# *R optimization tips & tricks (Benchmarked)*

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## Why optimize ?

- "Return on investment" for "Code Optimization" is +ve if:
  - The code is/will be re-used several times
    - It runs in a workflow / pipeline
    - You're deploying it for end-users
  - The "vanilla" way takes too damn long
  - You want to learn more about the language.

- "Fast software is the best software" – Craig Mod

  https://craigmod.com/essays/fast_software/

## When not to optimize ?

- You're on a deadline
- You're just waiting for it to be over

# Description of data

- Catalog of Somatic Mutations in Cancer COSMIC v91
  - https://cancer.sanger.ac.uk/cosmic/download#download-3
  - Complete size 16 GB (≈4G gzip RDS)
  - Processed to host 2 databases at:
    https://eleniuslabtools.utu.fi/main/HotspotExplorer.html
- 40 columns x millions of rows (*literally!!*)
- For these benchmarks → subset files were used with:
  - 10, 100, 1 000, 10 000, 100 000, 1 000 000 rows each
  - Max file size: 350M

# Test bench

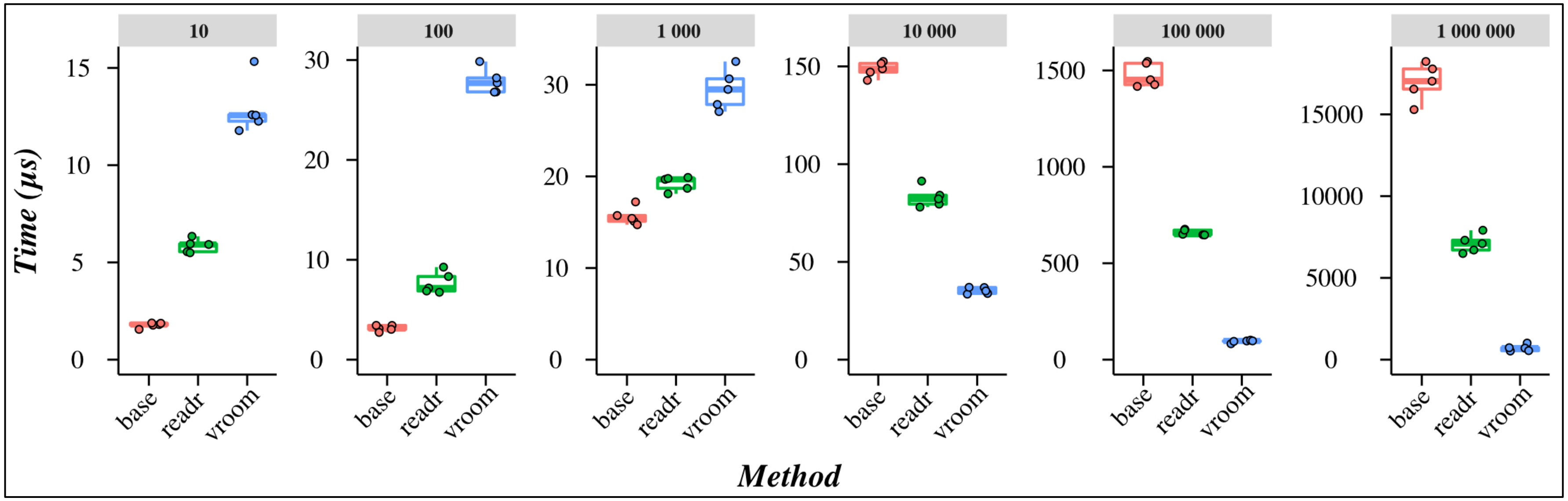
- Tested on iMac running Mac OS Catalina
  - **Proc:** 3.2 GHz x 4 physical cores x 1 thread  [i.e. *no SMT*]
  - **RAM** 24 GB 1600 MHz

- R version 3.6.3
  - vroom – 1.3.0
  - readr – 1.3.1
  - ggplot2 - 3.3.2
  - stringi  - 1.4.6
  - parallel - 3.6.3
  - doParallel – 1.0.15
  - snow  - 0.4-3
  - plyr – 1.8.6
  - microbenchmark – 1.4-7

## Disclaimer !

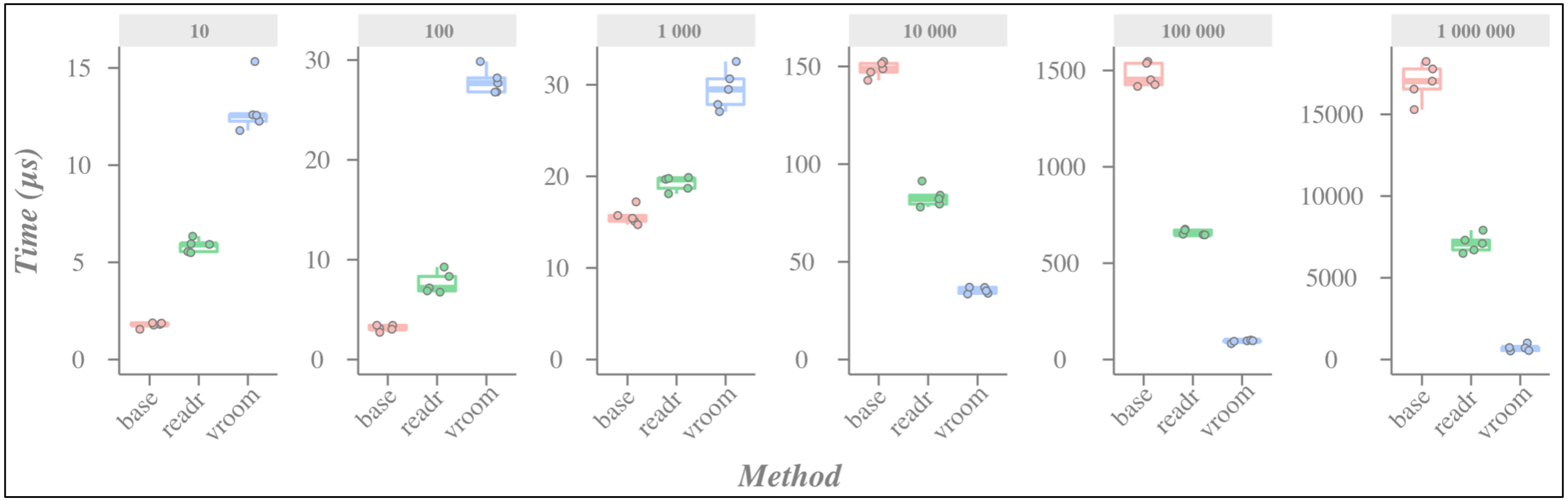
- Tested on Mac OS (**2** machines)
- Based on **my** experience
- Examples: some are *real*, **MOST** are *fabricated*
- I'm **NOT** here to tell you what is the "right way".
  Your way IS the right way for you.
  I'm just offering alternative(s).
- These are definitely **NOT** the "fastest" way.
  That would be to **write something in C**, etc.!

