

Taking R to its limits: 70+ tips

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ABSTRACT

R has many capabilities most of which are not known by many users, yet waiting to be discovered. For this reason we provide more tips on how to write really efficient code without having to program in C++, programming advices, and tips to avoid errors and numerical overflows.

INTRODUCTION

Efficient code is really important in large scale datasets, computations, or simulation studies. R may not be a scripting language or computationally efficient when compared to other open source programs, yet it has strong capabilities not known however to most of its users.

We will show a few tips for faster computations. The speed-ups one will in small sample and or low dimensions will be small, but in bigger datasets the differences are observable. One might observe a time difference of only 5 seconds in the whole process. Differences from 40 seconds to 12 seconds for example, or to 22 seconds are still worthy. But not always this kinds of differences will be experienced. Some times, one tip gives 1 second and then another tip 1 second and so on until you save 5 seconds. If a researcher has to run 1000 simulations, then they can save 5000 seconds. Our moto is that every decrease in time or memory matters.

Some times the speed-ups will appear with large samples only. To put it simply, for someone who needs a simple car, a very expensive car or a jeep type might not be of such use, especially if they do not go off-road. But for the user who needs a jeep, every computational power, every second they can gain matters.

We have listed 70+ tips that can help the user write more efficient code, use less memory, become more familiar with R and its commands. The list is not exhaustive and we are sure there are tips we are not aware of. However, this is the first time such a long list is available.

1 DURATION OF A PROCESSES

In order to measure the time your process or computation or simulation needs, one can do the following in R

```
runtime <- proc.time()
## put your function here
runtime <- proc.time() - runtime
## runtime gives you 3 numbers (all in seconds) like the ones below
user  system elapsed
0.18   0.07   3.35
```

The elapsed is the desired metric. Alternatively the package microbenchmark (Mersmann, 2015) which allows for comparison between two or more functions measuring the execution time even in the nanoseconds scale.

2 GENERAL ADVICE

We begin with a list of of programming advices.

- 38 1. Avoid unnecessary calculations. In a discriminant analysis setting for example there is no need
 39 to calculate constant parts, such as $\log(2\pi)$, every time for each group and every iteration. This
 40 only adds time and takes memory and does not affect the algorithm or the result. The same for
 41 the Euclidean or the Hellinger distance. The square root and the multiplication by the same factor
 42 everywhere makes no difference and if can be avoided, then it should be avoided.
- 43 2. Try to make the mathematics and hence the operations as simple as possible. The partial correlation
 44 coefficient can be computed with many ways. Two of them are via two regression models, or via
 45 the simple correlation matrix. The second one is much faster.
- 46 3. If you have a function which uses many regression models, not necessarily from different down-
 47 loadable R packages, but even from R's built-in models you should not to create a function for each
 48 model. This seems like the obvious thing to do, simply because different regression models have
 49 different signatures and hypothesis test with each of them is different, *lm* uses *F* test, *glm* use *F* or
 50 χ^2 test and so on.
- 51 The optimal solution is to write one function which includes all regression models and their
 52 arguments. This way, you have one inclusive function for all models, instead of many. Every time
 53 you want to add a new regression model you add it in this function and do not have to create a new
 54 function. This way, you have less files and require less memory.
- 55 4. When writing code, leave space between operations, parentheses, indent the lines inside the *for*
 56 loops. Put comments at the end of every loop so as to know to which loop each bracket refers to.
 57 This is really helpful if your code is long. Make your code more readable and *clean*. The goal is
 58 not only to make it readable by someone else, but mainly by yourselves. Clean code is easier to
 59 understand and edit. A good programmer makes mistakes, but detects them fast. If your code is
 60 long, has no spaces and no comments, spotting any mistakes can become a difficult task.
- 61 5. Understand how R works and what operations do, what you can or are not allowed to do. The
 62 command *mahalanobis* for example uses this line to calculate the distances.
- ```
rowSums(x %*% cov * x)
```
- 63 The first key message is that the function performs one and not two (as one would expect) matrix  
 64 multiplications. Secondly, the user is given the chance to see that he can apply these types of  
 65 operations. Thirdly, he is given the chance to make this function faster.
- 66 6. Do not use object oriented programming (S3,S4 methods) . It is not necessary and makes the hole  
 67 program slow but if it is necessary then try make you own object using environments.
- 68 7. If you have a vector *x* with integer numbers, it is preferable to have it *as.integer(x)* than *as.numeric(x)*.  
 69 The former requires less memory than the latter.

