The simulator: An Engine to Streamline Simulations

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Abstract

The simulator is an R package that streamlines the process of performing simulations by creating a common infrastructure that can be easily used and reused across projects. Methodological statisticians routinely write simulations to compare their methods to pre-existing ones. While developing ideas, there is a temptation to write “quick and dirty” simulations to try out ideas. This approach of rapid prototyping is useful but can sometimes backfire if bugs are introduced. Using the simulator allows one to remove the “dirty” without sacrificing the “quick.” Coding is quick because the statistician focuses exclusively on those aspects of the simulation that are specific to the particular paper being written. Code written with the simulator is succinct, highly readable, and easily shared with others. The modular nature of simulations written with the simulator promotes code reusability, which saves time and facilitates reproducibility. The syntax of the simulator leads to simulation code that is easily human-readable. Other benefits of using the simulator include the ability to “step in” to a simulation and change one aspect without having to rerun the entire simulation from scratch, the straightforward integration of parallel computing into simulations, and the ability to rapidly generate plots, tables, and reports with minimal effort.

Keywords: simulations, reproducible code, parallel computing.

1. Introduction

Methodological statisticians spend an appreciable amount of time writing code for simulation studies. Every paper introducing a new method has a simulation section in which the new method is compared across several metrics to pre-existing methods under various scenarios. Given the formulaic nature of the simulation studies in most statistics papers, there is a lot of code that can be reused. The goal of the simulator is to streamline the process of performing simulations by creating a common infrastructure that can be easily used and reused. By infrastructure, we mean everything that is common across projects. This includes code for

- running simulations in parallel,
- proper handling of pseudorandom number generator streams (relevant when running simulations in parallel),
- storing simulation outputs at various stages to allow one to “step in” and change one aspect of a simulation (such as how a method is being evaluated) without having to rerun the entire simulation from scratch,
- summarizing simulation results with plots and tables showing how various methods compare across one or more metrics, and
- generating reports to easily communicate simulation results and code to others.

The simulator is an R (R Core Team 2016) package focused on all of these aspects of a
The simulator divides a statistical simulation study into four basic components or modules:

1) **Models**: The statistical model, determining how data is generated.

2) **Methods**: The statistical procedures being compared: Given the data, each method produces an output such as an estimate, prediction, or decision.

3) **Evaluations**: Metrics that evaluate a method’s output based on the input.

4) **Plots, Tables, Reports**: How one displays the evaluated metrics for various methods under various scenarios, and how one communicates the results and code to others.

When using the simulator, one codes the models, methods, and metrics particular to the problem at hand. These are then “plugged in” to the simulator.

After an initial look at the simulator in action (Section 2), we will then discuss each of the components of the simulator mentioned above in greater detail (Section 3). In Section 4, we discuss certain principles that informed our design choices for the package. Section 5 recommends a simple way to get started with the simulator. Section 6 gives credit to the R packages that are leveraged by the simulator, and Section 7 reviews other simulation packages. We conclude (in Section 8) with a discussion of the future of the simulator.

### 2. A first look: Betting on sparsity with the lasso

The easiest way to learn about the simulator is by example. For this reason, we have created a series of vignettes, available online, which show how the simulator can be used in the context of some of the most well-known papers in statistics. We provide here a first look at working
with the simulator, applying it to a simulation involving the lasso (an extended form of this example is available online as a vignette).

Hastie, Tibshirani, and Friedman (2009) put forward the “bet on sparsity” principle: “Use a procedure that does well in sparse problems, since no procedure does well in dense problems.” The authors perform simulations comparing the lasso (Tibshirani 1996) with ridge regression in sparse and dense situations. A simulation of this sort can be concisely coded in several easy-to-read lines of code using the simulator.

```r
library(simulator)

ew_simulation(name = "bet-on-sparsity", label = "Bet on sparsity") %>%
generate_model(make_sparse_linear_model, n = 200, p = 500,
    k = as.list(seq(5, 80, by = 5)), vary_along = "k") %>%
simulate_from_model(nsim = 5, index = 1) %>%
run_method(list(lasso, ridge)) %>%
evaluate(list(mse, bestmse, df))
```

The code above can be read as follows: Create a new simulation (with some name and label); add to it a sequence of sparse linear models where the sparsity level is varied from 1 to 80; simulate 5 random draws from this model; run the lasso and ridge on both of these; finally, compute the mean squared error, best mean squared error (over all values of the tuning parameter), and degrees of freedom for each of these. In coding this simulation, we only needed to define the problem-specific parts, which are

1) the function `make_sparse_linear_model`, which creates a Model object,
2) the Method objects `lasso` and `ridge`,
3) and the Metric objects `mse`, `df`, and `bestmse`.

