(A bit of) Advanced R

Efficient R programming

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http://github/jchiquet/CourseAdvancedR

1. Benchmark your code
2. Use all your cores when needed
3. Good and bad practices in `R`
4. Remember that R is object oriented
5. Mind your vocabulary: `R` fast built in function
6. Interface with lower-level languages

Resources

- Gillespie & Lovelace (2016): efficient R programming
- Wickham (2014)

Outline

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
##   0.012   0.000   0.010
```

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

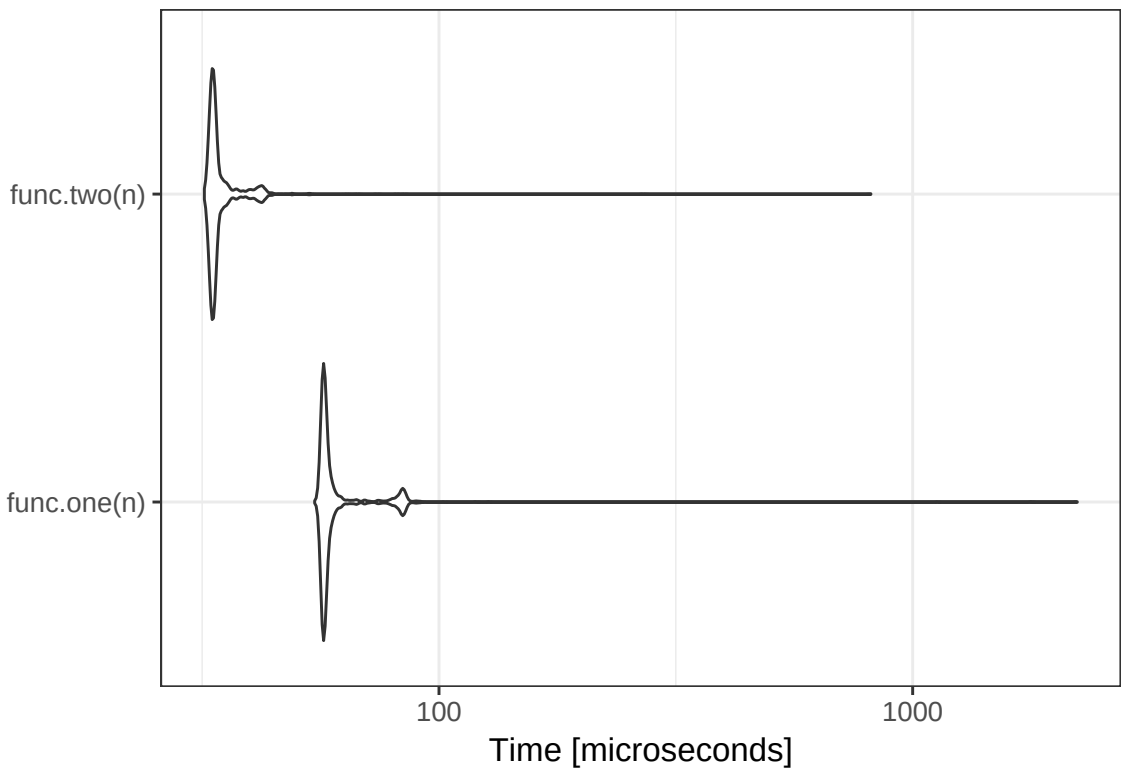
```
##    user  system elapsed
##   0.008   0.000   0.007
```

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 I

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"             1.05    77.78       1.10     81.48
## "matrix"             0.15    11.11       0.15     11.11
## "aperm.default"      0.05     3.70       0.05      3.70
## "apply"              0.05     3.70       0.05      3.70
## "[.data.frame"       0.05     3.70       0.05      3.70
```

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

Profile your code with base Rprof II

```
##                       total.time total.pct self.time self.pct
## "block_exec"                1.35    100.00      0.00     0.00
## "call_block"                1.35    100.00      0.00     0.00
## "eval"                      1.35    100.00      0.00     0.00
## "evaluate"                  1.35    100.00      0.00     0.00
## "evaluate_call"             1.35    100.00      0.00     0.00
## "evaluate::evaluate"        1.35    100.00      0.00     0.00
## "FUN"                       1.35    100.00      0.00     0.00
## "handle"                    1.35    100.00      0.00     0.00
## "in_dir"                    1.35    100.00      0.00     0.00
## "knit"                      1.35    100.00      0.00     0.00
## "knitr::knit"               1.35    100.00      0.00     0.00
## "lapply"                    1.35    100.00      0.00     0.00
## "my_func"                   1.35    100.00      0.00     0.00
## "process_file"              1.35    100.00      0.00     0.00
## "process_group"             1.35    100.00      0.00     0.00
## "process_group.block"       1.35    100.00      0.00     0.00
## "rmarkdown::render"         1.35    100.00      0.00     0.00
## "timing_fn"                 1.35    100.00      0.00     0.00
## "withCallingHandlers"       1.35    100.00      0.00     0.00
## "withVisible"               1.35    100.00      0.00     0.00
## "lm.ridge"                  1.15     85.19      0.00     0.00
## "La.svd"                    1.10     81.48      1.05    77.78
## "svd"                       1.10     81.48      0.00     0.00
## "matrix"                    0.15     11.11      0.15    11.11
## "scale"                     0.10      7.41      0.00     0.00
## "scale.default"             0.10      7.41      0.00     0.00
```

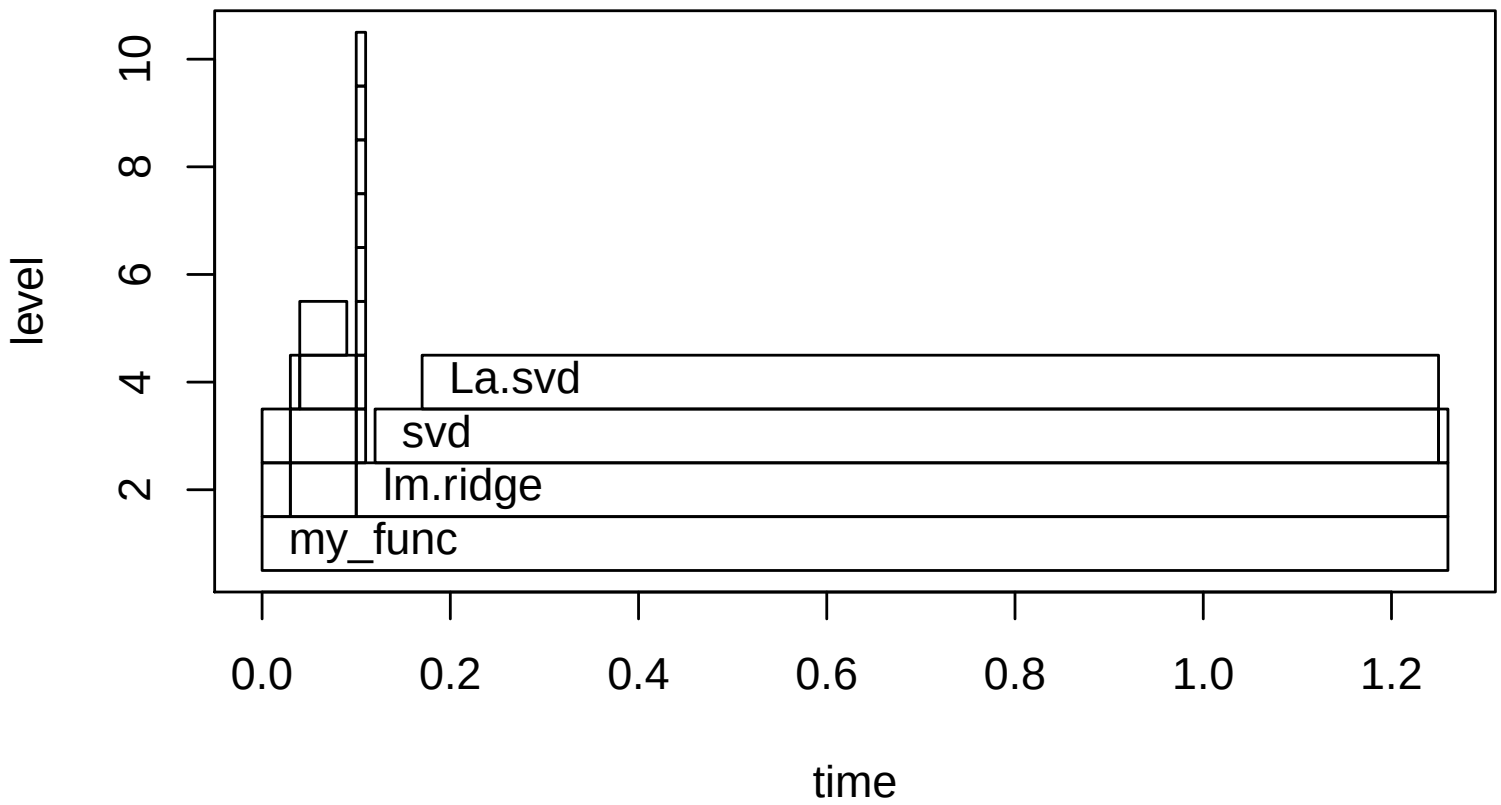
Profile your code with base Rprof III

```
## "aperm.default"           0.05      3.70      0.05      3.70
## "apply"                   0.05      3.70      0.05      3.70
## "[.data.frame"            0.05      3.70      0.05      3.70
## "["                       0.05      3.70      0.00      0.00
## "aperm"                   0.05      3.70      0.00      0.00
## "eval.parent"             0.05      3.70      0.00      0.00
## ".External2"              0.05      3.70      0.00      0.00
## "model.frame.default"     0.05      3.70      0.00      0.00
## "na.omit"                 0.05      3.70      0.00      0.00
## "na.omit.data.frame"      0.05      3.70      0.00      0.00
## "stats::model.frame"      0.05      3.70      0.00      0.00
## "sweep"                   0.05      3.70      0.00      0.00
```

