

# Reproducible workflows at scale with drake

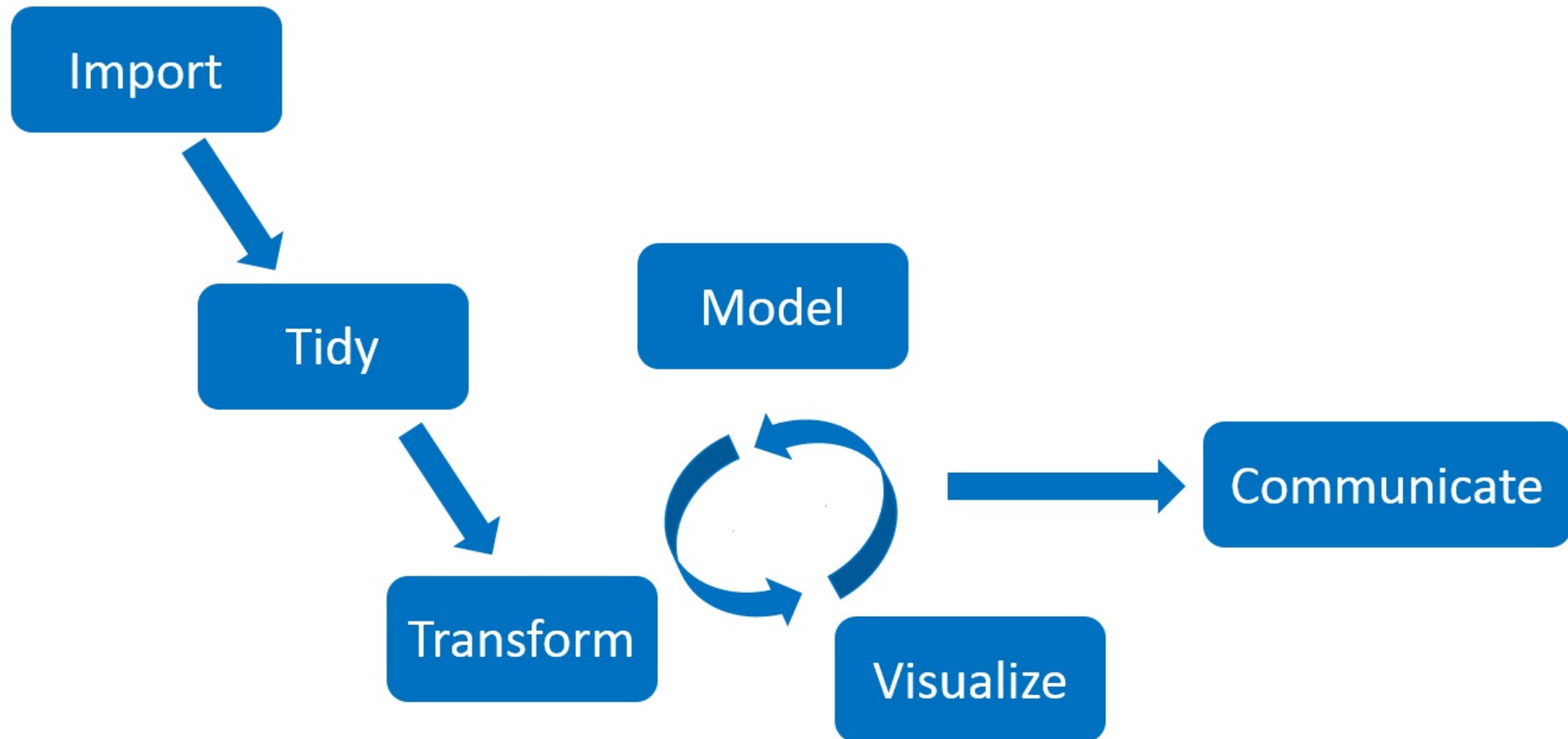


Will Landau

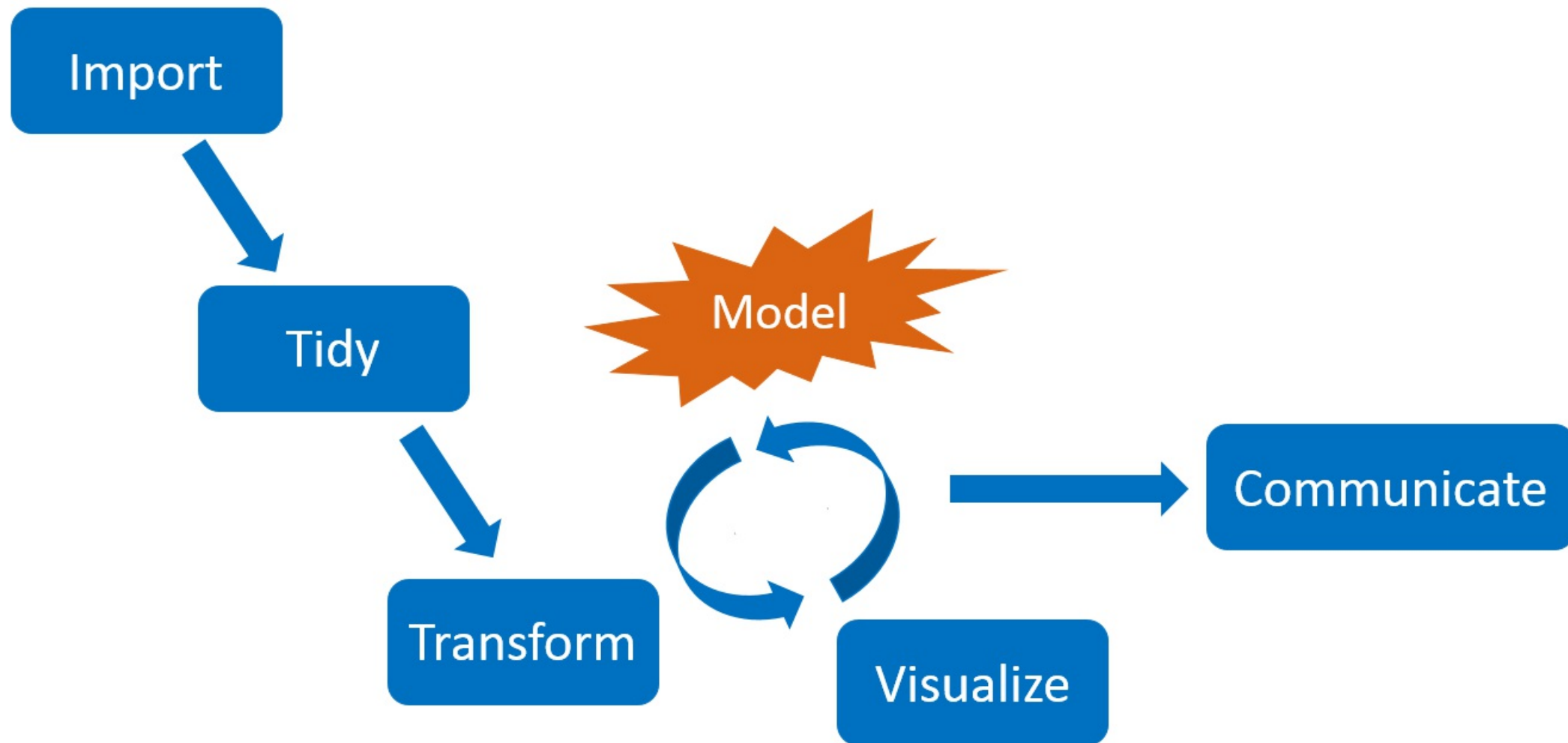
# Large data science workflows

- Struggles
  1. Long runtimes.
  2. Many tasks.
  3. Interconnected tasks.
- Examples
  - Deep learning
  - Classical machine learning.
  - Bayesian computation via Markov chain Monte Carlo (`rjags`, `rstan`, etc.)
  - Spatial data analysis.
  - Clinical trial modeling and simulation.
  - Subgroup identification.
  - Graph-based multiple comparison procedures.
  - Genomics pipelines.
  - PK/PD modeling (`mrgsolve`, `nlmixr`, etc.)

