STAT 215A Fall 2022 Week 7

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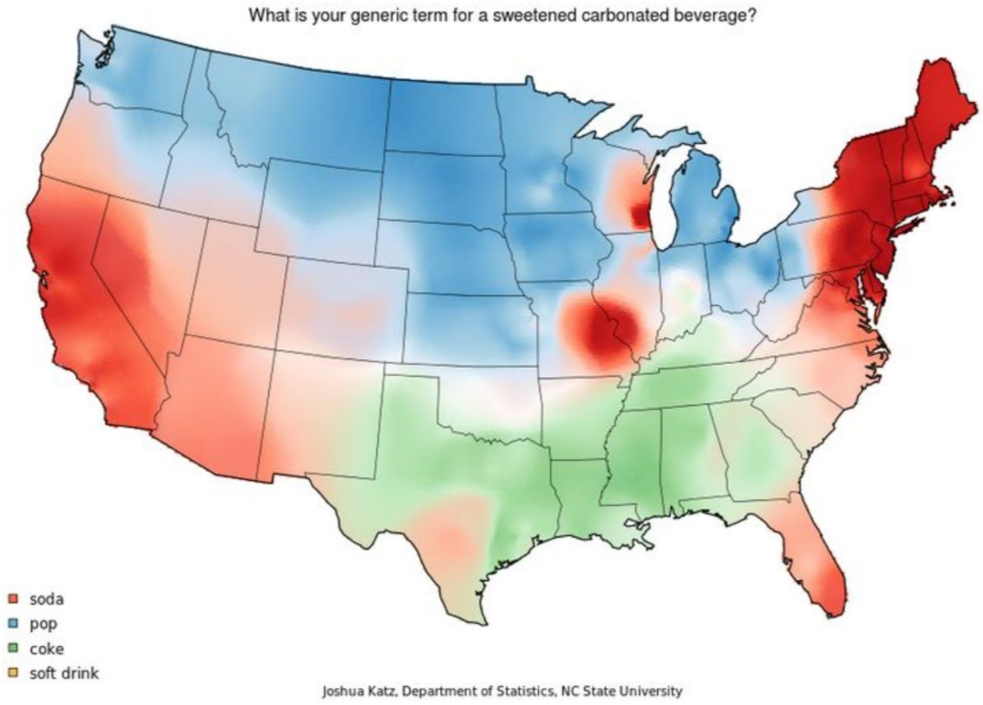
Slides in part thanks to past 215A GSIs (Tiffany Tang, Zoe Vernon, Rebecca Barter, and others.)

Announcements

- Discussion section feedback survey results
- Lab 3 will be released on Sunday 10/09
    - DUE: **10/21 at 11:59pm** (only 10 days!)
- Midterm: 10/27
    - more info / practice midterm to come

How did Lab 2 go?

- Challenges?
- Likes & dislikes?
- What clustering method did you use?


What is your generic term for a sweetened carbonated beverage?
🟥 soda
🟦 pop
🟩 coke
🟨 soft drink
Joshua Katz, Department of Statistics, NC State University

https://www.businessinsider.com/22-maps-that-show-the-deepest-linguistic-conflicts-in-america-2013-6#ok-this-one-is-crazy-everyone-pronounces-pecan-pie-differently-10

Outline for today

- Introduce **Lab 3: Stability and Computability**
- Parallelization
- Statistical Computing Facility (SCF)
- Rcpp