Profile your code with `profr`

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

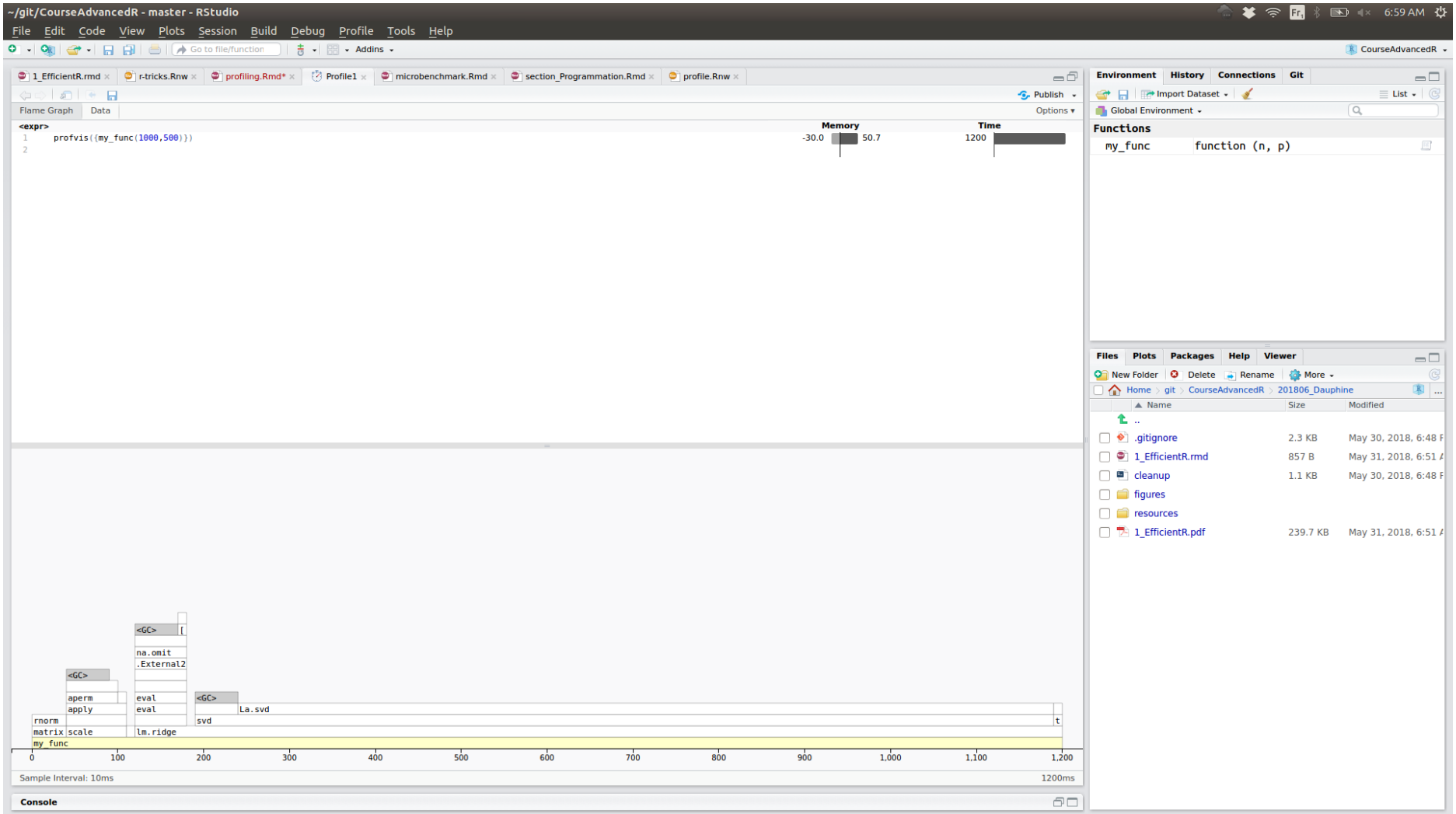
```
library(profr)
profiling <- profr({my_func(1000,500)}, interval = 0.01)
plot(profiling)
```



Profile your code within R Studiow with `profvis`

Profvis integrates the profiling to the Rstudio API

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



Outline

Parallel computing

Usual Roadmap

1. Start up and intialize 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

$\rightsquigarrow$ 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

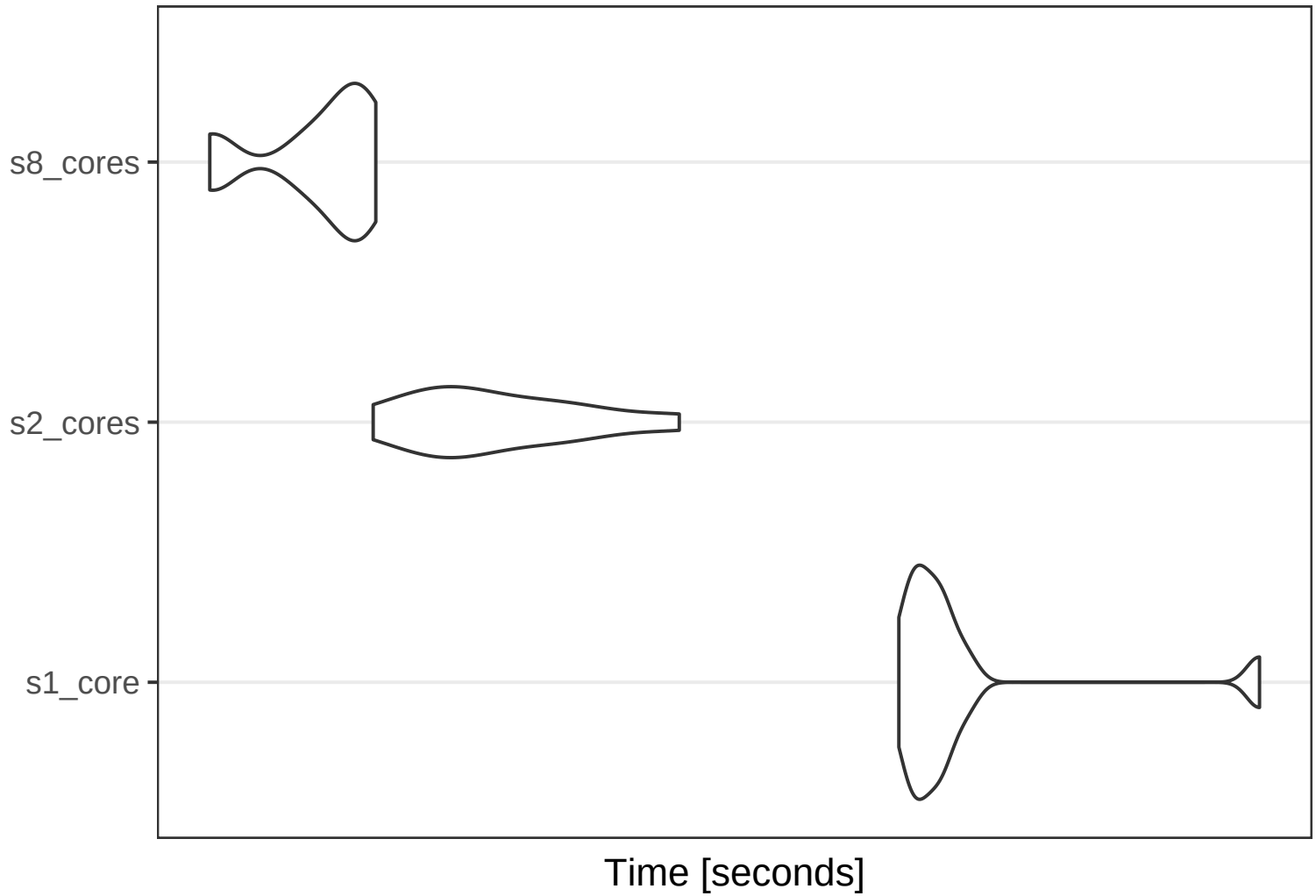
```
one.simu <- function(i) {
  ## draw data
  n <- 1000; p <- 500
  x <- matrix(rnorm(n*p),n,p) ; y <- rnorm(n)
  ## return ridge's coefficients
  train <- 1:floor(n/2)
  test  <- setdiff(1:n,train)
  ridge <- MASS::lm.ridge(y~x+0,lambda=1,subset=train)
  err <- (y[test] - x[test, ] %*% ridge$coef )^2
  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,] 14.45796 19.79301
## [2,] 10.3222  14.86089
## [3,] 12.15729 16.8608
```

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 11.86539 11.26563 8.845916 14.37104 12.91292 13.25386 12.50689
## sd  16.6455  15.63073 12.32548 18.74685 18.49328 17.62274 16.61861
##     [,8]
## err 8.508118
## sd  12.48525
```

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 `pbmcapply` (progress bar)

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

