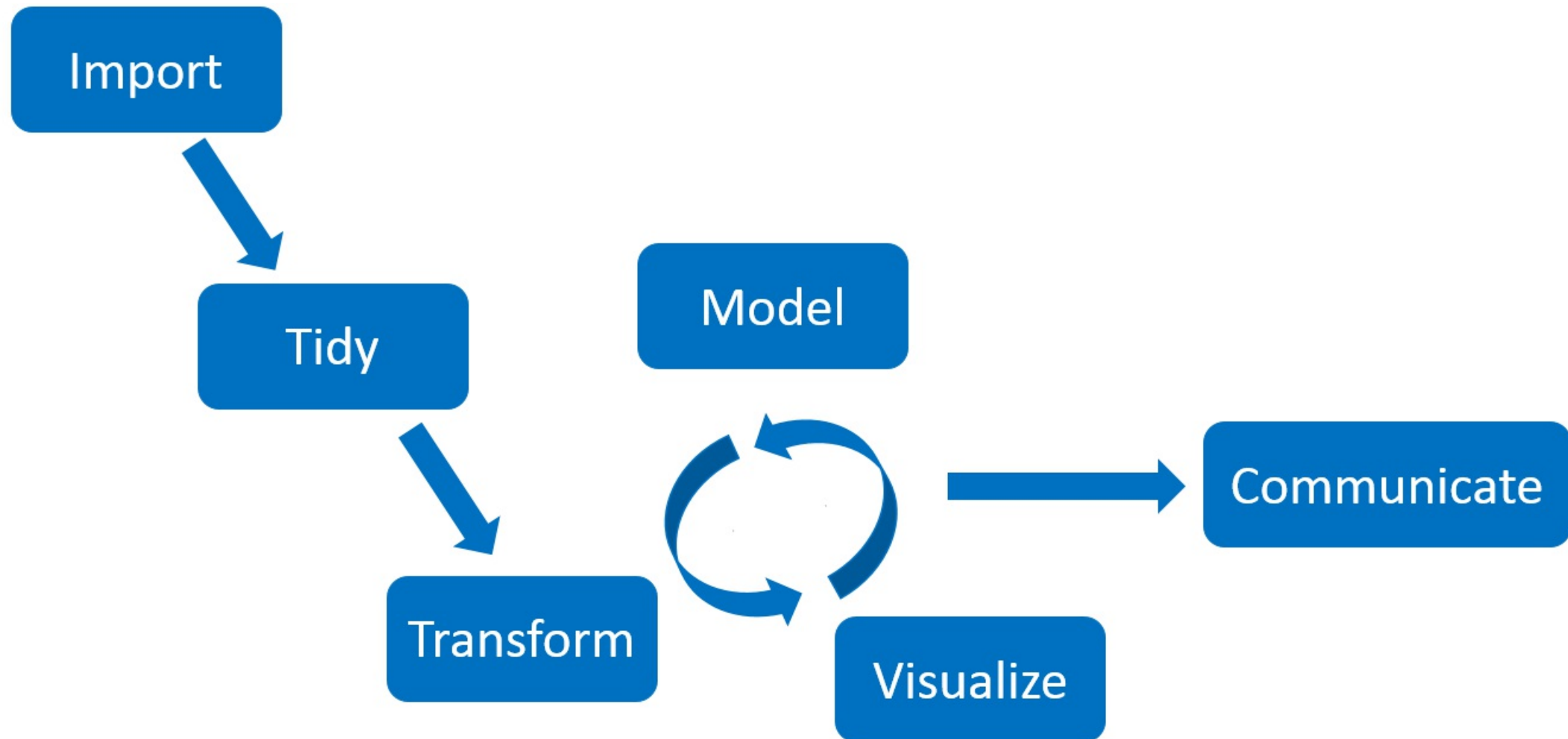


# Machine learning workflow management in R

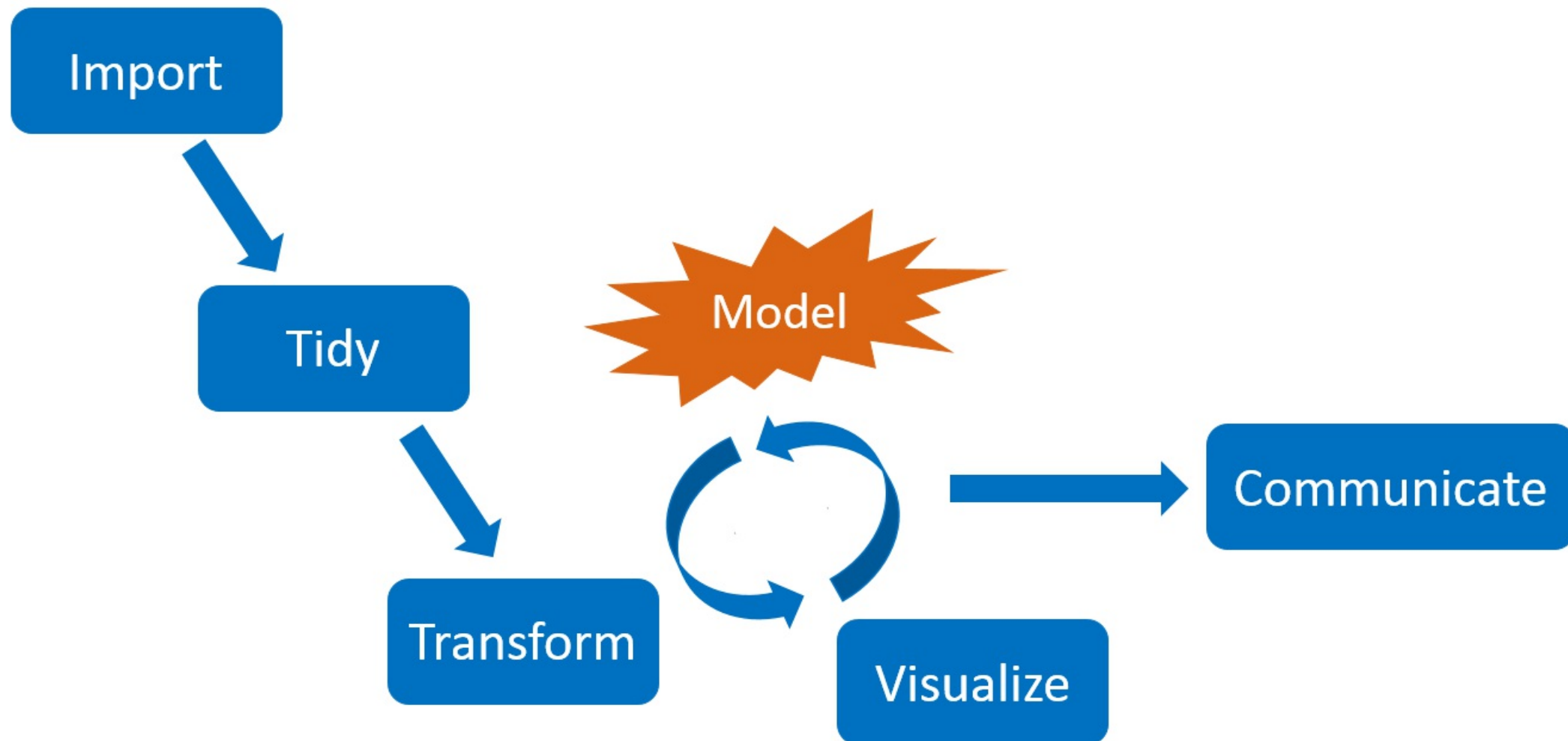


Will Landau

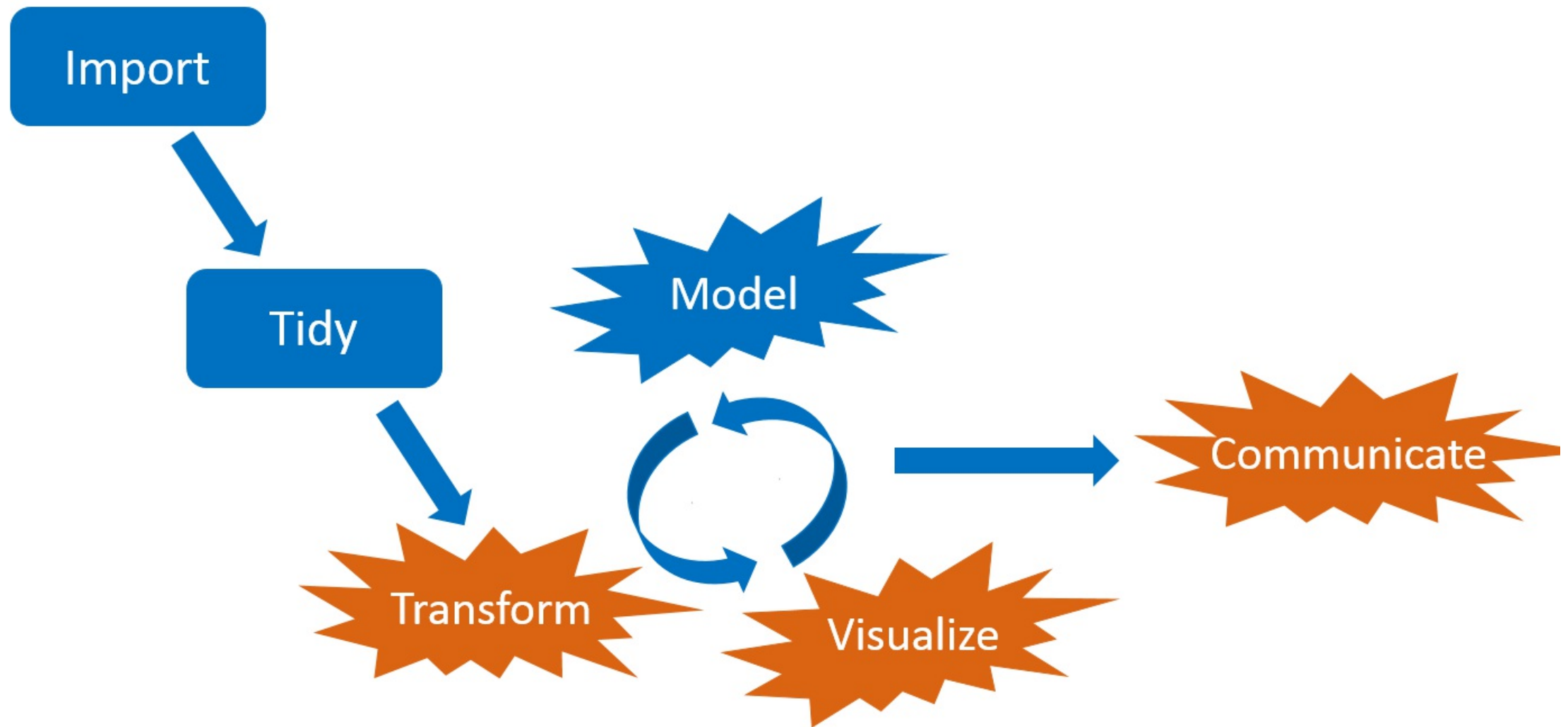
# Workflows have interconnected steps.



# When you change something...



...the downstream steps are no longer valid.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>

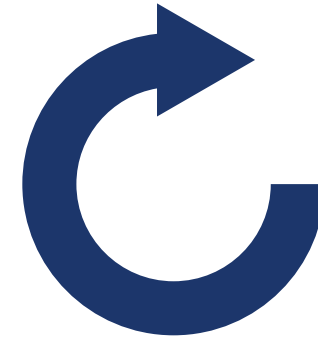
# Pipeline tools



**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 makes drake different?



- Aggressively designed for R.
  - Think **functions**, not script files.
  - Think **variables**, not output files.
  - Think **data frames**, not Makefiles.
- Major improvements in late 2018 and early 2019:
  - A **domain-specific language** for workflows.
  - Massive improvements in speed and memory usage.
  - Special **functions and checks** to safeguard reproducibility.



# Relevance to pharma

- 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 data analysis.



