Performance and Parallel Evaluation

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15 July, 2016
Performance & Parallel Evaluation

My code is slow, how do I make it run faster?

Write better R code
- Correct, then efficient
- 10-1000× speed-up, great satisfaction

Parallel evaluation
- Computer: 5-10× speed-up, 2-5× frustration
- Cluster: 10-100× speed-up, 10-20× frustration
- Cloud: 100+× speed-up, 20-50× frustration
Priorities

1. Correct!
2. Robust – works for most realistic inputs
3. Simple
4. Fast
R code: deadly sins

1. Unnecessary iteration

```r
x <- 1:10000; for (i in seq_along(x)) x[i] = log(x[i])
```

2. Copy-and-append iteration

```r
answer <- numeric()
for (i in 1:10000) answer <- c(answer, 1/i)
for (i in 1:10000) answer[i] <- 1/i
```

3. Unnecessary evaluation

```r
x <- 1:1000000
for (i in seq_along(x)) x[i] = x[i] * sqrt(2)
```

4. Re-implementation
fun1 <- function(n) {
    ## How many sins?
    x <- numeric()
    for (i in 1:n)
        x <- c(x, log(i) * sqrt(2))
    x
}

fun2 <- function(n)
    log(seq_len(n)) * sqrt(2)
R code: saving graces II

1. Validation – `identical()`, `all.equal()`

```r
identical(fun1(1000), fun2(1000))
## [1] TRUE
```

2. Timing – `system.time()`, `microbenchmark()`

```r
library(microbenchmark)
microbenchmark(fun1(1000), fun2(1000))
```

```r
## Unit: microseconds
##    expr     min      lq median      uq     max neval
## fun1(1000) 1573.650 1587.4655 2406.3808 1628.533 17768.803 100
## fun2(1000)   21.088   21.8585   23.3476   22.882   40.376 100
```
3. ‘Experience’ – available packages & functions
4. Profiling – `Rprof()`
5. Foreign languages – e.g., C, *Rcpp*
Parallel evaluation

- Most often: ‘embarassingly parallel’ evaluation of iterative for loops / `lapply()`

Other packages
- `parallel` – a base package; single computer
- `foreach` – popular ‘for’ loop paradigm
- `BatchJobs` – clusters with job schedulers
- `Rmpi` – classic HPC

**BiocParallel**
- Consistent interface
- Plays well with many **Bioconductor** packages
library(BiocParallel)
fun <- function(i) {
    Sys.sleep(1)
    i
}

system.time(res1 <- lapply(1:5, fun))

## user  system elapsed
## 0.000  0.000   5.006

system.time(res2 <- bplapply(1:5, fun))

## user  system elapsed
## 0.024  0.028   3.487

identical(res1, res2)

## [1] TRUE
Parallel evaluation: **BiocParallel**

- Different *Param()* objects for styles of computing, e.g.,
  - `SerialParam()`: no parallel evaluation
  - `MulticoreParam()`: separate forked processes on one computer
  - `BatchJobsParam()`: jobs submitted to a cluster queuing system
- `register()` a param or provide it as an argument for use in `bplapply()`.
- Sensible default values.
Parallel evaluation: errors and debugging

- `bptry()` to see errors.
- `BPRED0` argument to `bplapply()` to evaluate just the errors.
- `BPPARAM=SerialParam()` to make problematic code run locally for easy debugging.
- See the vignette Errors, Logs, and Debugging
Parallel evaluation: processing large genomic files

Restrict input to minimum necessary data

- Select columns or fields of files to import, e.g., colClasses argument to read.table(); ScanBamParam() and ScanVcfParam().
- Use a data base, hdf5, or other file format that allows queries or slices of the data to be imported.

Iterate through files to manage memory use

- File connections in base R
  - BamFile("my.bam", yieldSize=1000000)

GenomicFiles

- Functions to help manage collections of genomic files
Parallel evaluation: extended example

Goal: for a vector of paths to bam files, \( \text{fls} \), summarize GC content of each aligned read.

```r
library(Rsamtools); library(GenomicFiles)
bfls <- BamFileList(fls, yieldSize=100000)
yield <- function(bfl) # input a chunk of alignments
  readGAlignments(bfl, param=ScanBamParam(what="seq"))
map <- function(aln) {
  # GC content, bin & cummulate
  gc <- letterFrequency(mcols(aln)$seq, "GC",
                        as.prob=TRUE)
  cumsum(tabulate(1 + gc * 50, 51))
}
reduce <- `+`

gc <- bplapply(bfls, reduceByYield, yield, map, reduce)
```
Summary

- **Correct** first, performance second
- No need to worry about code that doesn’t take very long!
- ‘Embarassingly’ parallel (\texttt{lapply()}-like) problems easily parallelized, especially on a single computer.
- Opportunity for very scalable computations, e.g., via AMI & StarCluster.
Acknowledgments

- Core: Valerie Obenchain, Hervé Pagès, (Dan Tenenbaum), Lori Shepherd, Marcel Ramos, Yubo Cheng.
- The research reported in this presentation was supported by the National Cancer Institute and the National Human Genome Research Institute of the National Institutes of Health under Award numbers U24CA180996 and U41HG004059. The content is solely the responsibility of the authors and does not necessarily represent the official views of the National Institutes of Health or the National Science Foundation.

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