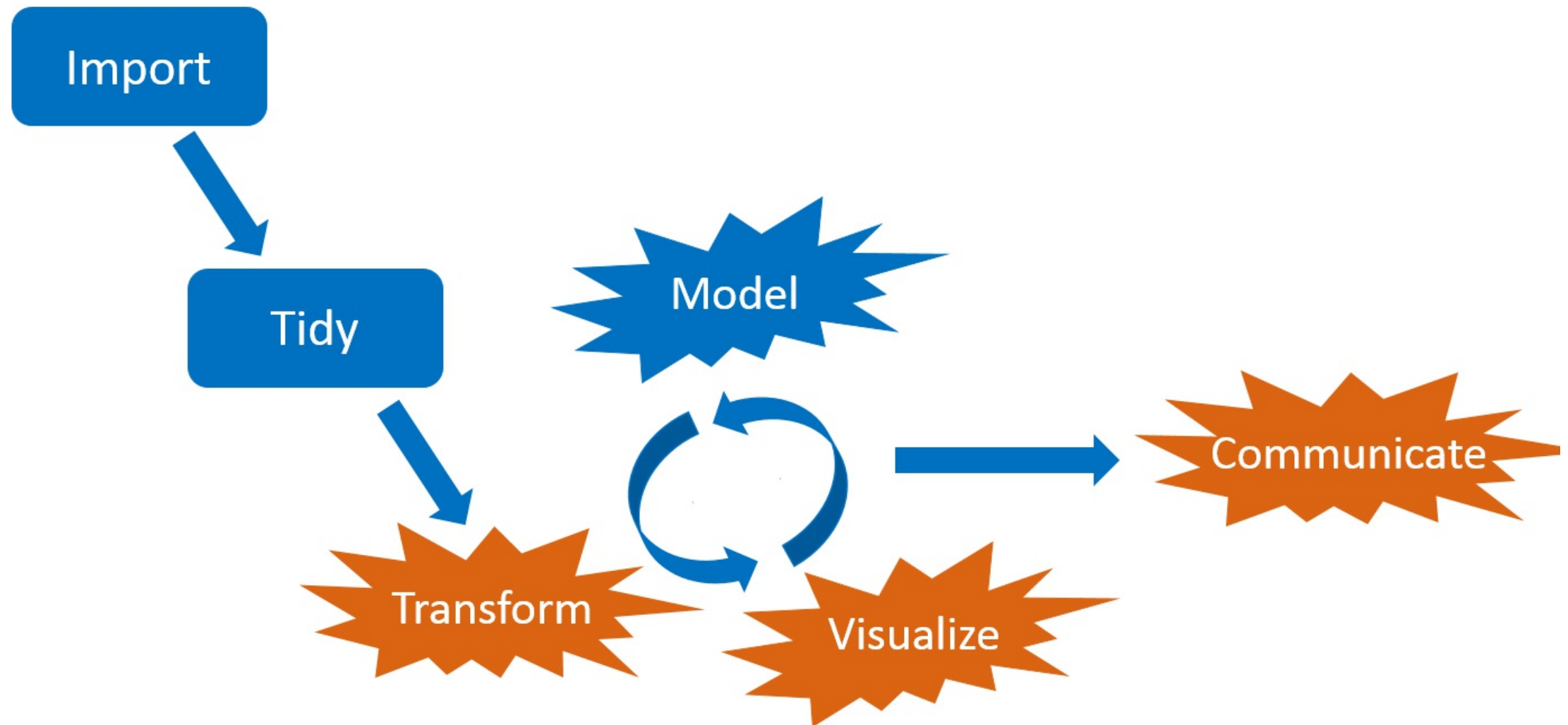
# Interconnected tasks



# When you change something...



...the downstream output is no longer valid.



# Do you rerun everything from scratch?

- Not if you deal with long runtimes!



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

# Do you pick and choose what to update?

- Messy.
- Prone to human error.
- Not reproducible.



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

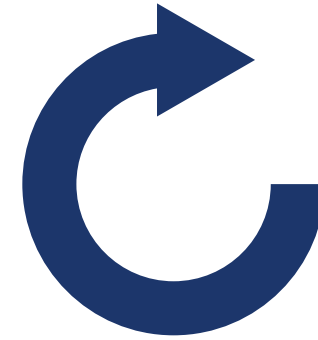
# Solution: pipeline tools



**Scale** up the  
work you need.



**Skip** the  
work you don't.



**See** evidence of  
reproducibility.

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



# What distinguishes `drake`?



- Aggressively designed for R.
  1. Think **functions**, not script files.
  2. Think **variables**, not output files.
  3. Think **data frames**, not `Makefiles`.
- `drake` borrows (1) and (2) from the `remake` package by Rich FitzJohn.
  - `remake` is no longer under development.
  - `drake` tries to extend `remake`'s ideas further and handle larger projects.

# Example: a 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 other industries.



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

# Projects like this get too big for numbered scripts!

```
run_everything.R
R/
├─ 01-data.R
├─ 02-munge.R
├─ 03-model.R
├─ 04-results.R
└─ 05-plot.R
data/
└─ customer_churn.csv
output/
├─ model_relu.h5
├─ model_sigmoid.h5
├─ confusion_matrix.rds
└─ metrics_plot.png
```

# Why not numbered scripts?

- The planning and the execution happen at the same time.
- Cumbersome, ad hoc, jumbled, muddled.

```
# 02-munge.R
library(recipes) # Package dependencies scattered across scripts.

rec <- data %>% # Single-use code, difficult to test.
  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()

saveRDS(rec, "recipe.rds") # Final output scattered across code.
```

# Instead, embrace functions!

- Separate the planning from the execution.
- Clarity: break down complicated ideas into manageable pieces.
- Reuse: define once, run whenever: testing, development, etc.

```
make.R
R/
├─ packages.R
├─ functions.R
├─ plan.R
data/
├─ customer_churn.csv
.drake/ # drake's cache
├─      # Output magically appears here.
```

