

(A bit of) Advanced R

Part 2 - faster R programming

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Outline I

- ① Benchmark
- ② Vectorize
- ③ Parallelize
- ④ Prefer simple objects
- ⑤ Use Rcpp and C++ code
- ⑥ Mind your vocabulary: R fast built in function, an others

References I

Advanced R (Wickham, 2014), <http://adv-r.had.co.nz/>

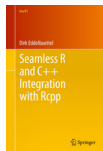


Efficient R programming (Gillespie & Lovelace, 2016),
<https://bookdown.org/csgillespie/efficientR/>



References II

Seamless R and C++ integration with Rcpp (Eddelbuettel, 2013), for sale but see <http://dirk.eddelbuettel.com>



The R inferno (Burns, 2012), <http://www.burns-stat.com/documents/books/the-r-inferno/>



Prerequisites

Data Structure in base R

- ① Atomic vector (integer, double, logical, character)
- ② Recursive vector (list)
- ③ Factors
- ④ Matrices and array
- ⑤ Data Frame

↪ Creation, Basic Operation, Manipulation, Representation

Basic R programming

- ① Control Statements
- ② Functions
- ③ Basics on Functionals

↪ Advanced R, Chapters I.6, II.10, II.11

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Quick (and dirty) benchmarking with `system.time()`

One usually relies on the command `system.time(expr)` to evaluate the timings:

```
func.one <- function(n) {return(rnorm(n,0,1))}  
func.two <- function(n) {return(rpois(n,1))}  
  
n <- 1000  
system.time(replicate(100, func.one(n)))
```

```
##      user  system elapsed  
##  0.008   0.000   0.011
```

```
system.time(replicate(100, func.two(n)))
```

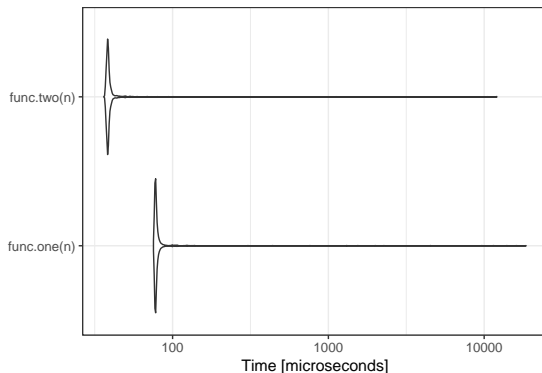
```
##      user  system elapsed  
##  0.008   0.000   0.009
```

Exercise

Write functions to compute the variance of a real vector, with and without loops. Benchmark them.

Quick benchmarking with microbenchmark

```
func.one <- function(n) {return(rnorm(n,0,1))}  
func.two <- function(n) {return(rpois(n,1))}  
  
library(microbenchmark)  
  
n <- 1000  
res <- microbenchmark(func.one(n), func.two(n), times=1000)  
ggplot2::autoplot(res)
```



Profile your code

Suppose you want to evaluate which part of the following function is hot:

```
## generate data, center/scale and perform ridge regression
my_func <- function(n,p) {

  require(MASS)

  ## draw data
  x <- matrix(rnorm(n*p),n,p)
  y <- rnorm(n)

  ## center/scale
  xs <- scale(x)
  ys <- y - mean(y)

  ## return ridge's coefficients
  ridge <- lm.ridge(ys~xs+0,lambda=1)

  return(ridge$coef)
}
```

Profile your code with base Rprof |

One can rely on the default Rprof function, with somewhat technical outputs

```
Rprof(file="profiling.out", interval=0.05)
res <- my_func(1000,500)
Rprof(NULL)
```

```
summaryRprof("profiling.out")$by.self
```

##	self.time	self.pct	total.time	total.pct
## "La.svd"	1.25	64.10	1.30	66.67
## "matrix"	0.20	10.26	0.20	10.26
## "aperm.default"	0.15	7.69	0.15	7.69
## "FUN"	0.10	5.13	1.95	100.00
## ".External2"	0.10	5.13	0.15	7.69
## "t.default"	0.10	5.13	0.10	5.13
## "na.omit"	0.05	2.56	0.05	2.56

```
summaryRprof("profiling.out")$by.total
```

Profile your code with base Rprof II

##	total.time	total.pct	self.time	self.pct
## "FUN"	1.95	100.00	0.10	5.13
## "block_exec"	1.95	100.00	0.00	0.00
## "call_block"	1.95	100.00	0.00	0.00
## "eval"	1.95	100.00	0.00	0.00
## "evaluate"	1.95	100.00	0.00	0.00
## "evaluate_call"	1.95	100.00	0.00	0.00
## "evaluate::evaluate"	1.95	100.00	0.00	0.00
## "handle"	1.95	100.00	0.00	0.00
## "in_dir"	1.95	100.00	0.00	0.00
## "knit"	1.95	100.00	0.00	0.00
## "knitr::knit"	1.95	100.00	0.00	0.00
## "lapply"	1.95	100.00	0.00	0.00
## "my_func"	1.95	100.00	0.00	0.00
## "process_file"	1.95	100.00	0.00	0.00
## "process_group"	1.95	100.00	0.00	0.00
## "process_group.block"	1.95	100.00	0.00	0.00
## "rmarkdown::render"	1.95	100.00	0.00	0.00
## "timing_fn"	1.95	100.00	0.00	0.00
## "withCallingHandlers"	1.95	100.00	0.00	0.00
## "withVisible"	1.95	100.00	0.00	0.00
## "lm.ridge"	1.55	79.49	0.00	0.00
## "La.svd"	1.30	66.67	1.25	64.10
## "svd"	1.30	66.67	0.00	0.00
## "scale"	0.25	12.82	0.00	0.00
## "scale.default"	0.25	12.82	0.00	0.00
## "matrix"	0.20	10.26	0.20	10.26