Lab 3: Stability of K-means and computability

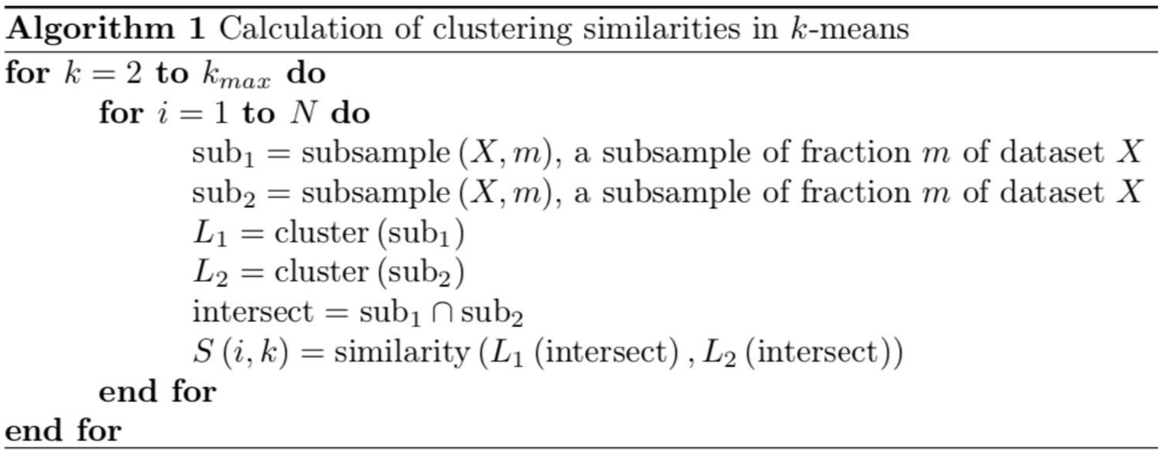
How to choose K using stability:

```
For each k = 2:kmax
    For each b = 1:B
        Perturb the data (e.g. bootstrap, subsample)
        Run K-means on the perturbed data
        Get cluster memberships
    Evaluate stability of the B cluster membership vectors
Choose k which gives the most stable clusters
```

How do we quantify the stability of clusters?

Lab 3: Stability of K-means and computability

- Ben-Hur (2002): A stability-based method for discovering structure in clustered data:



Algorithm 1 Calculation of clustering similarities in k-means

```
for $k = 2$ to $k_{max}$ do
    for $i = 1$ to $N$ do
        $\mathrm{sub}_1 = \mathrm{subsample}(X, m)$, a subsample of fraction $m$ of dataset $X$
        $\mathrm{sub}_2 = \mathrm{subsample}(X, m)$, a subsample of fraction $m$ of dataset $X$
        $L_1 = \mathrm{cluster}(\mathrm{sub}_1)$
        $L_2 = \mathrm{cluster}(\mathrm{sub}_2)$
        $\mathrm{intersect} = \mathrm{sub}_1 \cap \mathrm{sub}_2$
        $S(i, k) = \mathrm{similarity}(L_1(\mathrm{intersect}), L_2(\mathrm{intersect}))$
    end for
end for
```

- **Similarity metrics**: correlation, Jaccard, matching

Lab 3: Stability of K-means and computability

Your objectives:

1. Write efficient code to implement Algorithm 1 and speed up the computations.
2. Evaluate the stability of K-means using the binary-encoded data from Lab 2.

I will look at your code *closely* in this lab, so please be sure to follow an appropriate R style guide:

- https://style.tidyverse.org/
- https://google.github.io/styleguide/Rguide.html

How to speed up computation

- Easy:
  - Don’t repeatedly re-compute object that only need to be computed once.
  - Don’t define or store objects unnecessarily (intermediate variables)
- Other ways:
  - In R:
    - Base R: vectorize using the `apply()` and `Reduce()` family of functions
    - Tidyverse / `purrr`: use map() functions
  - Parallelize: use the multiple cores (or threads) on your laptop or the SCF cluster for larger jobs
  - Write functions in faster programming languages (e.g., C++) and read into R (using `Rcpp`)

Thanks to Tiffany Tang for her slides.

Key tools to speed up computation

- **Vectorized / functional programming**
- Parallelize
- SCF cluster
- C++ & `Rcpp`

Vectorizing code with `apply()`

Functions like `apply()`, `lapply()`, `Reduce()`, `map()`, and `map_*()` are useful for applying a function to each element of the input:

- `apply()` - applies a function to the margins of your input array/matrix

```
apply(X = df, MARGIN = 1, FUN = mean) # same as rowMeans(df)

apply(X = df, MARGIN = 1, FUN = function(x) {X - mean(X)}
```

- `lapply()` - given vector or list input, applies a function to each element and returns a list:
- Also see `sapply()` and `mapply()`

Vectorizing code with `apply()`

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- Also see `sapply()` and `mapply()`

Vectorizing code with `map()`

The `purrr` package provides the `map_*()` family of functions which provide similar utility with a few added niceties:

- `map()` - returns a list
- `map_dbl()` - returns a double vector
- `map_lgl()` - returns a logical vector
- See `?purrr::map`