# Write function-oriented R scripts.

```
# packages.R: all package dependencies
library(recipes)
# other packages...
```

```
# functions.R: pure reusable code
prepare_recipe <- function(data) {
  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()
}
# other functions...
```

# Conduct your analysis with your functions.

```
# run_everything.R
source("R/packages.R")
source("R/functions.R")
data <- read_csv(file_in("data/customer_churn.csv"), col_types = cols()) %>%
  initial_split(prop = 0.3)
saveRDS(data, "output/data.rds")
rec <- prepare_recipe(data) # Use your functions.
saveRDS(rec, "output/rec.rds")
model_relu <- train_model(rec, act1 = "relu")
save_model_hdf5(model_relu, "output/model_relu.h5")
model_sigmoid <- train_model(rec, act1 = "sigmoid")
save_model_hdf5(model_sigmoid, "output/model_sigmoid.h5")
conf_relu <- confusion_matrix(data, rec, model_relu)
saveRDS(conf_relu, "output/conf_relu.rds")
conf_sigmoid <- confusion_matrix(data, rec, model_sigmoid)
saveRDS(conf_sigmoid, "output/conf_sigmoid.rds")
metrics <- compare_models(conf_relu, conf_sigmoid)
saveRDS(metrics, "output/metrics.rds")
```

# But we can still do better...

- Avoid rerunning everything every time.
- Avoid micromanaging files. No more `saveRDS()`, `save_model_hdf5()`, etc.



<https://publicdomainvectors.org/en/free-clipart/Golden-magic-lamp/61683.html>



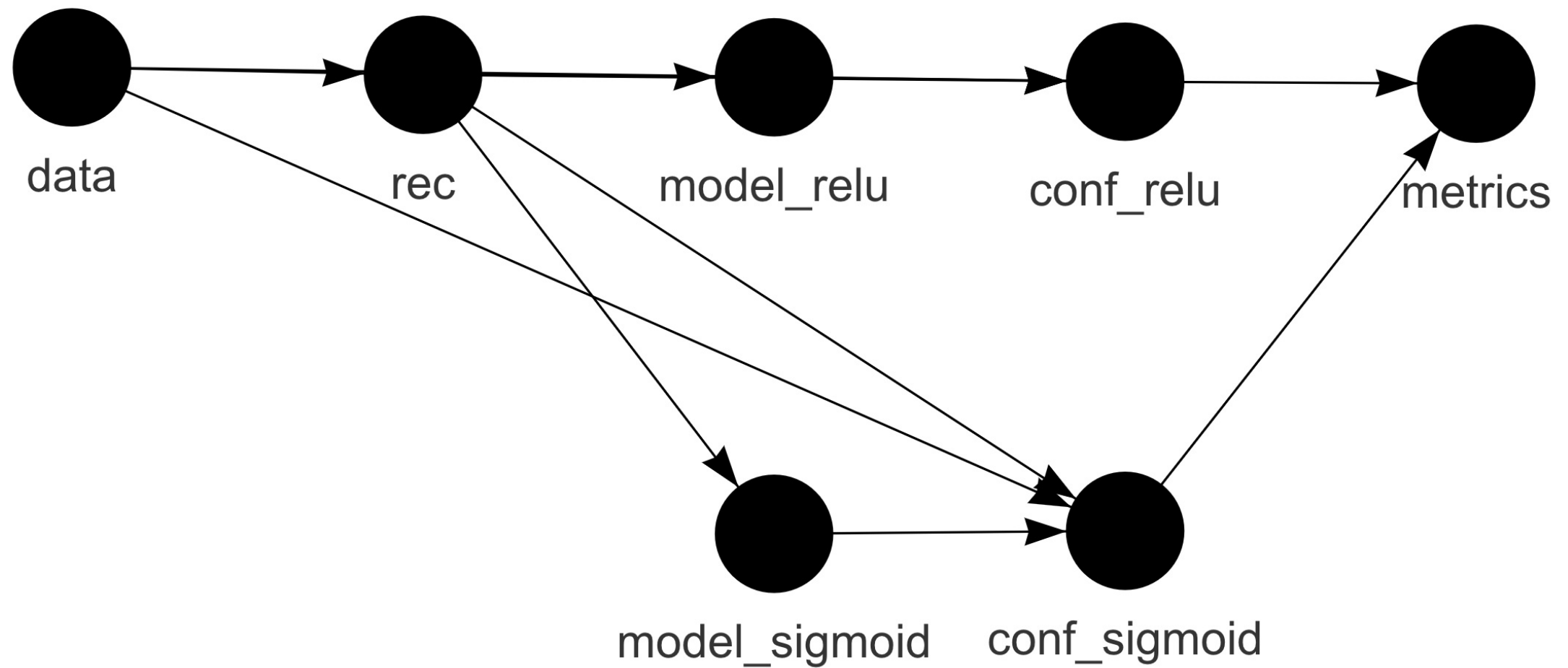
# Enter drake! Define a plan.

```
plan <- drake_plan(  
  rec = prepare_recipe(data), # Use your functions.  
  model = target(  
    train_model(rec, act1 = act),  
    format = "keras",  
    transform = map(act = c("relu", "sigmoid"))  
  ),  
  conf = target(  
    confusion_matrix(data, rec, model),  
    transform = map(model, .id = act)  
  ),  
  metrics = target(  
    compare_models(conf),  
    transform = combine(conf)  
  ),  
  data = read_csv(          # flexible target order,  
    file_in("data/customer_churn.csv"), # flexible commands  
    col_types = cols()  
  ) %>%  
    initial_split(prop = 0.3)  
)
```