This problem-specific code is provided in the Appendix.

The functions `new_simulation`, `generate_model`, `simulate_from_model`, `run_method`, and `evaluate` are simulator functions that take care of the details of bookkeeping, random number generation, parallel processing (if desired), saving outputs to file, etc.

It is useful to think of a simulation as a pipeline (see Figure 1), and this is emphasized by the simulator’s use of the magrittr pipe `%>%` (Bache and Wickham 2014). We discuss the pipe further in Section 4.4.

The results from all intermediate stages are saved to file. To get access to these results for further analysis, one loads the Simulation object that was created, using the name it was given.
The simulator

sim <- load_simulation("bet-on-sparsity")

This object only contains references to the simulation results (and not the results themselves) and thus is quick to load and remains lightweight even for large simulations.

We next make a plot showing how the best MSE of each method varies with sparsity level.

plot_eval_by(sim, "best_sqr_err", varying = "k", main = "Betting on sparsity")

The plot shows (a Monte Carlo estimate of) the best-achievable mean squared error of both methods. The rationale for the “bet on sparsity” principle is apparent from the plot. When \( k \) is low, we see large gains in performance using the lasso compared to ridge; when \( k \) is large, ridge does better—however, in this regime, neither method is doing particularly well (and in a relative sense, ridge’s advantage is only slight). Observe that the call to \texttt{plot_eval_by} is fairly simple considering that the simulator has labeled the axes and has identified the methods in a legend. This is an example of how the formulaic nature of most simulation studies allows for efficiency in coding.

The simulator is designed to make simulations as modular as possible so that one can easily add new parts, run various steps in parallel, etc. For example, if one later decides to compare to the minimax concave penalty (MCP) (Zhang 2010), one can simply call

sim <- run_method(sim, mcp)

and the earlier steps of generating data will not be repeated. If one decides to add more than 5 random draws to the simulation, one can do so without having to redo the earlier computation (this will be discussed in greater detail in Section 4.5).

Rather than looking at just the best MSE of each method, we might also like to examine how the MSE varies with degrees of freedom for each method. We look at the methods’ results when the true sparsity \( k \) is low and when it is high.
subset_simulation(sim, k == 20 | k == 80) %>% plot_evals("df", "sqr_err")

In practice, it is common to use cross-validation to select the tuning parameter, so we might also want to simulate the two methods when cross-validation is used. We organize this as a new simulation that shares the same models and simulated data as before, but with two new methods.

sim2 <- subset_simulation(sim, methods = "") %>%
  rename("bet-on-sparsity-cv") %>%
  relabel("Bet on sparsity (with cross validation)") %>%
  run_method(list(lasso + cv, ridge + cv)) %>%
  evaluate(mse)

We explain in the Appendix in greater depth the simulator construct that allows us to write lasso + cv, but for now we note that doing so allows us to avoid rerunning the lasso and ridge from scratch, which would be wasteful given that we have already computed them in these situations in the previous simulation. A plot reveals that qualitatively the results are quite similar.

plot_eval_by(sim2, "sqr_err", varying = "k", main = "Betting on sparsity")
3. A look at each component

In this section, we look more closely at the components of the simulator and give brief overviews of the functions pertaining to each component.

Thinking of a simulation as a pipeline, a Simulation object is what gets pushed through the series of pipes. Each of the main pipeline functions of the simulator (which can be thought of as the pipes) input and output a simulation object. Each main pipeline function creates new objects, saves them to file, and then records what was done in the Simulation object. Thus, the Simulation object serves as the memory of what has been done and as a handle for getting to the various intermediate stages of the simulation. Importantly, a Simulator object does not contain the results themselves, only references to them. This is discussed in greater detail in Section 4.

- **new_simulation** is used to create a new Simulation object. By default, when it is called, a record of its existence is saved to file.
- **save_simulation** is passed a Simulation object, it saves it to file. The location is given by the name and dir (short for directory) slot of the object.
- **load_simulation** when passed the name of a simulation loads the Simulation object into the R session.
- **subset_simulation** is useful for creating a new Simulation object from a preexisting one. For example, this is useful for focusing a plot on only certain models or for reusing only certain simulation results in a different context.

