

Lecture 9: Cluster computing

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BIOST 561: Computational Skills For Biostatistics I

29 May 2019

Motivation

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In Lecture 8, you learned how to compute without R.

Today, you'll learn how to transfer those skills to computing on a **cluster**.

Examples from my research

Large-scale simulation studies:

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Large-scale simulation studies:

- proof-of-concept examples

Examples from my research

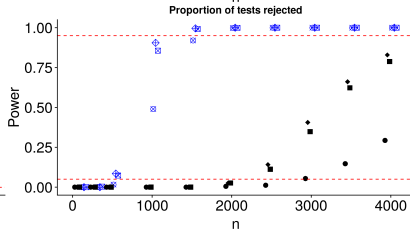
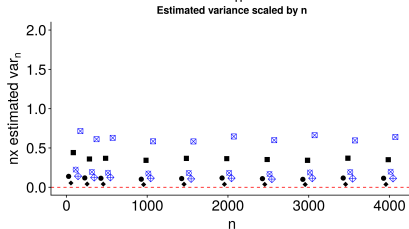
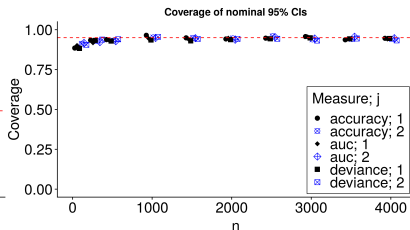
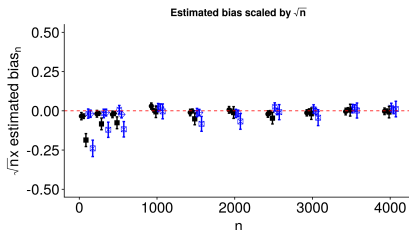
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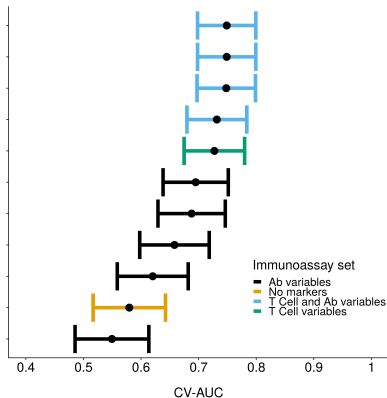
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Assay combination	CV-AUC [95% CI]
IgG + IgA + IgG3 + T Cells	0.749 [0.698, 0.799]
IgG + IgA + T Cells	0.749 [0.698, 0.799]
All markers	0.748 [0.697, 0.799]
T Cells + Fx Ab	0.732 [0.680, 0.784]
T Cells	0.727 [0.675, 0.780]
IgG3	0.695 [0.638, 0.751]
IgG + IgA + IgG3	0.688 [0.629, 0.746]
IgG + IgA + IgG3 + Fx Ab	0.658 [0.598, 0.718]
IgG + IgA	0.620 [0.559, 0.682]
No markers	0.580 [0.517, 0.643]
Fx Ab	0.550 [0.485, 0.614]



The problem

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The solution

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- allow you to submit multiple **jobs*** at once

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*: we will discuss this further!

Running example: robust standard errors (SEs)

Consider a sample of n observations generated iid according to

$$X \sim N(0, 1),$$

$$u \sim N(0, 1), \text{ independent of } X;$$

$$Y \mid X, u = \beta_0 + \beta_1 X + \epsilon, \text{ where}$$

$$\epsilon = |X|u.$$

Questions: can we use

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We will use the cluster to do this!

Part I: coding for the cluster

Coding for the cluster

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Today, I'll provide an alternative method (this should not always replace the simulator!).

Coding for the cluster: modular code

Modular code: each file has a single task

Coding for the cluster: modular code

Modular code: each file has a single task

Your turn!

Go to the code subdirectory. Then answer these questions **with a partner**:

1. what does `do_one` do? What are its arguments?
2. what does `generate_data` do? What are its arguments?
3. Write effective comments in each file so that **future you** understands each!