### 70 3 SIMPLE FUNCTIONS

- 71 We continue with a list of simple functions which will help you make your code more efficient and faster.
- 72 1. Do not expect that all packages or R itself have fast implementations. The function *mean* is slower  
 73 than *sum(x)/length(x)*. If you type *sum* you will see it is a *.Primitive* function whereas *crossprod* for  
 74 example is an *.Internal* function. Another example of a more advanced function is to perform many  
 75 univariate logistic regressions and each time calculate the deviance of the model. Create your own  
 76 functions, you will be surprised to see that you may do faster than R's built-in functions (it doesn't  
 77 always work that way).
- 78 2. The commands *cor* and *cov* are two very fast functions which can be used to calculate the correla-  
 79 tions or covariances between a vector and a matrix very efficiently. Many simple regression models  
 80 can be calculated using these two commands.
- 81 3. Search for functions that take less time. For example, the command *lm.fit(x,y)* is a wrapper for  
 82 *lm(y x)*, which means that the former is used by the latter. If you need only the coefficients, for  
 83 example, then use the first one. The syntax is a bit different, *x* must be the design matrix, and the  
 84 speed is also very different, especially in the big cases. The command *.lm.fit(x,y)* is even faster.

- 85 4. It's your algorithm. In a recent paper, Tsagris (2017) showed that conditional  $G^2$  tests of independence can become 3-4 faster if they are run using Poisson log-linear models and not by constructing the appropriate tables using *for* loops. There are many ways to perform your computations. Choose or implement the most appropriate and most efficient. For example, in order to generate vectors from the multivariate normal distribution you can either use spectral or Cholesky decomposition. The latter is faster. In general, try to find the optimal mathematical method or way for your problem.
- 91 5. Suppose you want to center some data. You can try with *apply*
- ```
cent <- function(x) x - mean(x)
a1 <- apply(data, 2, cent)
```
- 92 or use one of these
- ```
a2 <- scale(data, center = TRUE, scale = FALSE)
m <- colMeans(data)
a3 <- sweep(data, 2L, m)
a4 <- t(t(data) - m) ## this is from the previous tip
dm <- dim(data)
n <- dm[1]
p <- dm[2]
a5 <- data - rep(m, rep(n, p)) ## looks faster
```
- 93 6. If you want to extract the mean vector of each group you can use a loop (*for* function) or
- ```
a1 <- aggregate(x, by = list(ina), mean)
```
- 94 where *ina* is a numerical variable indicating the group. A faster alternative is the built-in command
- 95 *rowsum*
- ```
a2 <- rowsum(x, ina) / as.vector(table(ina))
a bit faster option is a3 below
a3 <- rowsum(x, ina, reorder = FALSE) / as.vector(table(ina))
```
- 96 7. Use *which.min(x)* and *which.max(x)* instead of *which( x == min(x) )* *which( x == max(x) )* to find the position of the minimum and maximum number respectively.
- 97
- ```
x <- array( dim = c(1000,10,10) )
for (i in 1:10) x[, , i] = matrix( rnorm(1000* 10), ncol = 10 )
a1 <- apply(x, 1:2, mean)
a2 <- t( colMeans( aperm(x) ) )
```
- 98 8. Incremental calculations. An example of this is the first order partial correlations, which can be computed from the simple correlations with fewer calculations. In general, if your function can perform calculations incrementally, the boost in the speed can be very high.
- 99
- 100
- 101 9. If you have a vector *x* and want to put it in a matrix with say 10 columns, do not write *as.matrix(x, ncol = 10)*, but *matrix(x, ncol = 10)*. The first method creates a matrix and puts the vector in. The second method, simply changes the dimension of *x*, instead of 1 column, it will now have 10. Again, about 2 times faster.
- 102
- 103
- 104
- 105 10. When it comes to calculating probabilities or p-values more specifically, do not do $1 - pchisq(stat, dof)$, but do *pchisq(stat, dof, lower.tail = FALSE)* as is a bit faster. In the tens of thousands of repetitions (simulation studies for example or an algorithm that requires p-values repeatedly), the differences become seconds.
- 106
- 107
- 108
- 109 11. When calculating operations such as *sum(a * x)*, where *x* is a vector or a matrix and *a* is a scalar (number) do *a * sum(x)*. In the first case, the scalar is multiplied with all elements of the vector (many multiplications), whereas in the second case, the sum is calculated first and then a multiplication between two numbers take place.
- 110
- 111
- 112

- 113 12. Suppose you want to calculate the factorial of some integers and most (or all) of those integers
 114 appear more than once (Poisson, beta binomial, beta geometric, negative binomial distribution for
 115 example). Instead of doing the operation for each element, do it for the unique ones and simply
 116 calculate its result by its frequency. See the example below. **Note however**, that this trick does not
 117 always work. It will work in the case where you have many integers and a *for* or a *while* loop and
 118 hence you have to calculate factorials all the time.

```
x <- rpois(10000, 5)
sum( lgamma(x + 1) )
y <- sort( unique(x) )
ny <- as.vector( table(x) )
sum( lgamma(y + 1) * ny )
```

- 119 13. If you use the *glm* or *lm* commands multiple times, then you should do

```
glm(y ~ x, family = ..., y = FALSE, model = FALSE)
lm(y ~ x, y = FALSE, model = FALSE)
```

120 The two extra arguments *y = FALSE, model = FALSE* reduce the memory requirements of the *glm*
 121 object.

- 122 14. When calculating $\log(1+x)$ use *log1p(x)* and not *log(1+x)* as the first one is faster.