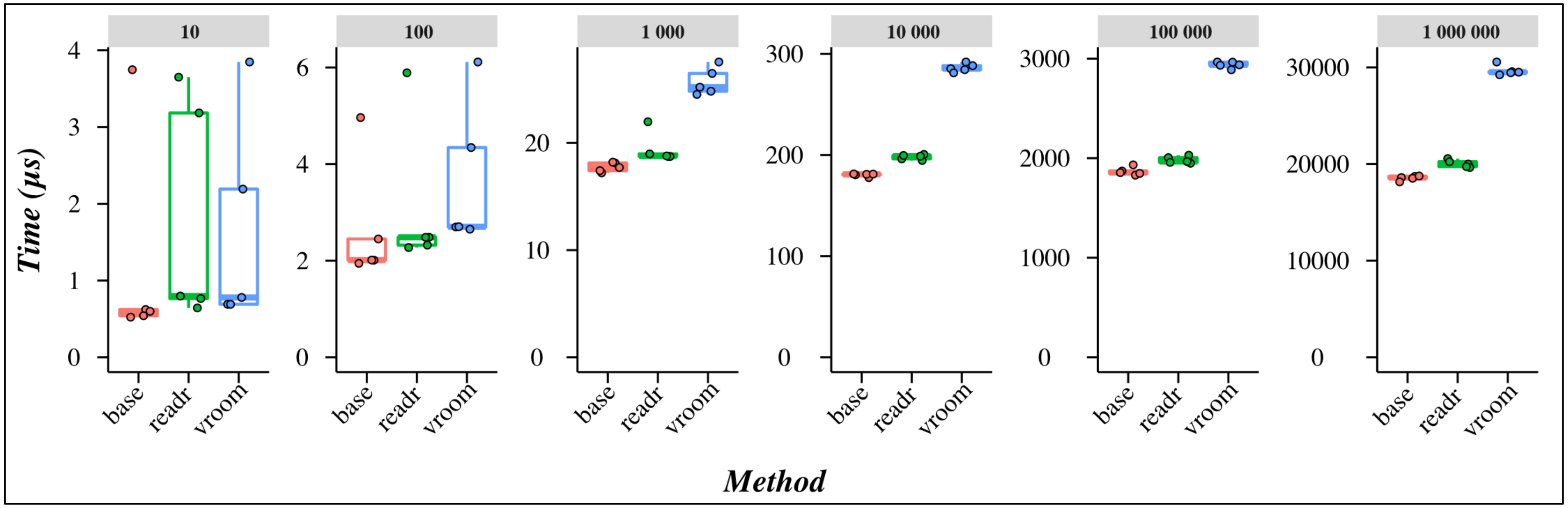
# Reading files



```r
# base
dat <- utils::read.table(file = file.name,header = T,sep = "\t",as.is = T,stringsAsFactors = T)
; rm(dat)
-------------------------------------------------------------------------------------
# readr
dat <- readr::read_delim(file = file.name,delim = "\t",progress=F) ; rm(dat)
-------------------------------------------------------------------------------------
# vroom
dat <- vroom::vroom(file = file.name,delim = "\t",progress = F) ; rm(dat)
```

# Reading files → Writing files

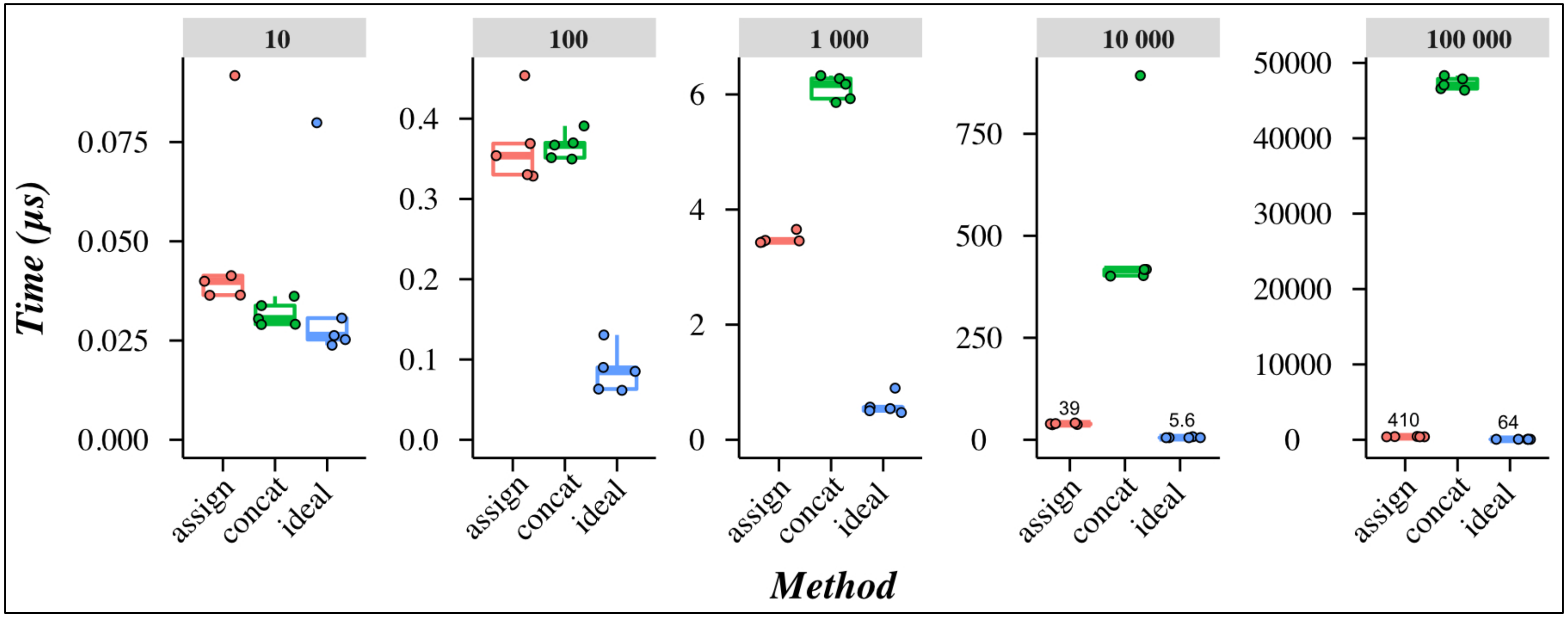




# Populating a vector

```
strings <- dat[1:i,"HGVSC"]  # ENST00000357360.4:c.*22C>T

# concat: concatenation
ENS_ID <- c()
for(idx in seq_along(strings)){
   ENS_ID <- c(ENS_ID, unlist(strsplit(x = strings[idx], split = ".", fixed =T),
use.names = F)[1])
}
-------------------------------------------------------------------------------

# assign
ENS_ID <- rep(NA,length(strings))
for(idx in seq_along(strings)){
   ENS_ID[idx] <- unlist(strsplit(x = strings[idx], split = ".", fixed =T),
use.names = F)[1]
}
-------------------------------------------------------------------------------

# ideal: vectorization (i.e. skip the for loop)
ENS_ID <- unlist(strsplit(x = strings,split = ".", fixed =T), use.names = F)[seq(1,
3 * length(strings), by = 3)]
```