<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, units1, units2, act1, act2, act3) {  
  # ...  
}  
  
train_model <- function(data, rec, units1, units2, act1, act2, act3) {  
  # ...  
}  
  
confusion_matrix <- function(data, rec, serialized_model) {  
  # ...  
}  
  
compare_models <- function(...) {  
  # ...  
}
```

# plan.R

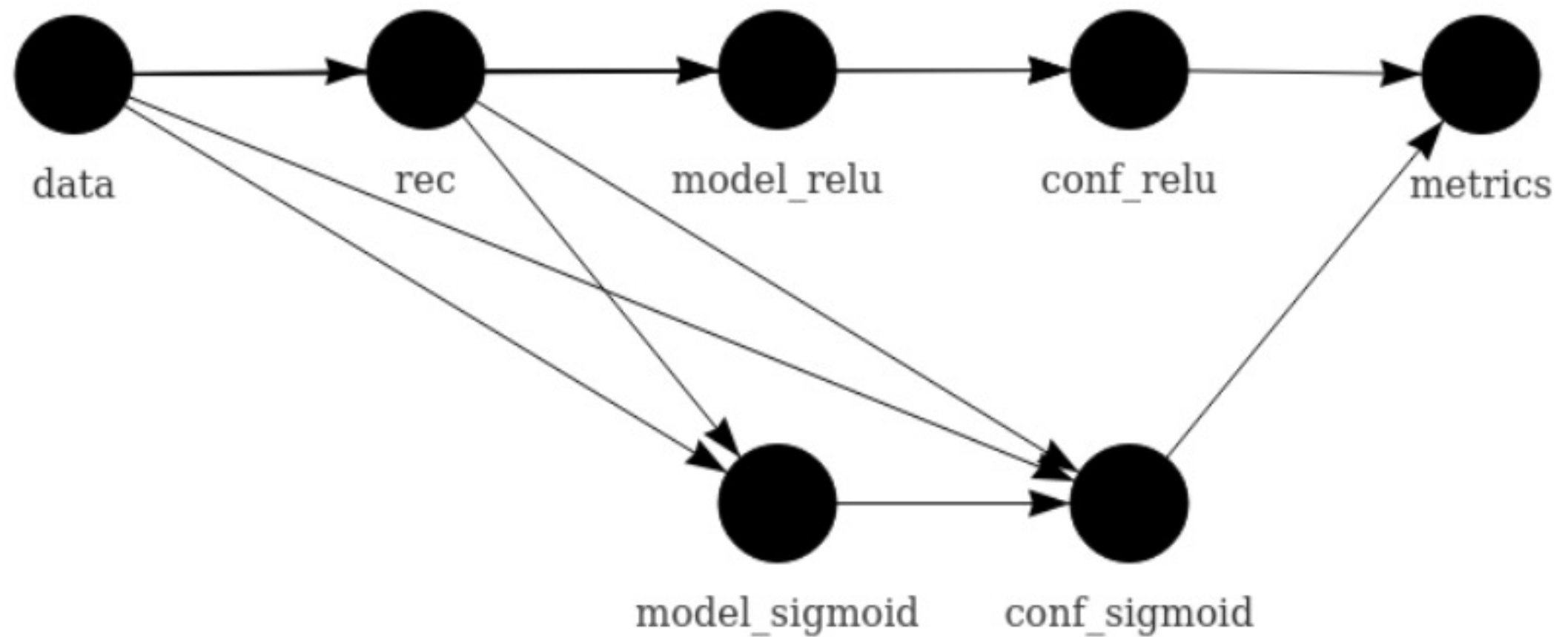
```
activations <- c("relu", "sigmoid")