# The plan is a data frame of skippable tasks.

```
plan
## # A tibble: 7 x 3
##   target      command      format
##   <chr>      <expr>      <chr>
## 1 rec        prepare_recipe(data)    ... <NA>
## 2 model_relu  train_model(rec, act1 = "relu")    ... keras
## 3 model_sigm... train_model(rec, act1 = "sigmoid")  ... keras
## 4 conf_relu   confusion_matrix(data, rec, model_relu)    ... <NA>
## 5 conf_sigmo... confusion_matrix(data, rec, model_sigmoid)  ... <NA>
## 6 metrics     compare_models(conf_relu, conf_sigmoid)    ... <NA>
## 7 data        read_csv(file_in("data/customer_churn.csv"), col_type... <NA>
```

# The workflow

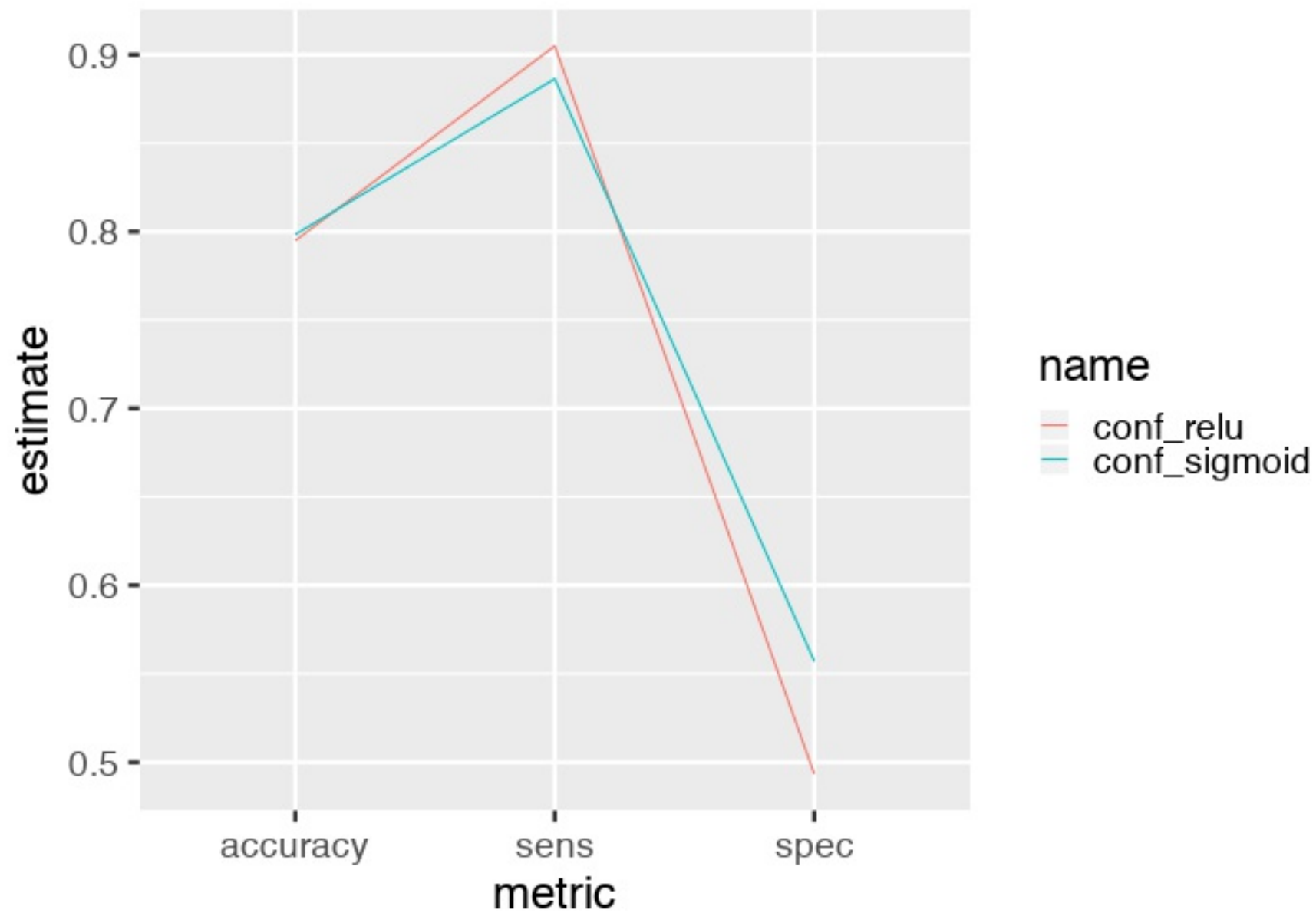


# Run the project in make.R.

```
source("R/packages.R")  
source("R/functions.R")  
source("R/plan.R")  
  
make(plan)  
## target data  
## target rec  
## target model_relu  
## target model_sigmoid  
## target conf_relu  
## target conf_sigmoid  
## target metrics
```

# Compare models.

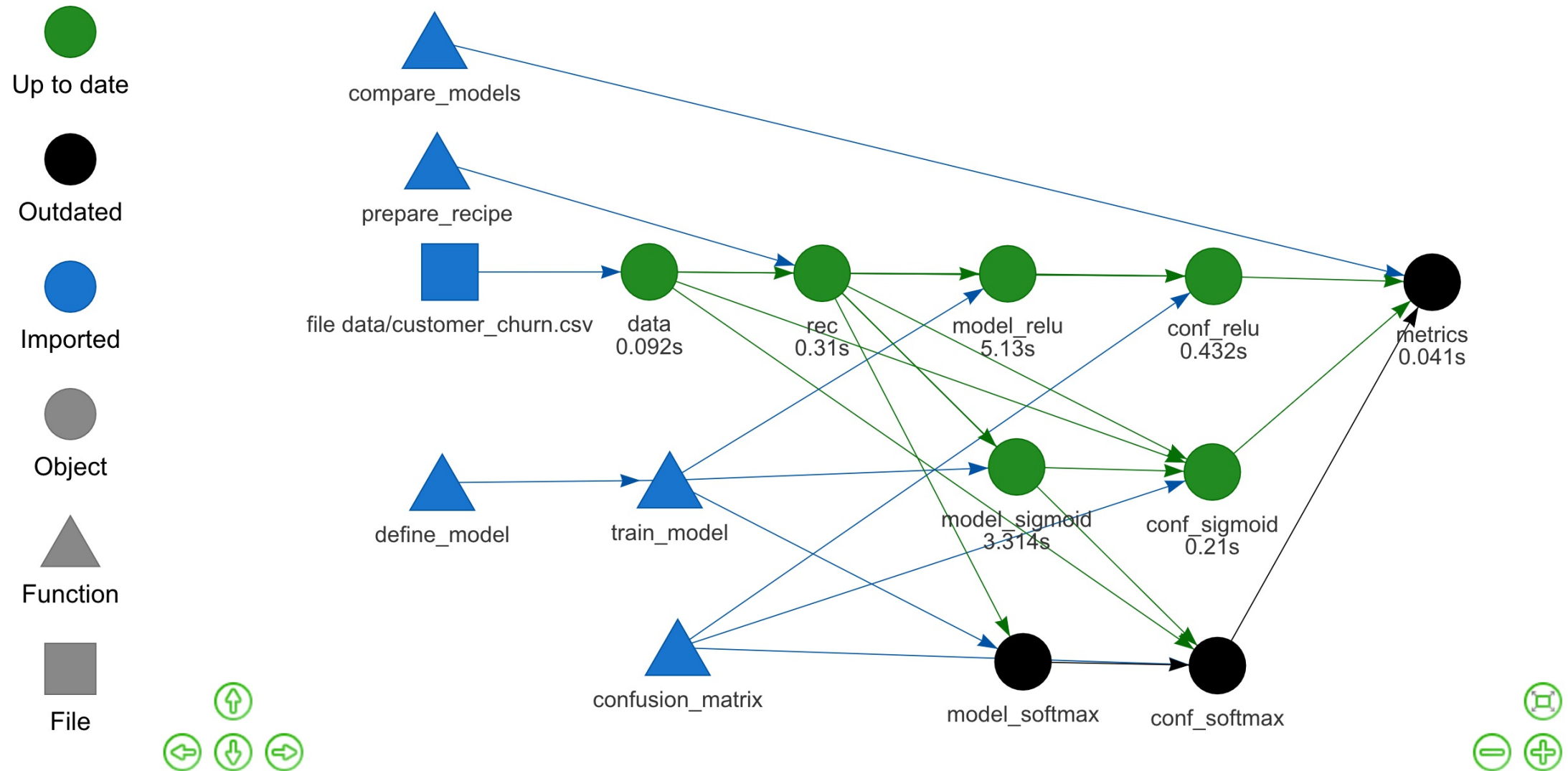
```
readd(metrics) # See also loadd()
```



