

# Reproducible computation at scale in R



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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

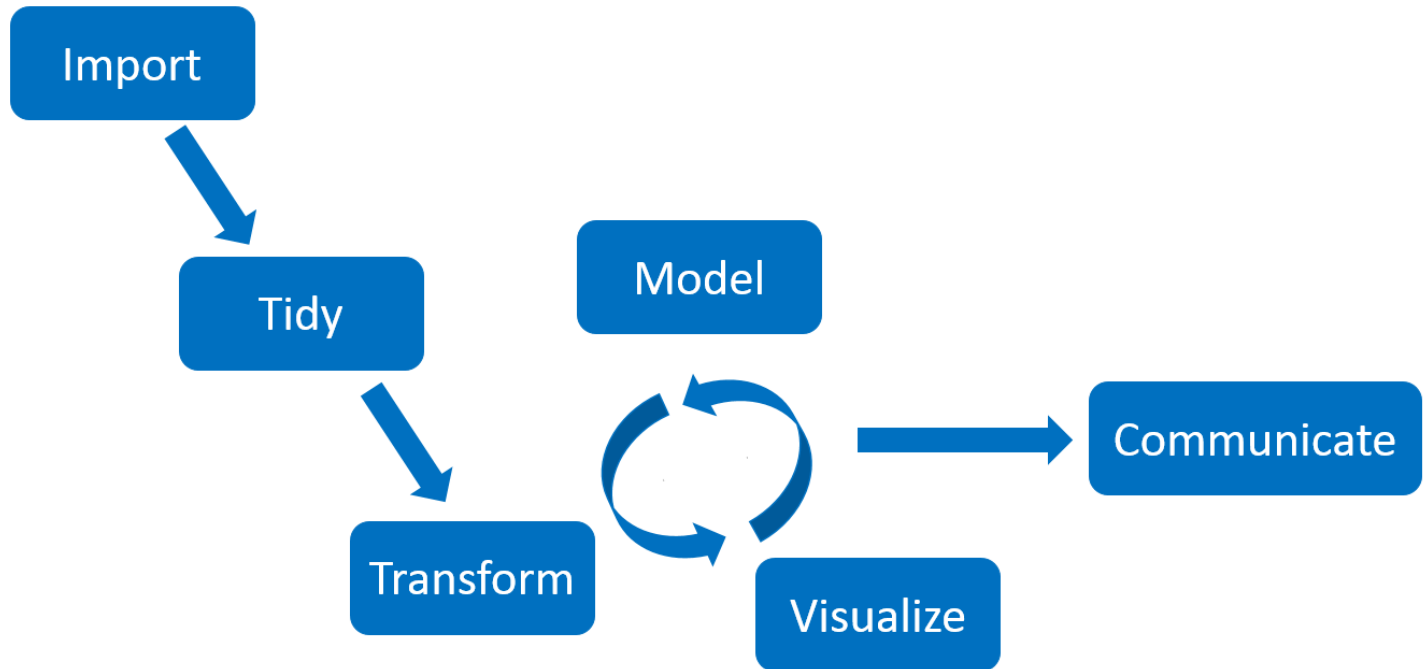
# Common features

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

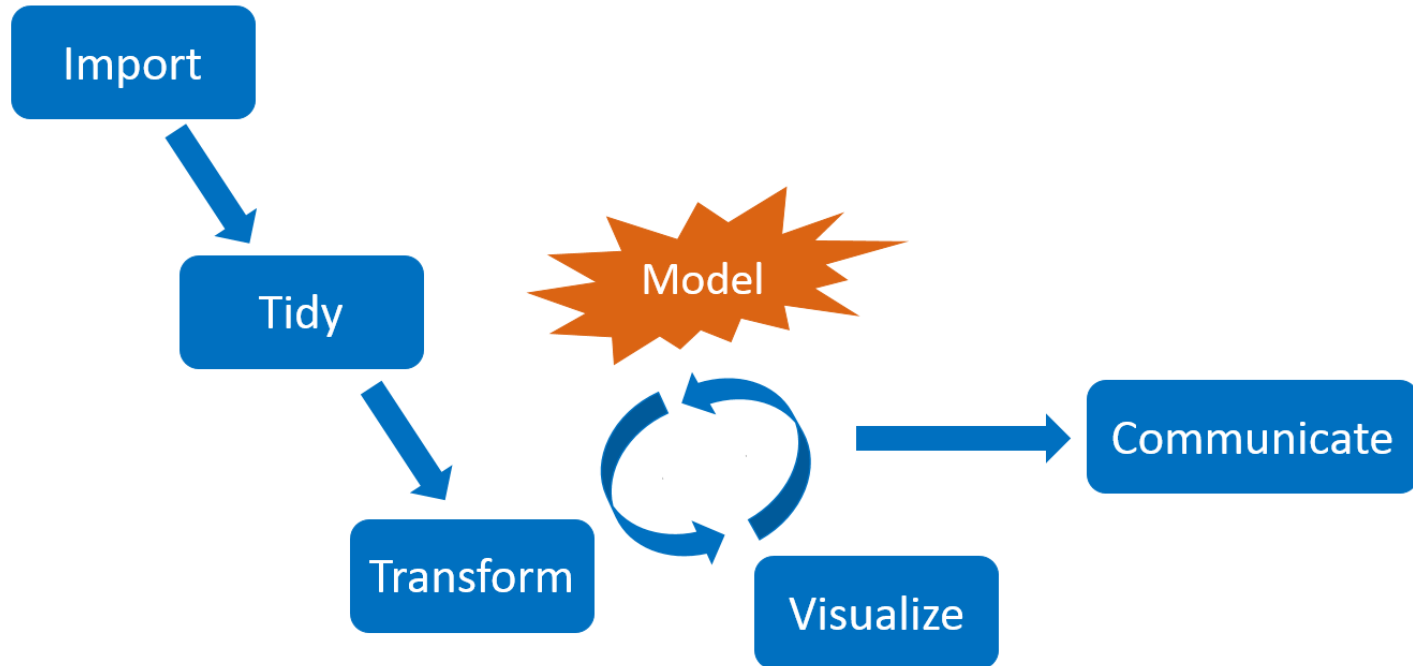


- <https://openclipart.org/detail/275842/sisyphus-overcoming-silhouette>

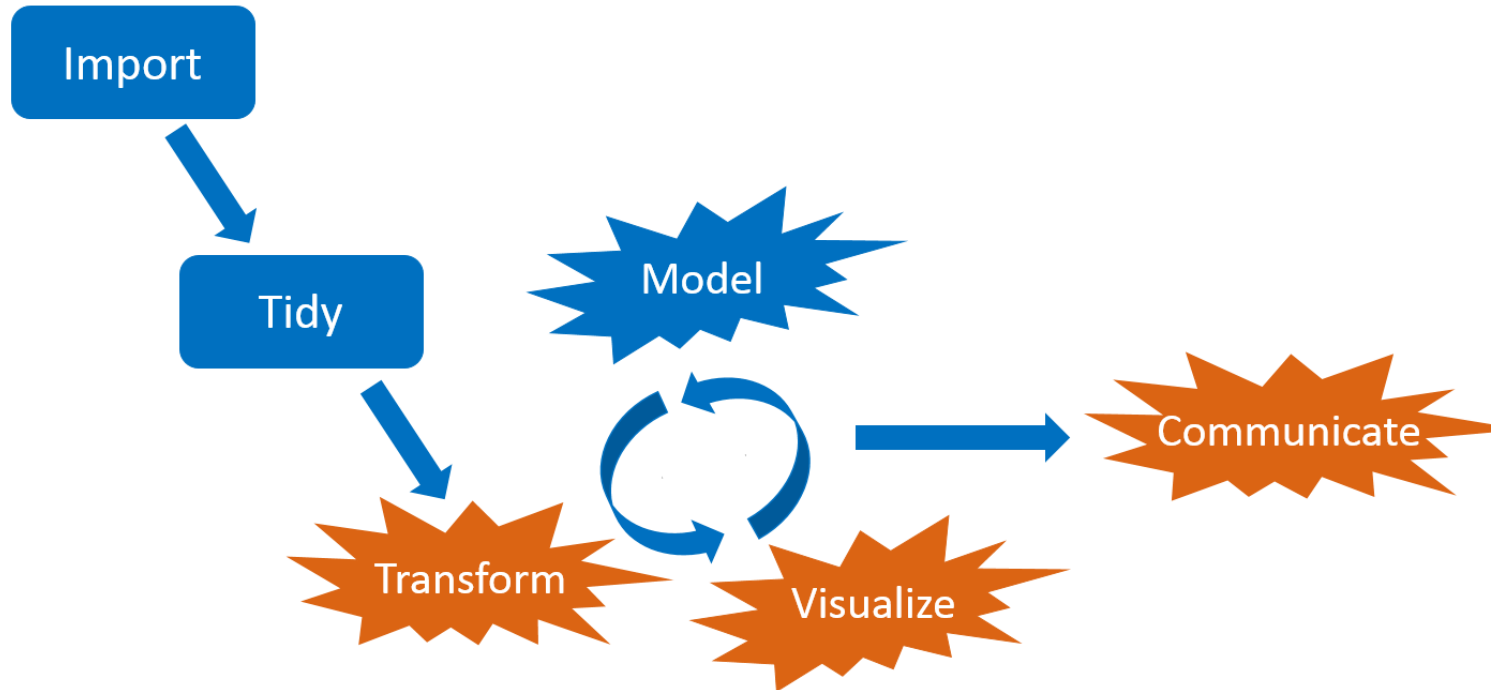
# Interconnected tasks



# Changes



# Consequences



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

# What distinguishes drake?



1. Respects the way R works.
2. Pushes you to write better code.



# Example drake 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 life sciences.



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

# ✗ Say goodbye to 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
```



# drake wants you to write **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
```

# Functions in a drake workflow

```
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()  
}
```

# Functions in a drake workflow

```
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, model) {
  # ...
}

test_model <- function(churn_data, churn_recipe, units1, units2, act1
  # ...
}

train_best_model <- function(best_run, churn_recipe) {
  # ...
}
```

# Typical project structure

- There are *many* variations on this theme.

```
make.R # Top-level script
R/
