Advanced R Programming - Lecture 6

Krzysztof Bartoszek (slides by Leif Jonsson and Måns Magnusson)

Linköping University

krzysztof.bartoszek@liu.se

20 September 2017



Today

Performant Code

Computational complexity

Parallelism

Improving R code

Parallelism in R

Rcpp

Memoization



Questions since last time?



Writing fast code

Speed is important! (do not forget memory)



Performant Code

Speed is important! (do not forget memory)

Time to write code



Writing fast code

Speed is important! (do not forget memory)

Time to write code Time to maintain (understand) code



Speed is important! (do not forget memory)

Time to write code Time to maintain (understand) code Time to execute code

Old Adage About Software

"You can have it Good, Fast, Cheap. Pick any two."

Performance

Performant Code

- 1. Performance
- 2. Complexity

Complexity affects performance



Theoretical worst case (but what about average case?)

Big-Oh notation

Basic operations

Relationship: operations to problem size



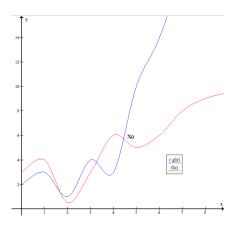
"How fast does a function grow?"

$$f(n) = O(g(n))$$
 or $f(n) \in O(g(n))$
$$\exists_{C>0} \exists_{N_0 \in \mathbb{N}} \forall_{\mathbb{N} \ni n > N_0} |f(n)| \le C * |g(n)|$$
 or
$$\limsup_{n \to \infty} \frac{|f(n)|}{|g(n)|} < \infty$$

number of operations f does not (up to a scaling constant) grow faster than g



Big Oh



https://en.wikipedia.org/wiki/Big_O_notation



Example

$$f(n) = n^2 + 100n + 100$$



Big Oh

Example

$$f(n) = n^2 + 100n + 100$$
$$f(n) = O(n^2)$$



Other Oh

$$f = o(g) \quad \forall_{C>0} \exists_{N_0 \in \mathbb{N}} \forall_{\mathbb{N} \ni n > N_0} | f(n) | \leq C | g(n) | \quad \lim_{n \to \infty} \frac{|f(n)|}{|g(n)|} = 0$$

$$f = O(g) \quad \exists_{C>0} \exists_{N_0 \in \mathbb{N}} \forall_{\mathbb{N} \ni n > N_0} | f(n) | \leq C | g(n) | \quad \lim_{n \to \infty} \sup_{n \to \infty} \frac{|f(n)|}{|g(n)|} < \infty$$

$$f = \omega(g) \quad \forall_{C>0} \exists_{N_0 \in \mathbb{N}} \forall_{\mathbb{N} \ni n > N_0} | f(n) | \geq C | g(n) | \quad \lim_{n \to \infty} \frac{|f(n)|}{|g(n)|} = \infty$$

$$f = \Omega(g) \quad \exists_{C>0} \exists_{N_0 \in \mathbb{N}} \forall_{\mathbb{N} \ni n > N_0} f(n) \geq C | g(n) | \quad \lim_{n \to \infty} \frac{f(n)}{|g(n)|} > 0$$

$$f = \Theta(g) \quad f = O(g) \text{ and } f = \Omega(g)$$

$$f \sim g \quad \lim_{n \to \infty} \frac{f(n)}{g(n)} = 1$$

Complexities (the data size is a lower bound)

Big Oh	Name	Example, optimal
O(1)	constant	assignments, $O(1)$
$O(\log N)$	logarithmic	binary search (sorted input), $O(\log N)$
O(N)	linear	max., $O(N)$
$O(N \log N)$	log–linear	sorting, $O(N \log N)$
$O(N^2)$	quadratic	naive vector-matrix mult., preprocessing
$O(N^3)$	cubic	naive matrix inversion, $O(n^{2.373})$
$O(N^3)$	cubic	naive matrix-matrix mult., $O(n^{2.373})$
$O(N^c)$	polynomial	
$O(c^n)$	exponential	brute force cracking of password, ???