Key tools to speed up computation

- Vectorized / functional programming
- **Parallelize**
- SCF cluster
- C++ & `Rcpp`

Parallelizing code

The Statistics Department has a resident expert in computation: **Chris Paciorek**

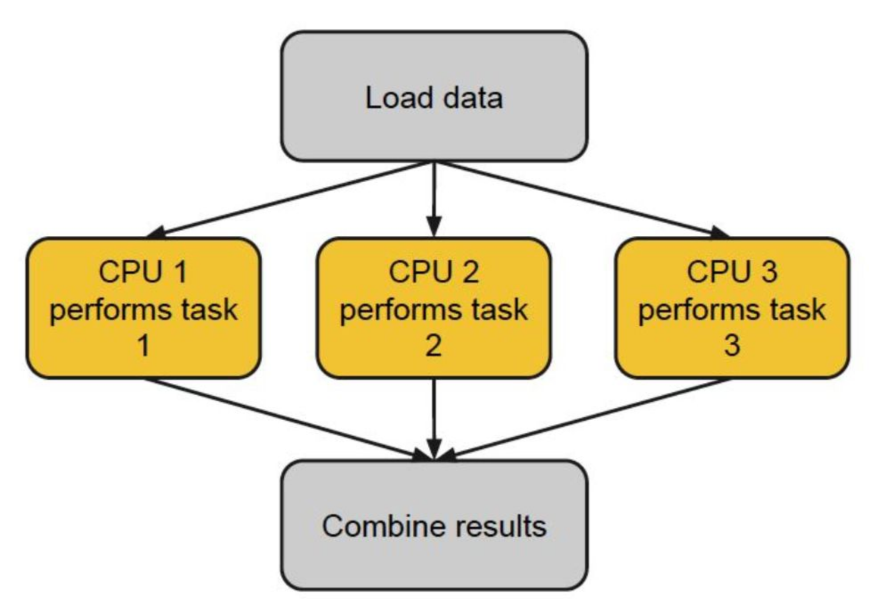
Useful resources prepared (mostly) by Chris:

- https://statistics.berkeley.edu/computing/training
- https://github.com/berkeley-scf/tutorial-parallel-basics

Thanks to Rebecca Barter for her slides on this as well.

Parallelizing code:

- Parallelization: doing things simultaneously
- However, parallel tasks cannot talk to one another
- Usually parallelize to speed up computation by
  - Doing loops simultaneously
  - Computing on multiple subsets of a large dataset at the same time
- Our focus: **embarrassingly parallel** tasks



A simple example

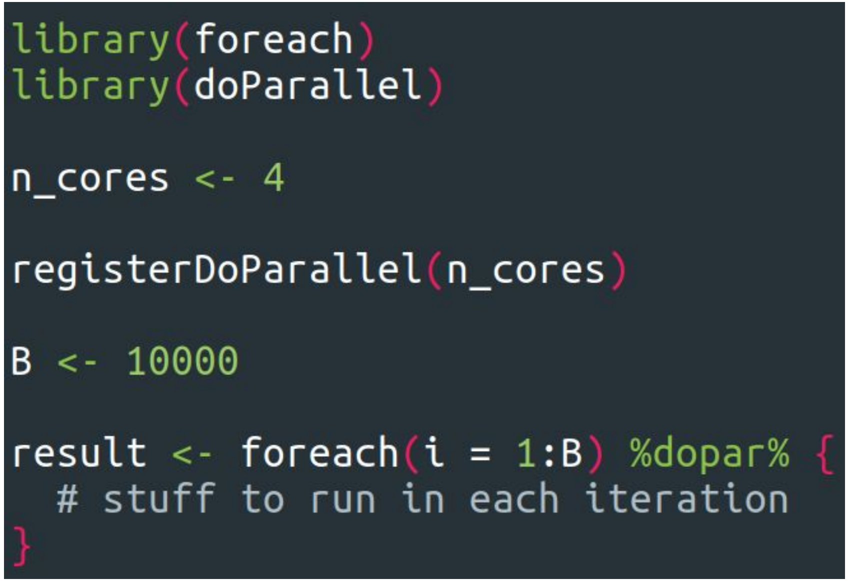
- Imagine you have a for loop where each iteration of the for loop does not depend on any other iteration of the for loop, e.g.,

```
for each b = 1:B
    Take a subsample of your data matrix X
    Do something with that subsample
end for loop
```

- Rather than doing this for loop iteratively, can run each iteration of this for loop “in parallel” (i.e., simultaneously)
- This is a simple example of parallelization, but even here it is a incredibly powerful tool

How to parallelize your R code?