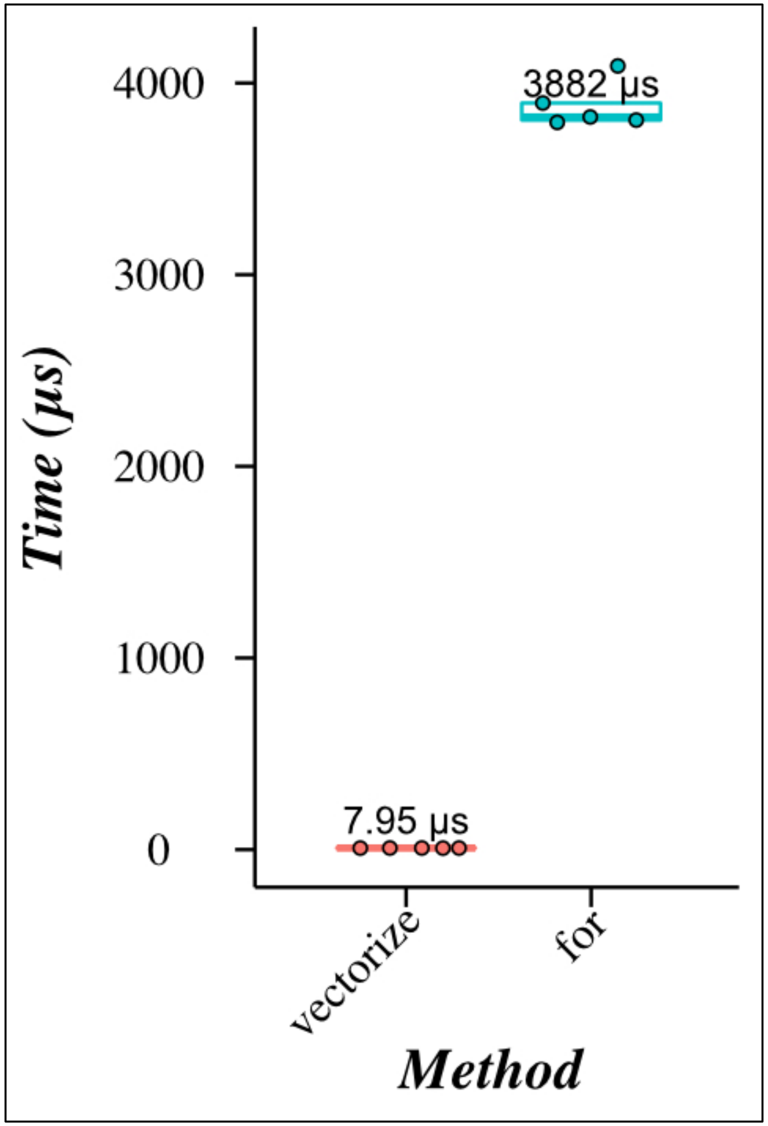
# Populating a vector



```
# concat: concatenation
ENS_ID <- c() # declare vector
for(loop){
   ENS_ID <- c(ENS_ID, new_value)
}

# assign: assign to different indices
ENS_ID <- rep(NA,length(strings)) # Initialize an empty vector
for(loop){
   ENS_ID[index] <- new_value
}

# ideal: vectorization (i.e. skip the for loop)
ENS_ID <- unlist(strsplit(x = strings, split = ".", fixed =T), use.names = F)[seq(1, 3 * length(strings), by = 3)]
```

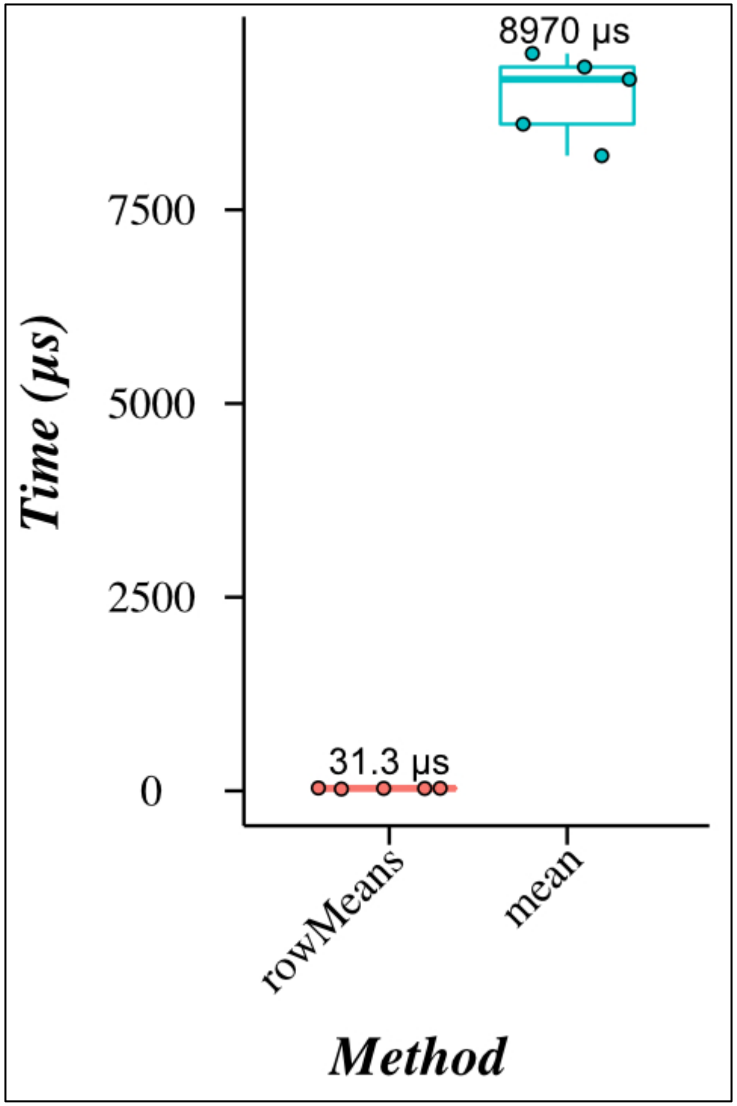
# Vectorization

```r
# calculations with 3 numeric columns

# vectorization
calc_vec <- ((dat$ID_tumour + dat$ID_sample)/
dat$HGNC.ID)



# for loop
calc_for <- rep(NA,length(dat$Gene.name))
for(i in seq_along(dat$Gene.name)){
    calc_for[i] <- ((dat$ID_tumour[i] +
dat$ID_sample[i]) / dat$HGNC.ID[i])
}
```

