MY472 – Week 10: Parallel Computing

Pablo Barberá & Akitaka Matsuo

MY 472: Data for Data Scientists

December 12, 2018

Course website: lse-my472.github.io

Course outline

1. Introduction to data
2. The shape of data
3. Cloud computing
4. Basics of HTML and CSS
5. Using data from the internet
6. (Reading week)
7. Working with APIs
8. Creating and managing databases
9. Interacting with online databases
10. Exploratory data analysis
11. Parallel computing

Seminar schedule

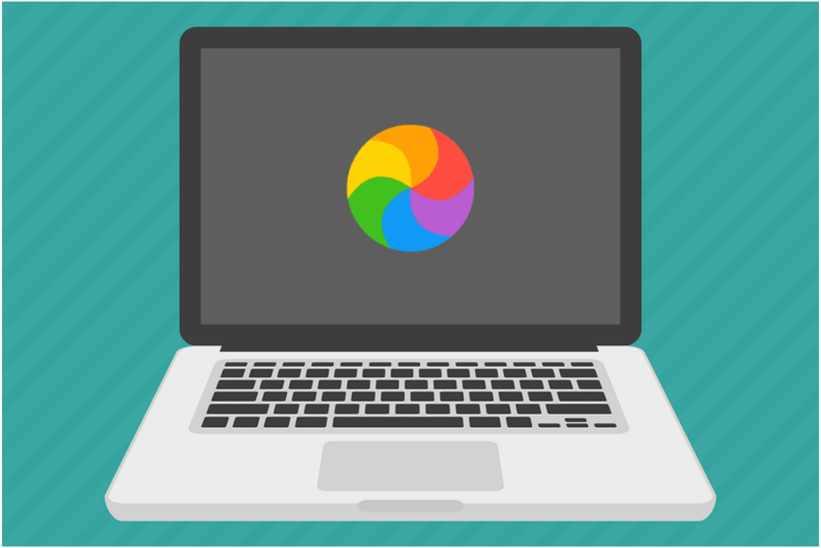
9. Online databases
   - 4th marked assignment (in groups)
   - Deadline: December 14th
10. Exploratory data analysis
11. Course wrap-up
    - 5th marked assignment (individual)
    - Deadline: January 11th

Take-home exam released December 18 and due January 18

Plan for today

- Efficient data analysis with R
  - Loops
  - Vectorized functions
  - Parallel computing
- Basic concepts and logic
- Split-apply-combine framework
- Parallel computing with R

Efficient data analysis with R



Myths about R as programming language

1. R is an interpreted language, so it must be slow
   - Interpreted = executes code directly without compiling
   - Compiled code = code executed natively on CPU (fast!)
   - BUT: many functions are written in C and C++ and thus run in fast machine code
   - Slow code can be written more efficiently
2. All objects in R are stored in memory
   - You cannot open datasets larger than RAM
   - BUT: most laptops now have 8+ GB of RAM (+virtual mem)
   - `bigmemory` package: work with files on disk
   - Easy to work with large databases in the cloud
3. R only uses one core of your CPU
   - Unlike STATA, no multi-core computing out of the box
   - BUT: many functions and packages now take advantage of multi-core computers
   - Easy to write your own code to do parallel computing

My data is too big! My code is too slow!

What to do?

1. Buy a better computer or expand RAM memory
2. Write more efficient code
3. Use parallel computing
4. Move your code/data to the cloud
5. Use out-of-memory storage: SQL databases, bigmemory package, Hadoop...

Writing efficient R code (Part I)

- Conventional wisdom: avoid for loops at all costs!
- But simply rewriting loops will not make code faster
- Key: use vectorized functions instead of loops
- What is slowing our code down?
  - Additional function calls: `for`, `:`, `[`, `<-`
  - `sapply` hides explicit loop, but loop is still there, and implemented in R code
- Why was + so fast? Implements vectorization by vector filtering
  - Takes vector as input and return vector as output
  - Loop is done in machine native code
  - Other vectorized functions: `ifelse()`, `which()`, `rowSums()`, `colSums()`, `sum()`, `any()`, `rnorm()`...