- 123 15. A very useful command is *tabulate*.

```
table(iris[, 5])
tabulate(iris[, 5])
```

124 Two differences between these two are that *table* gives you a name with the values, but *tabulate*
 125 gives you only the frequencies. Hence, *tabulate(x) = as.vector(table(x))*. In addition, if you use
 126 *tabulate*, you can do so with factor variables as well. But, if you have numbers, a numerical vector,
 127 make sure the numbers are consecutive, and strictly positive, i.e. no zero is included.

```
x <- rep(0:5, each = 4)
table(x)
tabulate(x) ## 0 is missing
x <- rep(c(1, 3, 4), each = 5)
table(x)
tabulate(x) ## there is a 0 appearing indicating the absence of 2
```

128 The command *tabulate* is many times faster than *table*. For discriminant analysis algorithms,
 129 *tabulate* might be more useful, because of speed, when counting frequencies, it could be more
 130 useful as well, as it will return a 0 value if a number has a zero frequency. The drawback arises
 131 when you have negative numerical data, data with a zero or positive numbers but not consecutive.
 132 If you want speed, formulate your data to match the requirements of *tabulate*.

- 133 16. Vectorization can save tremendous amount of time even in the small datasets. Try to avoid *for* loops
 134 by using matrix multiplications. For example, instead of

```
for (i in 1:n) y[i] <- x[i]^2
```

135 you can use

```
y <- x^2
```

136 Of course, this is a very easy example, but our point is made. This one requires a lot of thinking
 137 and is not always applicable. But, if it can be done, things can be substantially faster.

- 138 17. Make use of the command *outer*. An example is where you have two vectors *x* and *y* and you want
 139 to add each element of *y* in *x*. The final item would be a matrix.

```
z <- matrix(0, nrow = length(x), ncol = length(y) )
for ( i in 1:dim(z)[1] ) z[i, ] <- x[i] + y
```

```
## The above task can take place a lot faster by typing
outer(x, y, "+")
```

- 140 18. The command `sort` has an extra feature, by specifying `index.return = TRUE`, the outcome is a list
 141 with the sorted numbers, along with their ordered indexes. That is, you call `sort(x, index.return =`
 142 `TRUE)` and the command sorts the numbers and returns their order as if you used `order` separately.
- 143 19. You can partially sort a vector. In the k-NN algorithm for example you want the k smallest distances.
 144 There is no need to sort all the distances, only the k smallest. Hence, `sort(x, partial=1:k)`.
- 145 20. When using `sort` select type `sort(x, method=quick)` in order to make it even faster, in most cases.
- 146 21. Many functions call internal function inside. `sort` for example calls `sort.int`, `sample` calls `sample.int`
 147 etc.
- 148 22. You are given many matrices in a list, "A", and wish to unlist all of them and create a new matrix,
 149 where the matrix of each element is added one under the other. The command to do this efficiently
 150 is
- ```
do.call(rbind, A)
```

#### 151 4 CALCULATIONS INVOLVING MATRICES

152 R is not designed to handle large scale datasets, yet there are many ways to efficiently handle matrices  
 153 and we present to you some tricks below.

- 154 1. Use `colMeans` and `rowMeans` instead of `apply(x, 1, mean)` and `apply(x, 2, mean)` as they are  
 155 extremely fast. In addition, many really fast functions can be produced using these two commands.
- 156 2. Avoid using `apply` or `aggregate` whenever possible. For example, use `colMeans` or `colSums` instead  
 157 of `apply(x, 2, mean)` to get the mean vector of a sample because it's faster. For the median though,  
 158 you have to use `apply(x, 2, median)` instead of a `for` going to every column of the matrix. The `for`  
 159 loop is not slower, but the `apply` is knitter.
- 160 3. If you have to use a `for` loop going through the rows of a matrix, consider transposing the matrix  
 161 and then go through its columns.
- 162 4. If you are given a matrix and by using a `for` loop you would like to extract some specific  
 163 columns/rows of the matrix each time. Instead of that, you can store the indices of the columns/rows  
 164 inside the `for` loop and outside simply extract the columns/rows and perform any operations you  
 165 want.
- 166 5. If you want to extract the number of rows or columns of a matrix **X**, do not use `nrow(X)` or `ncol(X)`,  
 167 but `dim(X)[1]` or `dim(X)[2]` as they are almost 2 times faster.
- 168 6. Suppose you have a matrix **X** and you want the position of the maximum for each row. The obvious  
 169 solution is `apply(X, 1, which.max)`. The efficient solution is `max.col(X)`.
- 170 7. If you want to subtract a vector from a matrix in a row-wise fashion, you should be aware of the fact  
 171 that R does it column-wise. This is because R reads, writes and stores data in a column-wise fashion.  
 172 For example, **X** is a matrix and **y** is a vector whose length is equal to the number of columns of **X**.  
 173 You should type
- ```
t(X) - y
```
- 174 8. If you take your input matrix and transpose it and never use the initial matrix in the subsequent
 175 steps it is best to delete the initial matrix, or even better store its transpose in the same object. That
 176 is, if you have a matrix **X**, you should do the following

```

Y <- t(X)  ## not suggested
X <- t(X)  ## suggested

```

177 We repeat that this in the case when x is not used again in latter steps. The reason for this is memory
 178 saving. If x is a big and you have a second object as big as the first one, you request your computer
 179 to use extra memory with no reason.

