Reproducible computation at scale in R

Will Landau

Large statistical computation

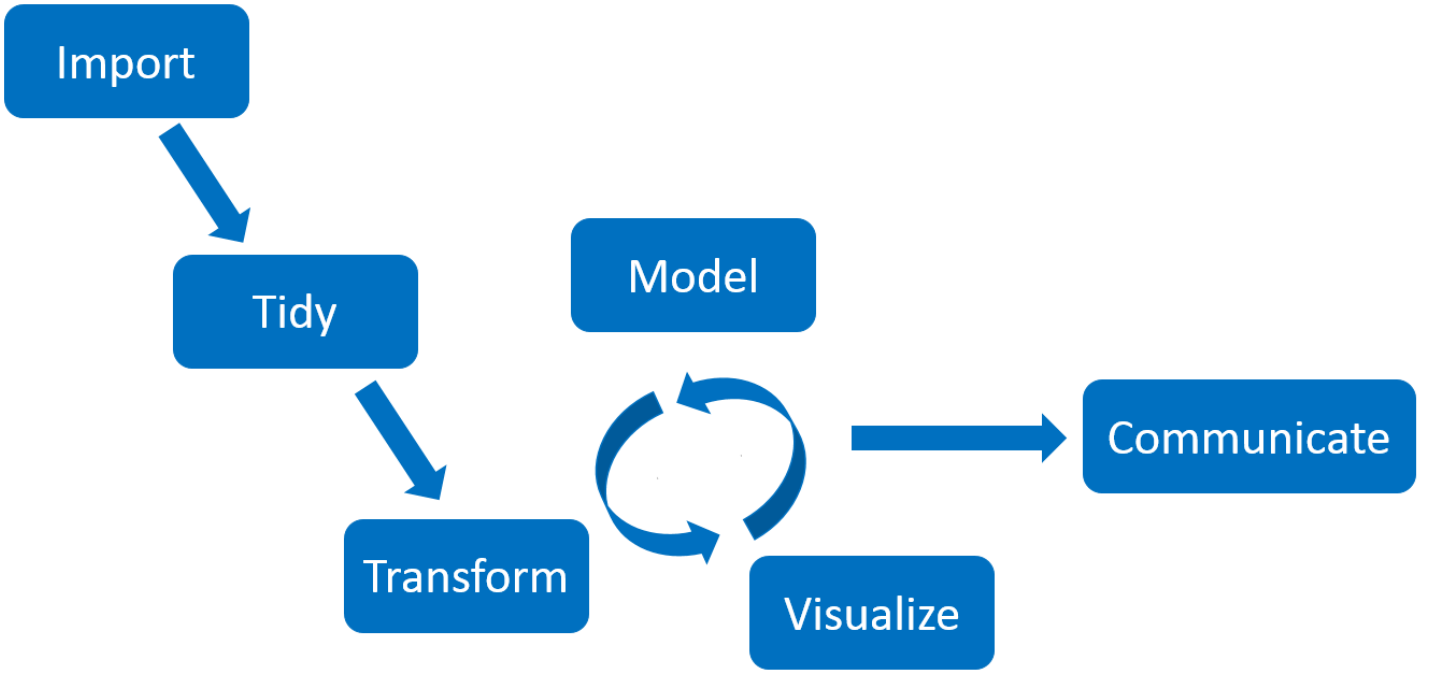
- Bayesian data analysis
- Bayesian network meta-analysis
- Graph-based multiple comparison procedures
- Subgroup identification
- Predictive modeling
- Deep neural networks
- PK/PD modeling
- Clinical trial simulation
- Target identification

Common features

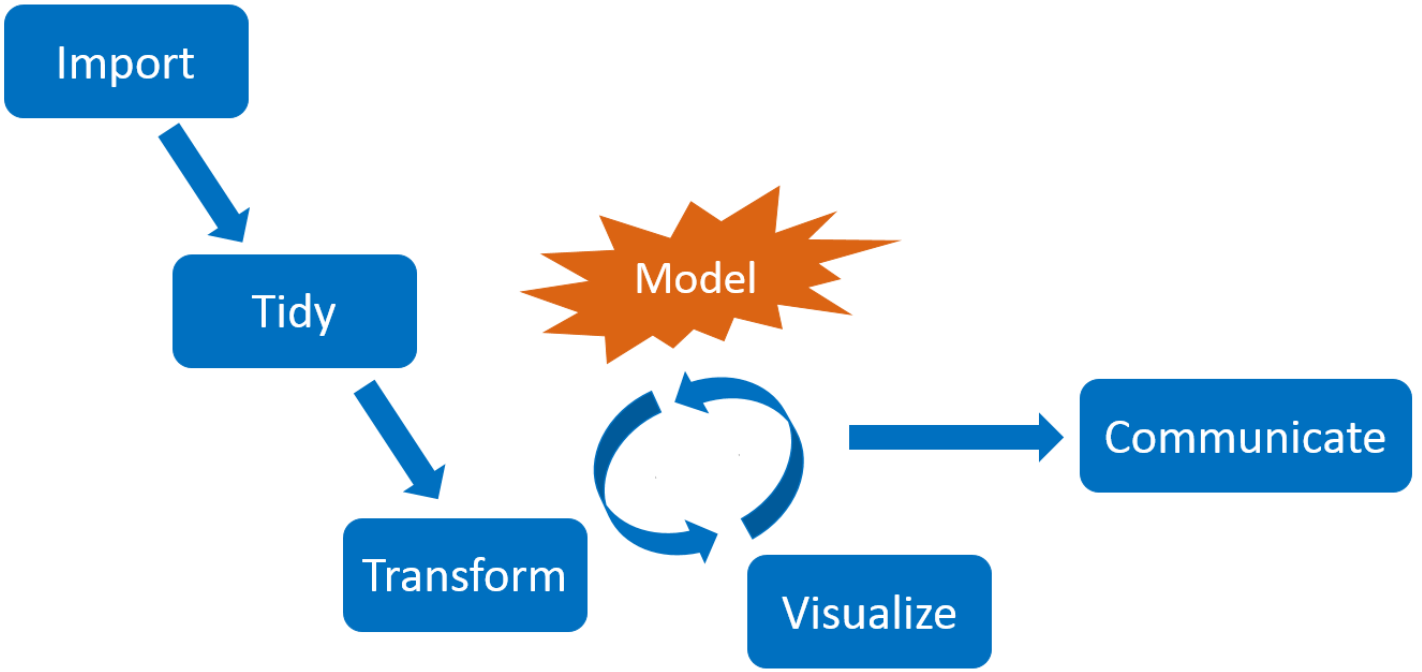
1. Heavy use of the R language.
2. Long runtimes.
3. Multiple sub-tasks.
4. Frequent changes to code and data.