```
##     [,1]     [,2]     [,3]     [,4]     [,5]     [,6]     [,7]     [,8]
## err 10.72632 14.25714 9.77985  9.589137 10.90891 11.8773  10.73228 11.2432
## sd  13.99144 18.25551 13.08587 14.26683 15.5244  15.03568 16.37883 15.9956
```

Outline

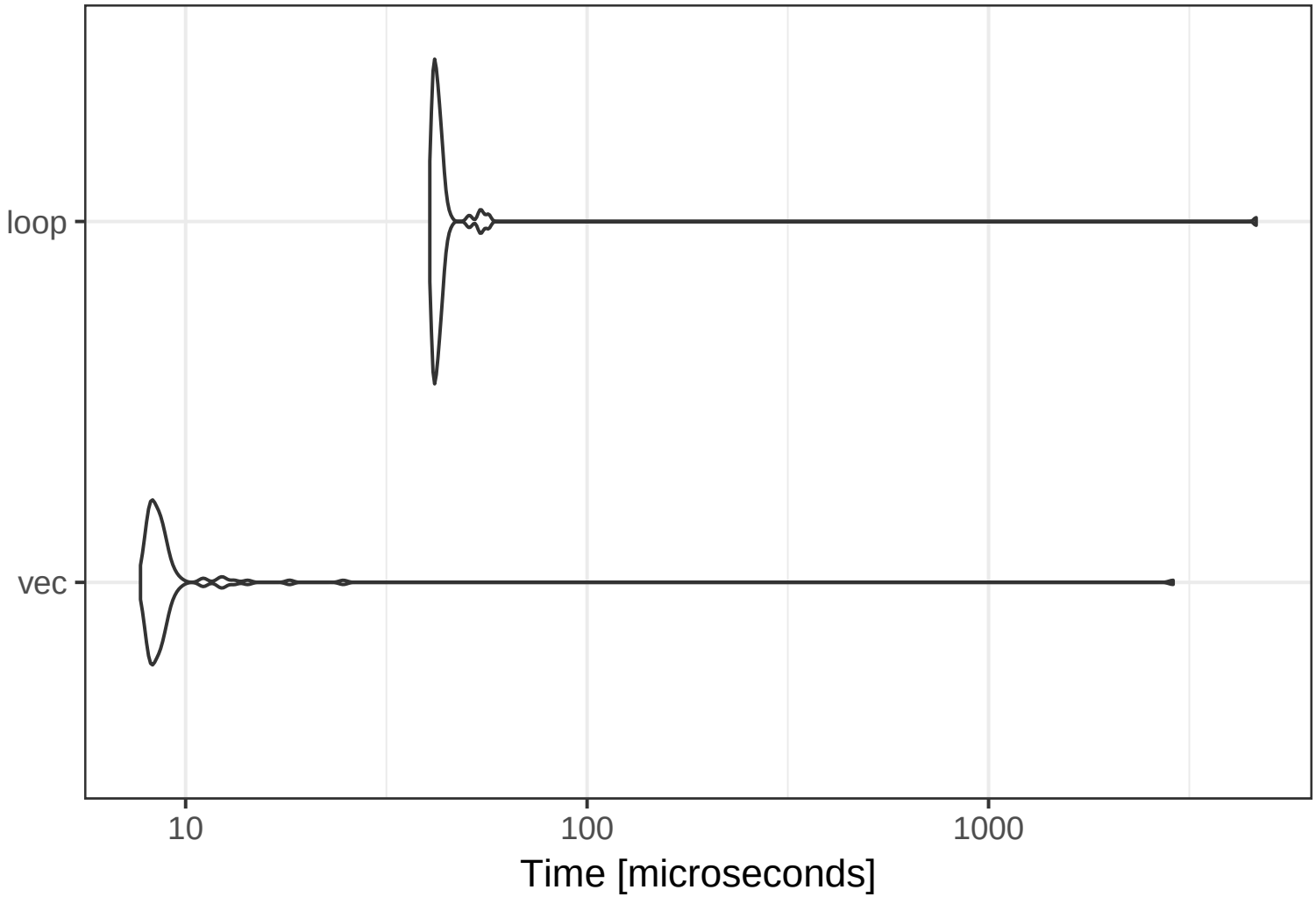
Vectorize any algebraic operation I

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

```
## the good way
exp_vec <- function(x, n){
  res <- sum(x^(0:n)/c(1,cumprod(1:n)))
  res
}
## the sad/bad/less readable way
exp_loop <- function(x, n){
  res <- 1
  for (k in 1:n) res <- res + 2^k/factorial(k)
  res
}
```

```
autoplot(microbenchmark(vec = exp_vec(2, 100), loop = exp_loop(2, 100)))
```

Vectorize any algebraic operation II



Vectorize, even for non-algebraic operation I

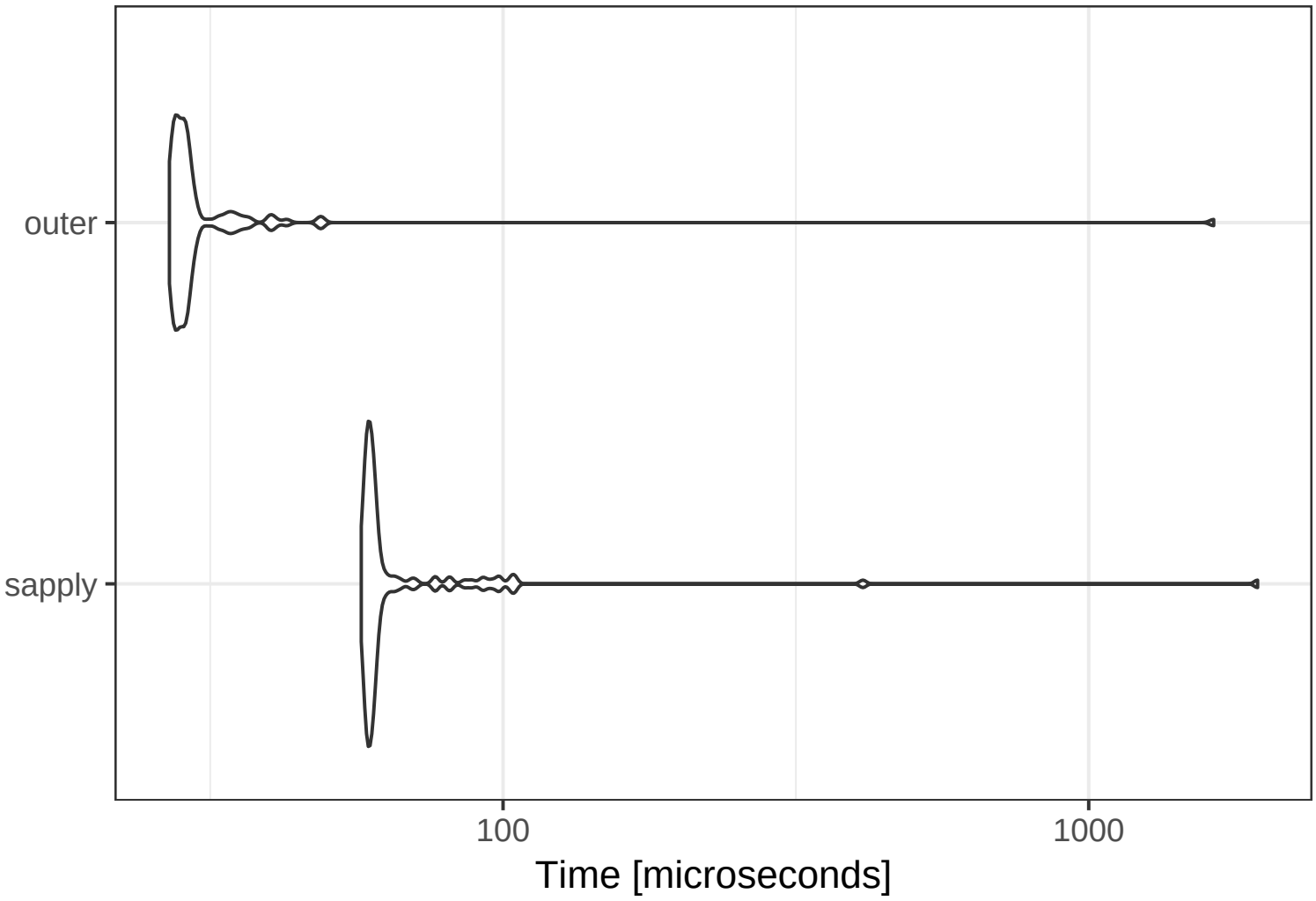
```
month_year_apply <- function(year) {
  sapply(month.name, function(month) paste(month, year, sep = "_"))
}

