Reproducible computation at scale in R

Will Landau

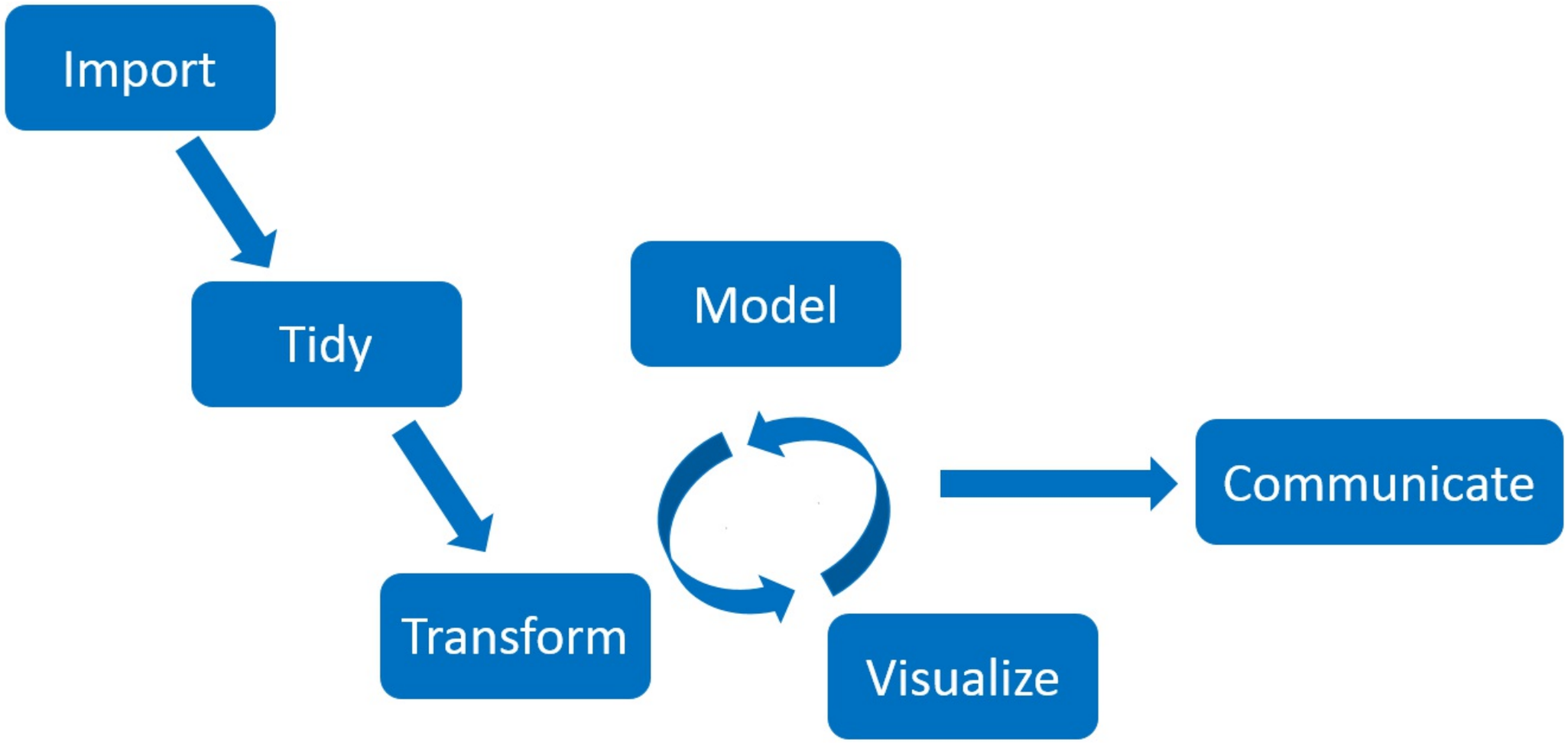
Purpose: manage data analyses with long runtimes

Scale up the work you need.