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

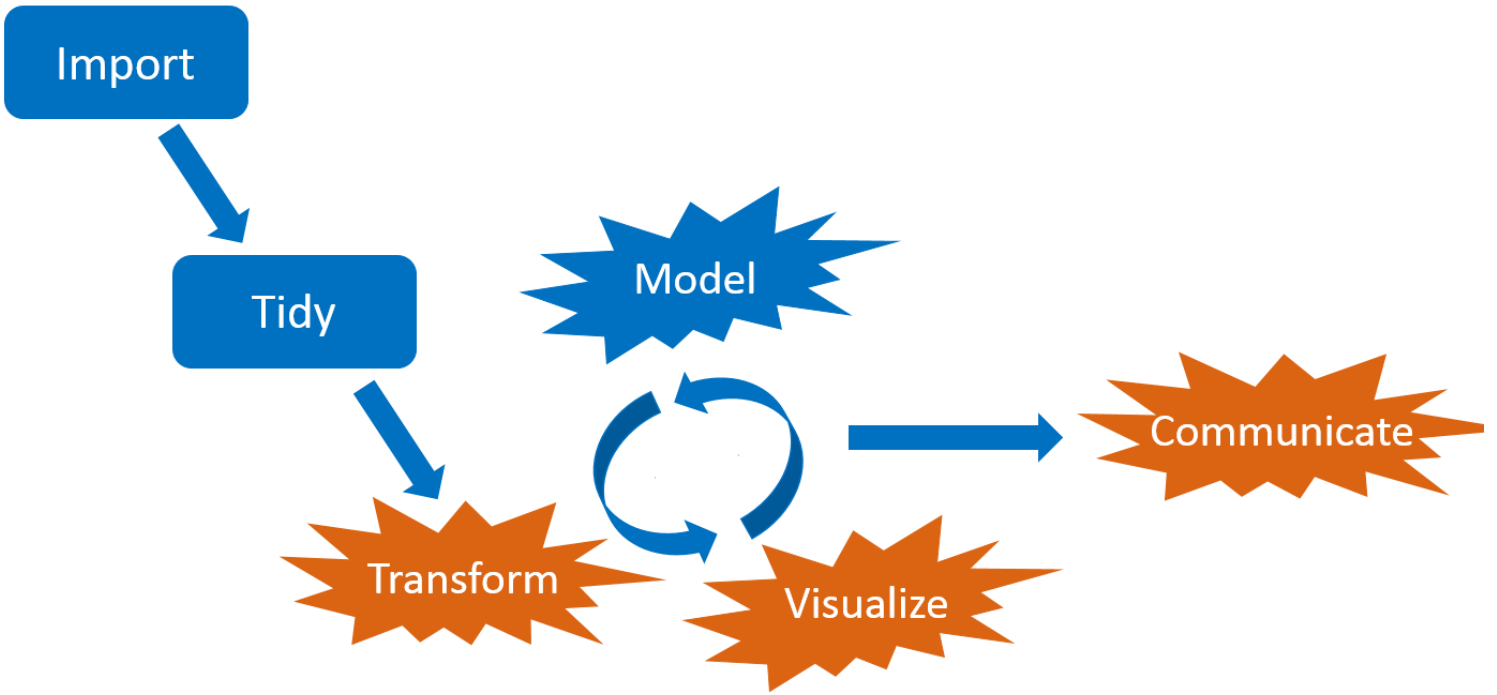
Interconnected tasks



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.
- 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, acti
  # ...
}

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

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

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

loadd(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    0.804     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    0.801     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) %>%
    top_n(1, accuracy) %>%
    head(1),
  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) %>%
    top_n(1, accuracy) %>%
    head(1),
  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   c4e1098c12c68254
#> 2 run_relu    relu    TRUE   54499b29ce0a42a9
#> 3 run_sigmoid sigmoid TRUE   85e7f77486f2fa9d
#> 4 run_sigmoid sigmoid TRUE   de127964495d752e
#> 5 run_softmax softmax TRUE   f1fef59da143747a
#> 6 run_softmax softmax TRUE   6938251661336f6b
```

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    0.804     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
- 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