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(
  sapply = month_year_apply(c(2011, 2013)),
  outer  = month_year_outer(c(2011, 2013)),
  times = 100))
```

Vectorize, even for non-algebraic operation II



Compile your functions with `base::compiler` I

If you cannot avoid a loop, you will save some time

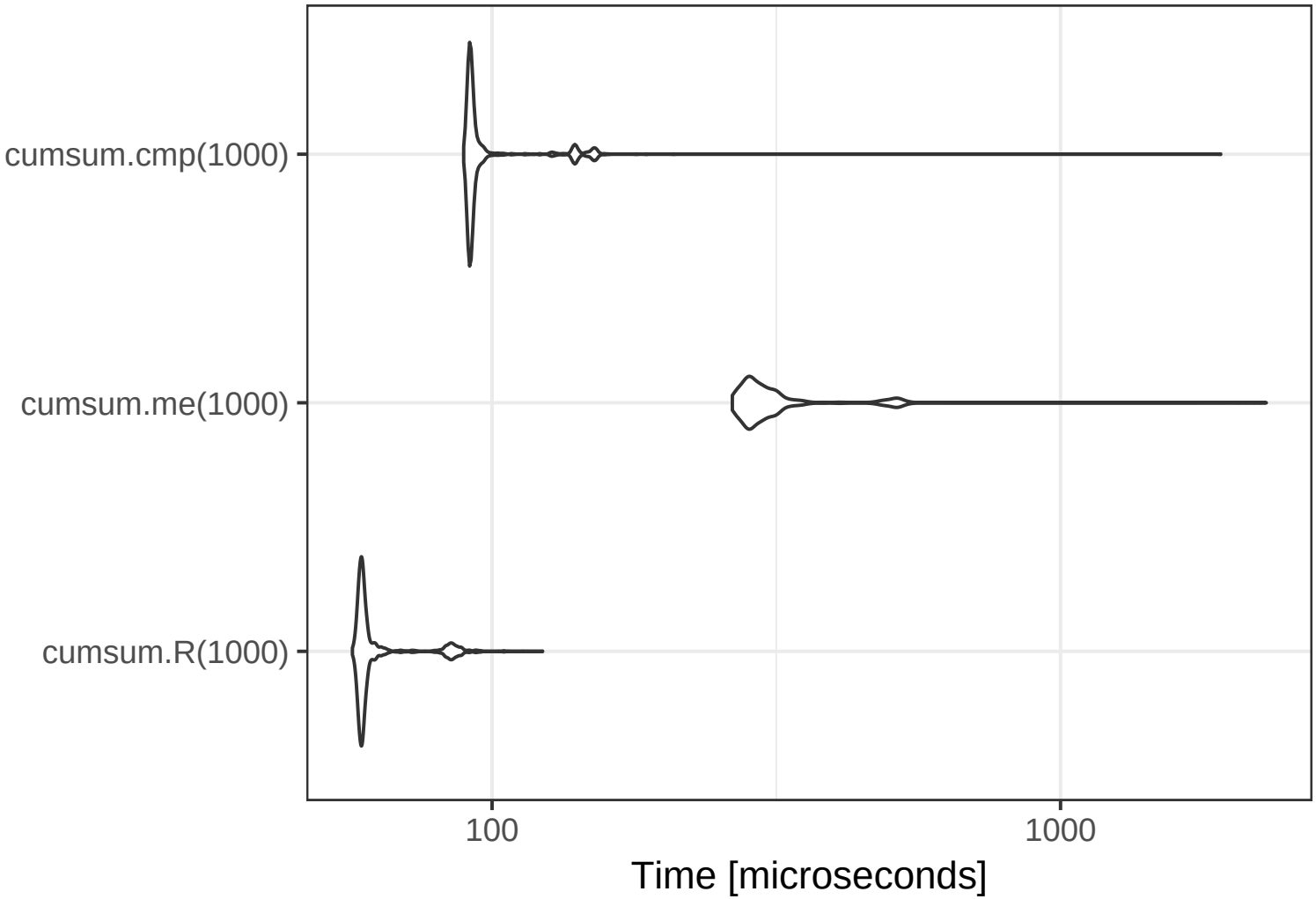
```
cumsum.R <- function(n) {
  x <- rnorm(n)
  cumsum(x)
}

cumsum.me <- function(n) {
  x <- rnorm(n)
  res <- 0
  for (i in 1:length(x))
    res <- res + x[i]
  res
}

cumsum.cmp <- compiler::cmpfun(cumsum.me)

autoplot(
  microbenchmark(
    cumsum.R(1000),
    cumsum.me(1000),
    cumsum.cmp(1000),
    times=1000)
)
```

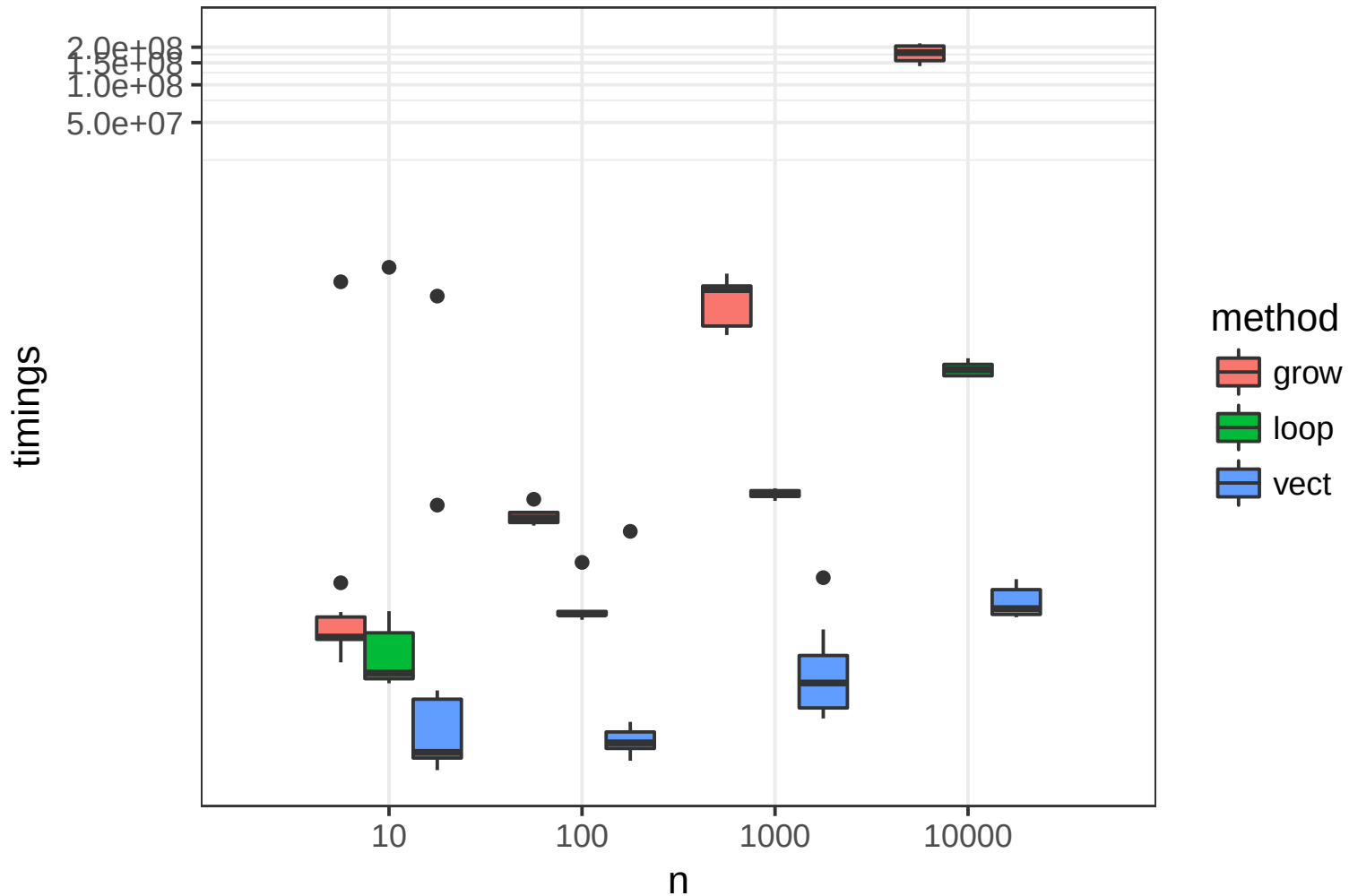
Compile your functions with `base::compiler` II



⇝ Can be set automatically with `compiler::enableJIT(3)`

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.

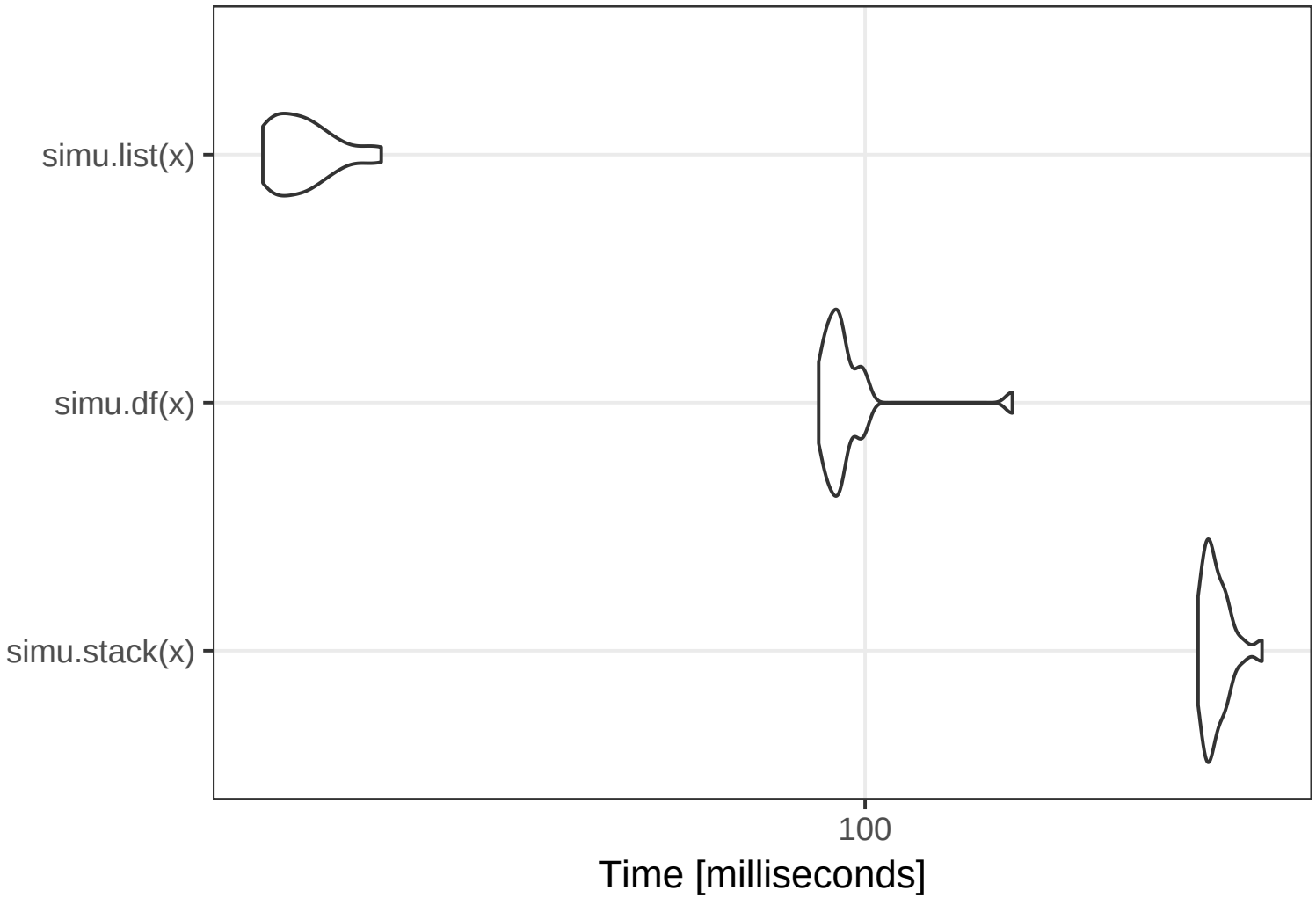
```
simu.stack <- function(x) { ## x is a n x p matrix
  out <- data.frame(mean = numeric(0), sd = numeric(0))
  for (i in 1:n)
    out <- rbind(out, data.frame(mean = mean(x[i,]), sd = sd(x[i, ])) )
  return(out)
}