plan <- drake_plan(
  data = read_csv(file_in("data/customer_churn.csv"), col_types = cols()) %>%
    initial_split(prop = 0.3),
  rec = prepare_recipe(data),
  model = target(
    train_model(data, rec, act1 = act),
    transform = map(act = !!activations)
  ),
  conf = target(
    confusion_matrix(data, rec, model),
    transform = map(model, .id = act)
  ),
  metrics = 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"), col_types = c
## 2 rec       prepare_recipe(data)
## 3 model_relu train_model(data, rec, act1 = "relu")
## 4 model_sigmo... train_model(data, rec, act1 = "sigmoid")
## 5 conf_relu  confusion_matrix(data, rec, model_relu)
## 6 conf_sigmoid confusion_matrix(data, rec, model_sigmoid)
## 7 metrics   compare_models(conf_relu, conf_sigmoid)
```

# The workflow



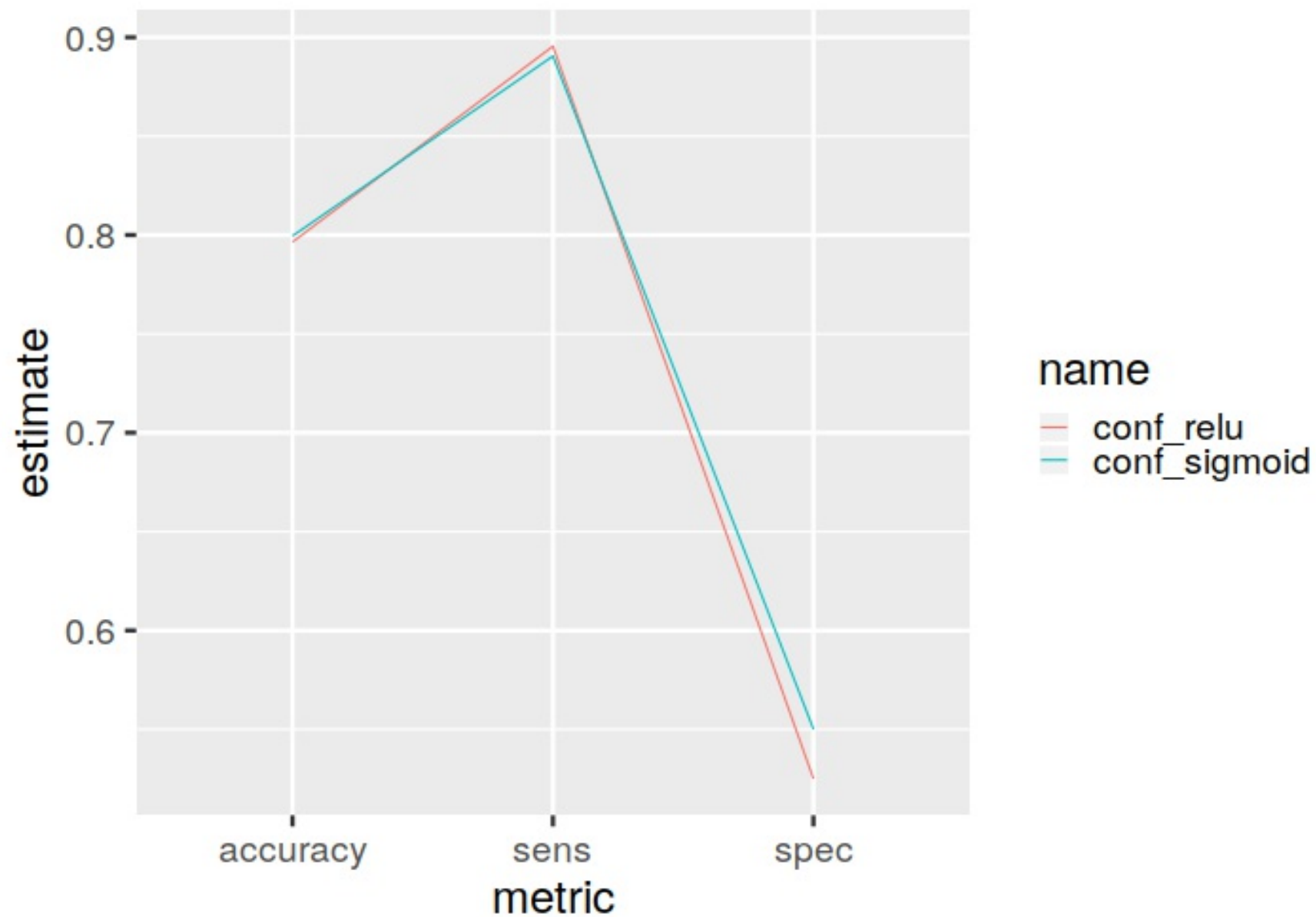


# Run the project in make.R.