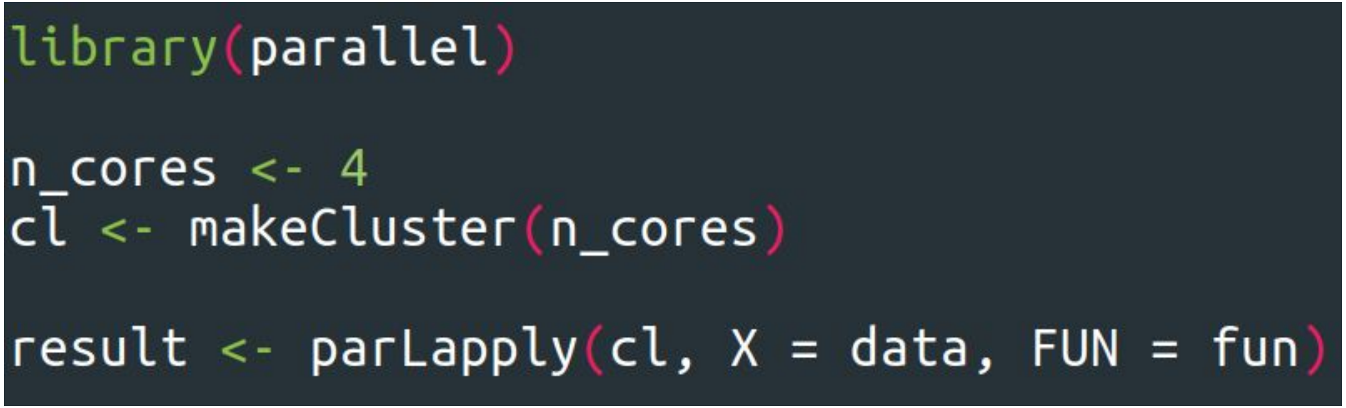
Option 1: `foreach` and `doParallel` packages



```r
library(foreach)
library(doParallel)

n_cores <- 4

registerDoParallel(n_cores)

B <- 10000

result <- foreach(i = 1:B) %dopar% {
  # stuff to run in each iteration
}
```

How to parallelize your R code?

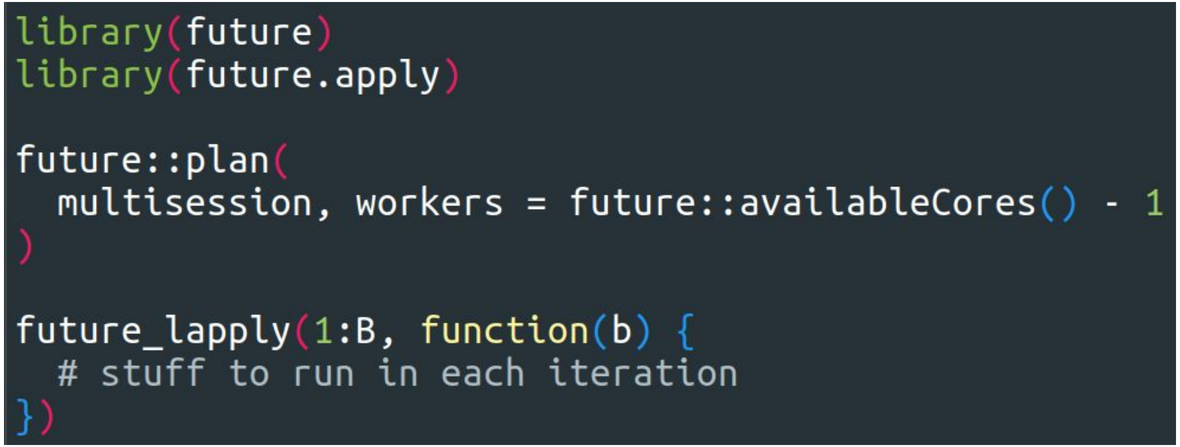
Option 2: `parallel` package



```r
library(parallel)

n_cores <- 4
cl <- makeCluster(n_cores)

result <- parLapply(cl, X = data, FUN = fun)
```

How to parallelize your R code?

