

A Regression Simulation as a Workflow Example

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1 Introduction

This example illustrates a workflow for a simple simulation. Consider a linear regression model with

$$y_i = \mathbf{x}_i^\top \boldsymbol{\beta} + \epsilon_i, \quad \epsilon_i \stackrel{\text{iid}}{\sim} \text{N}(0, \sigma^2), \quad i = 1, \dots, n, \quad (1)$$

where $\mathbf{x}_i \in \mathbb{R}^d$ is a given covariate which is considered to be fixed. Let $\boldsymbol{\theta} = (\boldsymbol{\beta}, \sigma^2)$ represent the unknown parameters and let $\hat{\boldsymbol{\theta}} = (\hat{\boldsymbol{\beta}}, \hat{\sigma}^2)$ be the maximum likelihood estimator (MLE). Here the MLE has well-known closed form expressions

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}, \quad \hat{\sigma}^2 = \frac{1}{n} \mathbf{y}^\top (\mathbf{I} - \mathbf{H}) \mathbf{y},$$

where \mathbf{X} is the $n \times d$ matrix with rows \mathbf{x}_i^\top and $\mathbf{H} = \mathbf{X}(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top$. A property of interest for the MLE is its mean-squared error

$$\text{MSE}(\hat{\boldsymbol{\theta}}, \boldsymbol{\theta}) = \text{E} \left[\|\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}\|^2 \right]$$

with respect to the true data generating parameter $\boldsymbol{\theta}$. We will prepare a small simulation to evaluate the MSE for $\boldsymbol{\beta} = (-1, 1)$, $\sigma \in \{1, 2, 3\}$, and $n \in \{50, 100, 200\}$. Each combination of (σ, n) will be referred to as a “level” of the simulation. For each level, we will repeat the following for $r = 1, \dots, R = 200$: first generate observations $\mathbf{y}^{(r)} = (y_1^{(r)}, \dots, y_n^{(r)})$ from model (1) using the current $\boldsymbol{\theta}$ and n , then obtain the MLE $\hat{\boldsymbol{\theta}}^{(r)}$. Using the empirical sampling distribution of $\hat{\boldsymbol{\theta}}^{(1)}, \dots, \hat{\boldsymbol{\theta}}^{(R)}$, we may then approximate

$$\text{MSE}(\hat{\boldsymbol{\theta}}, \boldsymbol{\theta}) \approx \frac{1}{R} \sum_{r=1}^R \|\hat{\boldsymbol{\theta}}^{(r)} - \boldsymbol{\theta}\|^2.$$

The end result will be a table with the following form.

	$n = 50$	$n = 100$	$n = 200$
$\sigma = 1$
$\sigma = 2$
$\sigma = 3$

This simple simulation can be run within an R script in a matter of seconds. We can create nested loops to iterate through the crossed levels of σ and n , and then loop through the R repetitions. Now imagine a more involved study where computing each estimate takes on the order of minutes or hours. Also, instead of having only 9 levels of the simulation, perhaps we have hundreds. Rather than saving just the MLE repetitions, we may also want to save the generated data $\mathbf{y}^{(r)}$, and diagnostics from each fit so that unanticipated results can be investigated after the run. This motivates the following workflow:

- Each level of the simulation will be placed into its own dedicated folder with a launcher script. Any logging and output relevant to the level will be saved here as well.
- The folders and launcher scripts will be generated by a script that we write.

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- We will utilize one or more “workers”, whose job is to search the folders for available work. A folder is reserved and has its launcher executed by at most one worker.
- If a level fails, or if we wish to investigate its result, we can manually enter the folder and run the launcher or load the results.
- We will write a script to extract results from the folders and produce the desired results (a table of MSEs).

This kind of “embarrassingly parallel” computing is typical in many statistical projects: no communication is needed across levels during the simulation. Coordination is only needed to initially generate the workload and in post-processing. We may therefore take advantage of multiple CPUs to process our workload faster without requiring more sophisticated tools available for parallel and distributed computing. In contrast, individual computations which are too CPU or memory intensive for a single processor or compute node may benefit greatly from these tools; for example, the `pbdr` package provides an MPI implementation in R while the `parallel` package supports parallel computing which offers less control over communication but is simpler to use.

2 Workflow Implementation

The following scripts are used to implement our workflow for the regression simulation:

- `gen.R` generates the folder structure and creates a `launch.R` script in each folder.
- `util.R` contains several utility functions used by other scripts.
- `sim.R` contains the main logic to run each level of the simulation. The program sleeps for a few moments after each repetition to give the feeling of a more computationally demanding simulation.
- `launch.R` is responsible for setting variables specific to the simulation level and running `sim.R`.
- `worker` is a Python script that seeks simulation levels which have not yet run and attempts to run them.
- `analyze.R` handles post-processing after the simulation is completed. A table of MSEs is presented as the final result.

All scripts mentioned above, except for `worker`, are specific to this simulation and must be rewritten or customized for other applications.