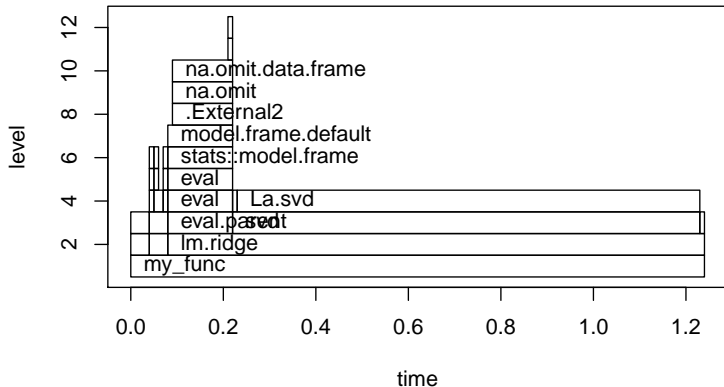
Profile your code with base Rprof III

## "aperm.default"	0.15	7.69	0.15	7.69
## ".External2"	0.15	7.69	0.10	5.13
## "aperm"	0.15	7.69	0.00	0.00
## "sweep"	0.15	7.69	0.00	0.00
## "t.default"	0.10	5.13	0.10	5.13
## "apply"	0.10	5.13	0.00	0.00
## "model.matrix"	0.10	5.13	0.00	0.00
## "model.matrix.default"	0.10	5.13	0.00	0.00
## "t"	0.10	5.13	0.00	0.00
## "na.omit"	0.05	2.56	0.05	2.56
## "eval.parent"	0.05	2.56	0.00	0.00
## "model.frame.default"	0.05	2.56	0.00	0.00
## "stats::model.frame"	0.05	2.56	0.00	0.00

Profile your code with profr

The *profr* package is maybe a little easier to understand...

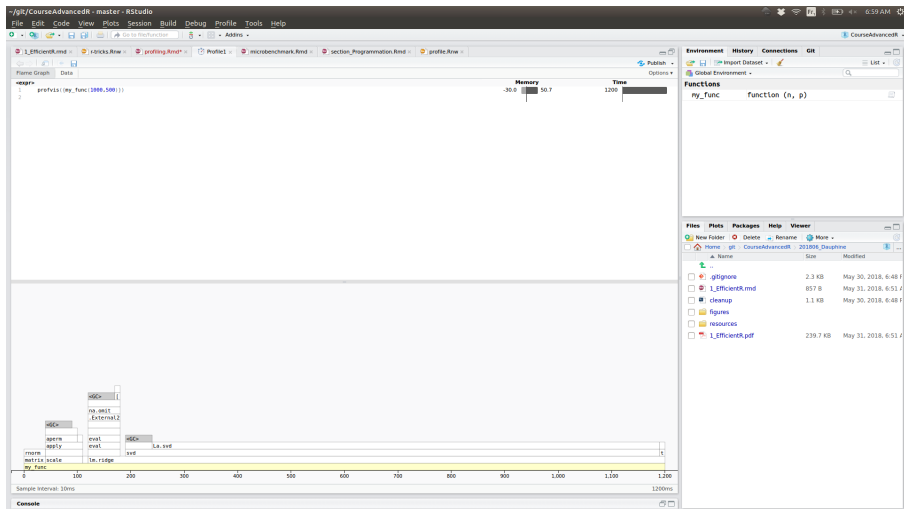
```
library(profr)
profiling <- profr({my_func(1000,500)}, interval = 0.01)
plot(profiling)
```



Profile your code within Rstudio with profvis

Profvis integrates the profiling to the Rstudio API: try it!

```
library(profvis)
profvis({my_func(1000,500)})
```



Outline

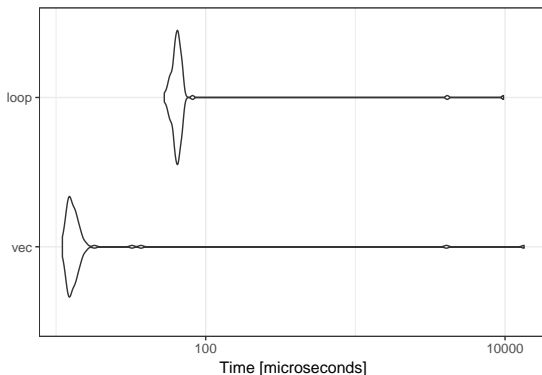
- 1 Benchmark
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Vectorize any algebraic operation

Example: compute $\exp(x) = \sum_{k=0}^n \frac{x^k}{k!}$

```
exp_loop <- function(x, n){ ## the sad/bad/less readable way
  res <- 1
  for (k in 1:n) res <- res + 2^k/factorial(k)
  res
}
```

```
## the good way
exp_vec <- function(x, n) sum(x^(0:n)/c(1,cumprod(1:n)))
```

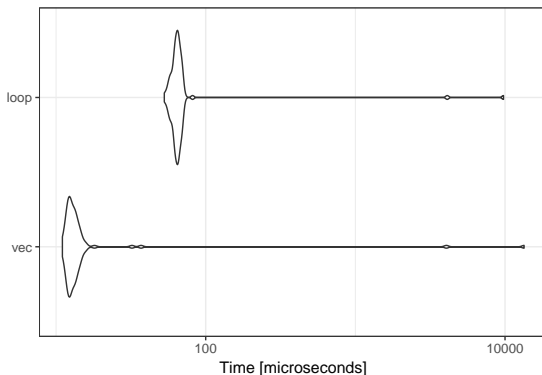


Vectorize any algebraic operation

Example: compute $\exp(x) = \sum_{k=0}^n \frac{x^k}{k!}$

```
exp_loop <- function(x, n){ ## the sad/bad/less readable way
  res <- 1
  for (k in 1:n) res <- res + 2^k/factorial(k)
  res
}
```

```
## the good way
exp_vec <- function(x, n) sum(x^(0:n)/c(1,cumprod(1:n)))
```