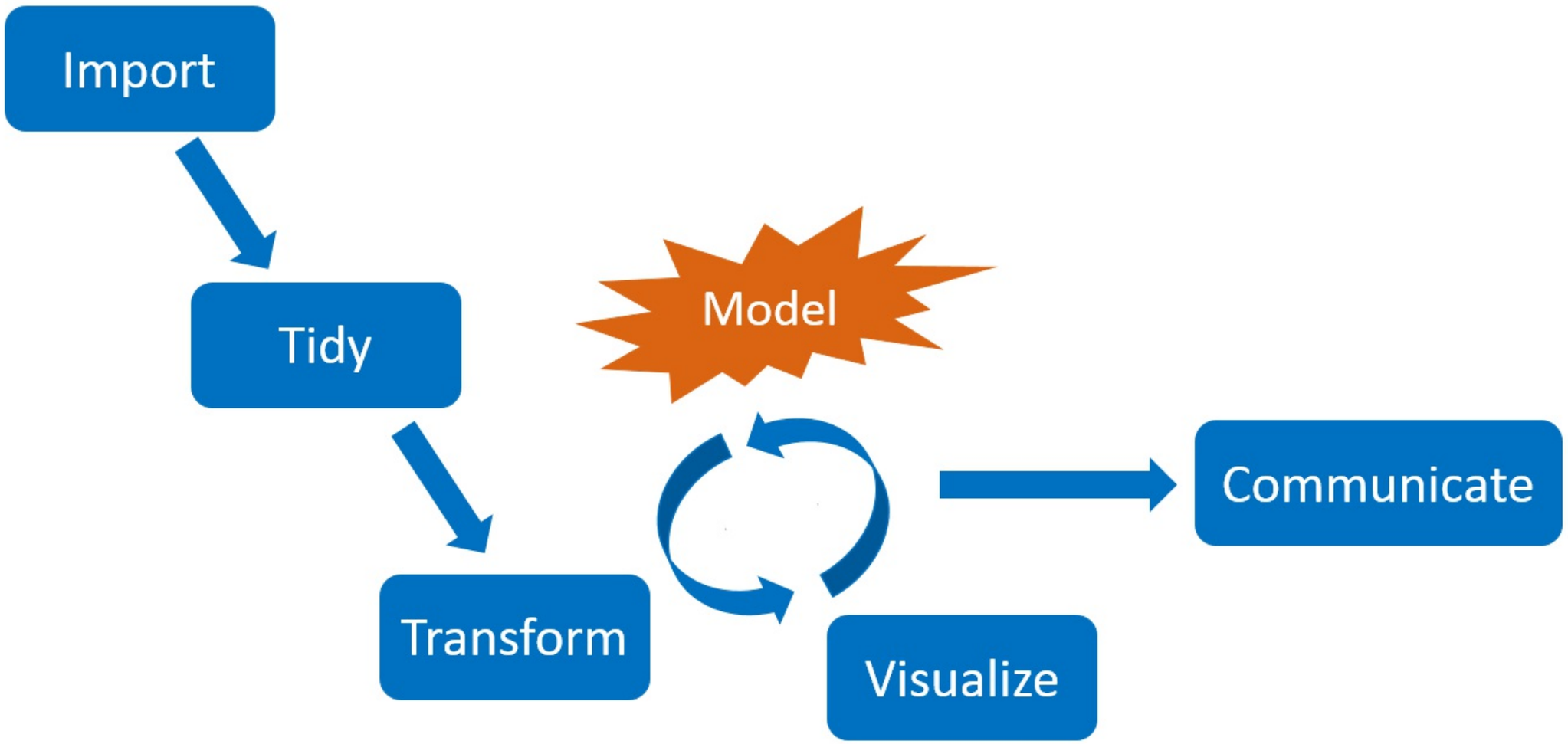
Skip the work you don't.

See evidence of reproducibility.