Coding for the cluster: modular code

Answers:

1. `do_one` runs the simulation a single time for a given n and β_1 ; it returns a tibble with n , β_1 , $\hat{\beta}_1$, a confidence interval for β_1 , and the type of SE estimator (model-based, sandwich). Argument are n (sample size) and β (true β_1).
2. `generate_data` generates a single dataset with n observations from the specified data-generating mechanism and returns this dataset. Argument are n (sample size) and β (true β_1).
3. Brian's comments are on GitHub in the `code/` directory

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Executables (e.g., /bin/sh):

- actually run your code
- other examples: /bin/bash, /usr/local/bin/Rscript, /usr/local/bin/python3

Coding for the cluster: saving output

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This is important regardless of whether or not you use the simulator!

Handy functions for saving output: `saveRDS`.

Coding for the cluster: saving output

Your turn!

In the robust SEs example, our goal is to compare model-based to robust SEs. **With a partner**, answer the following questions:

1. What output should we save?
2. How should we evaluate performance of the SEs?

Coding for the cluster: robust SEs

Check out `run_sim_robust_se.R` in the code directory!

Coding for the cluster: debugging

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Best practices (in my opinion):

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Best practices (in my opinion):

- debug **everything** on your machine first
- modular code (isolate bugs)
- run one job for subset of parameters prior to cluster

Coding for the cluster: compiling output

Check out `load_sim_robust_se.R` in the code directory!

Part II: using the cluster

Using the cluster

Department resources for HPC*:

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- cox: 12-core computer

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A cluster consists of:

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A cluster consists of:

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- cox: 12-core computer (not a cluster)
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Using the cluster

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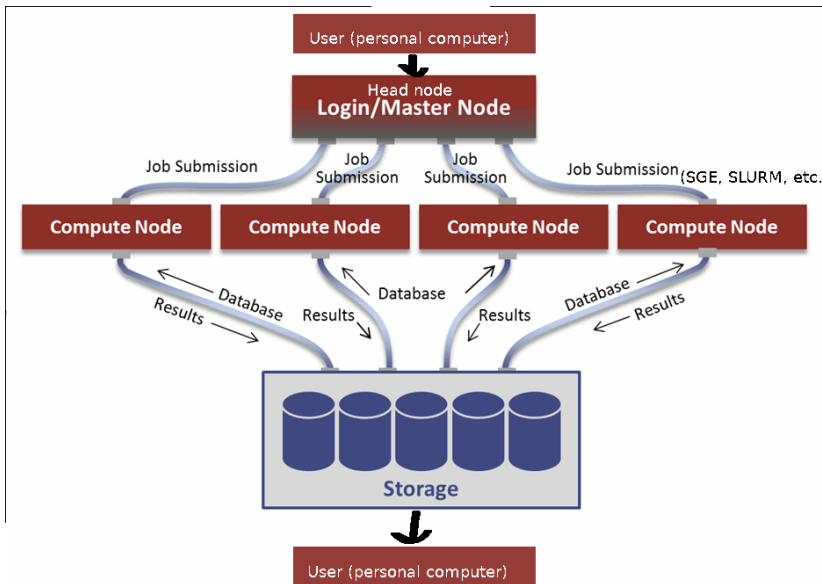
A cluster consists of:

- a head node (where you are)
- compute nodes (where your code gets run)
- submission system (how your code gets run)

*other groups have similar resources, e.g.,

- **hyak** (managed by UW-IT)
- pearson (statistical genetics group only)
- gizmo (Fred Hutchinson Cancer Research Center only)
- Microsoft Azure, Amazon Web Services (AWS)

Using the cluster



Using the cluster: bayes

More specifically, bayes

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- has 4 department-wide compute nodes, each with 12 cores

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Since this is a shared resource, being nice is important:

- don't run simulations on the head node
- don't flood the cluster

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Since this is a shared resource, being nice is important:

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We'll practice good habits for being nice as we go along.

Using the cluster: logging in

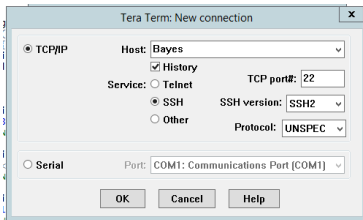
First step: make sure you are through the department firewall.