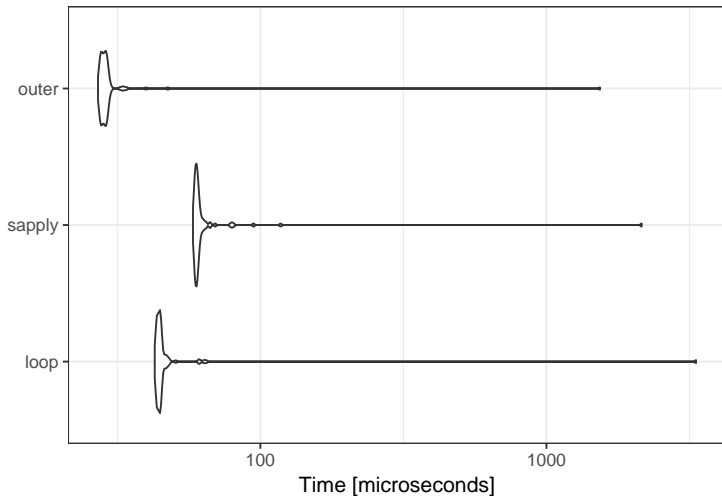
Vectorize, even for non-algebraic operation I

```
month_year_loop <- function(year) {  
  res <- c()  
  for (month in month.name)  
    res <- c(res, paste(month, year, sep = "_"))  
  res  
}  
  
month_year_apply <- function(year) {  
  sapply(month.name, function(month) paste(month, year, sep = "_"))  
}  
  
month_year_outer <- function(year) {  
  outer(month.name, year, FUN = paste, sep = '_')  
}  
head(month_year_outer(c(2010, 2013)), 3)
```

```
##      [,1]      [,2]  
## [1,] "January_2010" "January_2013"  
## [2,] "February_2010" "February_2013"  
## [3,] "March_2010"   "March_2013"
```

```
autoplot(microbenchmark(  
  loop    = month_year_loop(c(2011, 2013)),  
  sapply  = month_year_apply(c(2011, 2013)),  
  outer   = month_year_outer(c(2011, 2013))  
)  
)
```

Vectorize, even for non-algebraic operation II

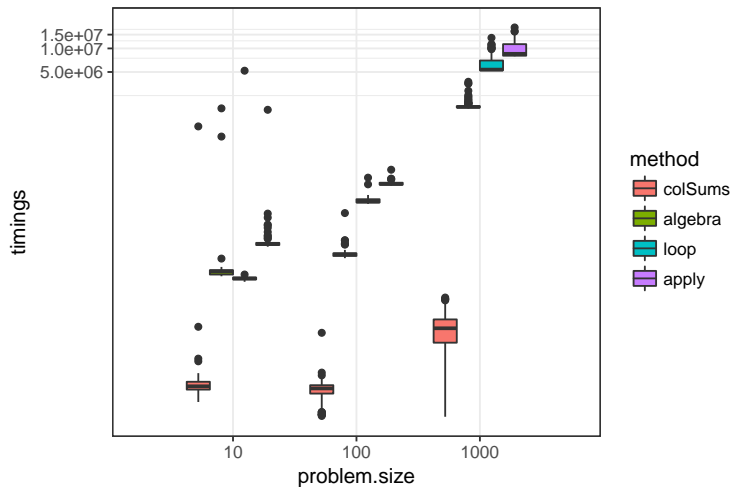


The row/colSums family I

col/rowSums, col/rowMeans and their extensions in the matrixStats package (rank,max,min, etc.) are very efficient.

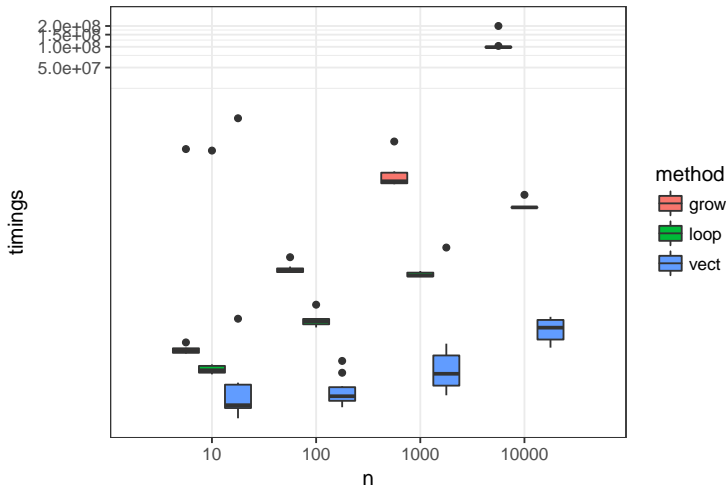
```
colSums.default <- function(x) return(colSums)
colSums.algebra <- function(x) return(crossprod(rep(1,nrow(x)), x))
colSums.apply <- function(x) return(apply(x,2,sum))
colSums.loop <- function(x) {
  res <- rep(0,ncol(x))
  for (i in 1:ncol(x)) {
    res[i] <- sum(x[,i])
  }
  res
}
```

The row/colSums family II



Preallocate whenever it is possible

```
grow <- function(n) {vec <- numeric(0); for (i in 1:n) vec <- c(vec,i)}  
loop <- function(n) {vec <- numeric(n); for (i in 1:n) vec[i] <- i}  
vect <- function(n) {1:n}
```



Do not stack objects I

Even if it is tempting when the final size is unknown.

