(A bit of) Advanced R

Efficient R programming

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http://github/jchiquet/CourseAdvancedR

Resources

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

Part 0: Prerequesties

- xpply family, do.call, Reduce

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)))
```

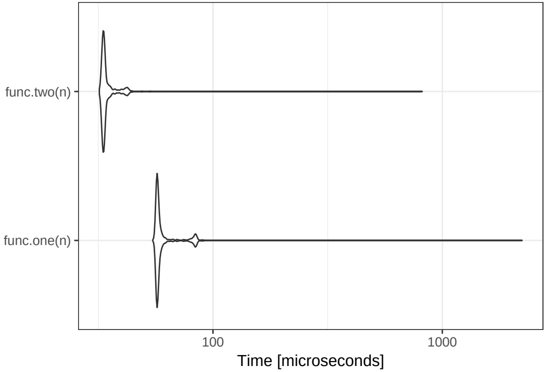
```
##    user  system elapsed
##   0.008   0.000   0.007
```

Quick benchmarking with `microbenchmark`

```r
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:

```r
## 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
```

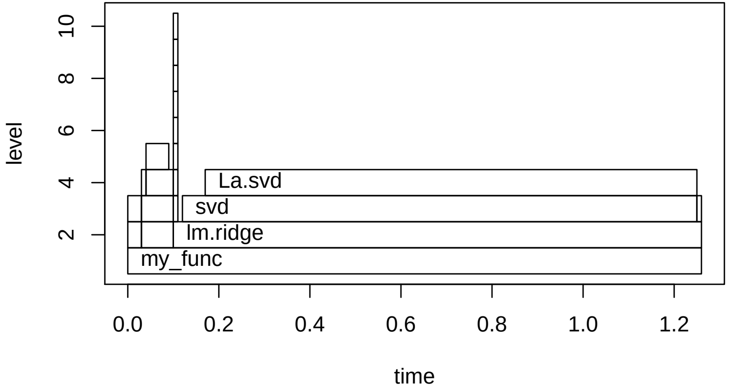
Profile your code with base Rprof III

```
## "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...

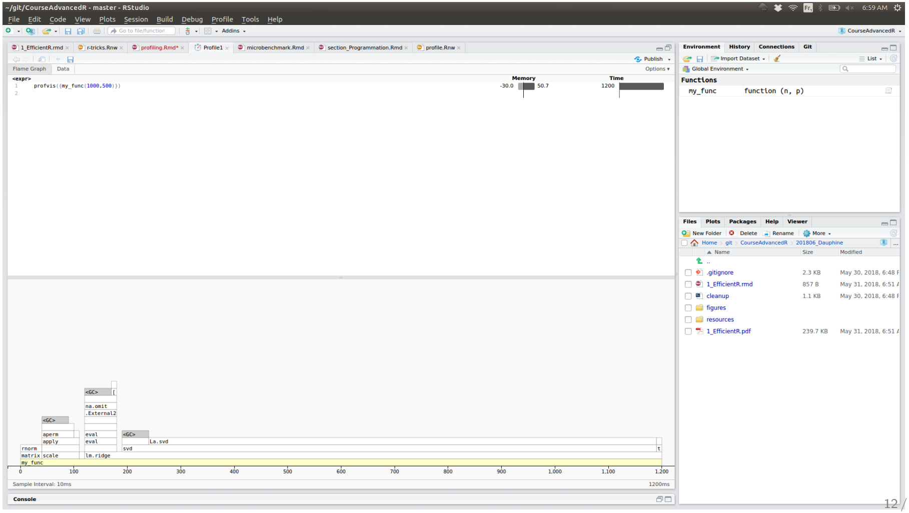
```r
library(profr)
profiling <- profr({my_func(1000,500)}, interval = 0.01)
plot(profiling)
```



Profile your code within R Studiow with `profvis`

Profvis integrates the profiling to the Rstudio API

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



~/git/CourseAdvancedR - master - RStudio