How: [OpenSesame](#) (on biost intranet)

1. Navigate to OpenSesame website
2. Select host (e.g., Bayes)
3. Click OpenSesame

Using the cluster: logging in (Windows, incl. box)

1. Open TeraTerm [or your favorite secure shell (SSH) client]
2. Enter the address of your favorite cluster, e.g.,
bayes.biostat.washington.edu
3. Make sure that the “New connection” window is filled out as in the figure, except for “Host” (screenshot from box)
4. Click OK, enter your UW BOST username and password when prompted (user and pass you use for box)



Using the cluster: logging in (Mac/Linux)

1. Open a Terminal window
2. Type `ssh mynetid@cluster.washington.edu`
 - replace `mynetid` with Your UW NetID, and
 - replace `cluster` with Your cluster, e.g., `bayes`
3. Enter password (same password as box) when prompted (the field will remain blank but your password will be received)

Using the cluster: logging in

Your turn! Take 2 minutes to complete this activity **by yourself** (if you don't have a computer, write down how you would do this).

1. Log into bayes
2. What is the name of the directory that you are when you log in? **answer: your home**
3. Create a directory called `robust_ses` in your home directory
4. Create a directory called `robust_ses` on **your** computer, under `biost561/lecture9`

Using the cluster: moving around

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Using the cluster: moving around

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- navigation,
- vim,
- commands, and
- shell scripts

are all used **in exactly the same way!**

Using the cluster: jobs

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Using the cluster: jobs

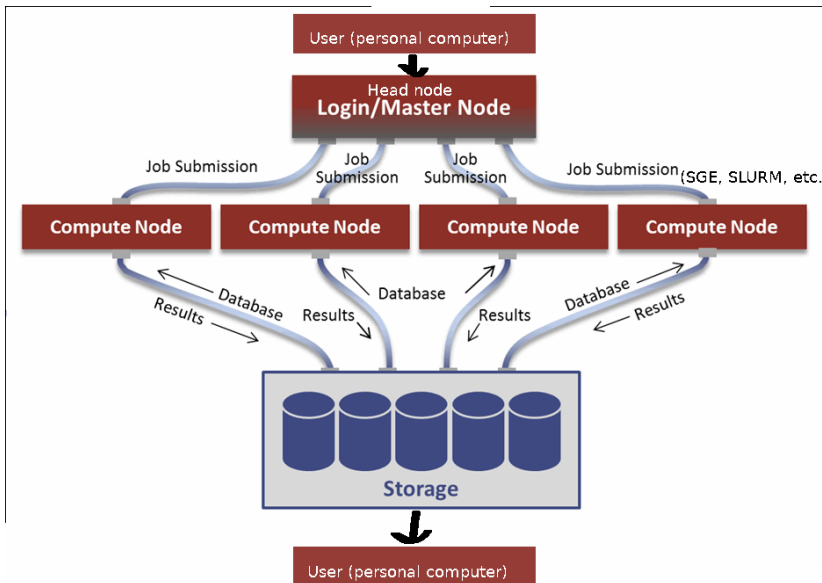
The basic unit of cluster computing is a **job**.

Jobs:

- perform a specified task
- can be submitted to the cluster compute nodes

Example job: `run run_sim_robust_se.R` with 50 replicates

Using the cluster: jobs



Using the cluster: calling your R script

Your turn!

Check out the file `call_sim_robust_se.sh`. **With a partner**, answer the following questions:

1. What does the `$` mean?
2. How many command-line arguments does `run_sim_robust_se.R` take?
3. What do the command-line arguments do?

Using the cluster: calling your R script

Answers:

1. Access a command-line arg (e.g., \$1 is command-line arg 1)
2. 3
3. Set the simulation name, the total number of replicates, and the number of replicates per job, respectively

Using the cluster: submitting jobs

Workhorse command on SGE: `qsub`

Many options, including:

Using the cluster: submitting jobs

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- `cwd`: execute script in current working directory

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- `e` and `o`: send error and output files to a folder, e.g., `iotrash/`

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- `t <task1-taskn>` submits a job array with `taskn-task1` tasks

Using the cluster: submitting jobs

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- `e` and `o`: send error and output files to a folder, e.g., `iotrash/`
- `t <task1-taskn>` submits a job array with `taskn-task1` tasks (more to come on this)

Options are specified with a single `-`, as you saw in Lecture 8.