```
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()
```

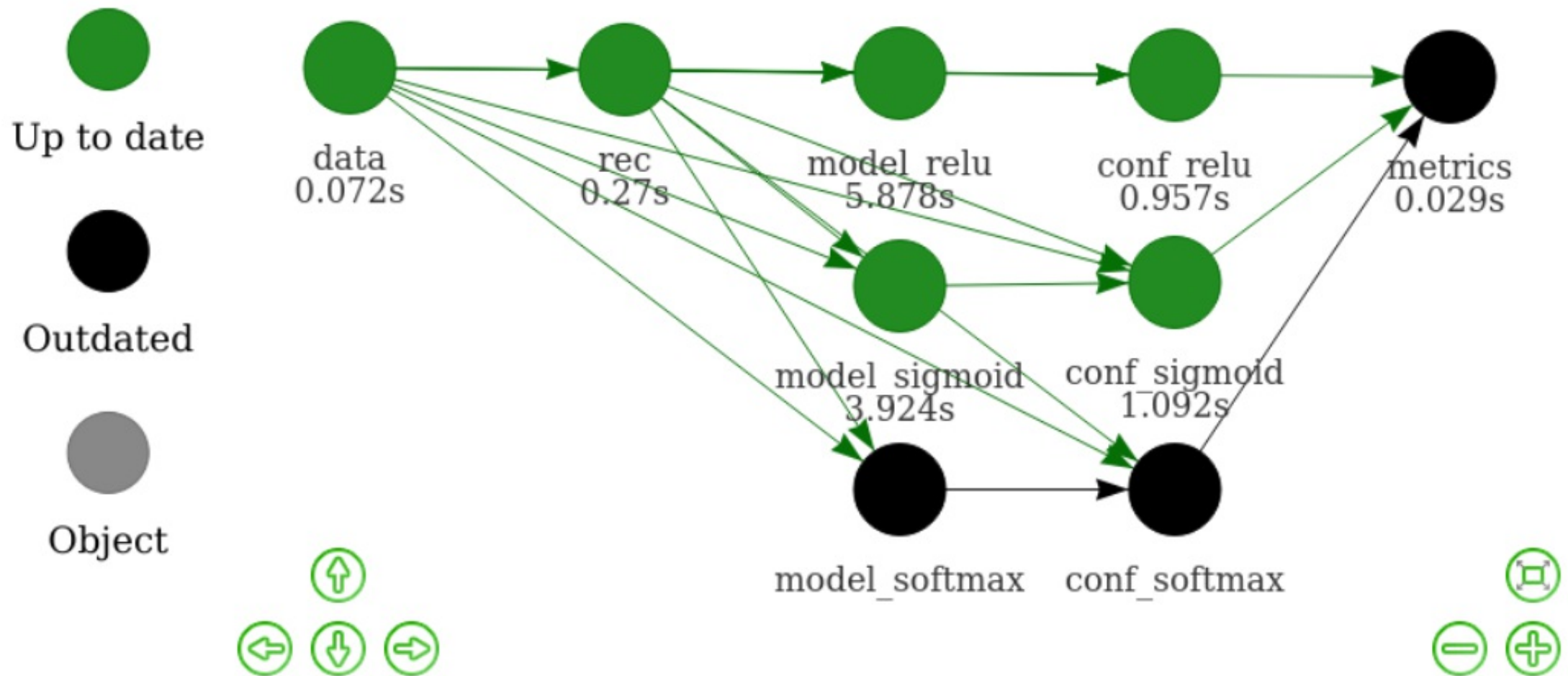


# Try another activation function.