180 9. Use the command *prcomp* instead of *princomp*. The first one should be used for principal component
 181 analysis when you have matrices with more than 100 variables. The more variables the bigger the
 182 difference (40 times for example) from using *eigen(cov(x))*.

183 10. Create the vectors or matrices from the start. Instead of making a vector longer each time, using *c()*
 184 create an empty vector with the required size. The commands *rbind* and *cbind* are useful, but come
 185 with a heavy price. They are very expensive when called a lot of times.

186 11. For the covariance matrices the command *by* could be used. The matrices are stored in a list and
 187 then you need the command *simplify2array* to convert the list to an array in order to calculate for
 188 example the determinant of each matrix. The *for* loop is faster, at least that's what we have seen in
 189 our trials.

190 12. What if you have an array with matrices and want to calculate the sum or the mean of all the
 191 matrices? The obvious answer is to use *apply(x, 1:2, mean)*. R works in a column-wise fashion
 192 and not in a row-wise fashion. Instead of the *apply* you can try *t(colSums(aperm(x)))* and *t(*
 193 *colMeans(aperm(x)))* for the *sum* and *mean* operations respectively.

194 13. If you want to calculate the logarithm of the determinant of a matrix \mathbf{X} , instead of *log(det(X))*, you
 195 can type *determinant(X, logarithm = TRUE)* as it is slightly faster for small matrices. In the big
 196 matrices, say of dimensions 100×100 or more, the differences become negligible though.

197 14. If you want the matrix of distances, with the zeros in the diagonal and the upper triangular do not
 198 use the command *as.matrix(dist(x))* but use *dist(x, diag = TRUE, upper = TRUE)*.

199 15. Suppose you want the Euclidean distance of a single vector from many others (say thousands for
 200 example). The inefficient way is to calculate the distance matrix of all points and take the row
 201 which corresponds to your vector. The efficient way is to use the Mahalanobis distance with the
 202 identity matrix and the covariance matrix.

```

x <- rnorm(50)
y <- matrix( rnorm(1000 * 50), ncol = 50 )
a1 <- dist( rbind(x, y) )  ## inefficient way
Ip <- diag(50)
## a2 is a better way
a2 <- mahalanobis( y, center = x, cov = Ip, inverted = TRUE )

```

203 Another way is the following

```

z <- y - x
a <- sqrt( colSums(z^2) )

```

204 16. Calculating $\mathbf{X}^T \mathbf{Y}$ in R as *t(X)%*%Y* instead of *crossprod(X, Y)* causes \mathbf{X} to be transposed twice;
 205 once in the calculation of *t(X)* and a second time in the inner loop of the matrix product. The
 206 *crossprod* function does not do any transposition of matrices.

207 17. If you want to calculate the product of an $n \times p$ matrix $\mathbf{X}^T \mathbf{X}$ for example. The command *crossprod(X)*
 208 will do the job faster than the matrix multiplication.

```

t(X) %*% Y      ## classical
crossprod(X, Y) ## more efficient
X %*% t(Y)     ## classical
tcrossprod(X, Y) ## more efficient

```

```
t(X) %*% X ## classical
crossprod(X) ## more efficient
```

209 18. Let \mathbf{X} and \mathbf{m} be a matrix and a vector and want to multiply them. There are two ways to do it.

```
sum(m * x)
sum(x %*% m) ## a bit faster
```

210 19. When working with arrays it is more efficient to have them transposed. For example, if you have K
 211 covariance matrices of dimension $p \times p$, you would create an array of dimensions $c(p, p, K)$. Make
 212 its dimensions $c(K, p, p)$. If you want for example to divide each matrix with a different scalar
 213 (number) in the first case you will have to use a for loop, whereas in the transposed case you just
 214 divide the array by the vector of the numbers you have.

215 20. If you want to only invert a positive definite matrix (e.g. covariance matrix) then you should use
 216 `chol2inv(chol(X))` as it is faster.

217 21. To invert a matrix (not necessarily positive definite) and multiply the result with a vector or another
 218 matrix, there are two ways to do that

```
solve(X) %*% Y ## classical
## a much more efficient way is not
## to invert the matrix X
solve(X, Y)
```

219 22. The trace of the square of a matrix $\text{tr}(\mathbf{X}^2)$ can be evaluated either via

```
sum( diag( crossprod(X) ) )
```

220 or faster via

```
sum(X * X) ## or
sum(X^2)
```

221 23. If you want to calculate the following trace involving a matrix multiplication $\text{tr}(\mathbf{X}^T \mathbf{Y})$ you can do
 222 either

```
sum( diag( crossprod(X, Y) ) ) ## just like before
```