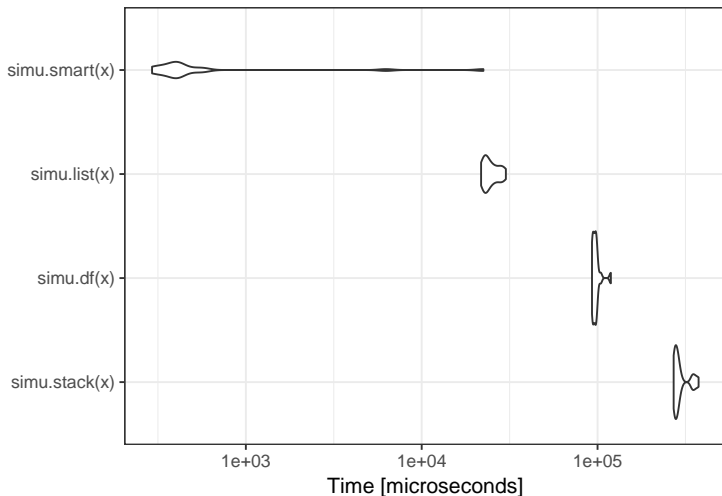
```
simu.stack <- function(x) { ## x is a n x p matrix
  out <- data.frame(mean = numeric(0), sd = numeric(0))
  for (i in 1:n) out <- rbind(out, data.frame(mean = mean(x[i,]), sd = sd(x[i, ])) )
  out
}
```

```
simu.df <- function(x) {
  out <- data.frame(mean = numeric(n), sd = numeric(n))
  for (i in 1:n) out[i, ] <- c(mean = mean(x[i,]), sd = sd(x[i, ]))
  out
}
```

```
simu.list <- function(x) {
  my.list <- lapply(1:nrow(x), function(i) c(mean(x[i,]), sd(x[i, ])))
  out <- data.frame(do.call(rbind, my.list))
  colnames(out) <- c("mean", "sd")
  out
}
```

```
n <- 1000; p <- 10; x <- matrix(rnorm(n*p), n, p)
autoplot(microbenchmark(simu.stack(x), simu.df(x), simu.list(x), simu.smart(x), times=20))
```

Do not stack objects II



Exercise: code the smart function (no loop)

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Parallel computing

Usual Roadmap

- ① Start up and initialize M 'worker' processes
- ② Send data required for each task to the workers
- ③ Split the task into M roughly equally-sized chunks and send them (including the R code needed) to the workers
- ④ Wait for all the workers to complete their tasks, and ask them for their results
- ⑤ Repeat steps (2–4) for any further tasks
- ⑥ Shut down the worker processes

Socketing vs Forking

Two approaches achieving the same goal

The socket approach

- launches a new version of R on each core
- connection is done via networking all happening on your own computer

The forking approach

- copies the entire current version of R and moves it to a new core
- several processes acheive the same task resulting in different outputs

↪ Forking is only possible on Unix systems (Linux, Mac OS)

Parallel computing with parallel

Package parallel

- merge of packages multicore and snow
- included in base R and maintained by the R Core team

Check your computer

```
library(parallel) ## embedded with R since version 2.9 or something
cores <- detectCores() ## How many cores do I have?
print(cores)
```

```
## [1] 4
```

~> parallel features both socketing (parLapply) and forking (mclapply)

Forking approach with `parallel::mclapply`

Very easy: use parallel features as soon as you do simulations !

Example: estimates the test error from ridge regression

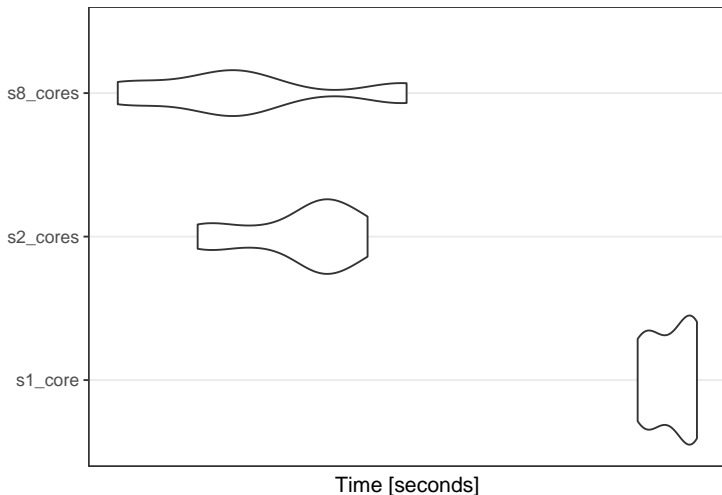
```
one.simu <- function(i) {  
  ## draw data  
  n <- 1000; p <- 500  
  x <- matrix(rnorm(n*p),n,p) ; y <- rnorm(n)  
  ## return ridge's coefficients  
  train <- 1:floor(n/2)  
  test  <- setdiff(1:n,train)  
  ridge <- MASS::lm.ridge(y~x+0,lambda=1,subset=train)  
  err <- (y[test] - x[test, ] %*% ridge$coef )^2  
  return(list(err = mean(err), sd = sd(err)))  
}
```

```
head(do.call(rbind, mclapply(1:8, one.simu, mc.cores = cores)), n = 3)
```

```
##      err      sd  
## [1,] 11.11148 16.45305  
## [2,] 13.43357 18.93762  
## [3,] 14.64665 20.64142
```