Quicksort: $O(N^2)$ worst case, but $O(N \log N)$ on average



```
statement 1
statement 2
...
Statement c
```

```
if(a)
   statement a
else
   statement b
```



Determine complexity

```
for(i in 1:N)
  statement i
```



```
for(i in 1:N)
  for (j in 1:M)     O?
     statement i,j
```

Determine complexity

```
for(i in 1:N)
                      O(N * M)
  for (j in 1:M)
    statement i,j
```



Determine complexity

$$g(n) = O(n^2)$$
$$O(n^3)$$

What is parallelism?

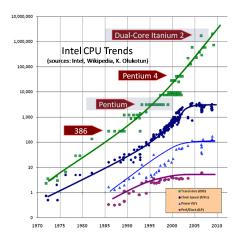
Multiple cores

Each core work with its own part

Cores can exchange information



Why parallelism?



http://www.gotw.ca/publications/concurrency-ddj.htm

Why parallelism?

Single core limits

Handling larger data

Solving problems faster

More and more important

Is there any **but** ...?



Types of parallelism

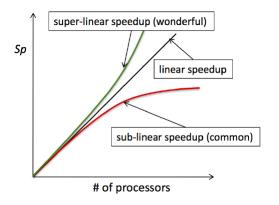
Multicore systems

Distributed systems

Graphical processing units (GPU)



Speedup



https://portal.tacc.utexas.edu/c/document_library/get_file?uuid=

e05d457a-0fbf-424b-87ce-c96fc0077099&groupId=13601



Theoretical limits

Strong scaling: Amdahl's law

Deals with fixed problem size, increasing resources

Weak scaling: Gustafsons law

Deals with increasing size problem along with increasing resources



Amdahl's law

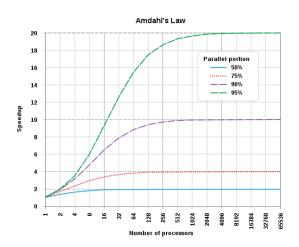
$$S_p = \frac{1}{f_s + \frac{f_p}{P}}$$

Where:

 f_s = serial fraction of code f_p = parallel fraction of code P = number of cores

For a fixed size problem!

Amdahl's law



https://en.wikipedia.org/wiki/Amdahl's_law



Gustafsons law

$$S_p = P - \alpha * (P - 1)$$

Where:

 $\alpha =$ the largest non-parallelizable fraction of any parallel process P = number of cores



Practical problems

Costs of parallelism communication load balancing scheduling

fine-grained vs embarrassingly parallel



Donald E. Knuth on Optimization

Programmers waste enormous amounts of time thinking about, or worrying about, the speed of noncritical parts of their programs, and these attempts at efficiency actually have a strong negative impact when debugging and maintenance are considered.

- Donald E. Knuth



Performance

Depends on many things

- 1. Code
- 2. Complexity
- 3. Compiler
- 4. Hardware
- 5. Language

If you don't measure, you don't optimize!



- Choose optimal algorithm
- 1. Write code that works with accompanying test suite
- 2. Profile your code for bottlenecks
- 3. Try to eliminate the bottle necks
- 4. Redo 2-3 until fast enough

proc.time() is a basic starting tool



Profiling

```
Rprof(tmp <- tempfile(),</pre>
  line.profiling = TRUE,
  memory.profiling = TRUE)
test_data <- pxweb::get_pxweb_data(</pre>
   nr1 =
     "http://api.scb.se/OV0104/v1/doris/sv/ssd/BE/BE0101
                                  /BE0101A/BefolkningNy",
   dims = list(Region = c('*'),
     Civilstand = c('*),
     Alder = c('*'),
     Kon = c('*').
     ContentsCode = c('*'),
     Tid = as.character(1970),
   clean = TRUE)
Rprof()
summaryRprof(tmp, lines = "show", memory = "both")
```