3.1. Models component
The first component in the simulator is the models component. An object of class Model defines a set of parameters and a function, called simulate, that takes these parameters and returns a specified number of random draws from this distribution. For example, in the “bet on sparsity” example of Section 2, we created a sequence of Model objects with varying sparsity level k. Loading one such object, we can have a look by printing it:

```r
m <- model(sim, k == 10)
m
```

Model Component
name: slm/k_10/n_200/p_500
label: n = 200, p = 500, k = 10
params: x beta mu sigma n p k

The parameters are stored in a named list m@params and the function to simulate data is m@simulate.

Here are some of the most useful functions related to the model component:

- **new_model** creates a new Model object. In the example, it is called in make_sparse_linear_model (see Appendix A.1).
- **generate_model** is one of the main pipeline functions of the simulator. The user supplies it with a function (make_sparse_linear_model, in the example) that returns an object of class Model, and generate_model then creates this model, saves it to file, and adds a reference to it to the Simulation object. In many simulation studies, one is interested in a sequence of models, indexed by several parameters. The vary_along parameter of generate_model is used to specify which parameters should be varied.
- **simulate_from_model** is another main pipeline function. Once the model has been generated, simulate_from_model creates a specified number of random draws from the distribution defined by the model. The Draws objects are saved to file and references to them are added to the Simulation object. These simulations can be broken into chunks and run either sequentially or in parallel (or a mix of the two). Parallelization is described in greater detail in Section 4.5.
- **model** loads one or more Model objects from a Simulation object into the R session.
- **draws** loads one or more Draws objects from a Simulation object into the R session.

The Draws objects have a simple structure.

```r
d <- draws(sim, k == 10)
d
```

Draws Component
name: slm/k_10/n_200/p_500
label: (Block 1:) 5 draws from n = 200, p = 500, k = 10

In this example, d@draws is a list of length 5 (since we had nsim = 5), with each element being a realization of the response vector y.
3.2. Methods component

The next component in the simulator is the methods component. An object of class Method defines a function that takes arguments model and draw. In the example, the design matrix $X$ is contained in the model (accessible via model$x), and the response vector $y$ comes from the draw argument. A Method object can also (optionally) include a list of settings.

- **new_method** creates a new Method object. In the example, the objects lasso and ridge were produced by the new_method function (see Appendix A.2).
- **run_method** is a main pipeline function. It runs one or more methods on the simulated data and creates Output objects, saves these to file, and adds references to these to the Simulation object.
- **output** loads one or more Output objects from a Simulation object into the R session.
- (for advanced usage—not needed in most simulations) **new_method_extension** and **new_extended_method** are used to create new MethodExtension and ExtendedMethod objects. An ExtendedMethod is an object that behaves like a method, but is allowed to use the output of another method. This can be useful when one method builds off of another. In the example, cv is a MethodExtension and lasso + cv is an ExtendedMethod (see Appendix A.4 for more).

At the core of an Output object is a list called out.

```
o <- output(sim, k == 10, methods = "lasso")
o
```

Output Component
- model_name: slm/k_10/n_200/p_500
- index: 1
- nsim: 5
- method_name: lasso
- method_label: Lasso
- out: beta, yhat, lambda, df, time

Each element of the list o@out corresponds to a random draw (i.e., realization) and gives the output of the lasso on this draw.

3.3. Metrics/Evaluation component

The next component in the simulator is the evaluations component, in which we evaluate each method based on some user-defined metrics. An object of class Metric defines a function with arguments model and out (the output of a method). In the example, the mean squared error is a metric of interest which measures how far the true coefficient vector $\beta$ (accessible via model$beta) is from a method’s estimate of this quantity (accessible via out$beta).

- **new_metric** creates a new Metric object. In the example, the objects mse, bestmse, and df are produced by the new_method function (see Appendix A.3).
• **evaluate** is a main pipeline function. It computes one or more metrics on the outputs of the methods and creates **Evals** objects, saves these to file, and adds references to these to the **Simulation** object. In addition to the metrics that are explicitly passed to **evaluate**, the computing time for a method is automatically saved as well.

- **evals** loads one or more **Evals** objects from a **Simulation** object into the R session.
- **as.data.frame** converts an **Evals** object (or list of **Evals** objects) to a **data.frame**.