Forking approach with parallel::mclapply (cont'd)

```
library(microbenchmark)
res <- microbenchmark(s1_core = mclapply(1:8, one.simu, mc.cores = 1),
                      s2_cores = mclapply(1:8, one.simu, mc.cores = 2),
                      s8_cores = mclapply(1:8, one.simu, mc.cores = 8), times = 10)
```



Socket approach with `parallel::parLapply`

Windows users need a bit more code to make it work

A possible option: export from base workspace

```
cl <- makeCluster(4)
clusterExport(cl, "one.simu")
res <- parSapply(cl, 1:8, one.simu) # several parLapply call are possible
stopCluster(cl)
res
```

```
##      [,1]      [,2]      [,3]      [,4]      [,5]      [,6]      [,7]
## err 13.77063 10.07072 9.917237 12.5304 12.11757 11.45066 19.36333
## sd  20.14429 14.80041 14.20996 17.55452 16.8775 16.28831 26.49789
##      [,8]
## err 11.21091
## sd  15.20287
```

Parallel computing with parallel: final remarks

- Parallelize pieces of code complex enough
- Do not choose stupidly the number of cores
- Screen outputs are lost in Rstudio: use `pbmccapply` (progress bar)

```
pbmccapply::pbmccapply(1:8, FUN = one.simu, mc.cores = 2)
```

```
##      [,1]      [,2]      [,3]      [,4]      [,5]      [,6]      [,7]
## err 11.22125 13.80911 13.38632 11.21224 13.20718 12.01847 13.46801
## sd  16.14348 20.30204 17.2794  15.06328 19.60637 16.5494  18.06206
##      [,8]
## err 13.14769
## sd  18.6168
```


Parallel computing: exercise

Here are two functions to bootstrap a table and to extract the R^2 from the output of `lm`, a linear model fit.

```
boot_df <- function(x) x[sample(nrow(x), rep = T), ]
rsquared <- function(mod) summary(mod)$r.squared
summary(lm(mpg ~ wt + disp, data = mtcars))
```

```
##
## Call:
## lm(formula = mpg ~ wt + disp, data = mtcars)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -3.4087 -2.3243 -0.7683  1.7721  6.3484
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  34.96055     2.16454   16.151 4.91e-16 ***
## wt          -3.35082     1.16413    -2.878  0.00743 **
## disp        -0.01773     0.00919    -1.929  0.06362 .
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 2.917 on 29 degrees of freedom
## Multiple R-squared:  0.7809, Adjusted R-squared:  0.7658
## F-statistic: 51.69 on 2 and 29 DF, p-value: 2.744e-10
```

Bootstrap the R^2 with `lapply`, `mclapply` and `replicate`.

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R is a typed language

R masks the numerical errors by printing a *convenient* summary of objects

```
7/13
```

```
## [1] 0.5384615
```

```
print(7/13, digits=16)
```

```
## [1] 0.5384615384615384
```

So do not use binary operator to compare floats because

```
.1 == .3/3
```

```
## [1] FALSE
```

```
print(.3/3, digits=16)
```

```
## [1] 0.09999999999999999
```

Try

```
all.equal(.1, .3/3)
```

```
## [1] TRUE
```

R is a typed language

R masks the numerical errors by printing a *convenient* summary of objects

```
7/13
```

```
## [1] 0.5384615
```

```
print(7/13, digits=16)
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.1 == .3/3
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## [1] FALSE
```

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print(.3/3, digits=16)
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## [1] 0.09999999999999999
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all.equal(.1, .3/3)
```

```
## [1] TRUE
```

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7/13
```

```
## [1] 0.5384615
```

```
print(7/13, digits=16)
```

```
## [1] 0.5384615384615384
```

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```
.1 == .3/3
```

```
## [1] FALSE
```

```
print(.3/3, digits=16)
```

```
## [1] 0.09999999999999999
```

Try

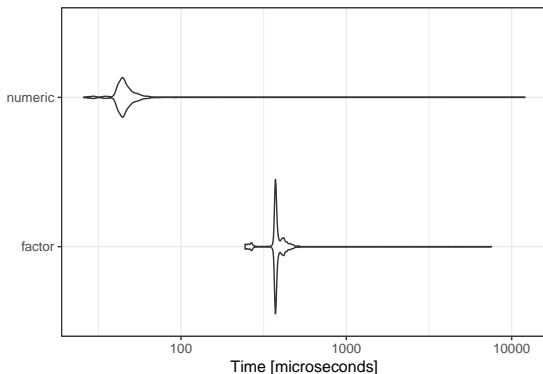
```
all.equal(.1, .3/3)
```