Writing efficient R code (Part II)

- A common bottleneck is memory re-allocation, e.g.:

```
result <- c()
for (i in 1:n){
   result[i] <- x[i] + y[i]
}
```

- In iteration, `R` re-sizes the vector and re-allocates memory
- For large operations (e.g. data frames), this can make your code really slow
- Solution: pre-allocate vector size:

```
result <- rep(NA, n)
for (i in 1:n){
   result[i] <- x[i] + y[i]
}
```

Parallel computing

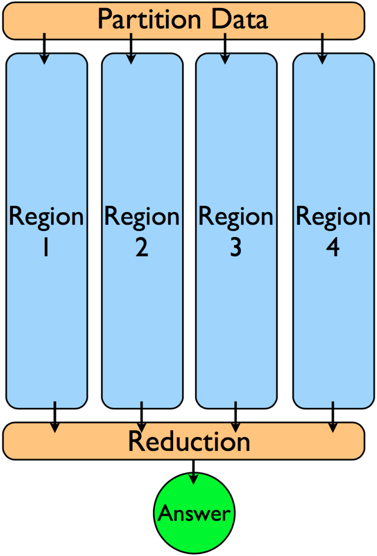
Some hardware terms:

- Node: a single motherboard, with possibly multiple processors
- Processor: silicon containing one or more cores
- Core: unit of computation
- Most modern CPUs (processors) have multiple cores

Logic of parallel computing

Split-apply-combine framework (Hadley Wickham and others):

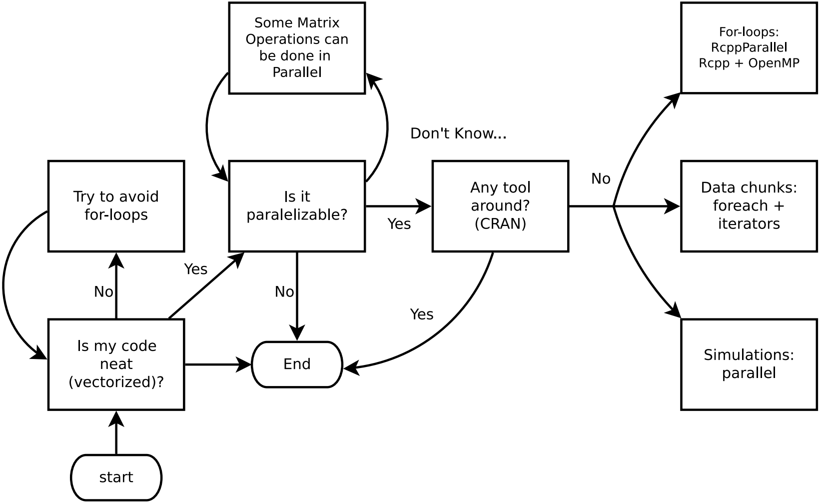
- Split your code and data across multiple nodes/processors/cores
- Apply computation in each region
- Combine the individual results into an aggregate answer



Logic of parallel computing

- BUT: overhead (e.g. splitting and combining data also take some time, no free lunch!)
- Works best with embarrassingly parallel problems:
  - Statistical simulation using multiple seeds
  - Word counts in documents
  - Cross-validation or ensemble learning
  - Rule-of-thumb: can you change the order of the iterations without altering the result?
- Sometimes problematic: applying on subsets of data, or when full dataset is needed in each node
- Not parallelizable: Markov-Chain Monte-Carlo methods, cumulative sums, etc.

Parallel computing



Source: Vega Yon and Garrett Weaver, 2017

Parallel computing in R

Two main approaches:

1. R packages
   - `parallel`: built-in package with support for parallel computation, including random-number generation (good for statistical simulation)
   - `foreach`: new type of loops that supports parallel execution (good for data analysis)
   - `iterators`: tools for iterating over various R data structures (more advanced)
2. Running C++ code in R:
   - `RcppArmadillo`: interact with C++ linear algebra library
   - `OpenMP`: utility to improve multiprocessing using shared memory; works across all platforms

And many others (e.g. Spark, Hadoop, RcppParallel...) we will not cover in this course. See the High-Performance and Parallel Computing Task View

For more: see slides+code by Vega Yon and Garrett Weaver