223 or faster

```
sum(X * Y) ## faster, like before
```

224 24. Moving in the same spirit, suppose you want the diagonal of the crossproduct of two matrices, then
 225 do

```
diag( tcrossprod(X, Y) ) ## for example
rowSums(X * Y) ## this is faster
```

226 25. Suppose you have two matrices \mathbf{A} , \mathbf{B} and a vector \mathbf{x} and want to find \mathbf{ABx} (the dimensions must
 227 match of course).

```
A %*% B %*% x ## inefficient way
A %*% (B %*% x) ## efficient way
```

228 The explanation for this one is that in the first case you have a matrix by matrix by vector calculations.
 229 In the second case you have a matrix by vector which is a vector and then a matrix by a vector. You
 230 do less calculations. The final tip is to avoid unnecessary and/or extra calculations and try to avoid
 231 doing calculations more than once.

232 26. As for the eigen-value decomposition, there are two ways to do the multiplication

```

s <- matrix( rnorm(100 * 100), ncol = 100 )
s <- crossprod(s)
eig <- eigen(s)
vec <- eig$vectors
lam <- eig$values
a1 <- vec %*% diag(lam) %*%t(vec)
a2 <- vec %*% ( t(vec) * lam ) ## faster way

```

- 233 27. The exponential term in the multivariate normal can be either calculated using matrices or simply
 234 with the command *mahalanobis*. If you have many observations and many dimensions and or many
 235 groups, this can save you a **lot** of time.

```

x <- matrix( rnorm(1000 * 20), ncol = 20 )
m <- colMeans(x)
n <- nrow(x)
p <- ncol(x)
s <- cov(x)
a1 <- diag( (x - rep(m, rep(n, p)) ) %*% solve(s)
%*% t(x - rep(m, rep(n, p)) ) )
a2 <- diag( t( t(x) - m ) %*% solve(s) %*% t(x) - m )
a3 <- mahalanobis(x, m, s) ## much faster

```

236 5 NUMERICAL OPTIMIZATION

- 237 1. The command *nlm* is much faster than *optim* for optimization purposes but *optim* is more reliable
 238 and robust. Try in your examples or cases, if they give the same results and choose. Or, use *nlm*
 239 followed by *optim*.
- 240 2. If you have a function for which some parameters have to be positive, do not use constrained
 241 optimization, but instead put an exponential inside the function. The parameter can take any values
 242 in the whole of R but inside the function its exponentiated form is used. In the end, simply take the
 243 exponential of the returned value. As for its variance use the δ -method (Casella and Berger, 2002).
 244 The trick is to use a link function, similarly to generalised linear models.
- 245 3. There are two ways to estimate the parameters of a distribution, Dirichlet for example. Either with
 246 the use *nlm* or via the Newton-Raphson algorithm. We performed some simulations and saw that
 247 the Newton-Raphson can be at least 10 times faster. The same is true for the circular regression
 248 (Presnell et al., 1998) when comparing *nlm* with the E-M algorithm as described by Presnell et al.
 249 (1998). Switching to E-M or the Newton-Raphson and not relying on *nlm* can save you a lot of
 250 time. If you want to write code and you have the description of the E-M or the Newton-Raphson
 251 algorithm available, then do it. Among these two, Newton-Raphson is faster.
- 252 4. If you have an iterative algorithm, such as Newton-Raphson, E-M or fixed points and you stop
 253 when the vector of parameters does not change any further, do not use *rbind*, *cbind* or *c()*. Store
 254 only two values, *vec.old* and *vec.new*. What we mean is, do not do for example

```

u[i, ] <- u[i - 1, ] + W%*%B ## not efficient
u.new <- u.old + W%*%B ## efficient

```

- 255 So, every time keep two vectors only, not the whole sequence of vectors. The same is true for the
 256 log-likelihood or the criterion of interest. Unless you want to keep track of how things change our
 257 advice is to keep two values only, the current and the previous one. Otherwise, apart from being
 258 faster, it also helps the computer run faster since less memory is used.

259 6 NUMERICAL OVERFLOWS

- 260 Numerical instabilities occur frequently when using real, not simulated, data. The reason why we mention
 261 these tricks is because one should not sacrifice numerical issues for the shake of speed. When trying to

262 speed-up code, we experienced numerical instabilities and overflows and we would like to share some of
263 the issues we faced.