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, ]))
  return(out)
}

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

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

Do not stack objects II

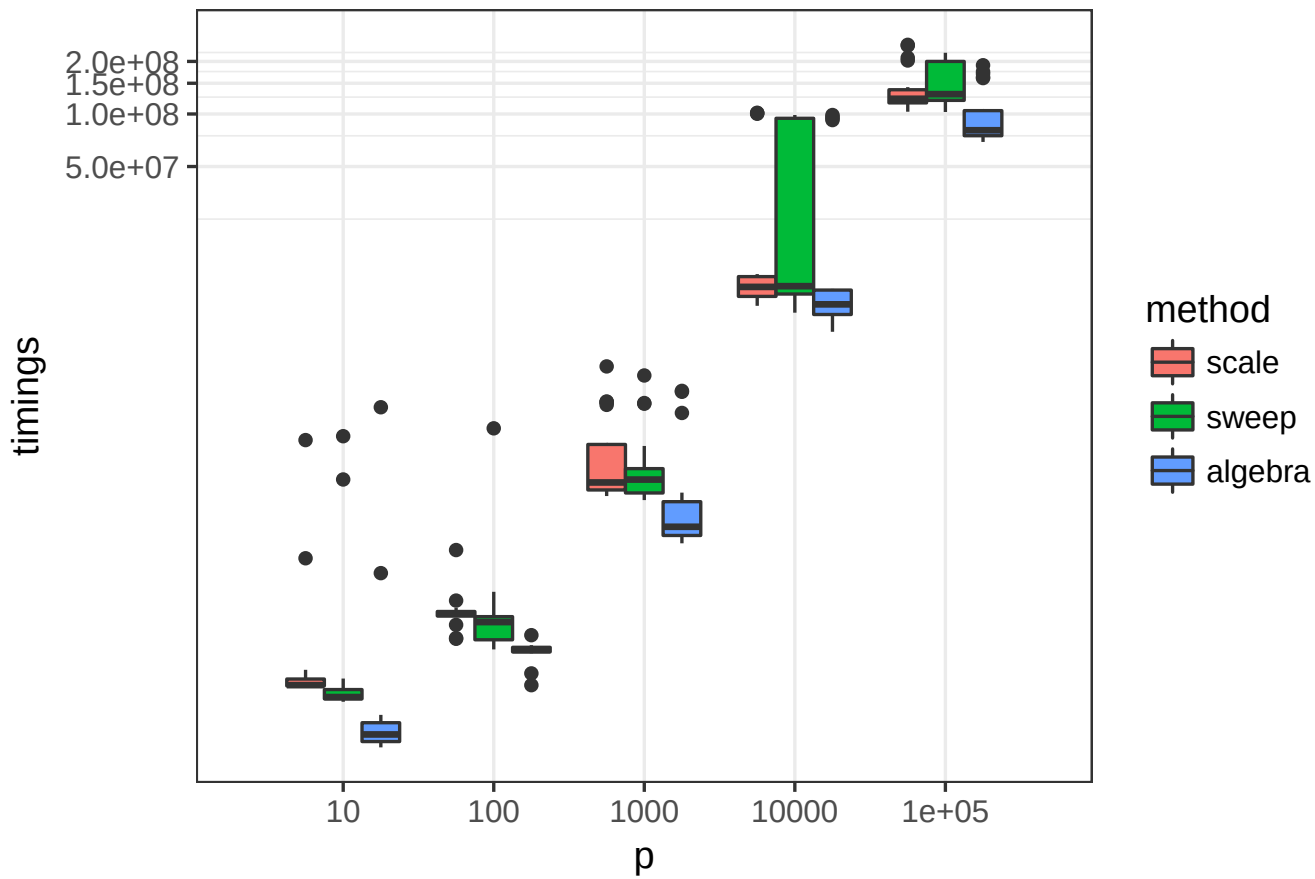


Mind some algebra

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
```

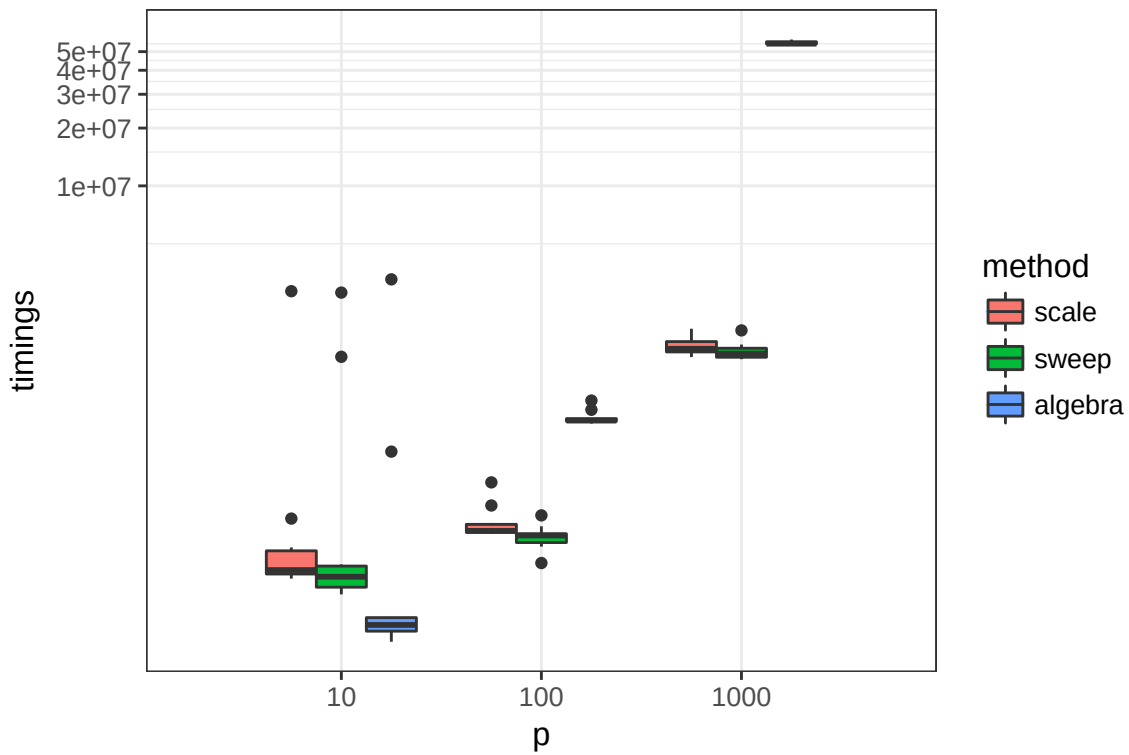


Algebra does not always pay

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
```