```
activations <- c("relu", "sigmoid", "softmax")

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

# vis\_drake\_graph()



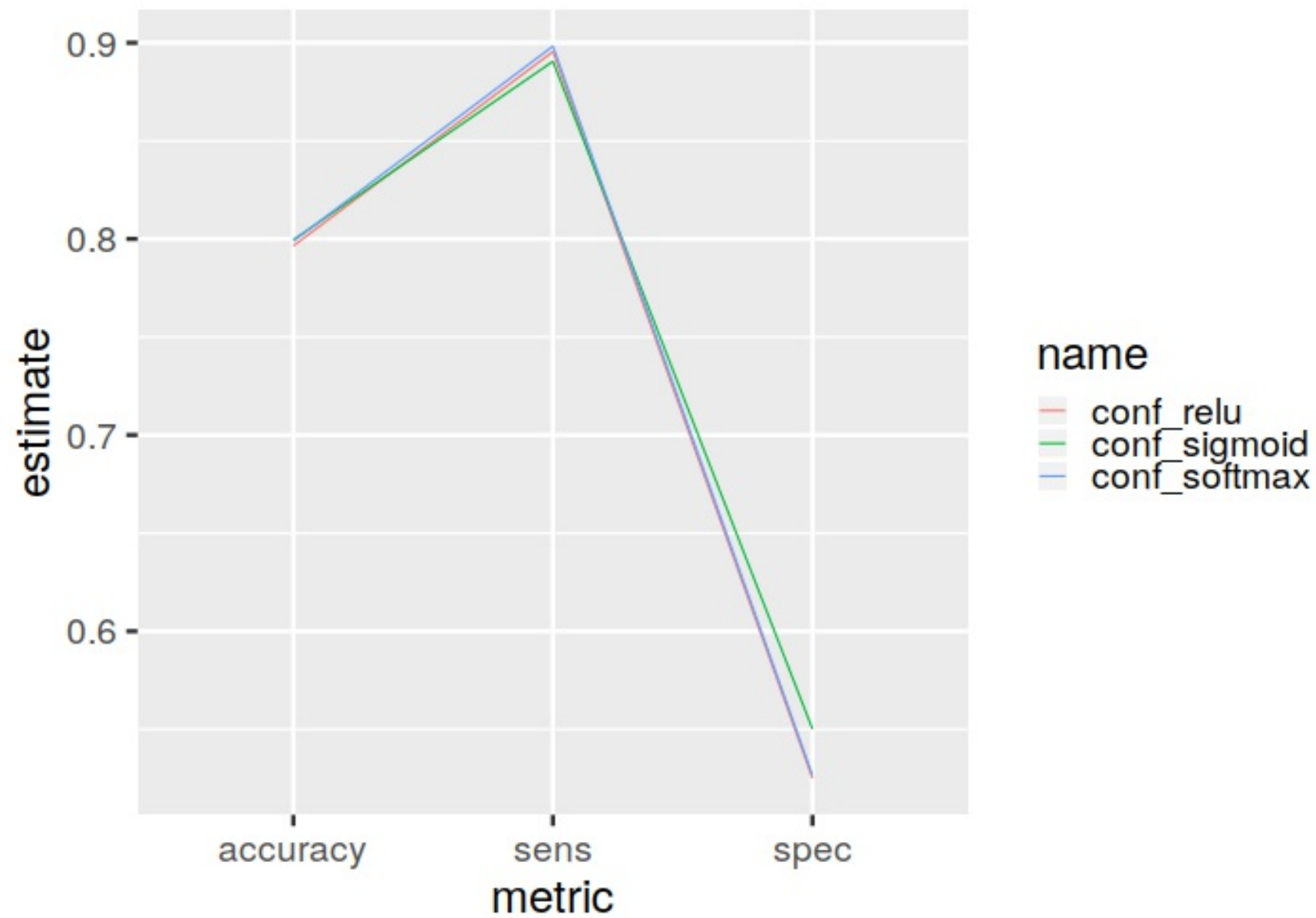
# Refresh the results in make.R.

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

```
make(plan)  
## target model_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()`.

# 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

- Get **drake**:

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

- Workshop materials:

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

- Example code from these slides:

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

# Links

- Development repository: <https://github.com/ropensci/drake>
- Full user manual <https://ropenscilabs.github.io/drake-manual>
- Reference website: <https://ropensci.github.io/drake>
- 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
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- 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