- 264 1. The fitted values in a logistic regression model make use of the inverse of the logit function $\frac{e^x}{1+e^x}$. If
265 x is a really high number, the numerator becomes infinity (*Inf*). If however you write this formula
266 in its equivalent form $\frac{1}{1+e^{-x}}$, then the result is 1 as it should be.
- 267 2. The same is true for the Poisson regression or other regression which use the log as their link
268 function. In those cases one uses e^x . Try using e^{-x} instead.
- 269 3. Kernel functions are of the form $e^{\frac{f(\mathbf{X})}{h}}$, where h is a scalar and \mathbf{X} is a matrix. In order to speed up
270 the calculations one could pre-calculate $e^{f(\mathbf{X})}$ and then raise the result to the power of the different
271 values of h . This can easily result in overflow and *Inf* values. Speed-up can lead to overflow, hence
272 caution must be taken.
- 273 4. By Taylor series we know that $\log(1 + e^x) \simeq x$, but when $x \geq 13$ the two terms are equal $\log(1 + e^x) =$
274 x . Even the command *log1p* will not avoid the *Inf* result.
- 275 5. The product $\prod_{i=1}^n x_i$, where $0 < x_i \leq 1$, becomes 0 very fast. In order to avoid this, you should use
276 $e^{\sum_{i=1}^n \log x_i}$.
- 277 6. Use the logarithm of the p-values and not the p-values. This can be very beneficial when your
278 algorithm calculates and compares p-values. When the p-value is smaller than the 2.220446e-16
279 (*.Machine\$double.eps*) are rounded to zero. R cannot sort, correctly, p-values less than that number
280 because they are all considered equal to zero. If you have requested the logarithm of the p-values
281 though, those negative numbers can be sorted correctly.

282 7 PARALLEL COMPUTING IN R

283 If you have a machine that has more than 1 cores, then you can put them all to work simultaneously and
284 speed up the process a lot. If you have tricks to speed up your code that is also beneficiary. We have
285 started taking into account tricks to speed up my code as we have mentioned before.

286 The idea behind is to use a library that allows parallel computing. We make use of the *doParallel*
287 package (which uses the *foreach* package). Below are some instructions on how to use the package in
288 order to perform parallel computing. In addition, we have included the parallel computing as an option in
289 some functions and in some others we have created another function for this purpose. So, if you do not
290 understand the notes below, you can always see the functions in R packages that use this package.

```
## requires(doParallel)
Create a set of copies of R running in parallel and communicating
## over sockets.
cl <- makePSOCKcluster(nc) ## nc is the number of cluster you
## want to use
registerDoParallel(cl) ## register the parallel backend with the
## foreach package.
## Now suppose you want to run R simulations, could be
## R <- 1000 for example
## Divide the number of simulations to smaller equally
## divided chunks.
## Each chunk for a core.
ba <- round( rep(R/nc, nc) )
## Then each core will receive a chunk of simulations
ww <- foreach(j = 1:nc, .combine = rbind) %dopar% {
## see the .combine = rbind. This will put the results in a matrix.
## Every results will be saved in a row.
## So if you have matrices, make them vectors. If you have lists
## you want to return,
## you have to think about it.
```

```

a <- test(arguments, R = ba[j], arguments)$results
## Instead of running your function "test" with R simulations
## you run it with R/nc simulations.
## So a stores the result of every chunk of simulations.
return(a)
}
stopCluster(cl) ## stop the cluster of the connections.

```

291 To see your outcome all you have to press is `ww` and you will see something like this

```

result.1 .....
result.2 .....
result.3 .....
result.4 .....

```

292 The object `ww` contains the results you want to see in a matrix form. If every time you want a number,
 293 the `ww` will be a matrix with 1 column. We will see more cases later on. Note that if you choose to use
 294 parallel computing for something simple, multicore analysis might take the same or a bit more time than
 295 single core analysis only because it requires a couple of seconds to set up the cluster of the cores. In
 296 addition, you might use 4 cores, yet the time is half than when 1 core is used. This could be because not
 297 all 4 cores work at 100%.

298 In this example we have given each chunk of simulations to a core. Alternatively, one can have a *for*
 299 loop going through all columns of a matrix, for example. The latter is slower, but the former is not always
 300 possible.

301 8 EFFICIENTLY WRITTEN FUNCTIONS IN R PACKAGES

302 The multinomial regression is offered in the package VGAM (Yee, 2010), but it also offered in the package
 303 `nnet` (Venables and Ripley, 2002). The implementation in the second package is much faster. The same is
 304 true for the implementation of the ordinal logistic regression in the VGAM and in the ordinal (Christensen,
 305 2015). The latter package does it much faster. Also, the package *fields* (Nychka et al., 2015) has a function
 306 called *rdist* which is faster than the built-in *dist* in R. These are just some examples where functions are
 307 available in more than one packages, but do not share the same computational cost.

308 Regression models, commands calculate distance matrices matrix, statistical tests, utility functions
 309 and many more can also be found in the package Rfast (Papadakis et al., 2017). This package contains
 310 many fast or really fast functions, either written in C++ or simply using R functions exploiting fast built-in
 311 functions. *colMedians* for example is much faster than *apply(x, 2, median)*. The same is true for the
 312 *colVars*. Functions for matrices, distribution fitting, utility functions and many more are there and we
 313 keep adding functions. We have also implemented regression functions as well, which can handle large
 314 sample sizes (50,000 or more, for example) efficiently. All codes are accessible in the .R or .cpp source
 315 files of the package.

316 9 MORE ADVANCED PROGRAMMING TIPS

317 There are programming languages that offer you extravagant features. We will mention some of those
 318 who support R, as well as their strengths and benefits.

319 1. Operator overloading.