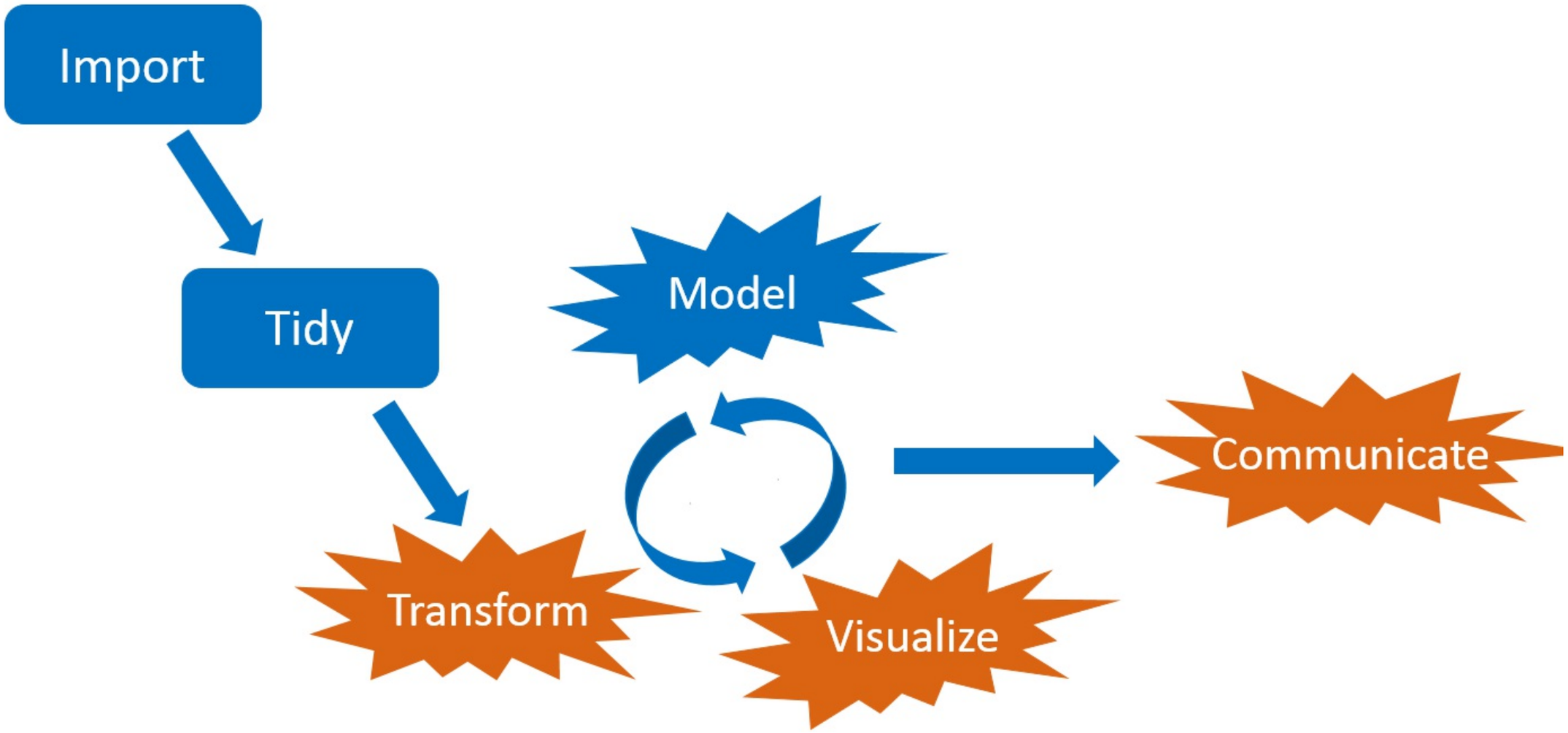
Workflows have interconnected steps.



When you change something...



...the downstream steps are no longer valid.



Do you rerun everything from scratch?