├─ packages.R # Calls to library(drake), library(keras), etc.
├─ functions.R
└─ plan.R
data/
├─ customer_churn.csv
.drake/ # drake's cache
└─      # Output automatically appears here.
```

# Build up your workflow in a **drake** plan.

- Usually goes in the `R/plan.R` script.

```
# R/plan.R
plan <- drake_plan(
  churn_recipe = prepare_recipe(churn_data),
  churn_data = split_data(file_in("data/customer_churn.csv"))
)
```

# The plan is a data frame of skippable *targets*.

```
plan
#> # A tibble: 2 x 2
#>   target      command
#>   <chr>      <expr>
#> 1 churn_recipe prepare_recipe(churn_data)
#> 2 churn_data   split_data(file_in("data/customer_churn.csv"))
```



# drake understands code and data dependencies.

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

```
vis_drake_graph(plan)
```

# Build your first targets.

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

```
make(plan)  
#> ► target churn_data  
#> ► target churn_recipe
```

# Check the targets for problems

- `loadadd()` and `readd()` get targets from the cache.

```
ncol(training(readd(churn_data)))
```

```
#> [1] 21
```

```
loadadd(churn_recipe)
```

```
ncol(juice(churn_recipe))
```

```
#> [1] 36
```

# Keep building up the plan.

- Continue on and fit some models.

```
# R/plan.R
plan <- drake_plan(
  churn_recipe = prepare_recipe(churn_data),
  churn_data = split_data(file_in("data/customer_churn.csv")),