# Add a new model.

```
plan <- drake_plan(  
  rec = prepare_recipe(data),  
  model = target(  
    train_model(rec, act1 = act),  
    format = "keras",  
    transform = map(act = c("relu", "sigmoid", "softmax"))  
  ),  
  conf = target(  
    confusion_matrix(data, rec, model),  
    transform = map(model, .id = act)  
  ),  
  metrics = target(  
    compare_models(conf),  
    transform = combine(conf)  
  ),  
  data = read_csv(  
    file_in("data/customer_churn.csv"),  
    col_types = cols()  
  ) %>%  
    initial_split(prop = 0.3)  
)
```

# vis\_drake\_graph()



# Refresh the results in make.R.

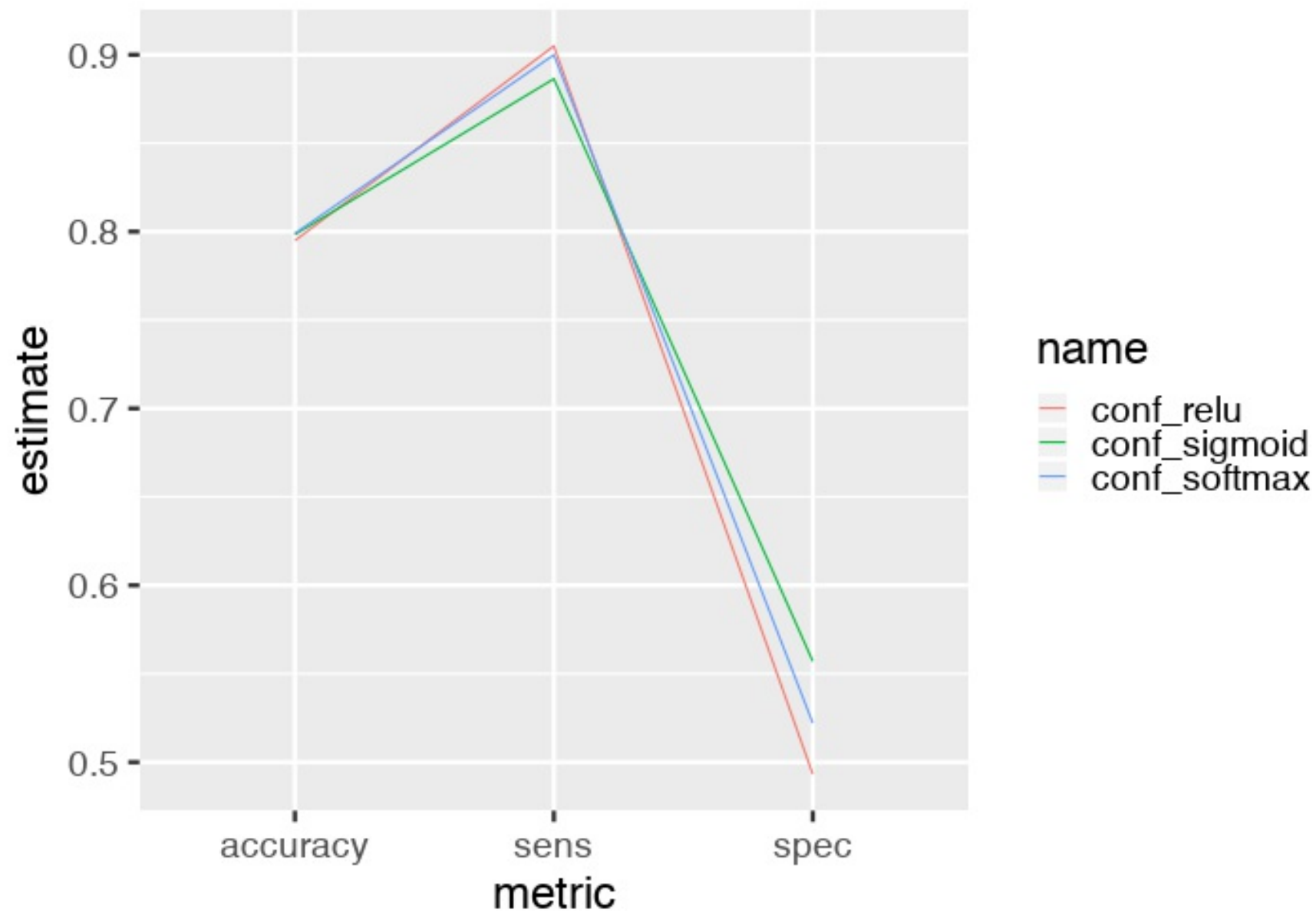
```
source("R/packages.R")  
source("R/functions.R")  
source("R/plan.R") # modified
```

```
make(plan)  
## target model_softmax  
## target conf_softmax  
## target metrics
```