Option 3: `future` / `future.apply` packages



```r
library(future)
library(future.apply)

future::plan(
  multisession, workers = future::availableCores() - 1
)

future_lapply(1:B, function(b) {
  # stuff to run in each iteration
})
```

More info: https://github.com/HenrikBengtsson/future.apply

How to parallelize your R code?

- See example in parallel_example.R
- To check how many cores your machine has

  ```
  future::availableCores()
  ```

  or

  ```
  parallel::detectCores(all.tests = FALSE, logical = TRUE)
  ```

- If running on your home computer, good idea to leave at least one core free for your operating system (and you) to use.

Key tools to speed up computation

- Vectorized / functional programming
- Parallelize
- **SCF cluster**
- C++ & `Rcpp`

Using the SCF clusters

- If you haven’t already, sign up for an SCF account at https://scf.berkeley.edu/account

- Information on submitting jobs to the cluster can be found here: http://statistics.berkeley.edu/computing/servers/cluster

Using the SCF Clusters

1. **ssh into an SCF machine**
2. Copy your files to that computer
3. Set up a shell script that runs your job (e.g., `shell_example.sh`)
4. Submit your job using SLURM, e.g.

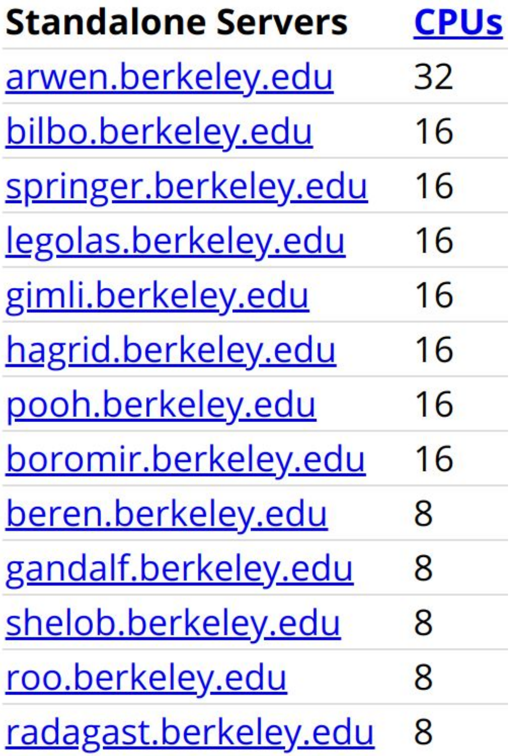
```
sbatch shell_example.sh
```

Step 1: ssh into an SCF machine

- The SCF cluster contains the following LOTR-named machines that you can ssh into. Check https://scf.berkeley.edu/ingrid
- To SSH into a machine, type in your terminal:

```
ssh theo_s@gimli.berkeley.edu
```

- Use your SCF username/password
- Once you ssh, you are logged in remotely to the SCF machine and can start using it.



Standalone Servers	CPUs
arwen.berkeley.edu	32
bilbo.berkeley.edu	16
springer.berkeley.edu	16
legolas.berkeley.edu	16
gimli.berkeley.edu	16
hagrid.berkeley.edu	16
pooh.berkeley.edu	16
boromir.berkeley.edu	16
beren.berkeley.edu	8
gandalf.berkeley.edu	8
shelob.berkeley.edu	8
roo.berkeley.edu	8
radagast.berkeley.edu	8

Using the SCF Clusters

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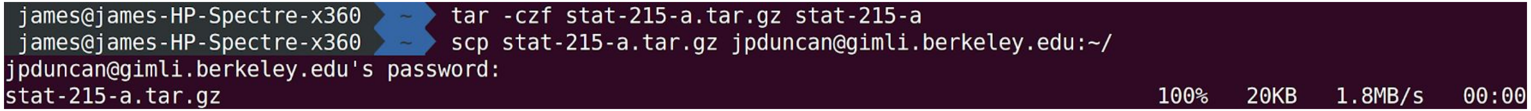
```
sbatch shell_example.sh
```

