units1, units2, act1, act2, ac
  input_shape <- ncol(
    juice(churn_recipe, all_predictors(), composition = "matrix")
  )
  keras_model_sequential() %>%
    layer_dense(
      units = units1,
      kernel_initializer = "uniform",
      activation = act1,
      input_shape = input_shape
    ) %>%
    layer_dropout(rate = 0.2) %>% # previously 0.1
    layer_dense(
      units = units2,
      kernel_initializer = "uniform",
      activation = act2
    ) %>%
    layer_dropout(rate = 0.1) %>%
    ...
```

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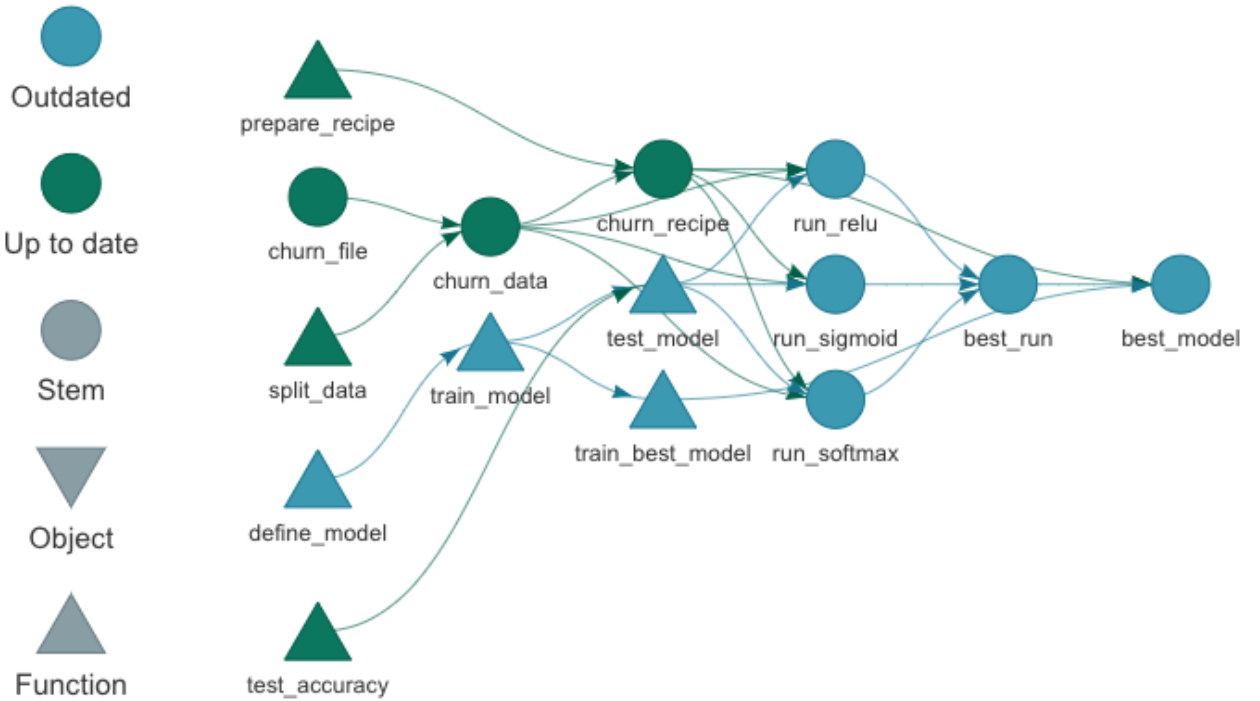
Show invalidated functions and targets.

```
tar_visnetwork()
```



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Rerun invalidated targets.

```
tar_make()
#> ✓ skip target churn_file
#> ✓ skip target churn_data
#> ✓ skip target churn_recipe
#> ● run target run_relu
#> ● run target run_sigmoid
#> ● run target run_softmax
#> ● run target best_run
#> ● run target best_model
```

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Similar story if the data file changes.