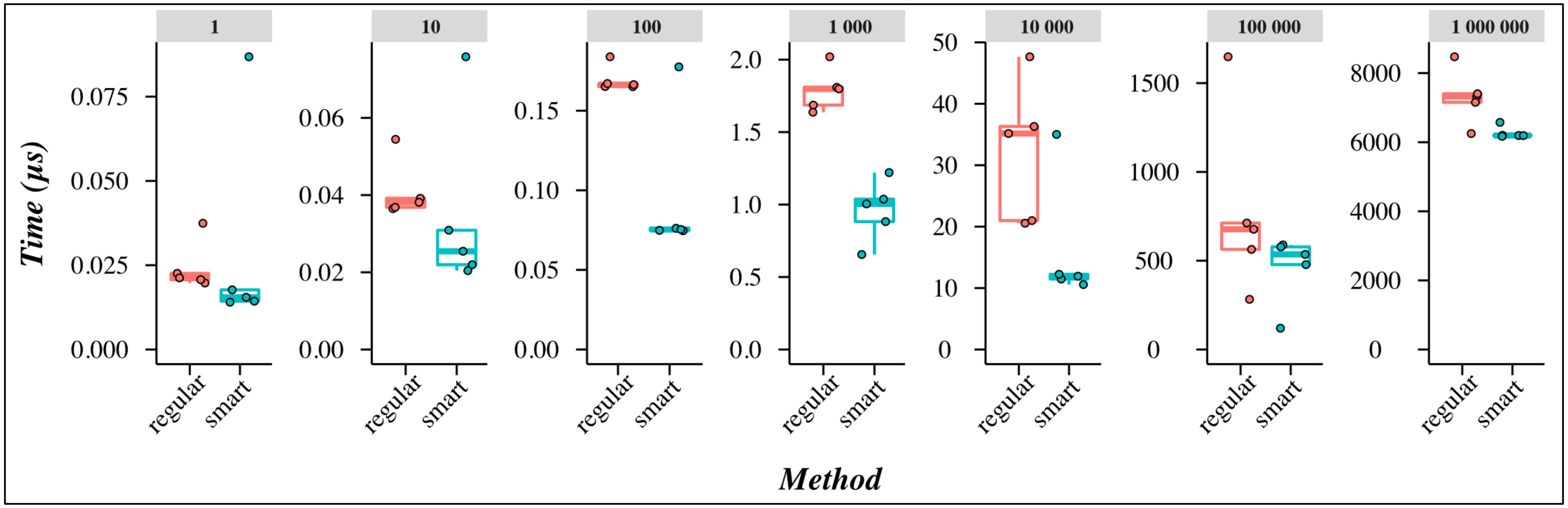


# Vectorization, better example

```r
# for each row calculate mean of value in 3 columns

# vectorized
rM <- rowMeans(dat[,c("ID_sample", "ID_tumour",
"MUTATION_ID")])
},

# for
M <- rep(NA,length(dat$Gene.name))
for(i in seq_along(dat$Gene.name)){
    M[i] <- ((dat$ID_tumour[i] + dat$ID_sample[i] +
dat$MUTATION_ID[i]) / 3)
}
```



# Utilizing specific function parameters



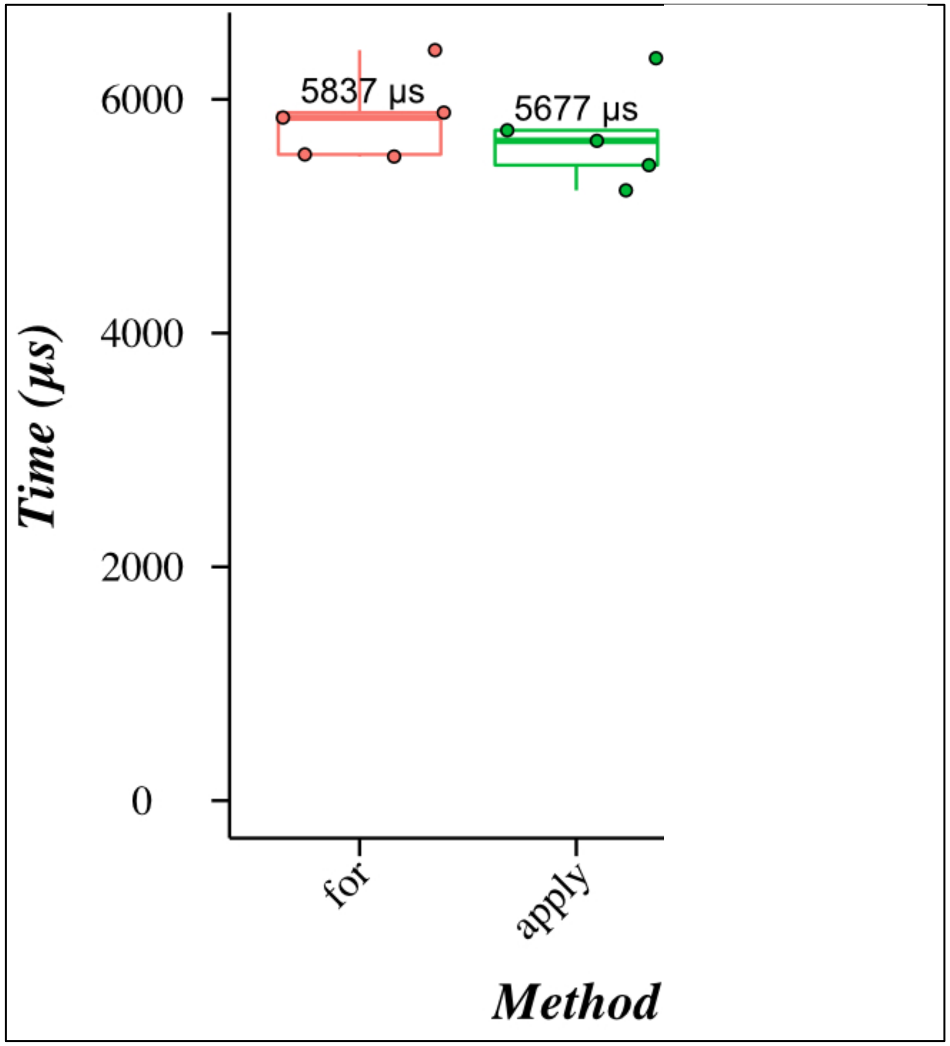
```
# "regular"
res_1 <-  base::substring(text = genomePos,first = {unlist(base::gregexpr(pattern = ":", text
= genomePos)) + 1})}

# smart
res_2 <- base::substring(text = genomePos,first = {unlist(base::gregexpr(pattern = ":",text =
genomePos, fixed = T), use.names = F) + 1})}


# fixed=T, if you’re not using regex [applicable in grep, gsub, etc.]
# use.names, if you don’t care about names of the values (or can add them later on as well).
```

# for() vs apply()

```
# chr1:1200312511-1587831227”  return -387518716

# for loop
res_for <- rep(NA,length(genomePosition))
for(i in seq_along(genomePosition)){
    genomePos <- base::substring(text = genomePosition[i],first = base::gregexpr(pattern = ":", text =
genomePosition[i], fixed = T)[[1]][1]+1)
    minus <- base::gregexpr(pattern = "-",text = genomePos, fixed = T)[[1]][1]
    res_for[i] <- as.integer(substring(text = genomePos,first = 1,last = minus-1))-as.integer(substring(text =
genomePos,first = minus+1))
}

# apply
find_length <- function(genomePos = NULL){
   genomePos <- base::substring(text = genomePos,first = base::gregexpr(pattern = ":",text = genomePos, fixed =
T)[[1]][1]+1)
   minus <- base::gregexpr(pattern = "-",text = genomePos, fixed = T)[[1]][1]
   return(as.integer(substring(text = genomePos,first = 1,last = minus-1))-as.integer(substring(text =
genomePos,first = minus+1)))
}
res_apply <- sapply(X = genomePosition,FUN = find_length,USE.NAMES = F)

# smart : define vectorized function that iterates by itself i.e. no need for apply
find_length_base <- function(genomePos = NULL){
    genomePos <- base::substring(text = genomePos,first = {unlist(base::gregexpr(pattern = ":",text =
genomePos, fixed = T),use.names = F)+1})
    minus <- unlist(base::gregexpr(pattern = "-",text = genomePos, fixed = T),use.names = F)
    return(as.integer(substring(text = genomePos,first = 1,last = minus-1))-as.integer(substring(text =
genomePos,first = minus+1)))
  }
  res_smart <- find_length_base(genomePos = genomePosition)
```