```
<expr>                                             Memory          Time
profvis({my_func(1000,500)})                  -30.0      50.7      1200
```

Functions

`my_func    function (n, p)`

	Name	Size	Modified
	..		
	.gitignore	2.3 KB	May 30, 2018, 6:48
	1_EfficientR.rmd	857 B	May 31, 2018, 6:51
	cleanup	1.1 KB	May 30, 2018, 6:48
	figures		
	resources		
	1_EfficientR.pdf	239.7 KB	May 31, 2018, 6:51

Sample Interval: 10ms

1200ms

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

```r
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

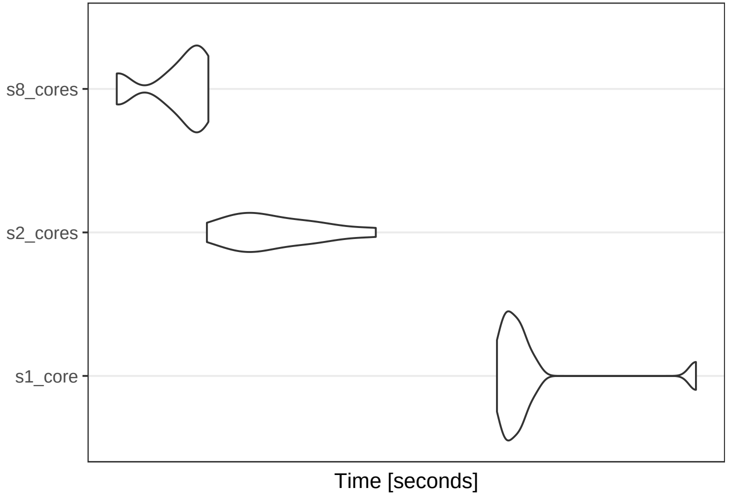
```r
one.simu <- function(i) {
  ## draw data
  n <- 1000; p <- 500
  x <- matrix(rnorm(n*p),n,p) ; y <- rnorm(n)
  ## return ridge's coefficients
  train <- 1:floor(n/2)
  test  <- setdiff(1:n,train)
  ridge <- MASS::lm.ridge(y~x+0,lambda=1,subset=train)
  err <- (y[test] - x[test, ] %*% ridge$coef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

```r
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

```r
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 piece 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

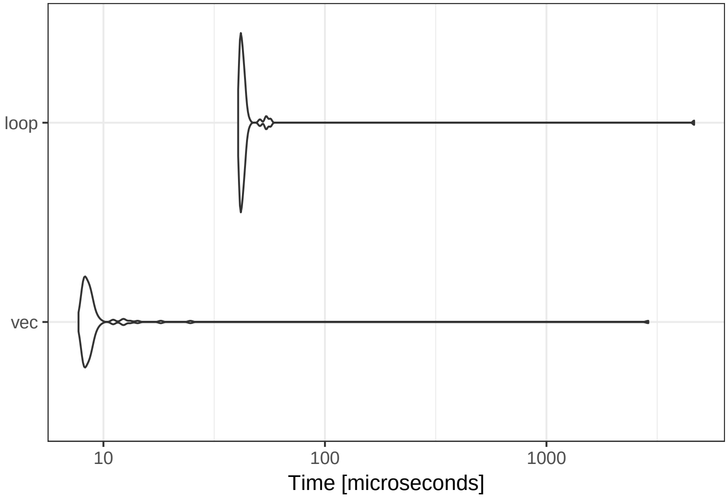
Vectorize any algebraic operation I

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