  run_relu = test_model(act1 = "relu", churn_data, churn_recipe),
  run_sigmoid = test_model(act1 = "sigmoid", churn_data, churn_recipe)
)
```

# Previous work is still up to date.

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

```
outdated(plan)  
#> [1] "run_relu"      "run_sigmoid"
```

# Previous work is still up to date.

```
vis_drake_graph(plan)
```

# drake skips up-to-date targets.

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

```
make(plan)  
#> ► target run_relu  
#> ► target run_sigmoid
```

# Inspect the newest targets.

```
readd(run_relu)
#> # A tibble: 1 x 6
#>   accuracy units1 units2 act1  act2  act3
#>   <dbl>   <dbl>   <dbl> <chr> <chr> <chr>
#> 1    0.801     16     16 relu  relu  sigmoid

readd(run_sigmoid)
#> # A tibble: 1 x 6
#>   accuracy units1 units2 act1    act2  act3
#>   <dbl>   <dbl>   <dbl> <chr>   <chr> <chr>
#> 1    0.802     16     16 sigmoid relu  sigmoid
```



# Find the best model

```
plan <- drake_plan(  
  churn_recipe = prepare_recipe(churn_data),  
  churn_data = split_data(file_in("data/customer_churn.csv")),  
  run_relu = test_model(act1 = "relu", churn_data, churn_recipe),  
  run_sigmoid = test_model(act1 = "sigmoid", churn_data, churn_recipe),  
  best_run = bind_rows(run_relu, run_sigmoid) %>%  
    filter(accuracy == max(accuracy)),  
  best_model = target(  
    train_best_model(best_run, churn_recipe),  
    format = "keras"  
  )  
)
```