An **Evals** object contains the computed metrics on each method-draw pair.

```r
e <- evals(sim, k == 10)
e
```

**Evals Component**

- model_name: slm/k_10/n_200/p_500  index: 1 (5 nsim)
- method_name(s): lasso, ridge (labeled: Lasso, Ridge)
- metric_name(s): sqr_err, df, best_sqr_err, time
- metric_label(s): squared error, degrees of freedom, best squared error, Computing time

In particular, `@evals$lasso` and `@evals$ridge` are lists of length 5 (one per random draw) and `@evals$lasso[[1]]$bestmse` gives the best MSE for the lasso on the first draw.

### 3.4. Plot/Table component

Making standard plots and tables of simulation results is a task that is particularly streamlined using the **simulator**. **plot_eval** takes the name of a metric and makes side-by-side box plots of each method. If multiple models are included, these are shown as a multifaceted plot.

```r
subset_simulation(sim, k == 20 | k == 80) %>% plot_eval("time")
```

![Plot Example](image-url)
• **plot_evals** takes the names of two metrics and plots the first versus the second with different colored/styled lines (or points) for each method. We used this function in Section 2.

• **plot_eval_by** plots a metric versus a model parameter that was varied across models (in our example, this corresponded to the sparsity level $k$ of the true coefficient vector). By default, a line with error bars is shown. The center and width of these error bars is by default the sample mean (across the random realizations) and standard error of the sample mean, respectively; however, one can pass custom-made `Aggregator` objects to have the center and width of the error bars represent different aggregates. Another option (with `type="raw"`) simply shows the raw values of the metric for each method at each value of the model parameter.

• **tabulate_eval** takes the name of a metric and creates a table (in latex, markdown, or html formats) in which each row is a model and each column is a method. As with **plot_eval_by**, the default is to show the sample mean (with its standard error in parentheses), and the user can provide custom `Aggregator` objects so that these represent more general aggregates.

• (for advanced usage—not needed in most simulations) `new_aggregator` can be used to create a custom `Aggregator`.

### 4. Design principles

#### 4.1. Modularity of components

As noted earlier, a simulation can be viewed as a pipeline of interlocking components. Each component can be easily inserted, modified, or removed without requiring one to change the structure of the overall simulation. For example, if one wishes to consider an additional model, include another method, or evaluate the methods using a different metric, this can all be easily done with minimal structural changes to the overall simulation. Each component in the pipeline has a standardized input and is responsible for providing output that will fit into the next component’s input. For example, at the heart of a `Metric` object is a function that takes in a method’s output and a `Model` and outputs a number or vector of numbers. The output of a metric can then be easily fed into the simulator’s plot or tabulation functions.

Another aspect of modularity is that the name (a short identifier used in file names) and the label (a longer human-readable string) of the component are stored as part of the component. This is in contrast to the typical practice of only labeling methods or models when plots or tables are made. Conceptually, it makes much more sense to label components at the location they are defined. A great benefit is that all downstream components have access to the labels. For example, the simulator’s plot functions automatically provide informative descriptions such as legends identifying the various methods, labeled axes, and titles describing the model.

Decoupling the components of a simulation is also important when certain aspects require more computing time than others. For example, applying statistical methods to simulated data is often the most computationally intensive aspect of simulations. This is similar in spirit to `roxygen2` (Wickham, Danenberg, and Eugster 2015), in which one documents functions in the same place where they are defined rather than writing separate `.Rd` files.
data is often much slower than computing metrics to evaluate their success. The modularity of the simulator disentangles these two parts so that if one changes a single metric, one does not have to rerun the statistical methods. Finally, the plotting and tabulating components are themselves separate from all previous parts—since one should not have to rerun any major computation as one makes slight modifications to plots or tables.

Finally, modularity makes it easier to share components across one’s projects with other researchers. A group of researchers might develop a set of common models and methods for, say, high-dimensional covariance estimation. When someone proposes a new covariance estimator, one simply needs to define this new Method object and then this can be easily plugged in to the preexisting code base, saving a lot of time and making for a more meaningful comparison.

4.2. Every component’s results saved to file

Every component of a simulation generates R objects that take time to compute and take space to keep in memory. When we modify a component of a simulation, we should not have to rerun the parts of the simulation that are “upstream” of the modification. Also, in analyzing a simulation, we might want to examine the generated objects at various stages in the simulation; again, we should not have to rerun anything to see an intermediate stage of the simulation. For all of these reasons, the simulator automatically saves all generated objects to files when one runs a simulation. The files are kept in an organized directory structure that is easy to interpret; however, the user never has to explicitly learn or pay attention to the particulars of the directory structure since there are a series of simulator functions that make it simple to load these saved files.