```
tar_make()
#> ● run target churn_file
#> ● run target churn_data
#> ● run target churn_recipe
#> ● run target run_relu
#> ● run target run_sigmoid
#> ● run target run_softmax
#> ● run target best_run
#> ● run target best_model
```

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Evidence of reproducibility

```
tar_make(plan)
#> ✓ skip target churn_file
#> ✓ skip target churn_data
#> ✓ skip target churn_recipe
#> ✓ skip target run_relu
#> ✓ skip target run_sigmoid
#> ✓ skip target run_softmax
#> ✓ skip target best_run
#> ✓ skip target best_model
#> ✓ Already up to date.
```

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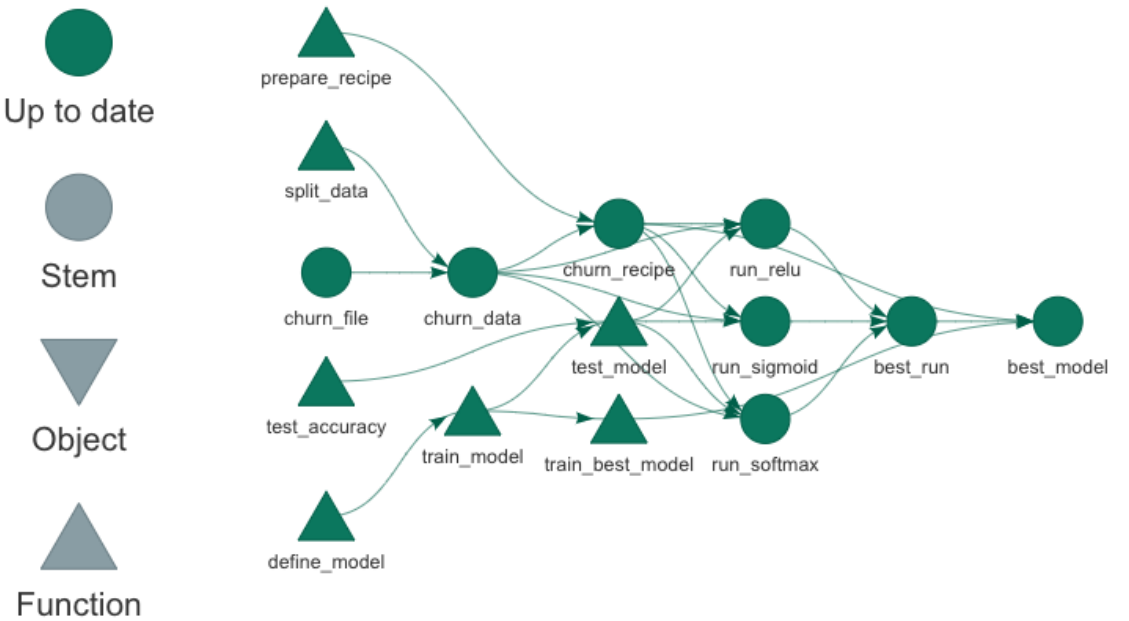
Evidence of reproducibility

```
tar_outdated()
#> character(0)

tar_visnetwork()
```



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Resources

- Get `targets`:

```
install.packages("remotes")
remotes::install_github("wlandau/targets")
```

- Code: https://github.com/wlandau/targets-keras
- RStudio Cloud workspace: https://rstudio.cloud/project/1430828/
- These slides: https://wlandau.github.io/targets-tutorial
- Tutorial materials: https://github.com/wlandau/targets-tutorial
- Development repository: https://github.com/wlandau/targets
- Full user manual: https://wlandau.github.io/targets-manual/
- Reference website: https://wlandau.github.io/targets/

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Thanks

- Edgar Ruiz
- example code

- Matt Dancho
- blog post

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The tutorial

1. Sign up for a free account at https://rstudio.cloud.
2. Log into https://rstudio.cloud/project/1512447.
3. Work through the R notebooks in order.
4. Optional: revisit the material again later at https://github.com/wlandau/targets-tutorial.

Topic	Notebook
Functions	`1-functions.Rmd`
Pipelines	`2-pipelines.Rmd`
Changes	`3-changes.Rmd`
Files	`4-files.Rmd`
Branching	`5-branching.Rmd`
Debugging	`6-debugging.Rmd`
Challenge	`7-challenge.Rmd`

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