# for() vs apply()

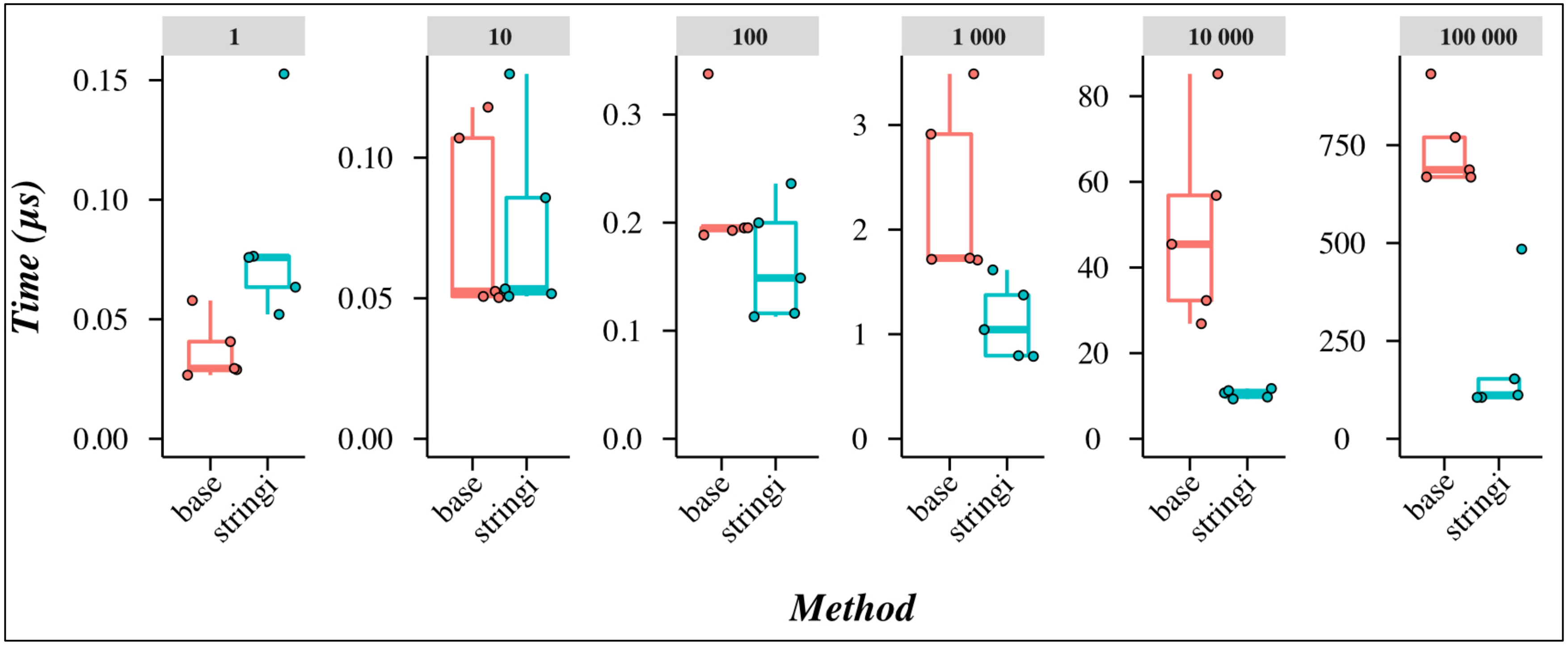
```r
# chr1:1200312511-1587831227"  return -387518716

# for loop
res_for <- rep(NA,length(genomePosition))
for(i in seq_along(genomePosition)){
    genomePos <- base::substring(text =
genomePosition[i],first = base::gregexpr(pattern =
":", text = genomePosition[i], fixed = T)[[1]][1]+1)
    minus <- base::gregexpr(pattern = "-",text =
genomePos, fixed = T)[[1]][1]
    res_for[i] <- as.integer(substring(text =
genomePos,first = 1,last = minus-1))-
as.integer(substring(text = genomePos,first =
minus+1))
}


# apply
res_apply <- sapply(X = genomePosition,FUN =
find_length,USE.NAMES = F)


# smart : define vectorized function that iterates
by itself i.e. no need of for or apply
  res_smart <- find_length_base(genomePos =
genomePosition)
```



# Even Faster string manipulation

```r
# chr1:1200312511-1587831227”  return -387518716

# base
find_length_base <- function(genomePos = NULL){
  genomePos <- base::substring(text = genomePos,first =
{unlist(base::gregexpr(pattern = ":",text = genomePos, fixed = T),use.names = F)+1})
  minus <- unlist(base::gregexpr(pattern = "-",text = genomePos, fixed = T),use.names
= F)
  return(as.integer(base::substring(text = genomePos,first = 1,last = minus-1))-
as.integer(base::substring(text = genomePos,first = minus+1)))
}

# stringi
find_length_stringi <- function(genomePos = NULL){
  genomePos <- stringi::stri_sub(str = genomePos,from
=  stringi::stri_locate_first_fixed(str = genomePos,pattern = ":")[,'start']+1,to = -
1)
  minus <- stringi::stri_locate_first_fixed(str = genomePos,pattern = "-")[,'start']
  return(as.integer(stringi::stri_sub(str = genomePos, from=1, to = minus-1))-
as.integer(stringi::stri_sub(str = genomePos, from=minus+1, to = -1)))
}
```