- Takes too long.
- Too frustrating.

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

Do you pick and choose pieces to update?

- Messy and prone to human error.
- Not reproducible.

https://openclipart.org/detail/216179/messy-desk

Pipeline toolkits solve this problem.

- Sophisticated, vibrant, active space of tools: github.com/pditommaso/awesome-pipeline.
- Most are language-agnostic or designed for other languages.
- **`drake`** is uniquely devoted to R.
  - A focus on ordinary R functions and variables rather than cumbersome files.
  - Heavy use of the data frame, even as a substitute for the traditional Makefile.
  - Native tidy evaluation support.
  - A domain-specific language (DSL) for creating large workflows.

Example uses in the pharmaceutical industry

- Clinical trial modeling and simulation
- Subgroup identification
- Bayesian network meta analysis
- Graph-based multiple comparison procedures
- Bayesian networks in genomics
- PK/PD modeling (e.g. `mrgsolve`)
- **Deep learning**

Example deep learning workflow

- Goal: predict customers who cancel their subscriptions with a telecom company.
- Data: IBM Watson Telco Customer Churn dataset.
- Workflow principles generalize to pharma, e.g. business analytics and genomics problems.

https://openclipart.org/detail/90739/newplus, https://github.com/rstudio/keras

File structure

```
make.R
R/
├── packages.R
├── functions.R
└── plan.R
data/
└── customer_churn.csv
```

packages.R

```
library(drake)
library(keras)
library(recipes)
library(rsample)
library(tidyverse)
library(yardstick)
```

functions.R

```
prepare_recipe <- function(data) {
  # ...
}

define_model <- function(rec) {
  # ...
}

train_model <- function(data, batch_size) {
  # ...
}

confusion_matrix <- function(data, rec, serialized_model) {
  # ...
}

compare_models <- function(...) {
  # ...
}
```

plan.R

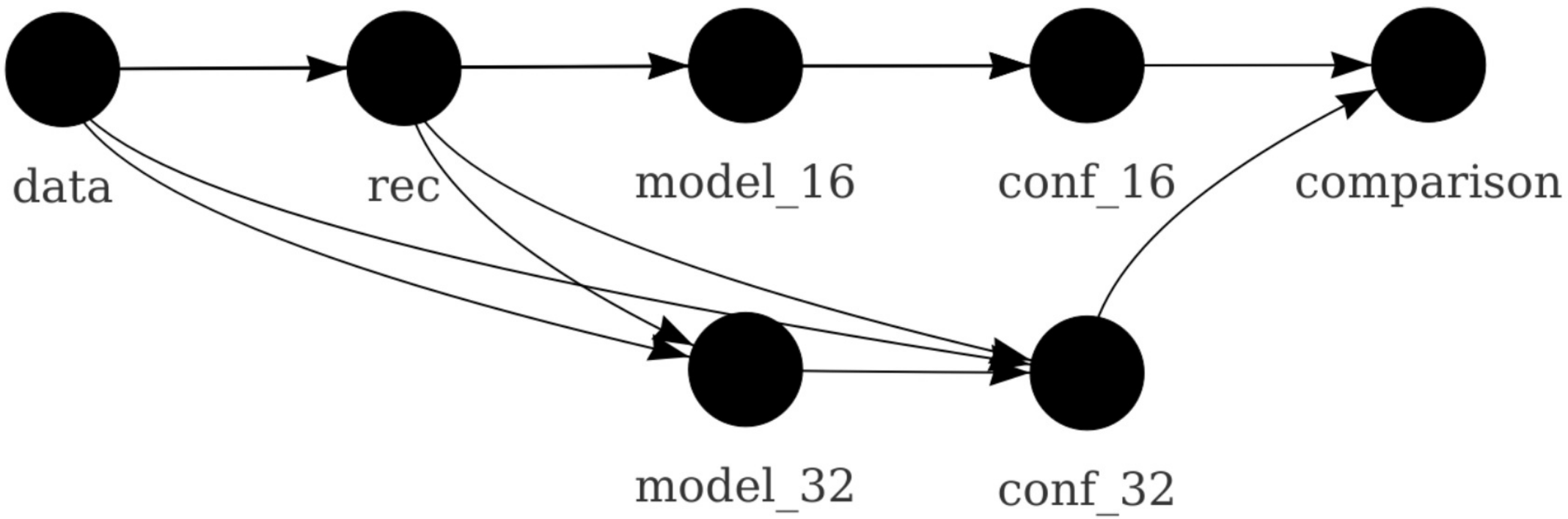
```
batch_sizes <- c(16, 32)

plan <- drake_plan(
  data = read_csv(file_in("data/customer_churn.csv")) %>%
    initial_split(prop = 0.3),
  rec = prepare_recipe(data),
  model = target(
    train_model(data, rec, batch_size),
    transform = map(batch_size = !!batch_sizes)
  ),
  conf = target(
    confusion_matrix(data, rec, model),
    transform = map(model, .id = batch_size)
  ),
  comparison = target(
    compare_models(conf),
    transform = combine(conf)
  )
)
```