```
## [1] TRUE
```

Factor conversion are slow (nlevels)

Do not convert large vector to factor if you need to perform just one operation on it.

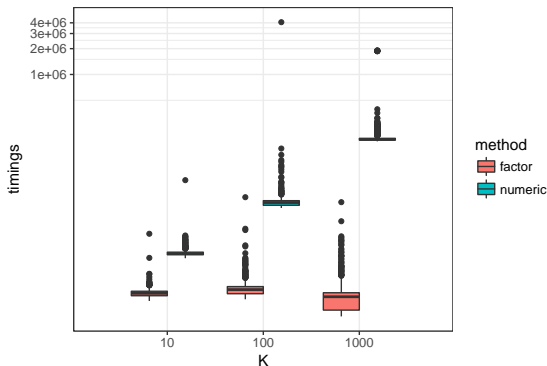
```
n <- 1000; K <- 10
autoplot(microbenchmark(
  factor = nlevels(factor(sample(1:K, n, rep=TRUE))),
  numeric = length(unique(sample(1:K, n, rep=TRUE))), times=1000)
)
```



Operations on factors are fast (e.g. nlevels)

Use factor if you need repeated operations on the same vector.

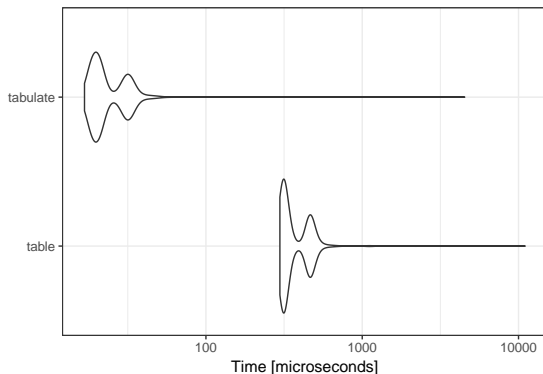
```
nk <- 20
seq.K <- c(10,100,1000)
res <- do.call(rbind, lapply(seq.K, function(K) {
  x1 <- rep(1:K,nk)
  x2 <- factor(x1)
  out <- microbenchmark(factor = nlevels(x2),
                        numeric = length(unique(x1)), times=1000)
  return(data.frame(method = out$expr, timings = out$time, K = factor(K)))
})))
```



Prefer tabulate to table whenever you can

`table` is a complex function that should not be used for simple operations like counting the occurrences of integers in a vector.

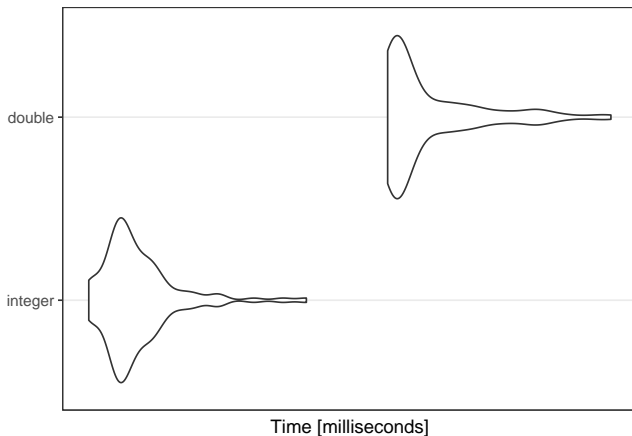
```
n <- 1000; K <- 10
autoplot(
  microbenchmark(
    table      = table      (sample(1:K, n, rep=TRUE)),
    tabulate   = tabulate(sample(1:K, n, rep=TRUE)),
    times=1000)
)
```



Variable type matters

Sorting a vector of integers is much faster than a vector of double, but R is so permissive that you might lose the gain if you do not take care:

```
x_int <- sample.int(1e7, 1e7)
x_dbl <- as.numeric(x_int)
res <- microbenchmark(integer = order(x_int),
                      double = order(x_dbl))
```



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Interfacing C++ with R is *really* easy I

For a vector $\mathbf{x} = (x_1, \dots, x_n)$, consider the simple task of computing

$$y_k = \sum_{i=1}^k \log(x_i), \quad k = 1, \dots, n.$$

One can easily integrate some C++ version of this code with Rcpp.

```
library(Rcpp)
rcpp <- cppFunction('NumericVector rcpp(NumericVector x) {
    using namespace Rcpp;

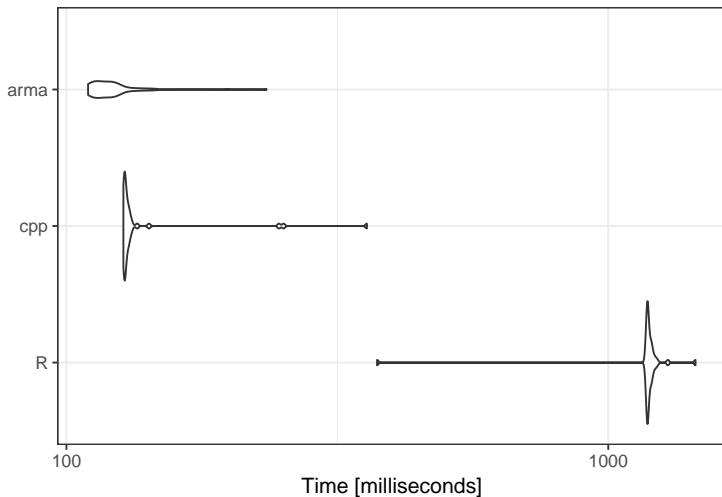
    int n = x.size() ;
    NumericVector res(x) ;
    res(0) = log(x(0));
    for (int i=1; i<n; i++) {
        res(i) = res(i-1) + log(x(i)) ;
    }
    return(wrap(res)) ;
}')
}
```

Interfacing C++ with R is *really* easy II

```
library(RcppArmadillo)
Arma <- cppFunction(depends = "RcppArmadillo", 'NumericVector Arma(NumericVector x) {
    using namespace Rcpp;
    using namespace arma;
    return(wrap(cumsum(log(as<vec>(x))))) ;
}')
```