Let us run `gen.R` on the command line. The following displays will shown as a Linux prompt, but other environments should work similarly.

```
$ R CMD BATCH gen.R
```

The following folders and directories are produced.

```
sigma1_n1  sigma1_n3  sigma2_n2  sigma3_n1  sigma3_n3  xmat-n2.rds
sigma1_n2  sigma2_n1  sigma2_n3  sigma3_n2  xmat-n1.rds  xmat-n3.rds
```

Folders of the form `sigmaA_nB` correspond to the simulation level for the A th value of σ and the B th value of n , for $A, B \in \{1, 2, 3\}$. Files of the form `xmat-nB.rds` represent the design matrix \mathbf{X} to be used when n is taken to be the B th value.

Let's inspect `launch.R` in the folder `sigma1_n1`.

```
N_sim = 200
beta_true = c(-1,1)
sigma_true = 2
xmat_file = "../xmat-n1.rds"

source("../sim.R")
```

It is a good practice to run one launch script manually to verify that our generated code is correct: all variables should be set and all external files and data should be in the appropriate place. Here we assume

the `sigma1_n1` folder is our current working directory, and that `sim.R` and `xmat-n1.rds` are in the parent directory.

Once we are certain the code and folders are laid out correctly, we will want to use a worker(s) instead of running the study manually. Suppose the path to our generated simulation folders is located at `/path/to/study`.

First make sure the worker script is executable.

```
chmod +x /path/to/worker
```

The following command invokes one worker.

```
/path/to/worker -b /path/to/study -p "sigma(.*)_n(.*)" -c 'R CMD BATCH launch.R'
```

- Option `-b` is used to specify one or more paths which contain work folders.
- Option `-p` is used to specify one or more patterns used to identify work folders (as opposed to other folders which we should ignore).
- Multiple paths and patterns may be specified. The count of each should match. The first pattern is considered coupled to the first path, the second pattern coupled to the second path, and so on.
- Option `-c` specifies a command to run if we find a work folder whose job has not yet been attempted.
- Use the `-h` flag to display a help message, including the command line format, and quit.

A worker logs its activity to stdout. This can be redirected to a file if desired.

```
2021-06-09 18:16:05 - Worker ID: 75e1421210cc92d62e5403313cab33f0
2021-06-09 18:16:05 - Home path: /sim-util/examples/regression-sim
2021-06-09 18:16:05 - Searching 1 basepaths for available work
2021-06-09 18:16:05 - Basepath[0]: /sim-util/examples/regression-sim
                        Pattern: sigma(.*)_n(.*)
2021-06-09 18:16:05 - Lockfile in sigma2_n2 exists, skipping
2021-06-09 18:16:05 - Lockfile in sigma1_n2 exists, skipping
2021-06-09 18:16:05 - Lockfile in sigma1_n3 exists, skipping
2021-06-09 18:16:05 - Lockfile in sigma2_n1 acquired
2021-06-09 18:19:25 - Processed 1 jobs and worked for 0.055721 total hours so far
2021-06-09 18:19:25 - Lockfile in sigma3_n1 acquired
```

Let us look in `sigma2_n1`, which was completed by the worker above.

```
$ ls sigma2_n1
launch.R launch.Rout results.Rdata worker.err worker.lock worker.out
```

The files `worker.out` and `worker.err` capture any output from stdout and stderr while running the job. The file `worker.lock` is placed as a marker to indicate that a job has been reserved by a worker. Only one worker may create this file. Furthermore, the worker who creates the file may only run the job immediately after creating it. When encountered afterward, the job is considered to have been reserved, whether it completed or not, and will be skipped. If a job has failed and you would like a worker to consider it again, delete the corresponding `worker.lock`.

The file `worker.lock` contains the ID of the worker that reserved it. This can be linked back to the `Worker` ID reported in the log output, which may help if it is necessary to determine which worker ran a job.

```
$ cat sigma2_n1/worker.lock
Reserved by worker: 75e1421210cc92d62e5403313cab33f0
```

When working on a remote server, it may not be possible to keep a persistent session open for long periods that may be needed for a simulation study. In a setting where a scheduler such as PBS or Slurm is used to allocate jobs to compute nodes, each worker may be submitted as a job to the scheduler. Example PBS and Slurm submission scripts are provided for this example in the files `worker.qsub` and `worker.slurm`.

In an environment without a scheduler, running workers via a terminal multiplexer such as `tmux` or `GNU`

screen allows terminal sessions to detach and reattach as needed to provide some persistence.

After the simulation is complete, we may run `analyze.R` to extract the estimates from each folder and build a table of MSEs.

```
R> source("analyze.R")
              n1          n2          n3
sigma1 0.07391762 0.03495352 0.01905428
sigma2 0.71125615 0.30743114 0.18523518
sigma3 3.15877261 1.32028399 0.82559688
```

As we may expect, the MSE increases as σ increases with n fixed, but decreases when n is increased and σ is fixed.