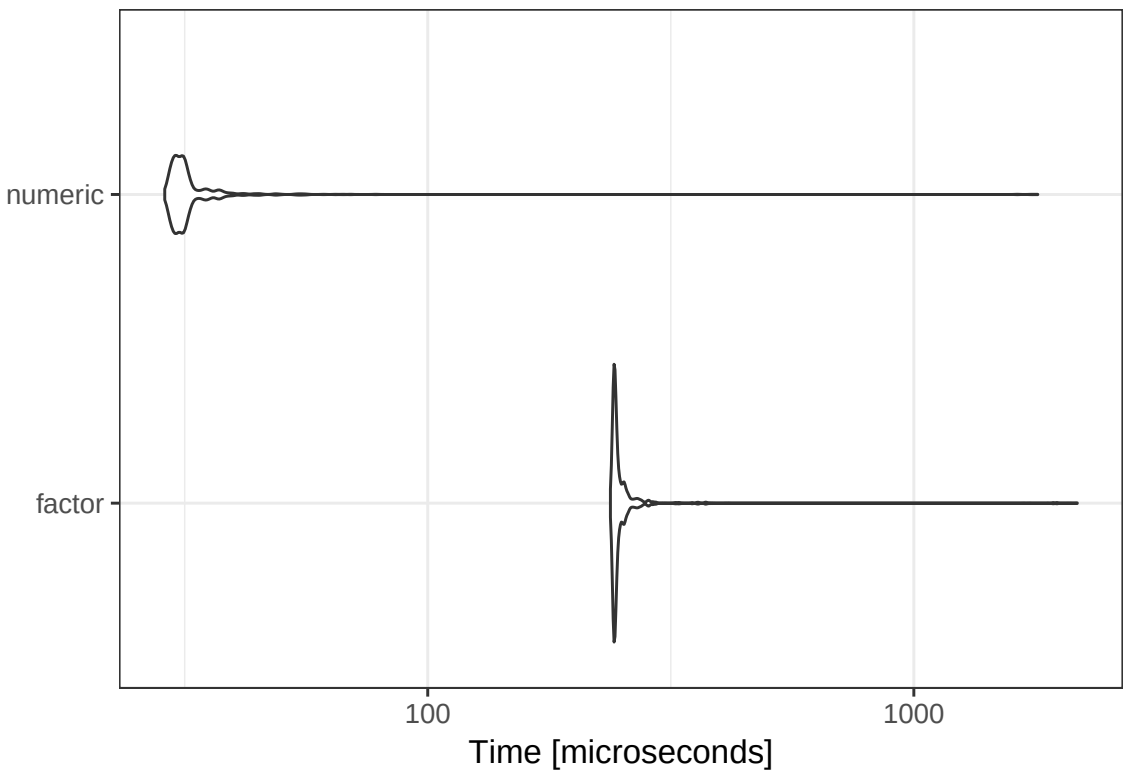


Outline

Factor conversion are slow (`nlevels`)

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

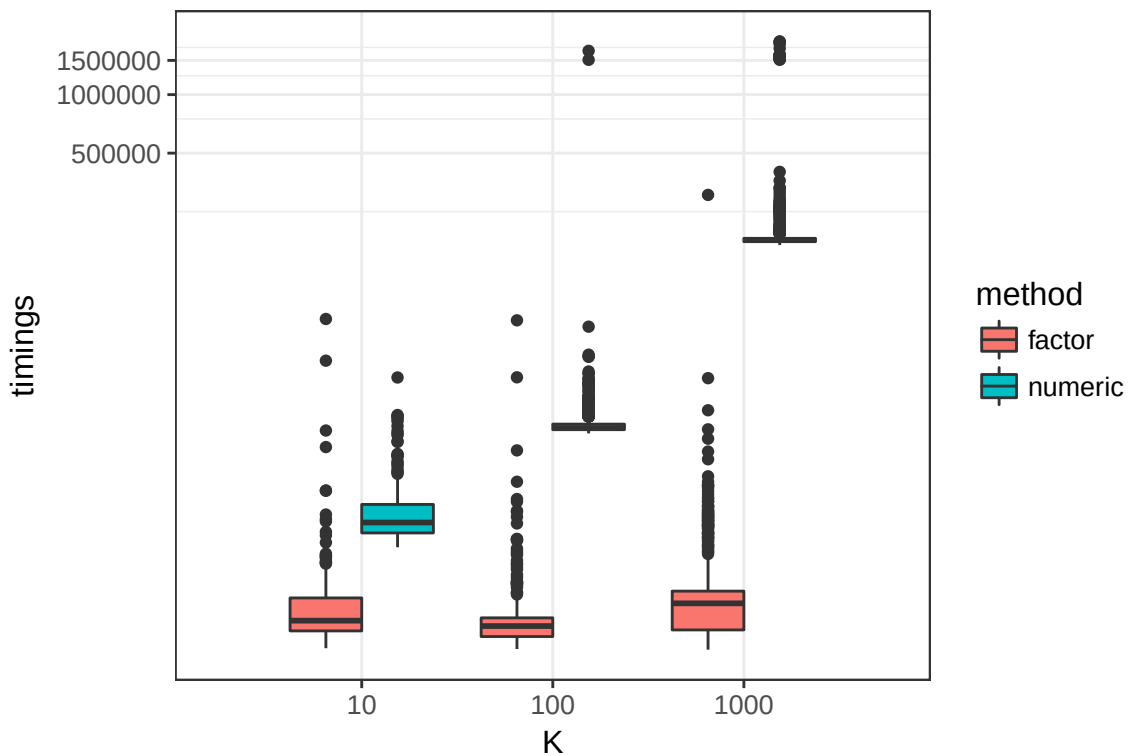
```
n <- 1000; K <- 10
autoplot(microbenchmark(
  factor = nlevels(factor(sample(1:K, n, rep=TRUE))),
  numeric = length(unique(sample(1:K, n, rep=TRUE))), times=1000)
)
```



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

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

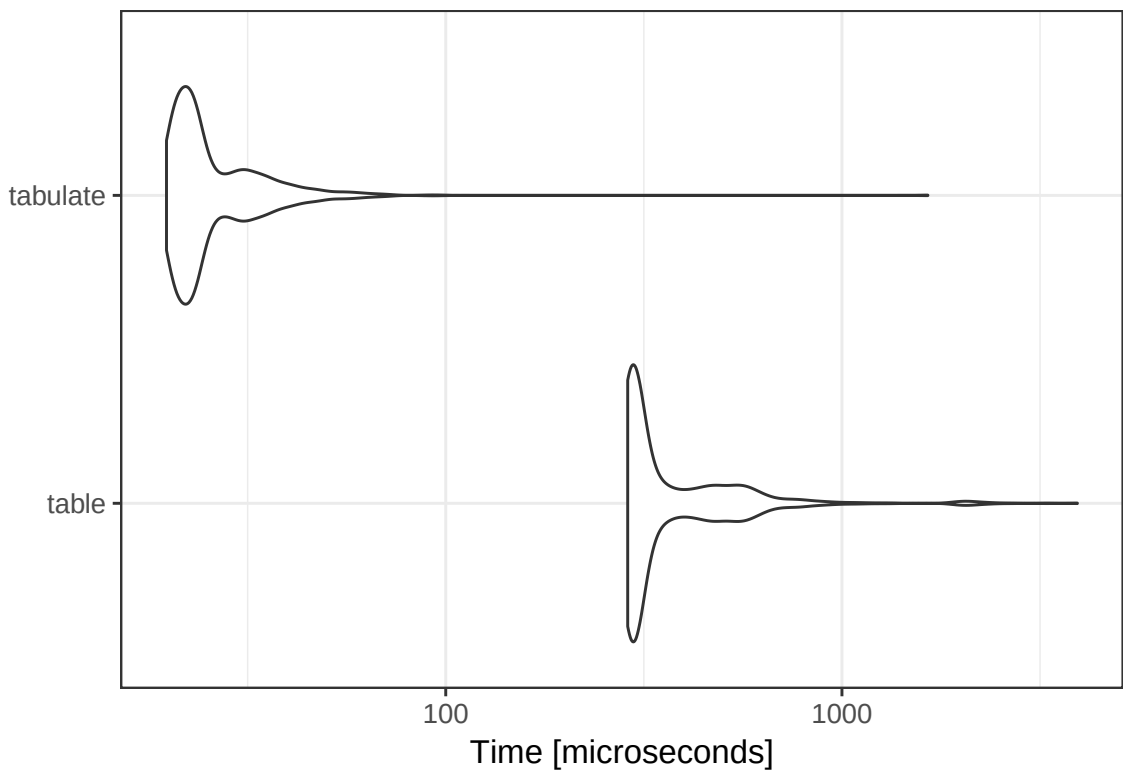
```
nk <- 20
seq.K <- c(10,100,1000)
res <- do.call(rbind, lapply(seq.K, function(K) {
  x1 <- rep(1:K,nk)
  x2 <- factor(x1)
  out <- microbenchmark(factor  = nlevels(x2),
                        numeric = length(unique(x1)), times=1000)
  return(data.frame(method = out$expr, timings = out$time, K =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



Prefer `tabulate` to `table` whenever you can

`table` is a complex function that should not be use 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)
)
```



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 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] 0.5384615384615384
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So do not use binary operator to compare floats because

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

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

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## [1] 0.09999999999999999
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Try

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

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

R masks the numerical errors

by printing a *convenient* summary of objects

```
7/13
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## [1] 0.5384615
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print(7/13, digits=16)
```

```
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```

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
```