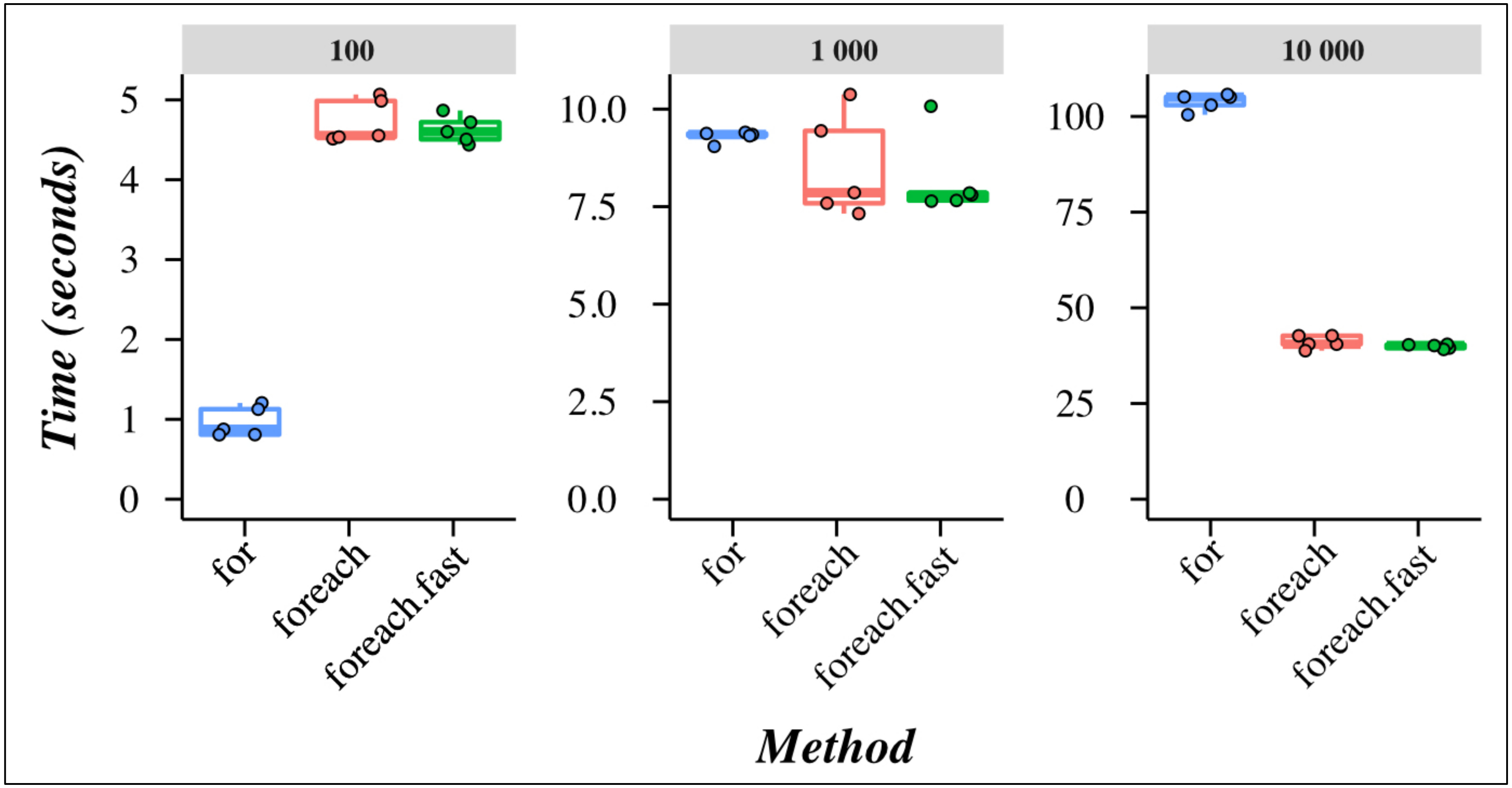
# String manipulation base vs stringi



# for vs foreach

```r
# For a given mutation “GENE A123R” → “lung:7387, kidney:4, prostate:4, breast:2, oesophagus:2,
small intestine:2, adrenal gland:1”

# foreach
myCluster <- makeCluster(4, type = "FORK",useXDR=F,.combine=cbind)
registerDoParallel(myCluster)
results_1 <- foreach(mut = mutations[1:i],.combine = cbind,.inorder = T) %dopar% {
  var1 <-  plyr::count(dat[dat$mutID==mut,],"Primary.site")
  var1 <- var1[order(var1$freq,decreasing = T),]
return(list(mut, sum(var1$freq), stringi::stri_paste(var1$Primary.site, ":", var1$freq,
collapse=',')))
}
stopCluster(myCluster)

# foreach.fast : use the .inorder = F if you do not care about the order
  # … same as “foreach” block …
  results_2 <- foreach(mut = mutations[1:i],.combine = cbind,.inorder = F) %dopar% {
  # … same as “foreach” block …
}

# for
results_3 <- list()
for(mut in mutations[1:i]){
  var1 <-  plyr::count(dat[dat$mutID==mut,],"Primary.site")
  var1 <- var1[order(var1$freq,decreasing = T),]
  results_3 <- cbind(results_3,list(mut, sum(var1$freq), stringi::stri_paste(var1$Primary.site,
":", var1$freq,collapse=',')))
}
```