```
x <- runif(1e7, 1,2)
res <- microbenchmark(R = cumsum(log(x)), cpp = rcpp(x), arma = Arma(x), times = 40)
print(autoplot(res))
```

Interfacing C++ with R is *really* easy III



Interfacing C++ with R is *really* easy I

Example that couples C++ + algebraic tricks

Let \mathbf{T} be an $n \times n$ lower triangular matrix with nonzero elements equal to one. We need fast computation of

$$\text{vec}(\mathbf{T}\mathbf{B}\mathbf{T}^\top) = (\mathbf{T} \otimes \mathbf{T}) \times \text{vec}(\mathbf{B}).$$

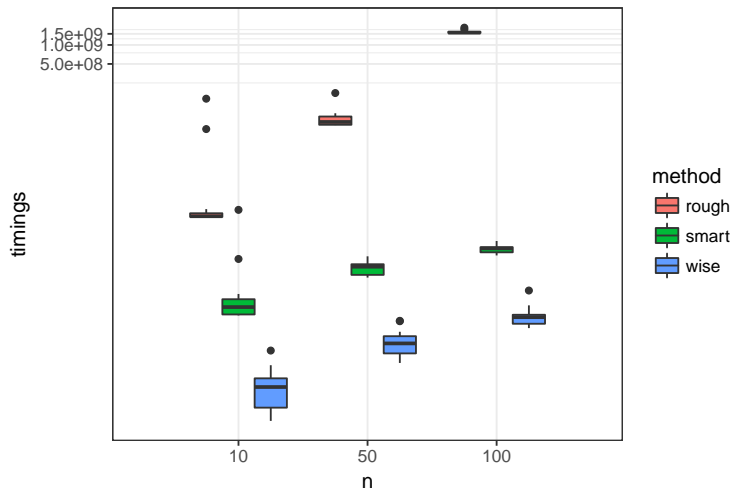
```
library(Matrix); library(inline); library(RcppArmadillo)

prod.rough <- function(B) {
  n <- ncol(B); T <- bandSparse(n,k=(-n+1):0)
  return(kronecker(T,T) %*% as.vector(B))}

prod.smart <- function(B) {
  return(as.vector(apply(apply(B,1,cumsum),1,cumsum))))}

prod.wise <- cxxfunction(signature(B="matrix"), '
  using namespace Rcpp;
  using namespace arma;
  return(wrap(vectorise(cumsum(cumsum(as<mat>(B),0),1)))) ;
  ' , plugin="RcppArmadillo")
```

Interfacing C++ with R is *really* easy II



Outline

- 1 Benchmark
- 2 Vectorize
- 3 Parallelize
- 4 Prefer simple objects
- 5 Use Rcpp and C++ code
- 6 Mind your vocabulary: R fast built in function, an others

The secret function rowsum I

`rowsum` (not to be confused with `rowSums`) computes sums in a vector split according a grouping variable (work for matrices).

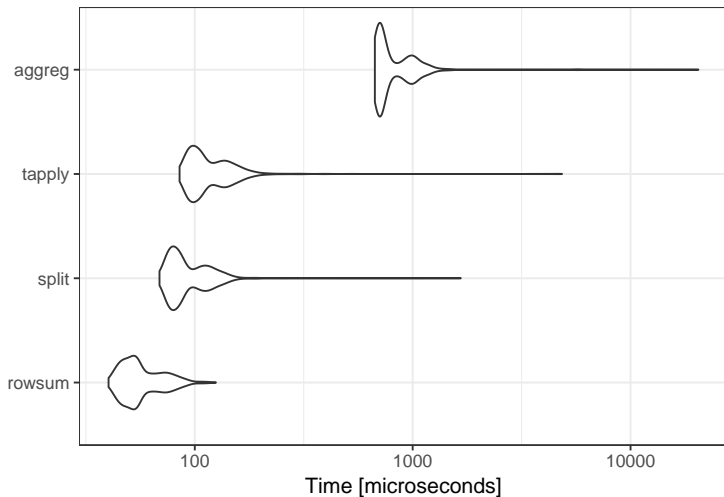
```
vec <- runif(1000)
grp <- sample(1:5, 1000, TRUE)
print(c(rowsum(vec, grp)))
```

```
## [1] 101.39001 96.82680 97.34139 99.04092 99.70550
```

There are many possibilities to perform the required task:

```
res <- microbenchmark(
  rowsum = rowsum(vec, grp),
  split  = sapply(split(vec, grp), sum),
  tapply = tapply(vec, grp, sum),
  aggreg = aggregate(vec, list(grp), sum),
  times = 1000)
```

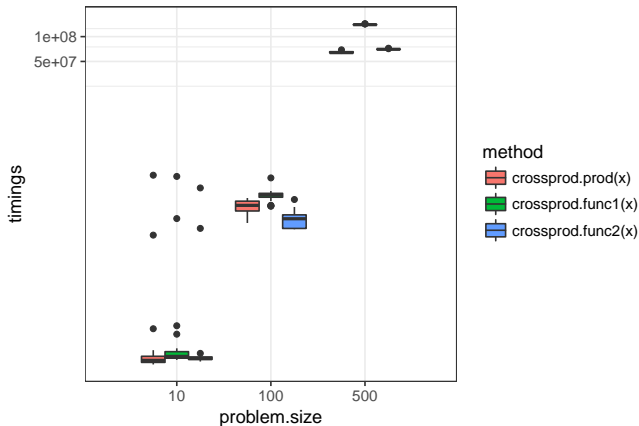
The secret function rowsum II



Dedicated function: cross-product

Generally (a bit) faster than `\% * \%` !

```
crossprod.prod <- function(x) return(t(x) %*% x)
crossprod.func1 <- function(x) return(crossprod(x,x))
crossprod.func2 <- function(x) return(crossprod(x))
```

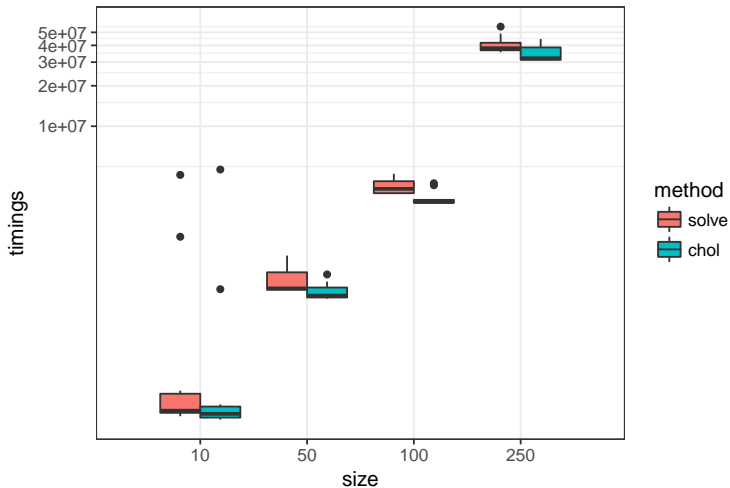


Dedicated function: inverting a PD matrices I

Use a Cholesky factorization