Data frame of workflow steps

```
plan
## # A tibble: 7 x 2
##   target     command
##   <chr>      <expr>
## 1 data       read_csv(file_in("data/customer_churn.csv")) %>% initial_spl
## 2 rec        prepare_recipe(data)
## 3 model_16   train_model(data, rec, 16)
## 4 model_32   train_model(data, rec, 32)
## 5 conf_16    confusion_matrix(data, rec, model_16)
## 6 conf_32    confusion_matrix(data, rec, model_32)
## 7 comparison compare_models(conf_16, conf_32)
```

The workflow



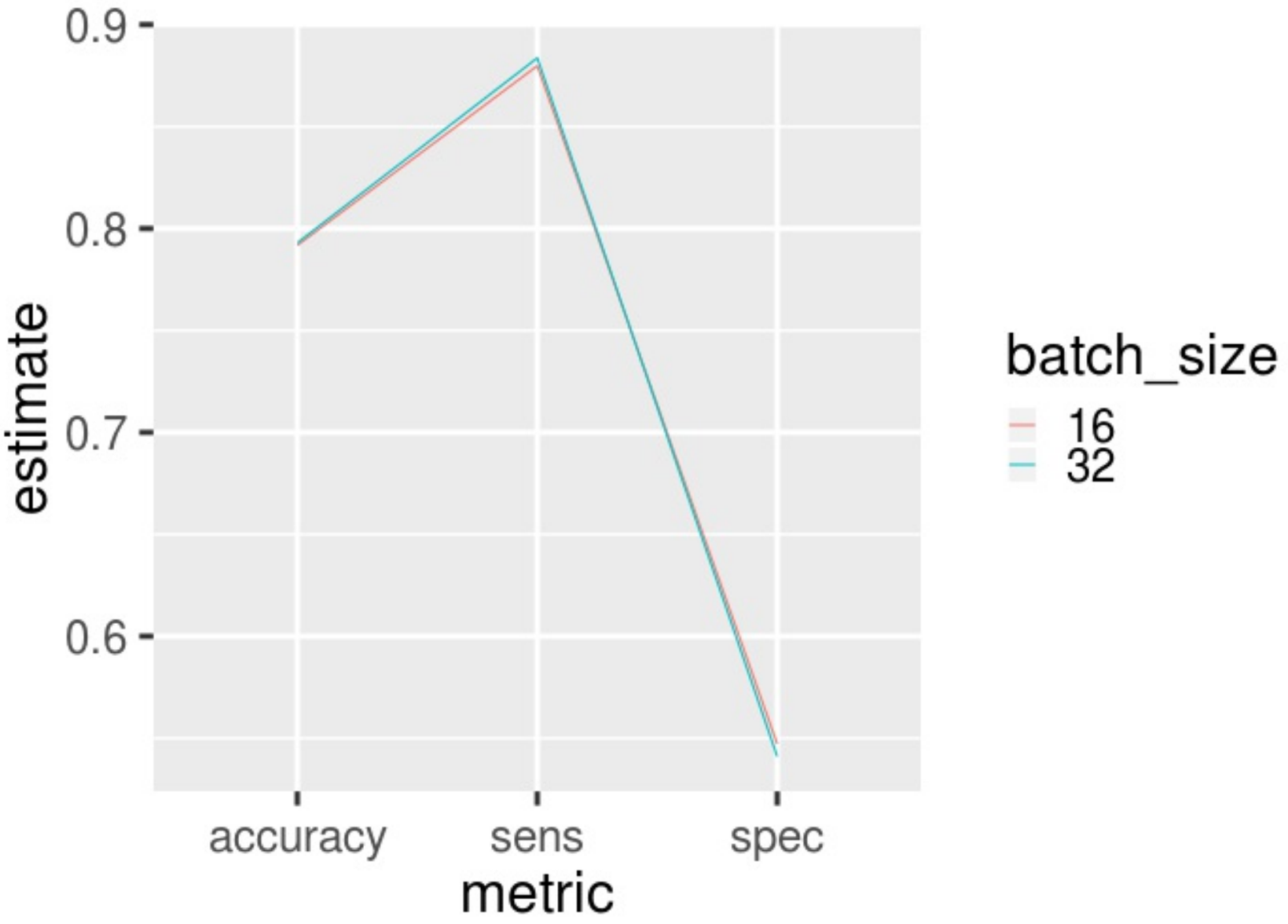
Run the project in make.R.

```
source("R/packages.R")
source("R/functions.R")
source("R/plan.R")

make(plan)
## target data
## target rec
## target model_16
## target model_32
## target conf_16
## target conf_32
## target comparison
```