# Compare models.

```
readd(metrics)
```



# 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()`.

# Fast big data formats

- Increased speed and reduced memory consumption.

```
library(drake)
n <- 1e8 # Each target is 1.6 GB in memory.
plan <- drake_plan(
  data_fst = target(
    data.frame(x = runif(n), y = runif(n)),
    format = "fst"
  ),
  data_old = data.frame(x = runif(n), y = runif(n))
)
make(plan)
#> target data_fst
#> target data_old
build_times(type = "build")
#> # A tibble: 2 x 4
#>   target      elapsed      user      system
#>   <chr>    <Duration>    <Duration>    <Duration>
#> 1 data_fst 13.93s      37.562s      7.954s
#> 2 data_old 184s (~3.07 minutes) 177s (~2.95 minutes) 4.157s
```

# History and provenance

```
drake_history()
## # A tibble: 10 x 10
##   target    current built exists hash  command      seed runtime  prop act
##   <chr>    <lgl>    <chr> <lgl> <chr> <chr>      <int>   <dbl> <dbl> <chr>
## 1 conf_r... TRUE    2019-... TRUE  8b54... confusio... 4.05e8  0.213   NA    <NA>
## 2 conf_s... TRUE    2019-... TRUE  8e03... confusio... 1.93e9  0.203   NA    <NA>
## 3 conf_s... TRUE    2019-... TRUE  c1ad... confusio... 1.80e9  0.408   NA    <NA>
## 4 data      TRUE    2019-... TRUE  ca84... "read_cs... 1.29e9  0.038   0.3   <NA>
## 5 metrics  FALSE   2019-... TRUE  6907... compare_... 1.21e9  0.0230  NA    <NA>
## 6 metrics  TRUE    2019-... TRUE  0c22... compare_... 1.21e9  0.021   NA    <NA>
## 7 model_... TRUE    2019-... TRUE  35f6... "train_m... 1.47e9  4.76    NA    rel
## 8 model_... TRUE    2019-... TRUE  4f8b... "train_m... 1.26e9  3.12    NA    sig
## 9 model_... TRUE    2019-... TRUE  d19a... "train_m... 8.05e8  3.26    NA    sof
## 10 rec      TRUE    2019-... TRUE  40e5... prepare_... 6.29e8  0.160   NA    <NA>
```

# Reproducible data recovery

```
clean() # Oops!

start <- proc.time()
make(plan, recover = TRUE)
## recover data
## recover rec
## recover model_relu
## recover model_sigmoid
## recover model_softmax
## recover conf_relu
## recover conf_sigmoid
## recover conf_softmax
## recover metrics

proc.time() - start
##      user  system elapsed
##    0.099    0.041    0.294
```

- Details + how to rename a target: <https://ropenscilabs.github.io/drake-manual/walkthrough.html#reproducible-data-recovery-and-renaming>

# Dependency-aware high-performance computing

- Just a little configuration...

```
# 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")
```

# Dependency-aware high-performance computing

# Resources

- Get **drake**:

```
install.packages("drake")
```

- Workshop materials:

```
remotes::install_github("wlandau/learndrake")
```

- Example code from these slides:

```
drake::drake_example("customer-churn")
```



# Links

- Development repository: <https://github.com/ropensci/drake>
- Full user manual <https://ropenscilabs.github.io/drake-manual>
- Reference website: <https://docs.ropensci.org/drake>
- Hands-on workshop: <https://github.com/wlandau/learndrake>
- Code examples: <https://github.com/wlandau/drake-examples>
- Discuss at rOpenSci.org: <https://discuss.ropensci.org>

## rOpenSci use cases

- Use **drake**? Share your use case at <https://ropensci.org/usecases>.



# Thanks



- Edgar Ruiz
- example code



- Matt Dancho
- blog post

# Thanks



- Maëlle Salmon
- Ben Marwick
- Julia Lowndes
- Peter Slaughter
- Jenny Bryan
- Rich FitzJohn
- Stefanie Butland

- Jarad Niemi
- Kirill Müller
- Henrik Bengtsson
- Michael Schubert
- Kendon Bell
- Miles McBain
- Patrick Schratz
- Alex Axthelm
- Jasper Clarkberg
- Tiernan Martin
- Ben Listyg
- TJ Mahr
- Ben Bond-Lamberty
- Tim Mastny
- Bill Denney
- Amanda Dobbyn
- Daniel Falster
- Rainer Krug
- Brianna McHorse
- Chan-Yub Park