```
use.chol <- function(n,p) {  
  x <- matrix(rnorm(n*p),n,p)  
  xtx <- crossprod(x)  
  return(chol2inv(chol(xtx)))  
}  
  
use.solve <- function(n,p) {  
  x <- matrix(rnorm(n*p),n,p)  
  xtx <- crossprod(x)  
  return(solve(xtx))  
}  
  
bench.p.fixed <- function(p, times) {  
  res <- microbenchmark(solve = use.solve(2*p,p),  
                        chol = use.chol (2*p,p), times=times)  
  return(data.frame(method = res$expr,  
                    timings = res$time,  
                    size = rep(as.character(p),times)))  
}
```

Dedicated function: inverting a PD matrices II

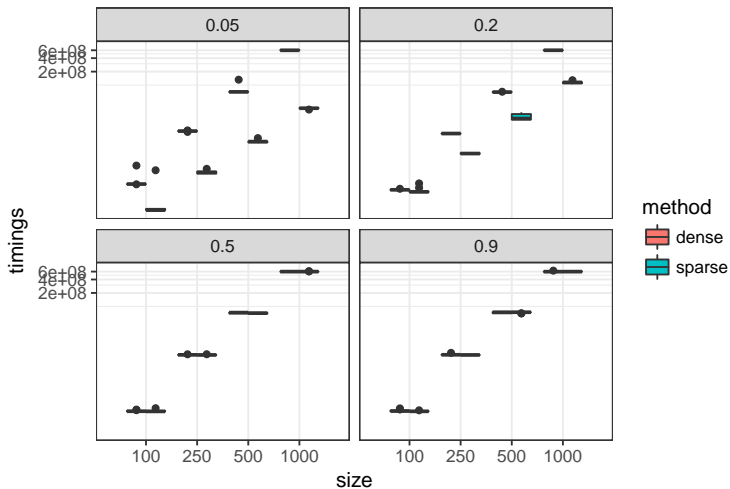


The Matrix package I

Propose a collection of functions for of matrix algebra adapted to the type of matrix at hand (sparse, diagonal, triangular, block diagonal, etc.)

```
library(Matrix)
bench.par.fixed <- function(par) {
  n <- par$n; density <- par$density
  data <- sample(c(0,1),n**2,rep=TRUE,prob=c(1-density,density))
  x.dense <- matrix(data,n,n)
  x.sparse <- Matrix(data,n,n)
  res <- microbenchmark(dense = crossprod(x.dense) ,
                        sparse = crossprod(x.sparse), times=10)
  return(data.frame(method = res$expr,
                    timings = res$time,
                    size = n ,
                    density = density ))
}
```

The Matrix package II

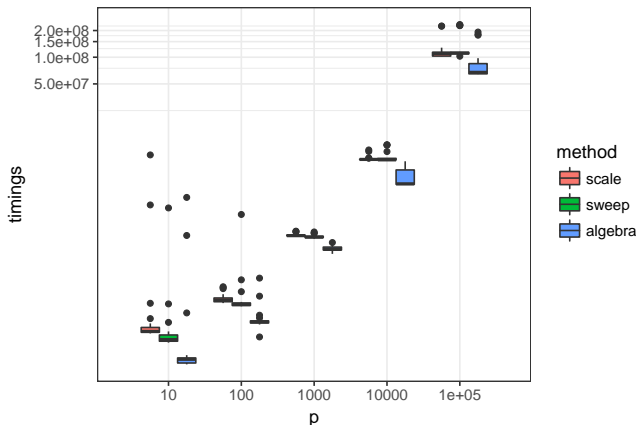


Mind some algebra

Sweep is a general way to apply a statistic on a given dimension of an array.

```
center1 <- function(x) return(scale(x, colMeans(x), FALSE))  
center2 <- function(x) return(sweep(x, 2, colMeans(x), "-", check.margin = FALSE))  
center3 <- function(x) return(x - outer(rep(1, nrow(x)), colMeans(x)) )
```

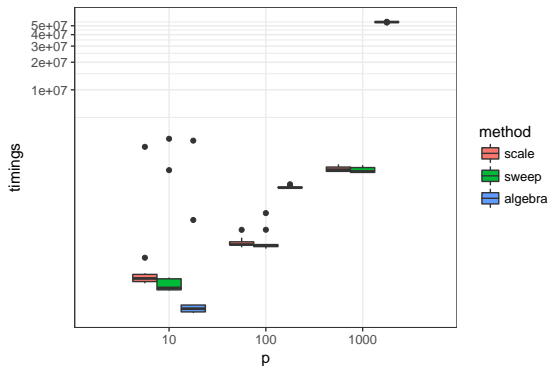
```
seq.p <- 10^(1:5); n <- 100; times <- 20
```



Algebra does not always pay

Example for scaling a matrix

```
scale1 <- function(x) return(scale(x, FALSE, colSums(x^2)))  
scale2 <- function(x) return(sweep(x, 2, colSums(x^2), "/", check.margin=FALSE))  
scale3 <- function(x) return(x %*% diag(1/colSums(x^2)) )  
  
seq.p <- 10^(1:3); n <- 100; times <- 20
```



References

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