4.3. Working with references

In the most common usage of the simulator, a Simulation object is passed through the simulator pipeline. As it gets fed through the various component functions, it accumulates more and more of a “record” of the simulation. An important aspect is that the Simulation object does not contain the objects generated from the various components themselves (which would be extremely memory intensive); rather, it contains references to these objects. A reference is an object containing the saved location of an object generated by the simulator. The fact that Simulation objects contain references rather than the objects themselves makes the simulator behave much more nimbly. One only loads the specific pieces of a simulation as needed. The functions models, draws, outputs, and evals allow one to load specific objects referred to in a simulation. A more advanced consequence is that multiple simulations can refer to the same set of saved objects (thus if multiple simulations have some common aspects, one can avoid recomputing these or creating multiple copies of them). The function subset_simulation is useful in this context.

4.4. Magrittr friendly

The first argument and the output of most simulator functions is a Simulation object. This is done to facilitate magrittr integration, which allows one to write succinct “one-liner” simulations that read (almost) like sentences. The pipe operator passes the output of its left-
hand-side to the first argument of the function on its right. Without the pipe, the example presented in Section 2 would be a bit more cumbersome.

```r
sim <- new_simulation(name = "bet-on-sparsity", label = "Bet on sparsity")
sim <- generate_model(sim, make_sparse_linear_model, n = 200, p = 500,
  k = as.list(seq(5, 80, by = 5)), vary_along = "k")
sim <- simulate_from_model(sim, nsim = 5, index = 1)
sim <- run_method(sim, list(lasso, ridge))
sim <- evaluate(sim, list(mse, bestmse, df))
```

4.5. Parallel processing and random seed streams

The simulator uses the parallel package (R Core Team 2016) to allow simulations to be run in parallel. In `simulate_from_model` one simulates draws in chunks, indexed by `index`. For example, `simulate_from_model(sim, nsim = 10, index = 1:10)` would lead to a total of 100 simulations performed in chunks of size 10. The `index` of a chunk is used to specify a distinct stream of pseudorandom numbers, using the “L’Ecuyer-CMRG” generator in R (L’ecuyer 1999). The use of streams is convenient because it compartmentalizes chunks of random draws, so that the starting state of one chunk does not depend on the end state of another chunk. In particular, the following three options all give identical results.

1) In sequence:

```r
simulate_from_model(sim, nsim = 10, index = 1:10) %>%
  run_methods(list_of_methods)
```

2) In parallel:

```r
simulate_from_model(sim, nsim = 10, index = 1:10) %>%
  run_methods(list_of_methods, parallel = list(socket_names = 4))
```

3) Mixed-and-matched with no particular order to `index`:

```r
simulate_from_model(sim, nsim = 10, index = 1:2) %>%
  run_methods(list_of_methods)
```

# perhaps a day later:

```r
sim <- load_simulation("bet-on-sparsity")
simulate_from_model(sim, nsim = 10, index = 5:10) %>%
  run_methods(list_of_methods, parallel = list(socket_names = 4))
```

# realize later you forgot two chunks:

```r
sim <- load_simulation("bet-on-sparsity")
simulate_from_model(sim, nsim = 10, index = 3:4) %>%
  run_methods(list_of_methods)
```

---

2For example, `matrix(rnorm(5 * 2), 5, 2)` could equivalently be written `5 * 2 %>% rnorm %>% matrix(5, 2)`.
Table 1: A comparison of Mean squared error (averaged over 5 replicates).

<table>
<thead>
<tr>
<th>n = 200, p = 500, k = 35</th>
<th>Lasso cross validated</th>
<th>Ridge cross validated</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.04 (0.00)</td>
<td>0.05 (0.00)</td>
<td></td>
</tr>
<tr>
<td>n = 200, p = 500, k = 40</td>
<td>0.06 (0.01)</td>
<td>0.06 (0.00)</td>
</tr>
<tr>
<td>n = 200, p = 500, k = 45</td>
<td>0.08 (0.01)</td>
<td>0.07 (0.00)</td>
</tr>
<tr>
<td>n = 200, p = 500, k = 50</td>
<td>0.09 (0.01)</td>
<td>0.08 (0.00)</td>
</tr>
<tr>
<td>n = 200, p = 500, k = 55</td>
<td>0.09 (0.00)</td>
<td>0.08 (0.00)</td>
</tr>
<tr>
<td>n = 200, p = 500, k = 60</td>
<td>0.11 (0.00)</td>
<td>0.09 (0.00)</td>
</tr>
</tbody>
</table>

When `simulate_from_model` creates a new `Draws` object (i.e., a chunk of random draws) the end state of the random number generator is saved to file. Whenever `run_method` is called on that `Draws` object, the random number generator is first set to that stored state. This ensures that we will get the same results regardless of the order in which we apply our methods (if any are randomized algorithms).