Profiling

\$by.self

	self.tlme	seli.pct	total.time	total.pct	mem.total
get_pxweb_data.R#102	1.96	39.2	1.96	39.2	579.2
<pre>get_pxweb_data_internal.R#42</pre>	1.16	23.2	1.16	23.2	405.0
get_pxweb_data.R#56	0.52	10.4	0.52	10.4	31.3
get_pxweb_data.R#80	0.38	7.6	0.38	7.6	29.1
get_pxweb_data.R#82	0.32	6.4	0.32	6.4	40.7
get_pxweb_data_internal.R#48	0.26	5.2	0.26	5.2	73.2
<pre>get_pxweb_data_internal.R#74</pre>	0.26	5.2	0.26	5.2	29.8
get_pxweb_data.R#83	0.08	1.6	0.08	1.6	17.2
api_catalogue.R#75	0.02	0.4	0.02	0.4	0.0
get_pxweb_data_internal.R#44	0.02	0.4	0.02	0.4	12.6
<pre>get_pxweb_data_internal.R#71</pre>	0.02	0.4	0.02	0.4	16.0



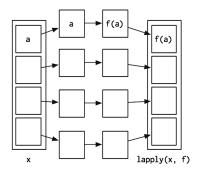
Improvements

- 0. Optimal data structure and algorithm
- 1. Look for existing solutions
- 2. Do less work
- 3. Vectorise
- 0. Optimal data structure and algorithm
- 4. Parallelize
- 0. Optimal data structure and algorithm
- Avoid copies



Parallelism in R

Based on lapply()



(H. Wickham, Advanced R, p. 201)



parallel package

Two approaches:

- 1. mclapply()
- parLapply()



mclapply()

Pros

Simple to use Low overhead (startup)

Cons

Does not work on Windows
Only multi core



Pros

Works everywhere Good for testing/developing

Cons

Slow on multiple nodes



parLapply(type="mpi")

Pros

Good for multiple computers Good for production

Cons

Can be used interactively Needs Rmpi package



Lecture 6

Example

https://github.com/STIMALiU/AdvRCourse/blob/master/Code/parallel_example.R
Parallel code example



Rcpp

Need C++ compiler (look
http://adv-r.had.co.nz/Rcpp.html)

Often called interfacing

Similar can be done with Java and Fortran

Extremely fast!

But just handle bottlenecks!



$$f(n) = \begin{cases} n, & \text{if } n < 2 \\ F(n-1) + F(n-2), & \text{otherwise} \end{cases}$$

Rcpp

Fibonacci R

```
fr <- function(n) {
   if (n < 2) return(n)
   f(n-1) + f(n-2)
}

system.time(fr(30))
user system elapsed
2.246  0.171  2.451</pre>
```

Rcpp

Fibonacci C++

```
library(Rcpp)
cppFunction(code = '
  int fcpp(int n) {
    if (n < 2) return(n);
    return(fcpp(n-1) + fcpp(n-2));
,)
system.time(fcpp(30))
          system elapsed
user
0.007000000 0.000000000 0.006999999
```

Memoization

A simple optimization technique Example of a general technique in optimization of trading memory for computation

Memoization stores (caches) results of function calls

If called again, returns old value

Depends on functional programming



Memoization

Memoise in R

```
> library(memoise)
> a <- function(x) runif(1)</pre>
> replicate(3, a())
[1] 0.6709919 0.3490709 0.4772027
> b <- memoise(a)</pre>
> replicate(3, b())
[1] 0.1867441 0.1867441 0.1867441
```



```
> c <- memoise(function(x) {Sys.sleep(1); runif(1)})</pre>
> system.time(print(c()))
[1] 0.7816399
      system elapsed
user
0.003 0.004 1.001
> system.time(print(c()))
[1] 0.7816399
user system elapsed
0.001 0.000 0.000
> forget(c)
[1] TRUE
> system.time(print(c()))
[1] 0.9234995
      system elapsed
user
0.003 0.004 1.001
```

The End... for today. Questions? See you next time!