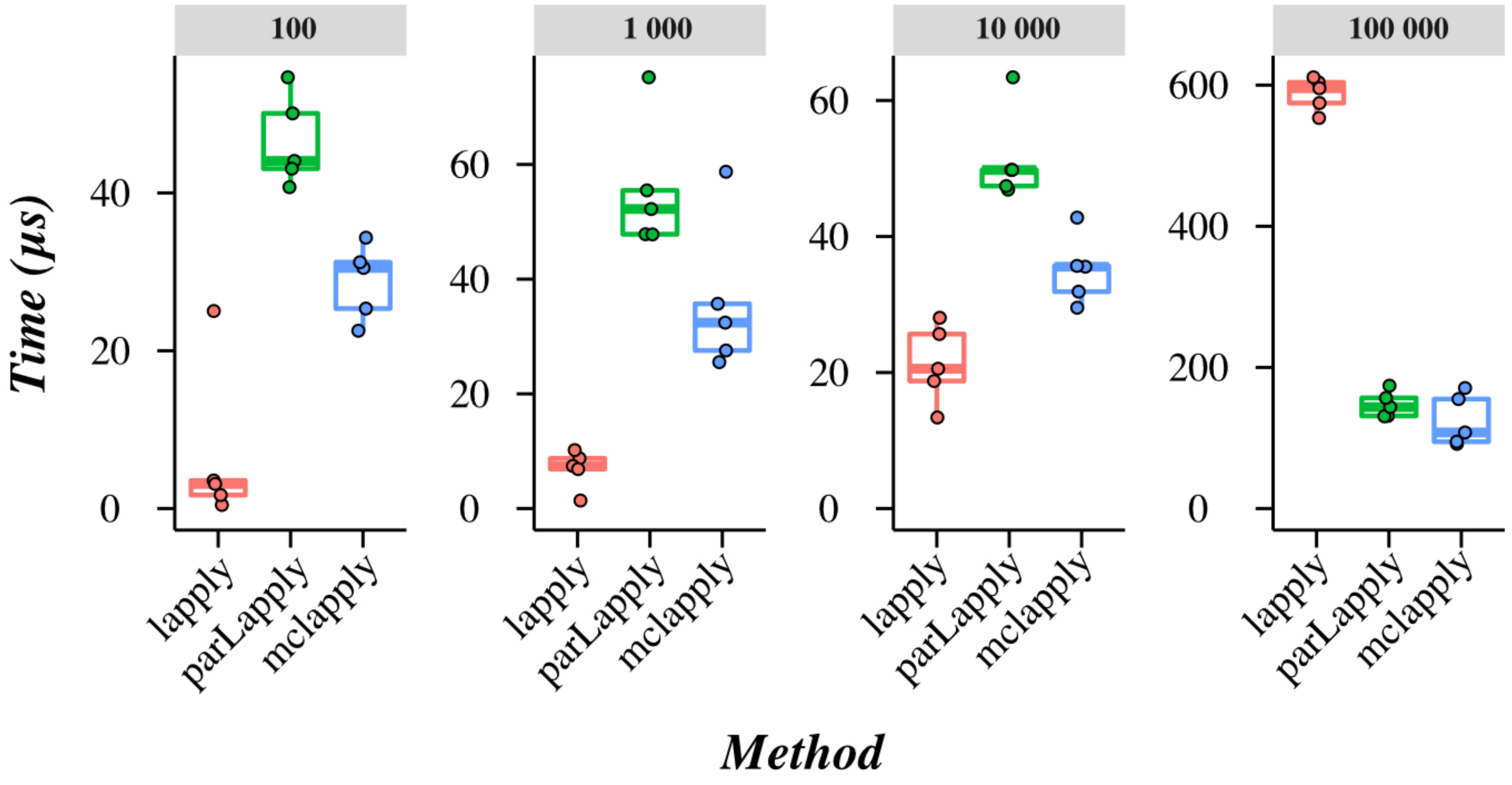
# for vs foreach



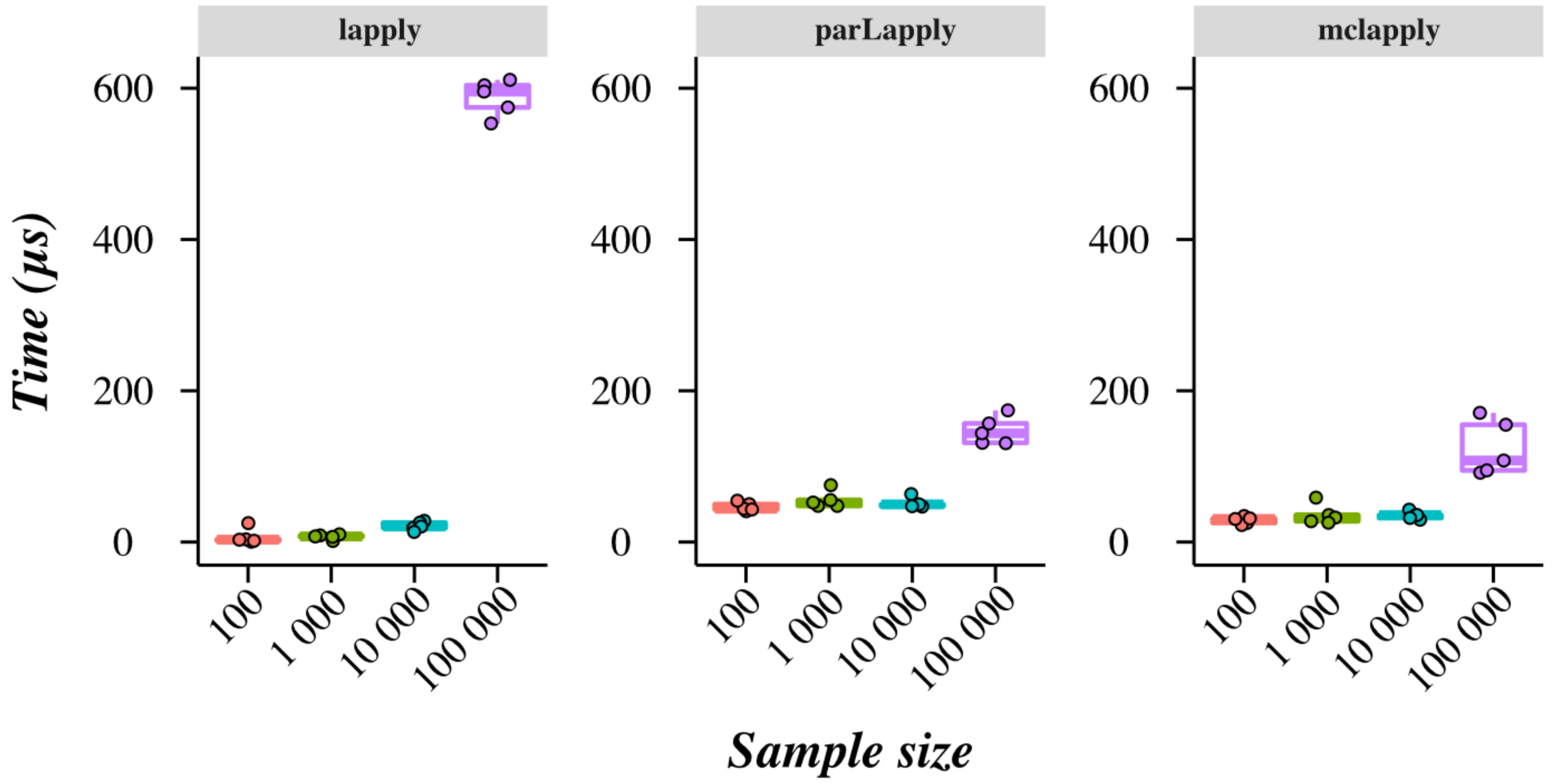
# lapply vs parLapply vs mclapply

```r
# Calculate mean FATHMM score for each gene

# lapply
res_l <- base::lapply(X = unique(dat$Gene.name), FUN = function(X)
mean(dat[dat$Gene.name == X, "FATHMM.score"], na.rm = T))


# parLapply (snow)
myCluster <- makeCluster(4,type = "FORK",useXDR=F,.combine=cbind)
registerDoParallel(myCluster)
res_par <- snow::parLapply(cl = myCluster, X = unique(dat$Gene.name),
        fun = function(X) mean(dat[dat$Gene.name == X, "FATHMM.score"], na.rm = T))
stopCluster(myCluster)


# mclapply (parallel)
res_mcl <- parallel::mclapply(X = unique(dat$Gene.name),
     FUN = function(X) mean(dat[dat$Gene.name==X,"FATHMM.score"],na.rm = T),
     mc.cores = parallel::detectCores())
```

# lapply vs parLapply vs mclapply



# Go parallel when there is "*critical mass*"



# saveRDS using multiple cores

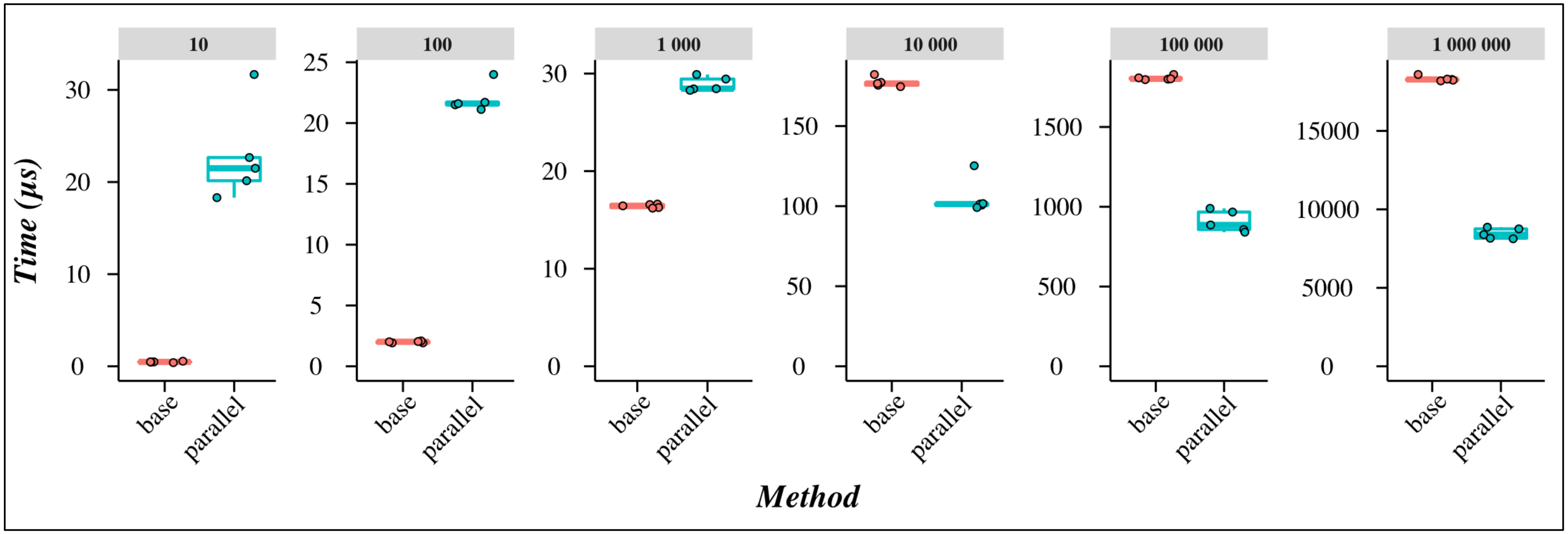
Parallelized version of saveRDS (uses parallelized .gz compression)
Get it: https://gist.githubusercontent.com/dchakro/8b1e97ba6853563dd0bb5b7be2317692/raw/parallelRDS.R

**Bottleneck**: disk I/O

```
# base::saveRDS
base::saveRDS(object = dat,
             compress = "gzip",
             file = "/dev/null")


# parallelized saveRDS
source("https://gist.githubusercontent.com/dchakro/8b1e97ba6853563dd0bb5b7be2317692
/raw/parallelRDS.R")

saveRDS.gz(object = dat,
           threads = parallel::detectCores(),
           compression_level = 6,
           file = "/dev/null")
```

# saveRDS using multiple cores

Parallelized version of saveRDS (uses parallelized .gz compression)
Get it: https://gist.githubusercontent.com/dchakro/8b1e97ba6853563dd0bb5b7be2317692/raw/parallelRDS.R



**Note**:

- It is possible to use `-T` in `xz` for multi-threaded compression (since xz version 5.2)
    - But the decompression (reading) isn't multi-threaded.