Step 2: Copy your files to SCF

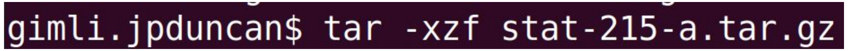
- Options:
  - Clone your GitHub repo on the remote machine:
    1. Change directories (cd) to where you want the copy of the repo
    2. `git clone https://github.com/USERNAME/stat-215-a`
- Another way: use **`scp`** to move files from your machine to the remote machine

On my computer:



```
 james@james-HP-Spectre-x360  ~  tar -czf stat-215-a.tar.gz stat-215-a
 james@james-HP-Spectre-x360  ~  scp stat-215-a.tar.gz jpduncan@gimli.berkeley.edu:~/
jpduncan@gimli.berkeley.edu's password:
stat-215-a.tar.gz                                                             100%   20KB   1.8MB/s   00:00
```

On the SCF machine:



```
gimli.jpduncan$ tar -xzf stat-215-a.tar.gz
```

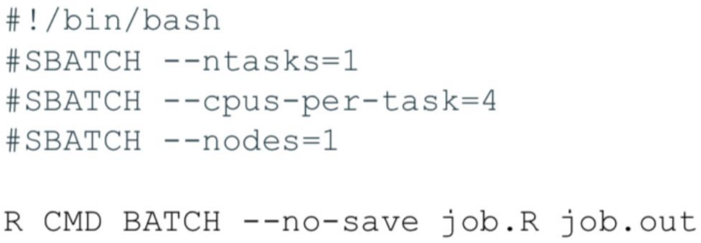
Using the SCF Clusters

1. ssh into an SCF machine
2. Copy your files to that computer
3. **Set up a shell script that runs your job (e.g., `shell_example.sh`)**
4. Submit your job using SLURM, e.g.

```
sbatch shell_example.sh
```

Step 3: Write shell script to run your job

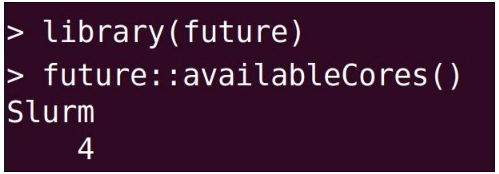
- See `shell_example.sh`



```
#!/bin/bash
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=4
#SBATCH --nodes=1

R CMD BATCH --no-save job.R job.out
```

- Make sure **`cpus-per-task`** is equal to the number of cores that you requested in your job.R script - typically, the number you used in **`registerDoParallel()`**, **`makeCluster()`**, or **`future::plan()`**



```
> library(future)
> future::availableCores()
Slurm
    4
```

Using the SCF Clusters

1. ssh into an SCF machine
2. Copy your files to that computer
3. Set up a shell script that runs your job (e.g., `shell_example.sh`)
4. **Submit your job using SLURM**, e.g.

```
sbatch shell_example.sh
```

Step 4: Submitting your job

```
sbatch shell_example.sh
```

- To cancel your job if you made a mistake:

```
scancel [job_id], e.g. scancel 475567
```

- To check that your jobs are running as expected on the SCF cluster:

```
squeue
```

- To see only my jobs:

```
squeue -u theo_s
```

Demo

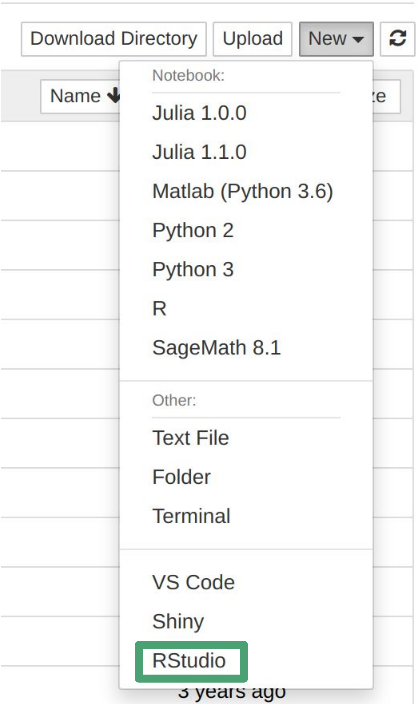
```
week7/scf_example/
```

Common mistakes

- If you are loading in data into R, set all file paths relative to the location of where you run your sbatch command
- Make sure **`cpus-per-task`** is equal to the number of cores that you requested in your job.R script – *typically*, the number inside **`registerDoParallel()`**, **`makeCluster()`**, or **`future::plan()`**
- Sometimes, functions that you call within your parallel loop are run in parallel by default. In this case, either request the appropriate number of cores or tell/force the function to use only one core. Ex. `ranger()`
- Don’t forget to save or write out your results when running on the SCF clusters!