### 4.6. Unified interface for plotting and tables

Gelman, Pasarica, and Dodhia (2002) go through every table appearing in an issue of the *Journal of the American Statistical Association* and conclude that plots are more effective than tables for most tasks. The `simulator` therefore focuses mostly on the generation of plots rather than tables. That said, the basic function for making tables (which can be in latex, html, or markdown format) is designed to have a very similar interface to one of the plotting functions, reflecting the similar task these two functions accomplish. For example, returning to the comparison of lasso and ridge with cross validation, one could tabulate the results (even though the plot generated in Section 2 seems more useful).

```r
subset_simulation(sim2, k > 30 & k <= 60) %>%
  tabulate_eval("sqr_err", format = list(nsmall = 2, digits = 0))
```

Everything about the table created by this command, including the caption, was automatically generated by `tabulate_eval`.

### 4.7. Easy extraction of data into data.frames

The `simulator` is intended to provide all the major functionality that is typically required when one performs a simulation study; however, users should not feel “locked in” to the `simulator`. In particular, since there may be specific situations in which a non-standard operation is required (e.g., generating an unusual sort of plot based on simulation results), the `simulator` makes it simple to extract simulation data into a `data.frame` which can then be manipulated outside the `simulator` framework.

### 5. Getting started

The easiest way to start using the `simulator` is to use the function `create`. The command
create("name/of/new/directory")

will produce the specified directory and the following files that make up the skeleton of a simulation:

- `model_functions.R` - file with a function that creates `Model` objects.
- `method_functions.R` - file that creates `Method` objects.
- `eval_functions.R` - file that creates `Metric` objects.
- `main.R` - file with the main simulation pipeline code (and that sources the three `_functions.R` files).
- `writeup.Rmd` - an `rmarkdown` file that lays out the code and results (showing the main code first and the definitions of various components later). The simulation code is not itself stored in `writeup.Rmd`, so that as one makes changes to the `.R` files, the report will remain up-to-date. Some basic caching logic is built into `writeup.Rmd` so that if the `.R` files of the simulation have not been changed since the simulation data was created, the simulation will not be rerun when one knits `writeup.Rmd`. This is convenient since one can see the effects of changes to the report without having to rerun the entire simulation.

A series of online vignettes for the `simulator` demonstrate its use in varied settings and may be useful for getting started with the `simulator`.

6. Dependence on other R packages

The `simulator` makes use of several R packages. The pipe operation, `%>%`, uses `magrittr` (Bache and Wickham 2014); the parallel processing capabilities are built upon the `parallel` (R Core Team 2016) package; file name formation is based on the `digest` package (with contributions by Antoine Lucas, Tuszyński, Bengtsson, Urbanek, Frasca, Lewis, Stokely, Muehleisen, Murdoch, Hester, Wu, and Onkelinx. 2016); `knitr` (Xie 2016) and `rmarkdown` (Allaire, Cheng, Xie, McPherson, Chang, Allen, Wickham, Atkins, and Hyndman 2016) are used for creating tables and report generation; plots are by default generated using `ggplot2` (Wickham 2009), although each plot function has a `use_ggplot2 = FALSE` setting for users preferring the basic plot functions provided through `graphics`; finally, although not directly involved in user-called functions, the packages `devtools` (Wickham and Chang 2016) and `testthat` (Wickham 2011) were instrumental in the development of the package.

7. Related work

A look into the literature and a search online for software packages reveal several packages similar in spirit to the `simulator`, which we briefly review here.

The packages `ezsim` (Chan 2014) and `simsalapar` (Hofert and Mächler 2016) are similar in spirit in many ways to the `simulator` and provide much of the same functionality (such as the ability to parallelize simulations, save results to files, generate plots, and vary model parameters). The major differences are in terms of design choices. For example, these packages’ approaches
are much less modular and less object-oriented. All aspects of the simulation are passed as functions to a single master function. By contrast, the simulator design encourages one to think of a simulation as a pipeline with replaceable parts that can be easily reused, swapped, and shared. Another difference is that ezsim does not appear well-suited for simulations that evolve over time (for example, if one later decides to add a method, increase the number of random draws, or add an additional metric, the simulator does not require one to rerun everything).