320

321 **General:** The overloading of operators is something incredibly handy and at the same time
 322 somehow dangerous. It allows you to manage your variables in the specific way that you declare.
 323 C++ supports overloading operators for a large number of operators, while others forbid it. R
 324 supports overload for a fairly large total (less than C++ since it contains fewer operators) of
 325 operators:

326 (a) brackets: `[]` (see in the special operators)

327 (b) double brackets: `[[]]` (see in the special operators)

328 (c) binary and unary operators:
`+, -, *, /, |, &, ^, %%, ==` (always 2 arguments)

329 (d) unary operators: (always 1 argument)

330 **Be careful:** Overloading is not supported for

`&&, ||, =, <-, ->, <<-, ->>.`

331 Although there is a way of overloading some of these operators that can be used together in a
 332 command, e.g. `[]` and `<-`, `[[]]` and `<-`.

333 The only drawback is that each operator is handled by a different set of arguments. However, there
 334 are no other drawbacks to R since all the above-mentioned operators (overloaded operators) are
 335 essential functions in relation to C++ that if you use overloading then the operators converted into
 336 functions (where you pay a penny as long as functions are called) while no surplus treatments are
 337 being handled in a completely different way. The advantage (for both R and C++) are: a) new ways
 338 of implementation, b) control of variables for error management (as does R in some cases) and c)
 339 perhaps even higher speed (depends on the algorithm).

340 **Implementation of overloading operators:** The algorithm for the implementation of the over-
 341 loading is the same for all overloaded operators (with some exceptions).

342 (a) Declare a variable (e.g. "x").

343 (b) Declare a variable with character value which represents anything you want.e.g. `new_class =`
 344 `"anything"`. This is the 1st important step for overloading operators.

345 (c) Change class for the variable from step (a): `class(x) <- new_class` This is the 2nd important
 346 step for overloading operators.

347 (d) Declare a function for the operator you want to overload. A general way is, let the operator
 348 be the "oper" which get values from the overloaded operators that R supports: "t.new_class"
 349 `<- function(whatever arguments the operator want)` a) Set class to null for its arguments. b)
 350 Execute the operator. c) Set class to `new_class_name`. *Be careful:* the function name is very
 351 important.

352 (e) Finished with the creation.

353 (f) Press: `x + x`

354 Special operators `[]` and `[[]]`: The operators `[]`, `[[]]` are used for access in some elements of a
 355 variable. There are 2 ways to use them, to extract an element and to import.

356 Extract:

```
357 []: ".new_class" <- function(x,i,...) {}
  [[]]: "[.new_class" <- function(x,i,...) {}
```

358 Import:

```
[[<- : "[<-.new_class" <- function(x, i, ..., value) { }
  [[]<- : "[[<-.new_class" <- function(x, i, ..., value) { return(x) }
```

359 **Be careful:** You don't have to write different functions for operators `<-`, `=`, `->`. You need only to
 360 use one of the three and R will understand the rest. Also you have to add one more argument for
 361 the import function because R uses it for the value to be stored. Finally, always return the argument
 362 "x".

363 E.g.

```

## OK
[]<- : "[<-.new_class" <- function(x, i, ..., v) { return(x) }

## will produce error
[]<- : "[<-.new_class" <- function(x, i) { return(x) }

## still OK but a bit risky
[]<- : "[<-.new_class" <- function(x, i, ...) { return(x) }

## for us, preferred way if you want to access more than one cells
[]<- : "[<-.new_class" <- function(x, ..., v) { return(x) }

```

364 Examples: Let's say we want to overload operator "+" for our own class.

365 (a) Declare a variable: `x |~ rnorm(10)`.

366 (b) Change class: `class(x) |~ "test_add"`.

367 (c) Create function.

```

"+.test_add" <- function(x, y) {
  class(x) <- class(y) <- NULL
  tmp <- x + y
  class(x) <- class(y) <- "test_add"
  tmp
}

```

368 (d) Create function for extract.

```

"|.test_add" <- function(x, ...){
  indices <- c(...)
  if (any (indices>length(x) ) ) {
    stop("Out of bounds in function '|~'")
  }
  class(x) <- NULL
  tmp <- x[indices]
  class(x) <- "test_add"
  tmp
}

```

369 (e) Create functions for import.

```

"<-.test_add"<-function(x, ...,v) {
  indices <- c(...)
  if ( any(indices>length(x) ) ) {
    stop("Out of bounds in function '<-'" )
  }
  class(x) <- NULL
  x[indices] <- v
  class(x) <- "test_add"
  x ## necessary step for R itself
}

```

370 2. Auto-printing your own class with your own style. In R you can print a variable using the functions
 371 "print";"cat" or just type the variables names and press the enter key. But what happened if you
 372 don't like the way that R treats the printing? that is the point of auto-printing. R support a general
 373 way to print your own class using its default function "print". The method is very simple but with
 374 one exception, you must change the class as we do in the 1st programming advise.

```
print.new_class_name(x, other_arguments_that_rs_print_passes) {
  cat("auto-printing my variable with class 'new_class_name'
    and value: ", x)
}
```

375 Example:

376 (a) Create a variable: `x`;-0

377 (b) Change its class: `class(x)`;- "anything"

378 (c) create the function to print the variable:

```
print.anything(x, other_arguments_that_rs_print_passes) {
  cat("Auto-printing variable of class anything: ", x)
}
```

379 (d) Press: `print(x)`

380 (e) That's it.