Using the SCF jupyterhub

- https://statistics.berkeley.edu/computing/jupyterhub
- Easier for those not familiar with command line
- Go to https://jupyter.stat.berkeley.edu and log in
  - You can run Rstudio:
- Convenient when you need to interact with your code or to debug your code.



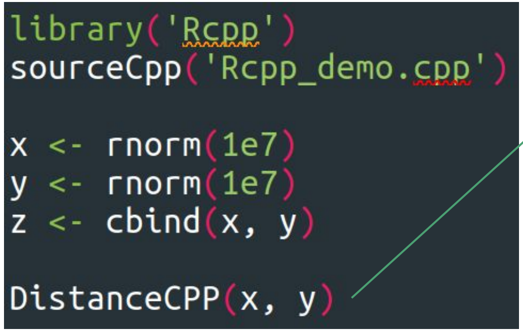
Key tools to speed up computation

- Vectorized / functional programming
- Parallelize
- SCF cluster
- **C++ & `Rcpp`**

Writing faster code with Rcpp

- Often times, C++ can be much faster than R
- Rcpp allows you to easily source C++ code into larger R functions

Rcpp_demo.R

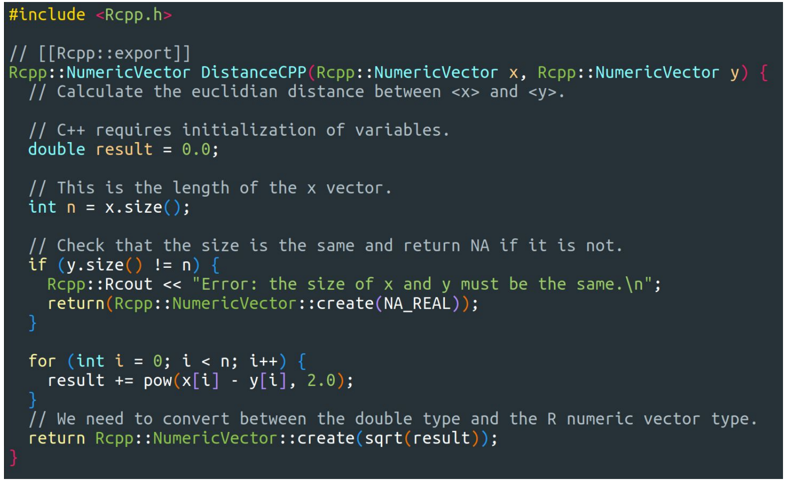


```r
library('Rcpp')
sourceCpp('Rcpp_demo.cpp')

x <- rnorm(1e7)
y <- rnorm(1e7)
z <- cbind(x, y)

DistanceCPP(x, y)
```

Rcpp_demo.cpp



```cpp
#include <Rcpp.h>

// [[Rcpp::export]]
Rcpp::NumericVector DistanceCPP(Rcpp::NumericVector x, Rcpp::NumericVector y) {
  // Calculate the euclidian distance between <x> and <y>.

  // C++ requires initialization of variables.
  double result = 0.0;

  // This is the length of the x vector.
  int n = x.size();

  // Check that the size is the same and return NA if it is not.
  if (y.size() != n) {
    Rcpp::Rcout << "Error: the size of x and y must be the same.\n";
    return(Rcpp::NumericVector::create(NA_REAL));
  }

  for (int i = 0; i < n; i++) {
    result += pow(x[i] - y[i], 2.0);
  }
  // We need to convert between the double type and the R numeric vector type.
  return Rcpp::NumericVector::create(sqrt(result));
}
```

Writing faster code with Rcpp

Some resources:

- https://adv-r.hadley.nz/rcpp.html
- http://heather.cs.ucdavis.edu/~matloff/158/RcppTutorial.pdf
- https://teuder.github.io/rcpp4everyone_en/index.html
- Google and Stack Overflow

Go to `week7/lab_week7`