Alfons, Templ, and Filzmoser (2010) develop the package simFrame as an object-oriented framework for simulation (and also include parallelization and plotting abilities). Their particular focus is on survey statistics (with associated issues of outliers and missing data), but the authors note that the framework is general and can be extended to many other applications. In the examples presented, it appears that the user writes a function that is passed to simFrame::runSimulation that has all the methods and metrics computed within it. This bundling of all methods and metrics together goes against the simulator design principle that methods should be decoupled from each other (so they can be run in parallel or at different times) and that the computation of metrics to evaluate the method objects should be viewed as a separate layer of the simulation.

The package harvestr (Redd 2014) focuses on the parallelization and caching infrastructure (and adds color with function names related to gardening!); the framework is quite general but less tailored to the sort of statistical simulations in which one is comparing methods across different models and wants to rapidly generate plots.

SimDesign (Chalmers 2016) has many aspects in common with the simulator and simFrame, for example its pipeline of generate-analyse-summarise is similar to the model-method-evaluate pipeline of the simulator. However, like the other simulation packages, SimDesign’s methods appear to be bundled together in the analyse step. Likewise all metrics are bundled together in the summarize step. Again, a distinguishing feature of the simulator is the modular organization of the Models/Methods/Metrics components.

8. Discussion

The simulator attempts to streamline an important yet often dreaded part of writing statistics papers. By taking care of the infrastructure and enforcing some structure on the process, we have found that it makes conducting simulation studies less tedious and less haphazard. Using this tool allows the user to focus time, energy, and thought on the problem-specific aspects, which hopefully leads to more carefully thought-out, insightful studies that might even be enjoyable to conduct. The foundation provided by the simulator can easily be built upon by developing domain-specific libraries of models, methods, and metrics. For example, the areas of high-dimensional regression, classification, multiple testing, graphical models, clustering, network science, etc, could each have a repository of simulator Model, Method, and Metric objects that can be easily shared. Building up such a library of components would greatly facilitate the sharing of simulation models, leading to greater consistency across the literature while at the same time requiring less effort.
Acknowledgments

The inspiration to take the large code base we had developed over years and turn it into an easy-to-use R package came from devtools, which was also used to make this package. We also acknowledge the book “R packages” (Wickham 2015) for influencing many of the design and code-style choices for the simulator package.

References


This appendix provides the problem-specific code required for the example shown in Section 2.

### A.1. The model

We simulate from a linear model

\[ Y = X\beta + \epsilon \]

where \( Y \in \mathbb{R}^n \), \( \beta \in \mathbb{R}^p \), and \( \epsilon \sim N(0, \sigma^2 I_n) \). We have taken \( X \) to have iid \( N(0, 1) \) entries and treat it as fixed in this simulation. We define a Model object, which specifies the parameters and, most importantly, describes how to simulate data.

```r
define_make_sparse_linear_model <- function(n, p, k) {
  x <- matrix(rnorm(n * p), n, p)
  beta <- rep(c(1, 0), c(k, p - k))
  mu <- as.numeric(x %*% beta)
  sigma <- sqrt(sum(mu^2) / (n * 2)) # fixes signal-to-noise at 2
  new_model(name = "slm", label = sprintf("n = %s, p = %s, k = %s", n, p, k),
            params = list(x = x, beta = beta, mu = mu, sigma = sigma, n = n,
                           p = p, k = k),
            simulate = function(mu, sigma, nsim) {
              y <- mu + sigma * matrix(rnorm(nsim * n), n, nsim)
              return(split(y, col(y))) # make each col its own list element
            })
}
```

We will typically put the code above in a file named `model_functions.R`.
A.2. The methods

We compare the lasso and ridge. Both of these methods depend on tuning parameters, so we compute a sequence of solutions.

```r
library(glmnet)
lasso <- new_method("lasso", "Lasso",
    method = function(model, draw, lambda = NULL) {
        if (is.null(lambda))
            fit <- glmnet(x = model$x, y = draw, nlambda = 50,
                intercept = FALSE)
        else {
            fit <- glmnet(x = model$x, y = draw, lambda = lambda,
                intercept = FALSE)
        }
        list(beta = fit$beta, yhat = model$x %*% fit$beta,
            lambda = fit$lambda, df = fit$df)
    })

ridge <- new_method("ridge", "Ridge",
    method = function(model, draw, lambda = NULL) {
        sv <- svd(model$x)
        df_fun <- function(lam) {
            # degrees of freedom when tuning param is lam
            sum(sv$d^2 / (sv$d^2 + lam))
        }
        if (is.null(lambda)) {
            nlambda <- 50
            get_lam <- function(target_df) {
                f <- function(lam) df_fun(lam) - target_df
                uniroot(f, c(0, 100 * max(sv$d^2)))$root
            }
            lambda <- sapply(seq(1, nrow(model$x),
                length = nlambda), get_lam)
        } else {
            lambda <- lambda
        }
        df <- sapply(lambda, df_fun)
        beta <- sapply(lambda, function(r) {
            d <- sv$d / (sv$d^2 + r)
            return(sv$v %*% (d * crossprod(sv$u, draw)))
        })
        list(beta = beta, yhat = model$x %*% beta,
            lambda = lambda, df = df)
    })
```