```r
## 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
}
```

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

Vectorize any algebraic operation II



Vectorize, even for non-algebraic operation I

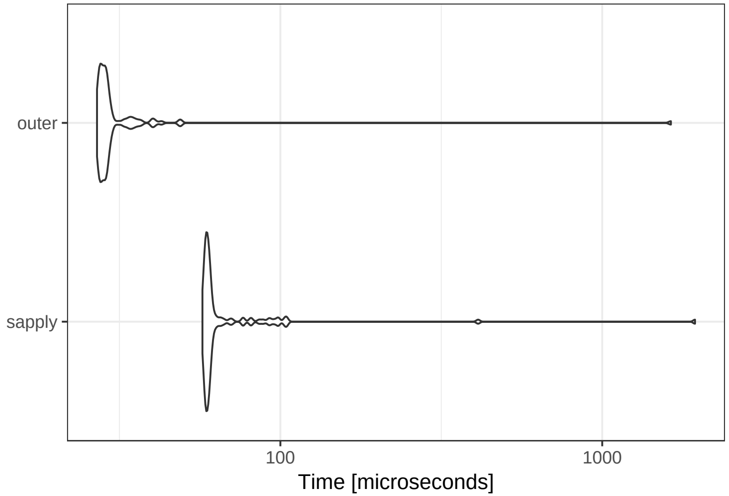
```r
month_year_apply <- function(year) {
  sapply(month.name, function(month) paste(month, year, sep = "_"))
}

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"
```

```r
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

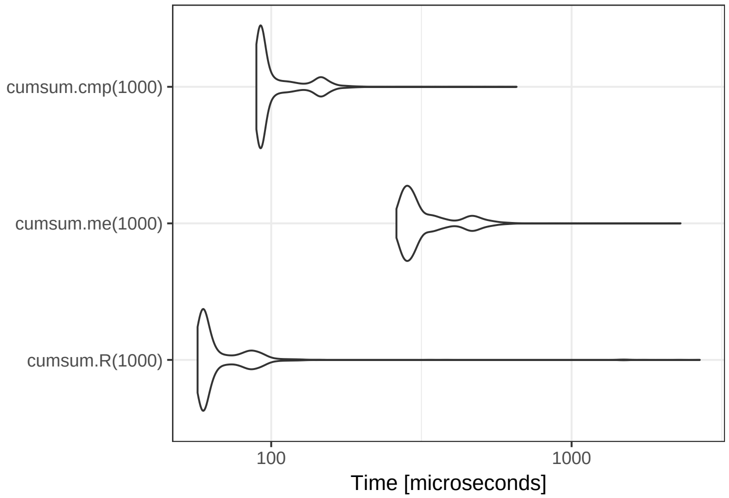
```r
cumsum.R <- function(n) {
  x <- rnorm(n)
  cumsum(x)
}

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)
)
```

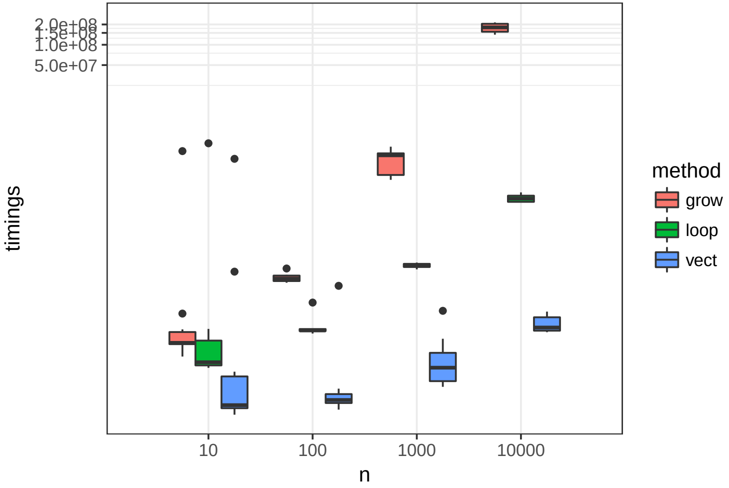
Compile your functions with `base::compiler` II



⇝ 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.