# Find the best model

```
make(plan)
#> ► target best_run
#> ► target best_model
```

# Find the best model

```
readd(best_model)
#> Model
#> -----
#> 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
#> -----
```

# Try another model.

```
# R/plan.R
plan <- drake_plan(
  churn_recipe = prepare_recipe(churn_data),
  churn_data = split_data(file_in("data/customer_churn.csv")),
  run_relu = test_model(act1 = "relu", churn_data, churn_recipe),
  run_sigmoid = test_model(act1 = "sigmoid", churn_data, churn_recipe),
  run_softmax = test_model(act1 = "softmax", churn_data, churn_recipe),
  best_run = bind_rows(run_relu, run_sigmoid, run_softmax) %>%
    filter(accuracy == max(accuracy)),
  best_model = target(
    train_best_model(best_run, churn_recipe),
    format = "keras"
  )
)
```

# What gets done stays done.

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

```
outdated(plan)  
#> [1] "best_model"  "best_run"    "run_softmax"
```

# What gets done stays done.

```
vis_drake_graph(plan)
```

# New best model?

- Only if the new run beats the old runs.
- Otherwise, drake does not bother to retrain the best model.

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

```
make(plan)  
#> target run_softmax  
#> target best_run
```

# 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) %>%
    layer_dense(
      units = 1,
      kernel_initializer = "uniform",
      activation = act3
    )
  )
```



# drake knows what to do.

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

# drake knows what to do.

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

```
make(plan)  
#> ► target run_relu  
#> ► target run_softmax  
#> ► target run_sigmoid  
#> ► target best_run  
#> ► target best_model
```

# Undo the change.

```
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 = 0.1) %>% # Changed back to 0.1.
    layer_dense(
      units = units2,
      kernel_initializer = "uniform",
      activation = act2
    ) %>%
    layer_dropout(rate = 0.1) %>%
    layer_dense(
      units = 1,
      kernel_initializer = "uniform",
      activation = act3
    )
  )
```

# Undo the change.

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

- Recover old targets instead of building new ones.

```
make(plan, recover = TRUE)  
#> ✓ recover run_relu  
#> ✓ recover run_softmax  
#> ✓ recover run_sigmoid  
#> ✓ recover best_run  
#> ✓ recover best_model
```

# Similar story if the data file changes.

```
source("R/packages.R")  
source("R/functions.R")  
source("R/plan.R") # Requires file_in() in the plan.
```

```
make(plan)  
#> target churn_data  
#> target churn_recipe  
#> target run_relu  
#> target run_sigmoid  
#> target run_softmax  
#> target best_run  
#> target best_model
```

# Evidence of reproducibility

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

```
make(plan)  
#> ✓ All targets are already up to date.  
  
outdated(plan)  
#> character(0)
```

# Evidence of reproducibility

```
vis_drake_graph(plan)
```

# History of past model runs

```
history <- drake_history() %>%  
  select(target, act1, exists, hash) %>%  
  filter(!is.na(act1)) %>%  
  print()  
#> # A tibble: 6 x 4  
#>   target      act1    exists hash  
#>   <chr>      <chr>    <lgl>  <chr>  
#> 1 run_relu    relu     TRUE   9e3e97fdee2e2629  
#> 2 run_relu    relu     TRUE   fbc97af3378e33e4  
#> 3 run_sigmoid sigmoid TRUE   d3467df3f1cc9cae  
#> 4 run_sigmoid sigmoid TRUE   924e53320c500e9b  
#> 5 run_softmax softmax  TRUE   a76e948282303ad3  
#> 6 run_softmax softmax  TRUE   a76e948282303ad3
```



# Recover an old model run.

```
drake_cache()$get_value(history$hash[1])  
#> # A tibble: 1 x 6  
#>   accuracy units1 units2 act1  act2  act3  
#>   <dbl>   <dbl>   <dbl> <chr> <chr> <chr>  
#> 1    0.801     16     16 relu  relu  sigmoid
```

# More highlights

- High-performance computing
- Efficient data formats
- Dynamic branching
- Memory management

```
# Run targets in parallel on a cluster:  
options(clustermq.scheduler = "slurm")  
make(plan, parallelism = "clustermq", jobs = 64)
```

# Resources

- Get **drake**:

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

- Example code from these slides:

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

- Workshop materials:

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

# Links

- Development repository: <https://github.com/ropensci/drake>
- Full user manual <https://books.ropensci.org/drake/>
- 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
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