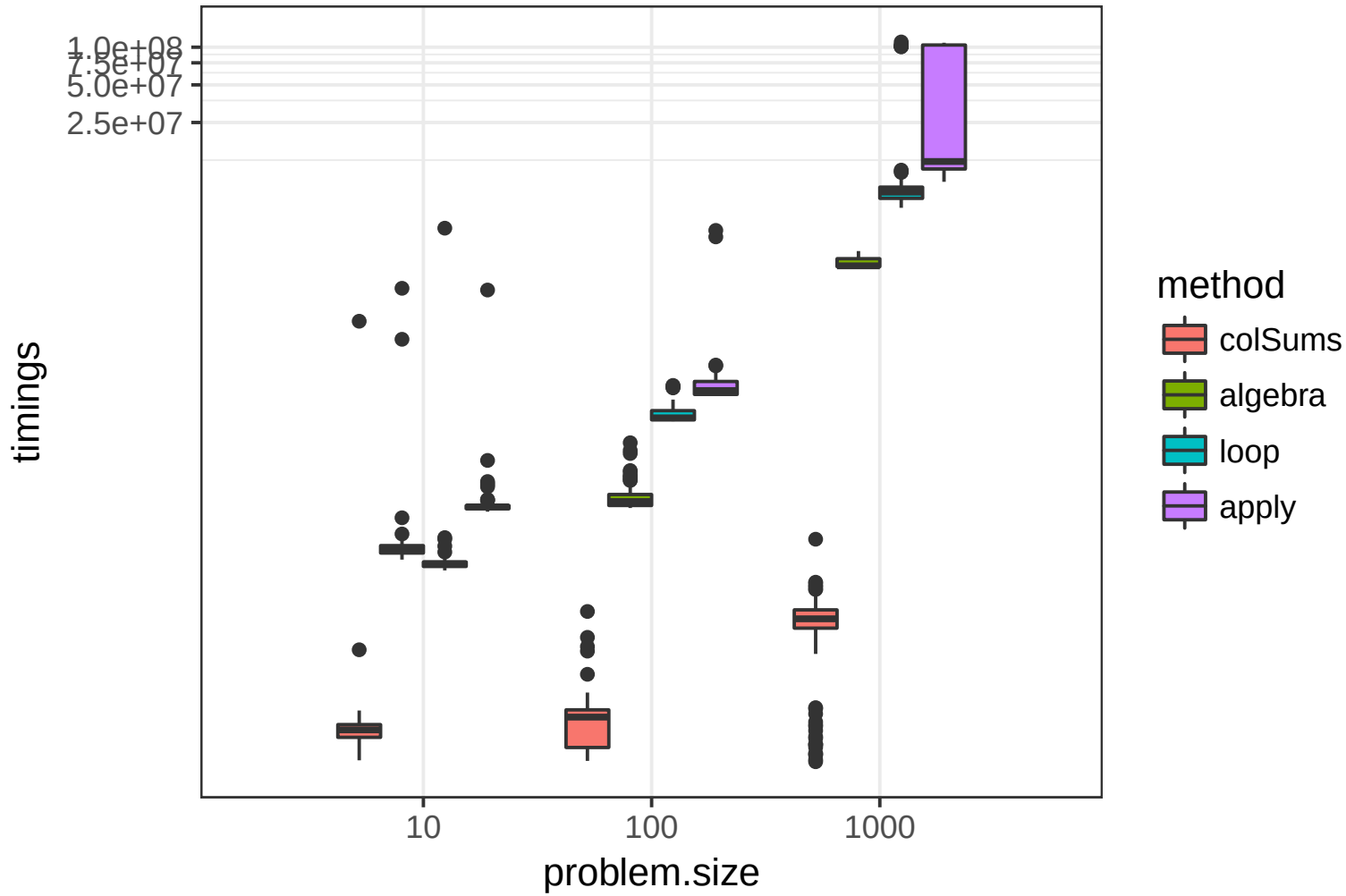
Outline

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



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).

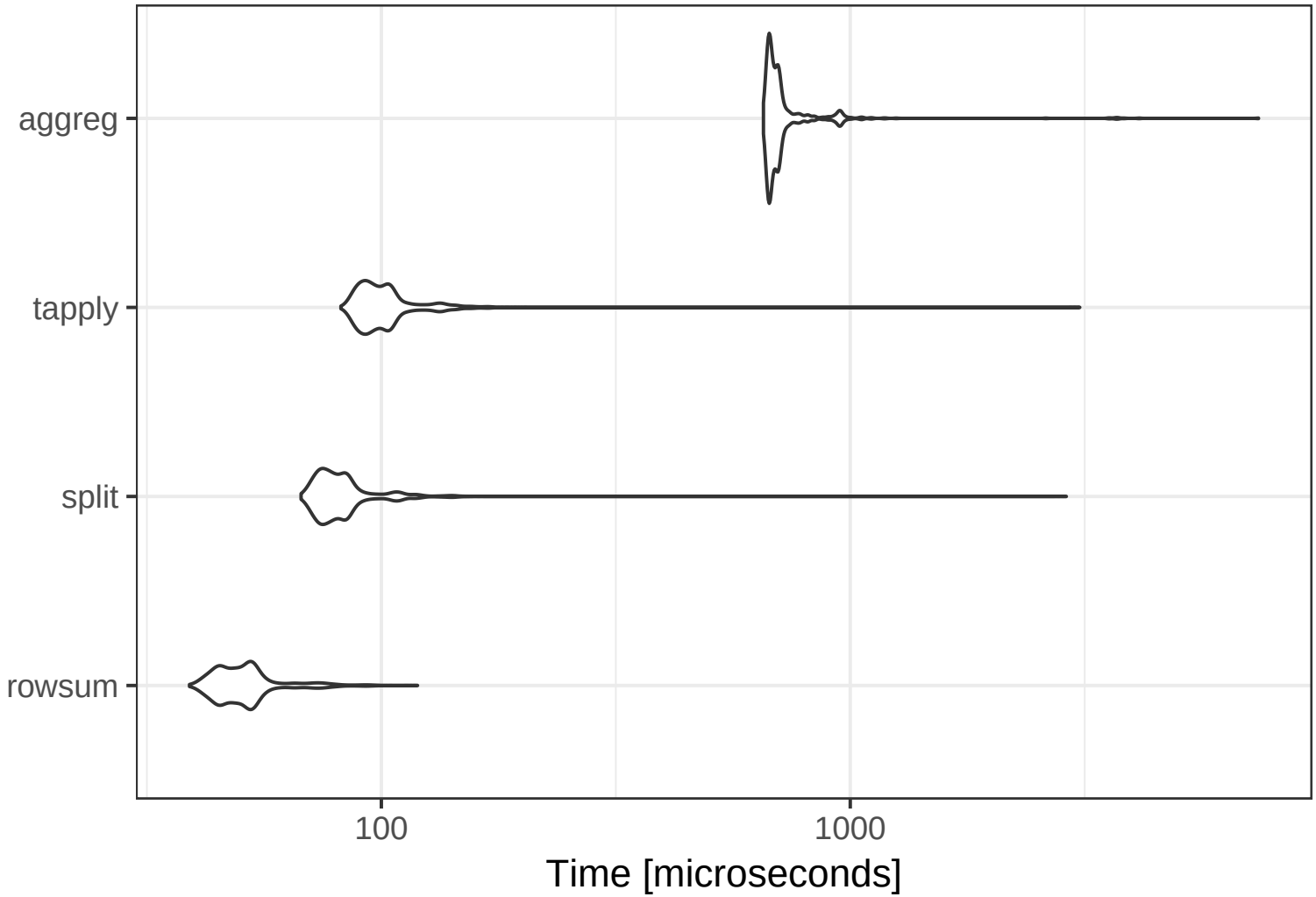
```
vec <- runif(1000)
grp <- sample(1:5, 1000, TRUE)
print(c(rowsum(vec, grp)))
```

```
## [1]  98.61321  82.57750  95.25504 111.53004 105.64565
```