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- embarrassingly parallel: can be split into sub-tasks run simultaneously (e.g., sim with varying parameters)
- inherently serial: cannot be split into concurrent sub-tasks (e.g., `run_sim_robust_se.R` with one replicate per job)

Using the cluster: job arrays

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- displays nicely on cluster (part of not flooding)

Using the cluster: batch submission scripts

Your turn!

Check out the file `submit_sim_robust_se.sh`. **With a partner**, answer the following questions:

1. What do lines 4 and 5 do?
2. How many jobs are in my array if I want 5000 total jobs and 50 replicates per job?

Using the cluster: batch submission scripts

Answers:

1. Create a variable called `num_n`, the number of unique sample sizes under consideration; create a variable called `njobs`, equal to the number of total replicates (arg 2) divided by the number of replicates per job (arg 3) multiplied by the number of unique sample sizes under consideration
2. $5000/50 \times 3 = 300$ jobs

Using the cluster: batch submission

Your turn!

Run the executable file `submit_sim_robust_se.sh`, with command line arguments

- `"robust_se"`
- `5000`
- `50`

Using the cluster: simulator

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```
list_of_names <- <get correct names>
simulate_from_model(nsim = 1000,
  index = 1:3,
  parallel = list(socket_names = list_of_names))
```


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- `qhold <job_id>[.tasklist]` puts a hold on job `job_id` (and optionally array elements in `tasklist`)
- `qrls <job_id>` removes a hold on a job
- `qdel <job_id>` deletes a job
- `qalter <job_id>` alters a job

Using the cluster: other helpful SGE commands

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Ways to help share the cluster:

- Submit batch jobs in job arrays
- Use holds on jobs, using `tc` argument in `qsub`
- Estimate timing of smallest job, consider this when creating and submitting job arrays

Using the cluster: checking and altering jobs

Your turn!

1. Check the status of **your** job array (replace my netid with yours): `qstat -f -u brianw26`
2. Allow only 20 jobs to run at a time (replace `<job_id>` with your job id): `qalter <job_id> -tc 20`

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Your turn!

1. Pull results files back to your computer
2. Run `load_sim_robust_se.R`
3. What can you conclude based on these results?

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These skills are easily portable to other cluster systems and your own coding projects (e.g., R packages).

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Remember to **be nice**: the cluster is a shared resource!

Appendix: other useful cluster things

Useful things: Windows file compatability

Editing files in Windows carries risks.

One such risk is adding *control characters* that cannot be processed on Unix systems (e.g., Linux on department cluster).

A helpful tool to remove this characters is dos2unix: to remove control characters from `myfile.sh`, run `dos2unix myfile.sh`.

Useful things: emails and other defaults

You can set default behavior (on bayes, but similar for other systems) by creating a file called `.sge_request`.

Mine reads

```
-j y  
-cwd  
-S /bin/bash  
-q normal.q  
-M brianw26@uw.edu  
-m e
```

Which means:

- submit either binary or script file
- run using bash
- email me
- email me at end of job

Useful things: aliases and functions (Mac/Linux)

You will probably end up logging into the cluster or sending files back and forth **quite often**.

Having *aliases* and *bash functions* set up makes this easier.

Creating aliases:

1. go to your `.ssh` folder (in your home directory on your computer)
2. create a file called `config` (using, e.g., `vim`)
3. edit it using the template below

```
Host <replace with, e.g., bayes>  
  HostName <replace with, e.g., bayes.biostat.washington.edu>  
  User <replace with, e.g., brianw26>
```

Useful things: Useful things: aliases and functions (Mac/Linux)

Creating functions:

1. go to your home directory
2. create a file called, e.g., `.bash_funcs`
3. edit it using the template below
4. edit your `.bashrc` file to include the lines

```
if [ -f ~/.bash_funcs ]; then
    . ~/.bash_funcs
fi
```

(makes sure that `.bash_funcs` is sourced when you open a new Terminal window)

```
function_name () {
    commands
}
```

E.g. : send R files from cwd to specified directory on bayes:

```
send_r_bayes () {
    scp *.R brianw26@bayes.biostat.washington.edu:~/$1
}
```

Useful things: FileZilla (all, but esp. Windows)

FileZilla is a nice program for pulling results back to your computer (via scp).

It can be used on all types of computers, but is especially helpful for Windows (since command prompt is strange!).