Compare models.

```
readd(comparison) # See also loadd()
```

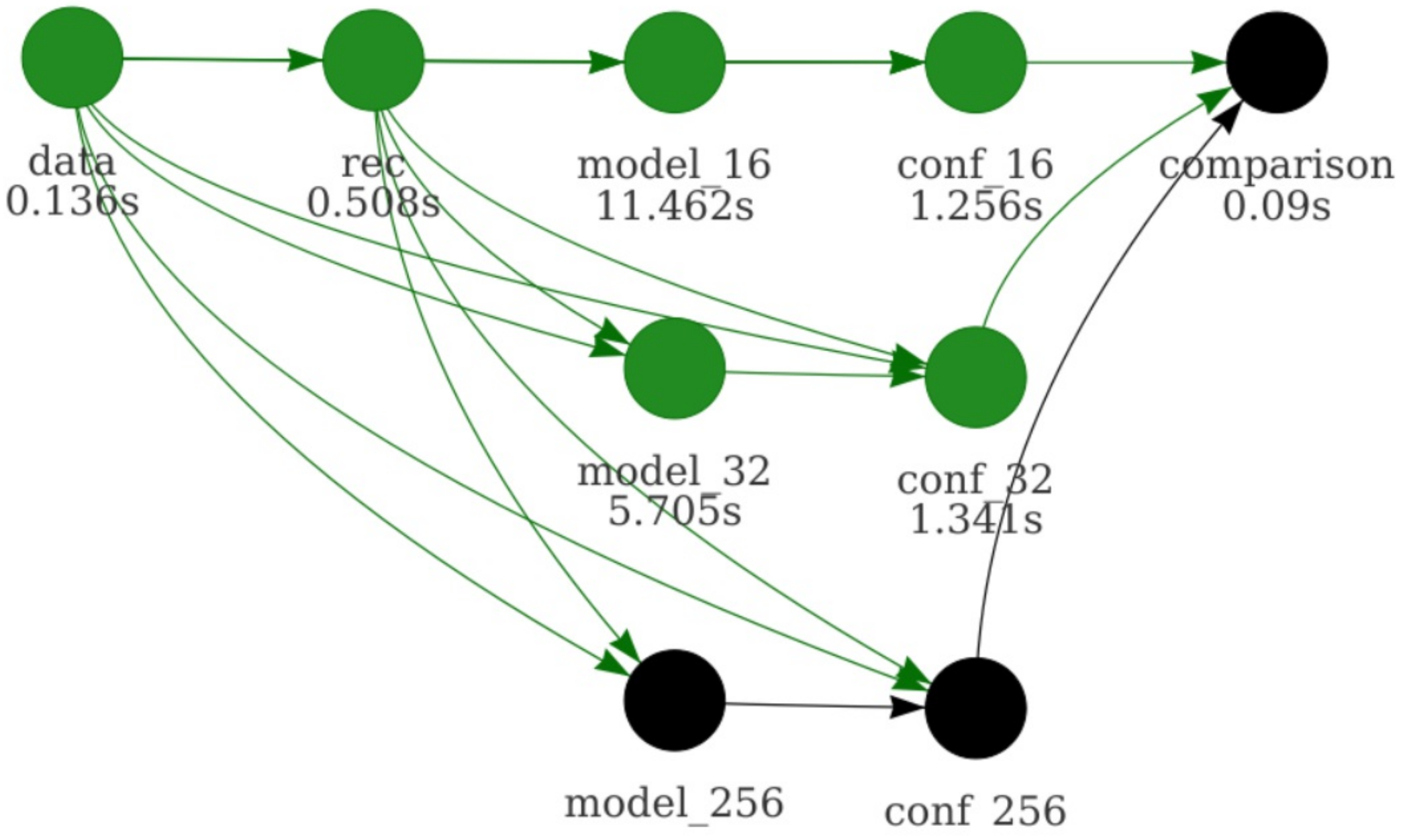


Try another batch size.

```
batch_sizes <- c(16, 32, 64)

plan <- drake_plan(
  data = read_csv(file_in("data/customer_churn.csv")) %>%
    initial_split(prop = 0.3),
  rec = prepare_recipe(data),
  model = target(
    train_model(data, rec, batch_size),
    transform = map(batch_size = !!batch_sizes)
  ),
  conf = target(
    confusion_matrix(data, rec, model),
    transform = map(model, .id = batch_size)
  ),
  comparison = target(
    compare_models(conf),
    transform = combine(conf)
  )
)
```

vis_drake_graph()