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)
```

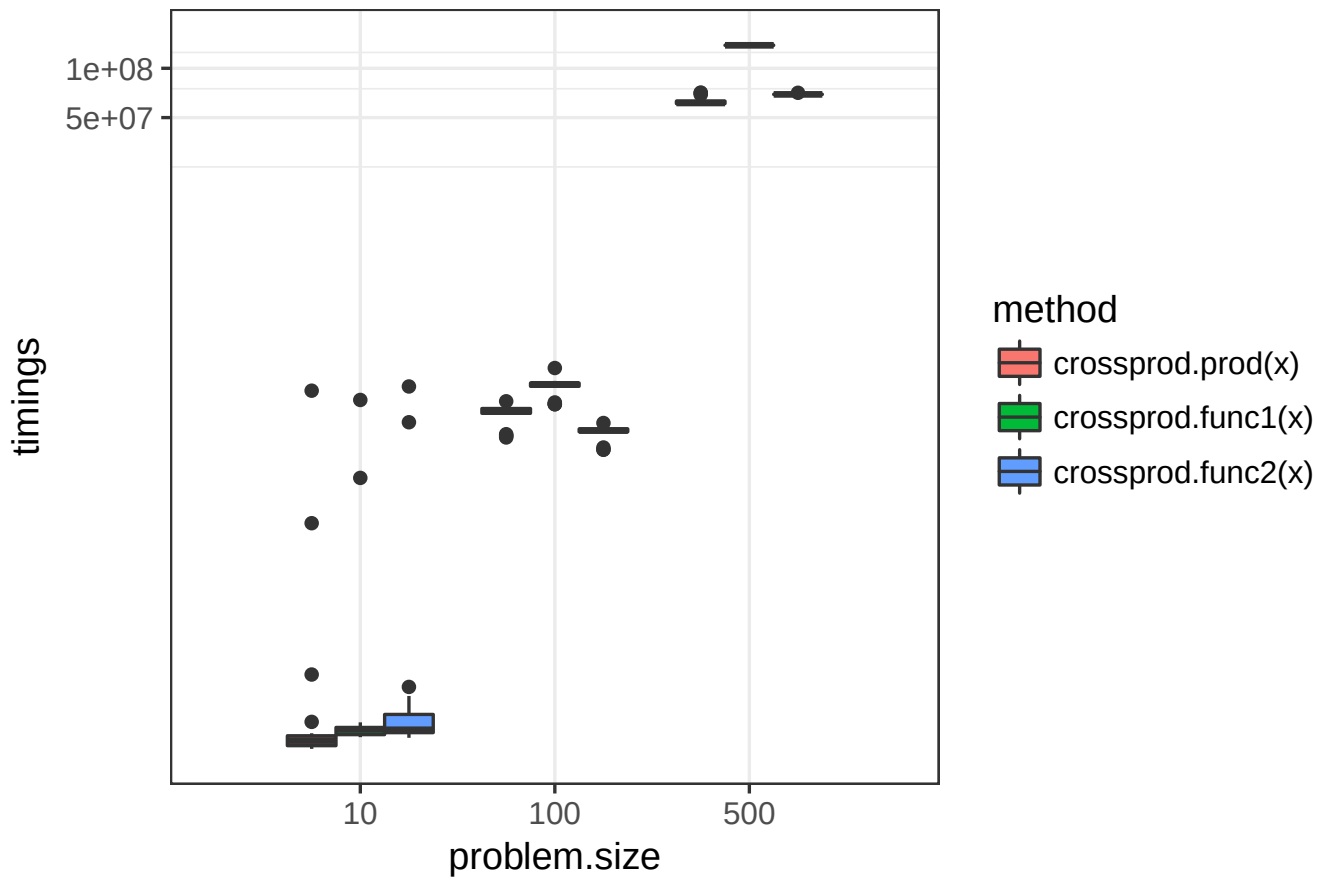
The secret function `rowsum` II



Dedicated function: cross-product

Generally (a bit) fastest 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

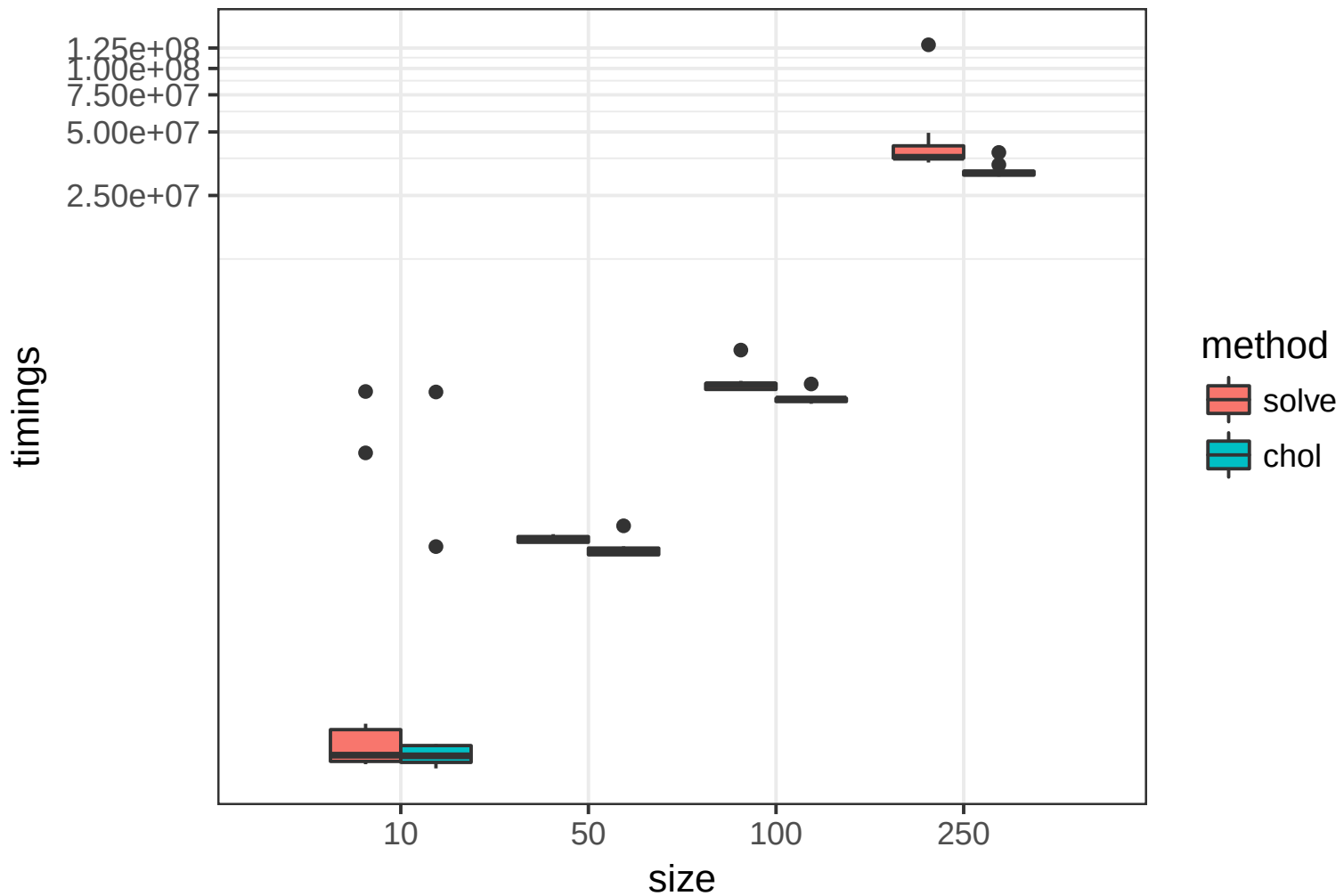
Use a Cholesky factorization

```
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

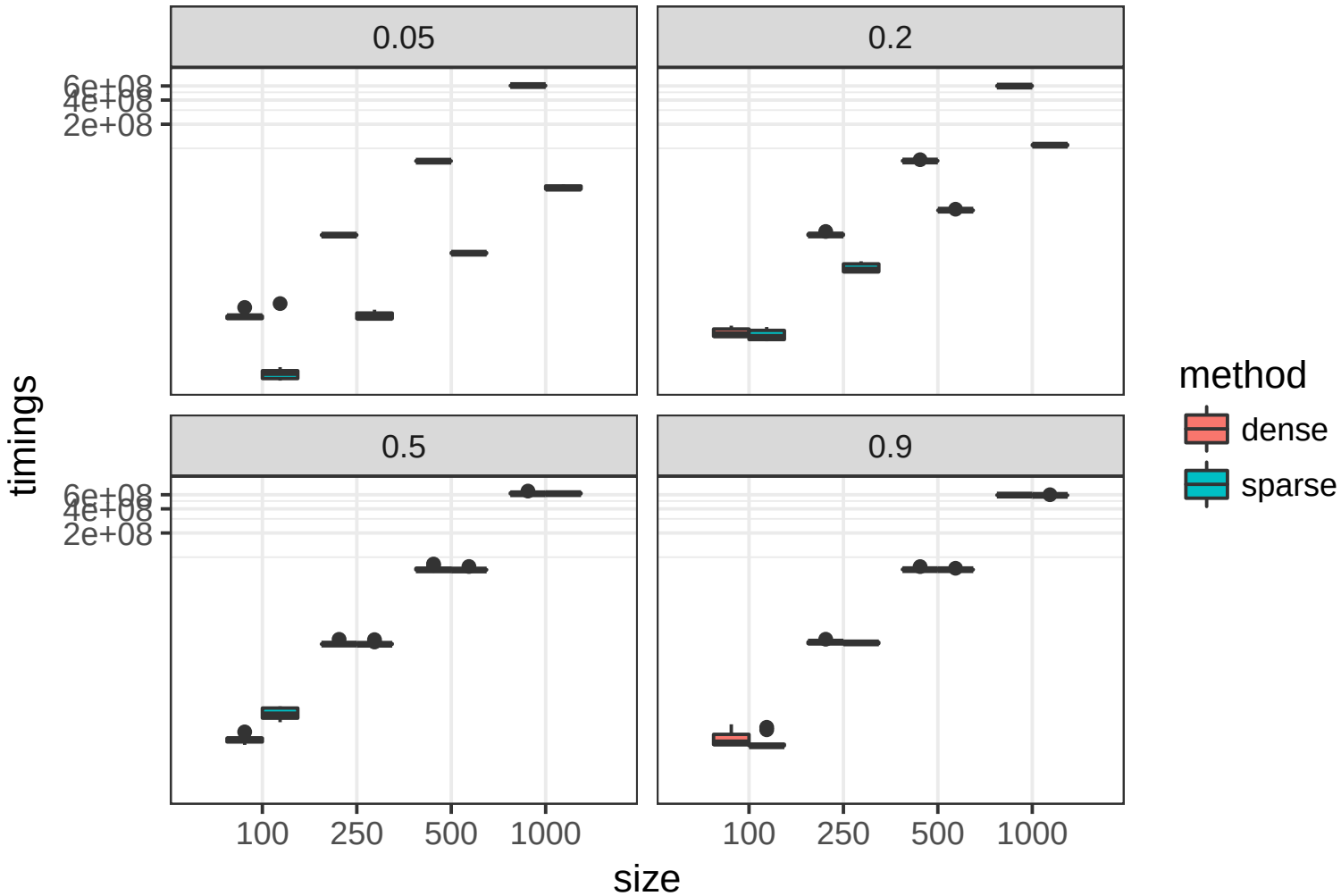


The Matrix package I

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



Outline

References

Gillespie, C., & Lovelace, R. (2016). *Efficient r programming*. " O'Reilly Media, Inc." Retrieved from https://bookdown.org/csgillespie/efficientR/

Wickham, H. (2014). *Advanced r*. CRC Press. Retrieved from http://adv-r.had.co.nz/