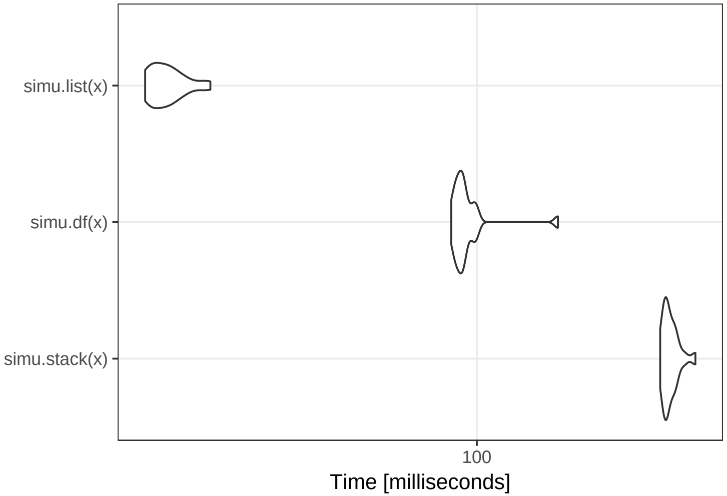
```r
simu.stack <- function(x) { ## x is a n x p matrix
  out <- data.frame(mean = numeric(0), sd = numeric(0))
  for (i in 1:n)
    out <- rbind(out, data.frame(mean = mean(x[i,]), sd = sd(x[i, ])) )
  return(out)
}

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)
}
```

```r
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

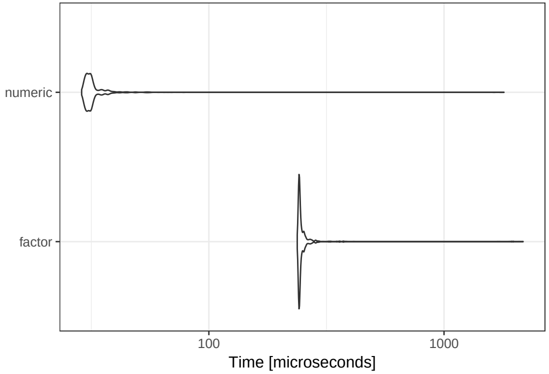


Outline

Factor conversion are slow (`nlevels`)

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

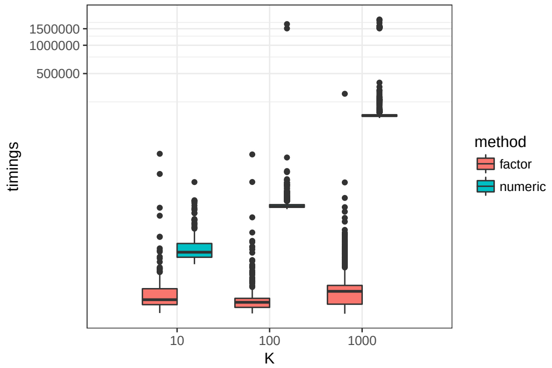
```r
n <- 1000; K <- 10
autoplot(microbenchmark(
  factor = nlevels(factor(sample(1:K, n, rep=TRUE))),
  numeric = length(unique(sample(1:K, n, rep=TRUE))), times=1000)
)
```



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

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

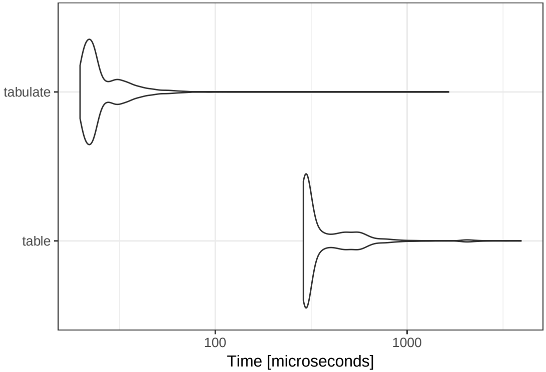
```r
nk <- 20
seq.K <- c(10,100,1000)
res <- do.call(rbind, lapply(seq.K, function(K) {
  x1 <- rep(1:K,nk)
  x2 <- factor(x1)
  out <- microbenchmark(factor  = nlevels(x2),
                        numeric = length(unique(x1)), times=1000)
  return(data.frame(method = out$expr, timings = out$time, K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

```r
7/13
```

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

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

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

So do not use binary operator to compare floats because

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

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

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

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

Try

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

```
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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by printing a *convenient* summary of objects

```
7/13
```

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

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

```
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```

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

```
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```

```
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```

Try

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

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

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/