- https://github.com/vasi/pixz - offers parallelized decompression.

# Did you know ?

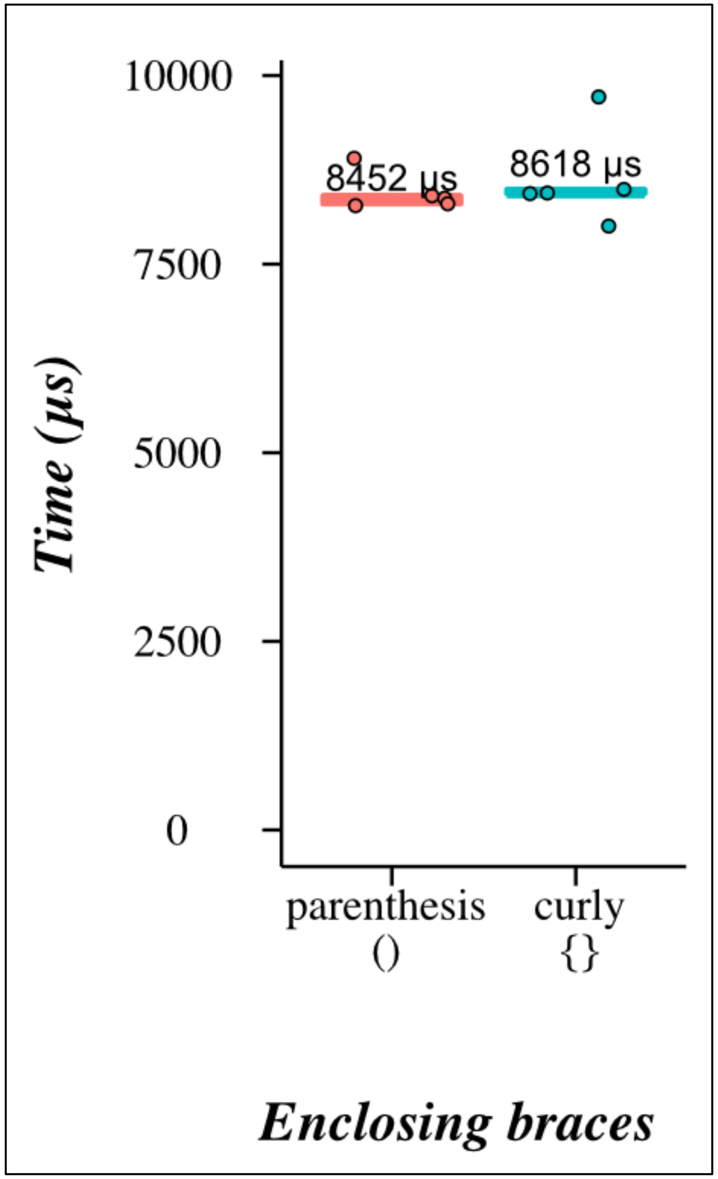
`utils::install.packages()` & `utils::update.packages()` support multiple processors in R.

Define the number of cores you want to use with the `Ncpus` parameter.

```
install.packages(c("affy","stringi","ggplot2","data.table"),
                 ...other arguments ... ,
                 Ncpus = parallel::detectCores())



update.packages(...package list... ,
                ...other arguments ... ,
                Ncpus = parallel::detectCores())
```

# { } vs ( ) – debunked ?

```r
# parenthesis
pM <- rep(NA,length(dat$Gene.name))
for(i in seq_along(dat$Gene.name)){

    pM[i] <- ((dat$ID_tumour[i] + dat$ID_sample[i] +
dat$MUTATION_ID[i]) / 3)

}

# curly
cM <- rep(NA,length(dat$Gene.name))
for(i in seq_along(dat$Gene.name)){

    cM[i] <- {{dat$ID_tumour[i] + dat$ID_sample[i] +
dat$MUTATION_ID[i]} / 3

}
```



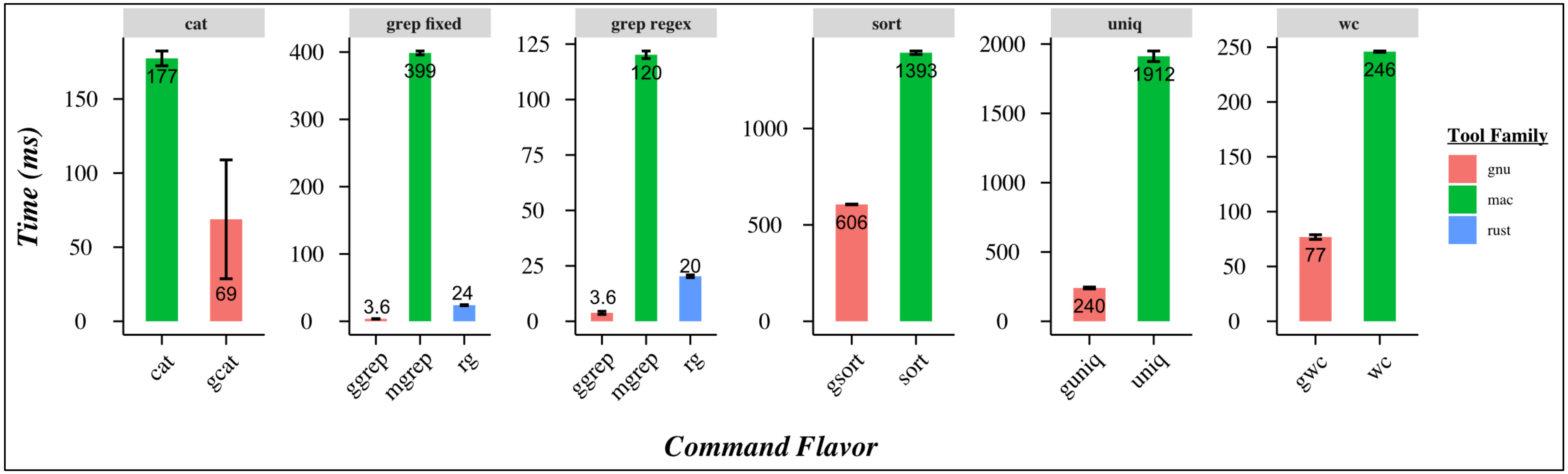
## **Summary / Tips** *(may depend on your use case)*

- Use vectorization
  - Use apply family of functions instead of iterating
- Remember, to check if you benefit from parallel computing
- Write a `function()` when possible:
  - Functions are compiled into byte-code by the JIT compiler in R
  - JIT is enabled by default since R version 3.4
- JIT also compiles `for()`, `while()` and `repeat()` structures
- Check function documentation for tips (e.g. `unlist` + `use.names`)
- Try to compile packages from source (optimized for your system).

# Bonus tips *(for Mac users)*

- Install Homebrew (https://brew.sh), and then install:
  - `brew install coreutils grep ripgrep`

- To log brew activity you can use: github.com/dchakro/brewlog
  - `brewlog install coreutils grep ripgrep`



Thank you!