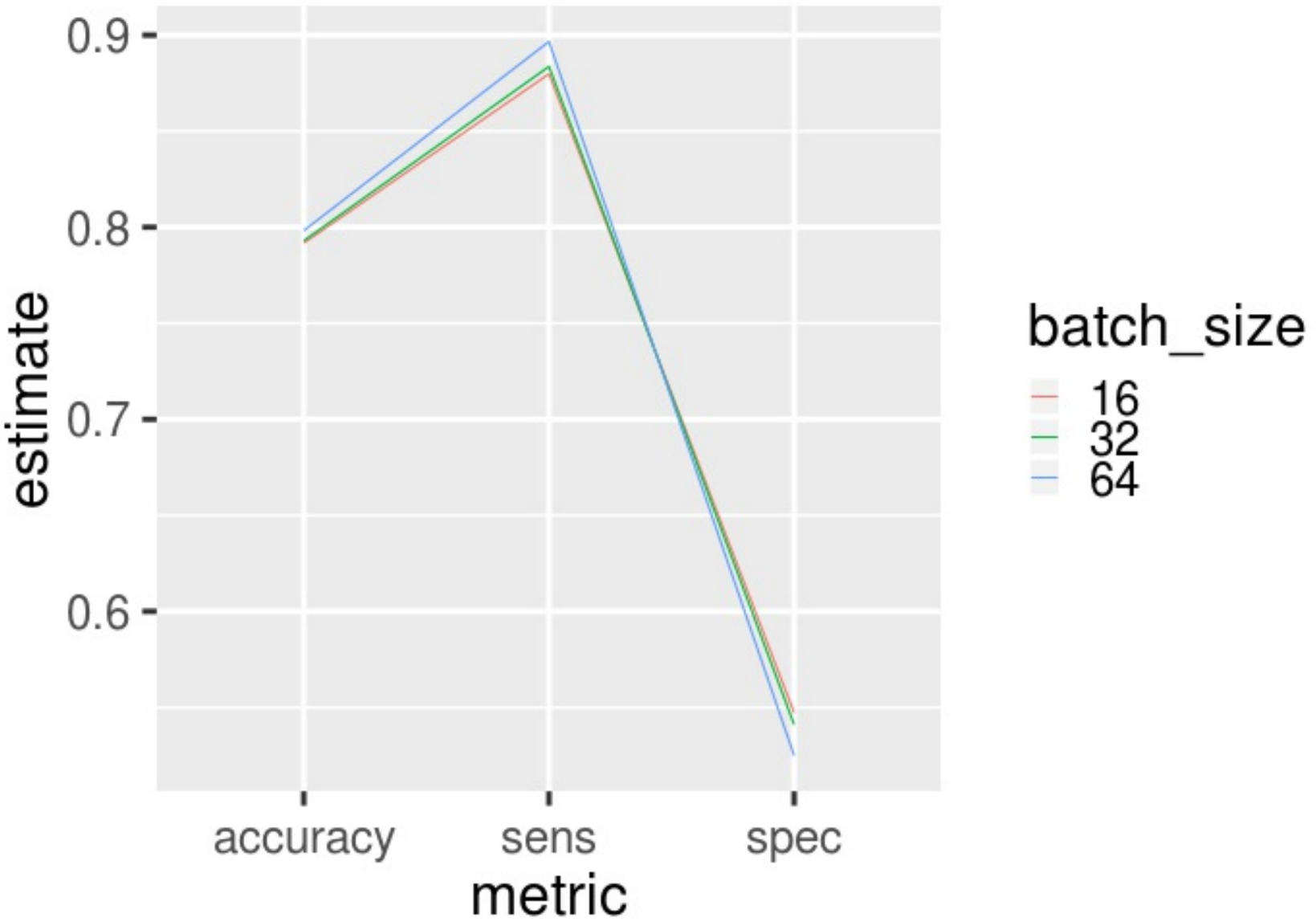
Refresh the results in make.R.

```
source("R/packages.R")
source("R/functions.R")
source("R/plan.R") # modified

make(plan)
## target model_64
## target conf_64
## target comparison
```

Compare models.

```
readd(comparison)
```



Evidence of reproducibility.

```
source("R/packages.R")
source("R/functions.R")
source("R/plan.R")

make(plan)
## All targets are already up to date.
```

- See also `outdated()`.

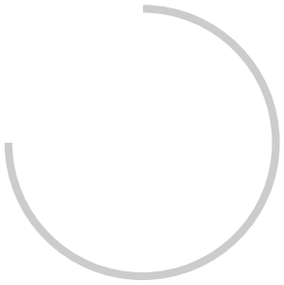
High-performance computing.

```
# template file with configuration
drake_hpc_template_file("slurm_clustermq.tmpl")

# Use SLURM resource manager with the template.
options(
  clustermq.scheduler = "slurm",
  clustermq.template = "slurm_clustermq.tmpl"
)

# make() is the basically the same.
make(plan, jobs = 2, parallelism = "clustermq")
```

High-performance computing.



Resources

```
install.packages("drake")                    # release
devtools::install_github("ropensci/drake") # development
```

- Today's code: `drake_example("deep-learning")`
- Reference website
- Full user manual
- Example workflows
- File an issue.
- Contribute code.
- Discuss at rOpenSci.org.

Thanks

- Edgar Ruiz
- example code

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- blog post

Thanks

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