381 3. Using if-else in one line. Another feature in C++ is the ternary operator (which is not overloaded).
 382 General is an if-else statement with different syntax, sometimes more fast than if-else and also with
 383 one more capability, it returns the last command. That means the ternary operator is an if-else
 384 assign syntax. R support it also in the default if-else syntax. This can reduce the length of the code.
 385 Example:

```
if (is true) {
  x <- 1
} else {
  x <- 2
}
```

386 The above example is very simple but it needs 5 lines to be written. Lets reduce it:

```
x <- if (is true) 1 else 2
```

387 In a single line we have the same code. *Be careful* with the syntax and the last returned statement to
 388 be the one you want to initialize the variable "x". For more than one commands use curly brackets.
 389 This works fine because of the if-else. The *if-else* in R is like a function which always return the
 390 last command if you write it with the way that functions uses to return a variable. Not using the
 391 "return" keyword, but just write the variable. *Note*: you can do the same exactly thing with *if-else-if*
 392 but do not forget to careful with the syntax.

393 4. Iterate vector. If you want to iterate a vector and use the variables for something you can do:

```
x <- rnorm(10)
for (i in 1:length(x) ) {
  cat(x[i])
}
```

394 This is classic. Another way to iterate through vector is:

```
x <- rnorm(10)
for ( i in x) {
  cat(i)
}
```

395 The second way is the same with the first one but instead of using the indices for the vector, then
 396 you use the vector itself. With the second way you eliminate one more action for each element of
 397 "x" in *for* loop. This means that the total eliminations is "length(x)". So, you can decrease your
 398 speed, not much but, satisfactorily.

399 5. Efficient implementation of R's factor using any build-in type. *Factor* is a clever implementation of
 400 an integer vector. It has for values integers that are indices to a character vector with values the
 401 initial that user gives. It uses low memory because a character value needs memory equal to its
 402 length but loses in speed because you have to convert from the initial type to character. This means
 403 that if someone wants to extract a value and convert to its real type then it is slow. Fortunately the
 404 build in `as.integer` functions are quite fast with one exception, the function `as.character` needs a lot of
 405 execution time for convert each number. It is reasonable but imagine a large data set. Also factor is
 406 a read-only vector (by default in R). Lets see the code:

407 (a) We are going to use an environment which is a reference struct so R will never copy it.

```
uf <- new.env()
## with this step we can apply all the above tricks
class(uf) <- "ufactor"
```

408 (b) Create local variables inside "uf" and a wrapper function:

```
ufactor <- function(x) {
  un <- sort( unique(x), method = "quick" )
  uf$values <- match(x, un)
  uf$levels <- un
  lockBinding("values", uf)
  lockBinding("levels", uf)
  lockEnvironment(uf)
  x
}
```

409 (c) Create function extract element extraction:

```
".ufactor" <- function(uf, i) {
  uf$levels[ uf$values[i] ]
}
```

410 Be careful: we don't need a function for import element because R doesn't support it. We
 411 want our variable to behave exactly like R's built-in.

412 (d) Create function for auto-printing the variable:

```
print.ufactor <- function(x) {
  cat("Levels:\n ")
  options(digits=15)
  cat( uf$levels[uf$values] )
  cat("Values:\n ")
  cat(uf$values)
}
```

413 And that's it. with this 5 steps we have a more general factor supporting the 4 built-in types
 414 (character, integer, numeric, logical) just like R. R might support more but we care for these mostly.
 415 So if you want to get the values and levels you don't need to use `as.integers/levels` but instead use
 416 the "\$" to access the local variables. We also use the lock functions to lock environment and local
 417 variables of our `ufactor` just to remind the user to do not change them at all. R will produce an error.
 418 In the end, our variable "uf" is an environment with class "ufactor" (for untyped factor) and you
 419 can use it for anything without losing speed with the copies that R might do or not. Example:

```
x <- sample( rnorm(10), 1000, replace = TRUE)
r_factor <- factor(x)
u_factor <- ufactor(x)
all.equal( as.integer(r_factor), u_factor$values) ## TRUE
all.equal( levels(r_factor), as.character(u_factor$levels) ) ## TRUE
```

```
print(r_factor)
print(uf_factor)
r_factor[1] == u_factor[1] ## TRUE
```

420 10 CONCLUSION

421 We have provided a long list of efficient coding tips to help the user make their programs faster. In some
422 cases, the user can benefit from having functions that use less memory, which is also another important
423 feature, apart from speed. We also provided tips to avoid numerical instabilities and numerical overflows.
424 These tips should not go unattended as one can easily face such errors when trying to optimize the
425 efficiency of their code.

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