Methods can return different items. However, aspects of the method that will be used downstream in the simulation and compared across methods should be in a common format. Thus beta, yhat, and df in each case are in the same format. These will be the items used when evaluating the methods’ performances.
We will typically put the code above in a file named `method_functions.R`.

### A.3. The metrics

When we compare methods in plots and tables, there are usually a number of “metrics” we use. An object of class `Metric` specifies how to go from a model’s parameters and the output of a method and return some quantity of interest.

```r
mse <- new_metric("mse", "Mean-squared error",
    metric = function(model, out) {
        colMeans(as.matrix(out$beta - model$beta)^2)
    })

bestmse <- new_metric("bestmse", "Best mean-squared error",
    metric = function(model, out) {
        min(colMeans(as.matrix(out$beta - model$beta)^2))
    })

df <- new_metric("df", "Degrees of freedom",
    metric = function(model, out) out$df)
```

Observe that `out` refers to the list returned by our methods and `model` refers to the `Model` object that is generated by `make_sparse_linear_model`. The `$` operator can be used to get parameters that are stored in the `Model` object.

We will typically put the code above in a file named `eval_functions.R`.

### A.4. Extensions of the methods

In Section 2, we wanted to study cross-validated versions of the lasso and ridge regression, so we inputed into `run_method` the objects `lasso + cv` and `ridge + cv`. These are `ExtendedMethod` objects, which behave much like `Method` objects, except they can get access to the output of another method.

If we only cared about relaxing the lasso, we could have directly created an `ExtendedMethod`; however, in this situation we wanted both methods to be cross-validated in an identical fashion. In the spirit of code reusability, we therefore created what we call a `MethodExtension` object, `cv`. A `MethodExtension` object when added to a `Method` object generates an `ExtendedMethod`.

```r
make_folds <- function(n, nfolds) {
    nn <- round(n / nfolds)
    sizes <- rep(nn, nfolds)
    sizes[nfolds] <- sizes[nfolds] + n - nn * nfolds
    b <- c(0, cumsum(sizes))
    ii <- sample(n)
    folds <- list()
    for (i in seq(nfolds))
        folds[[i]] <- ii[seq(b[i] + 1, b[i + 1])]
    folds
```
The simulator

```r

new_method_extension("cv", "cross validated",
  method_extension = function(model, draw, out,
    base_method) {
    nfolds <- 5
    err <- matrix(NA, ncol(out$beta), nfolds)
    ii <- make_folds(model$n, nfolds)
    for (i in seq_along(ii)) {
      train <- model
      train@params$x <- model@params$x[-ii[[i]],]
      train@params$n <- model@params$x[-ii[[i]],]
      train_draw <- draw[-ii[[i]]]
      test <- model
      test@params$x <- model@params$x[ii[[i]],]
      test@params$n <- model@params$x[ii[[i]],]
      test_draw <- draw[ii[[i]]]
      fit <- base_method@method(model = train,
                               draw = train_draw,
                               lambda = out$lambda)
      yhat <- test$x %*% fit$beta
      ll <- seq(ncol(yhat))
      err[ll, i] <- colMeans((yhat - test_draw)^2)
    }
    m <- rowMeans(err)
    se <- apply(err, 1, sd) / sqrt(nfolds)
    imin <- which.min(m)
    ioneserule <- max(which(m <= m[imin] + se[imin]))
    list(err = err, m = m, se = se, imin = imin,
         ioneserule = ioneserule,
         beta = out$beta[, imin],
         yhat = model$x %*% out$beta[, imin])
  })
```

Of course, if we later added `mcp` to the simulation, we could easily incorporate cross-validation into it as well with `mcp + cv`.

We will typically put the code above in the file named `method_functions.R`.