STATS 810 class 12: Introduction to parallel statistical computing in R on greatlakes

Edward L. Ionides

Outline

- Logging in to greatlakes
- 2 Moving files on and off greatlakes
- Working with batch jobs
- A R modules on greatlakes
- 6 A test for foreach
- 6 Editing text files on greatlakes
- Other ways to run R on greatlakes

Requirements

We follow Section 1.2 of the greatlakes user guide. As preliminaries, you need:

- A Slurm account. You should already have a primary account, stats_dept1, and a smaller backup account for if you exhaust your resourses, stats_dept2.
- A greatlakes cluster login account. If you have not yet filled in the form at https://arc-ts.umich.edu/greatlakes/user-guide/ then do so.
- A umich internet address. Use the umich VPN if you are not on campus.

Connecting to greatlakes with macOS or Linux

 Open a Terminal window (recall that, on a Mac, this can be done using Control-Spacebar and typing Terminal) and type

```
ssh uniqname@greatlakes.arc-ts.umich.edu
```

where uniquame is your uniquame.

2 Login with your Kerberos level-1 password, and Duo two-factor authentication.

This creates a remote terminal shell on greatlakes.

Connecting to greatlakes with Windows

This is essentially the same as for macOS.

- Follow instructions to install PuTTY at https://documentation.its.umich.edu/node/350
- 2 Launch PuTTY and enter greatlakes.arc-ts.umich.edu as the host name, then click open. If you receive a "PuTTY Security Alert" pop-up, this is completely normal, click the "Yes" option. This will tell PuTTY to trust the host the next time you want to connect to it. From there, a terminal window will open; you will be required to enter your UMICH uniqname and then your Kerberos level-1 password in order to log in. Please note that as you type your password, nothing you type will appear on the screen; this is completely normal. Press "Enter/Return" key once you are done typing your password.
- Omplete the request for Duo two-factor authentication.

This creates a remote terminal shell on greatlakes.

Moving files on and off greatlakes: scp

On Mac or Linux, you can use scp which has similar syntax to cp. To copy myfile on your laptop to a subdirectory mydir of your home directory on greatlakes:

```
scp myfile uniqname@greatlakes-xfer.arc-ts.umich.edu:mydir
```

To copy an entire directory, use the -r flag for recursive copy:

```
scp -r mydir uniqname@greatlakes-xfer.arc-ts.umich.edu:
```

These commands can also be reversed to copy files from greatlakes to your machine. The following copies mydir back to the current working directory:

```
scp -r uniqname@greatlakes-xfer.arc-ts.umich.edu:mydir .
```

You will need to authenticate via Duo to complete the file transfer. On Windows, you can use WinSCP or FileZilla.

Cluster batch workflow

- You create a batch script and submit it as a job
- Your job is scheduled, and it enters the queue
- When its turn arrives, your job will execute the batch script
- Your script has access to all applications and data
- When your script completes, anything it sent to standard output and error are saved in files stored in your submission directory
- You can ask that email be sent to you when your jobs starts, ends, or fails
- You can check on the status of your job at any time, or delete it if it's not doing what you want
- A short time after your job completes, it disappears

Useful batch commands

Submit a job

```
sbatch sample.sbat
```

Query job status

```
squeue -j jobid
squeue -u uniqname
```

Delete a job

scancel jobid

Check a job script and estimate its start time

sbatch --test-only sample.sbat

More Slurm commands to try

sacct -u user
seff jobid

show recent job history show cpu utilization for jobid

R modules on greatlakes

Sotware on greatlakes is packaged in modules which must be loaded

module load R

Other versions of R are available:

module avail R

We see that R4.0.1 is currently the default. For simple multicore computing, sending jobs to multiple cores on a single node, the default R module is appropriate. Other versions of R have been built and tested in other parallel environments, for example the Rmpi module runs R with mpi.

Set up test for foreach

- The gl subdirectory of the 810f21 git repository has a file test.sbat which submits a batch job running the parallel foreach test in test.R.
- A basic Linux exercise is to set up a directory on greatlakes with these files, at which point you can run

```
sbatch test.sbat
```

to submit the job.

 You can transfer the files from your laptop via scp, or by copy-paste, but it may be simplest to clone the class git repository into your greatlakes account,

```
git clone https://github.com/ionides/810f21.git
```

Editing text files on greatlakes

Inspect the text file test.sbat, for example by

```
more test.sbat
```

Is it fairly self-explanatory?

- One thing that needs changing is to set your email address for alerts about jobs beginning and ending.
- To make these edits on greatlakes, you need a text editor.
- It is convenient to use a text editor that runs in a terminal. Options include

```
vi test.sbat
emacs -nw test.sbat
nano test.sbat
```

• It is useful to have some familiarity with each of these editors.

Comparing results

You are now ready to run a batch job

sbatch test.sbat

- From inspecting the code in test.R, we see that the results are saved in test.csv
- Compare the run times with the results from running this code on your laptop, as done in homework 11.
- Also, try running the code in test2.R by

sbatch test2.sbat

What do you learn from comparing the outputs in test2.csv with test.csv on greatlakes and your laptop?

Other ways to run R on greatlakes

 It is sometimes useful to start an interactive session on greatlakes, particularly for debugging. This is done from the terminal as follows:

```
module load R
srun --nodes=1 --account=stats_dept1 --ntasks-per-node=8 \
    --pty /bin/bash
```

You can then run R in the terminal as usual, just by typing

R

- This R session will have access to the cores you have requested.
- Here, we require nodes=1 unless we use Rmpi since library(doParallel) alone cannot work with cores across different machines.
- You can also run web-based Rstudio. However, your task here is to run batch jobs, which remain the basic tool for intensive statistical computing.

Acknowledgments

- This lesson is prepared for STATS 810, Fall 2021.
- It builds on the Greal Lakes User Guide and notes by Charles Antonelli and John Thiels.
- Licensed under the Creative Commons Attribution-NonCommercial license. Please share and remix non-commercially, mentioning its origin.
- Compiled on November 12, 2021.