(A bit of) Advanced R

Part 1 - towards better R-base programming

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Outline

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

References

- R Core Team (2017): A Language and Environment for Statistical Computing https://www.R-project.org/
- Wickham (2014): Advanced R, retrieved from http://adv-r.had.co.nz/
- Gillespie & Lovelace (2016): efficient R programming https://bookdown.org/csgillespie/efficientR/

Prerequisites

Data Structure in base R

- 1 Atomic vector (integer, double, logical, character)
- Recursive vector (list)
- § Factors
- Matrices and array
- 6 Data Frame
- → Creation, Basic Operation, Manipulation, Representation

Resources

- Advanced R, chapters I.2, I.3 (Wickham, 2014, http://adv-r.had.co.nz/)
- An introduction to R programming http://julien.cremeriefamily.info/teachings_L3BI_ISV51.html

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The [a-z]*pply family I

Example with factors (tapply)

```
data <- rnorm(100)
sexe <- factor( sample(c("H","F"), 100, replace = TRUE))
mean.1 <- tapply(data, sexe, mean) ## good
mean.2 <- c() ## complicated
for (1 in levels(sexe))
   mean.2 <- c(mean.2, mean(data[sexe == 1]))</pre>
```

Example with list or data.frame (sapply/lapply)

The [a-z]*pply family II

[1] TRUE [1] TRUE [1] TRUE [1] FALSE

The do.call function I

2 ridge 0.6686981 0.9713040 ## 3 bayes 0.8816718 124.5252348

constructs and executes a function call from a name or a function and a list of arguments to be passed to it

Suppose you have the outputs of 100 simulations at your disposable, stored in a list like that

The do.call function II

[1] 300

```
## [1] 100
How would you store them in a single data frame?
all.res <- do.call(rbind, res)
dim(all.res)</pre>
```

The Reduce function

'Reduce' uses a binary function to successively combine the elements of a given vector

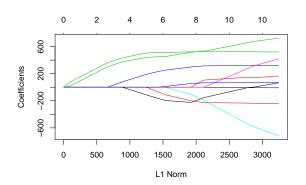
 \leadsto can be use to post-process your list of simulations obtained via mclapply just like do.call

Say more... (map, Reduce)

A Reduce example: "jacknifing" a lasso solution path

A single Lasso fit of the diabete data set

```
library(glmnet)
library(lars) # the diabetes data set (part of the lars package)
data(diabetes)
y <- diabetes$y
x <- diabetes$x
n <- length(y)
lasso <- glmnet(x,y)
plot(lasso)</pre>
```



A Reduce example: "jacknifing" a lasso solution path II I

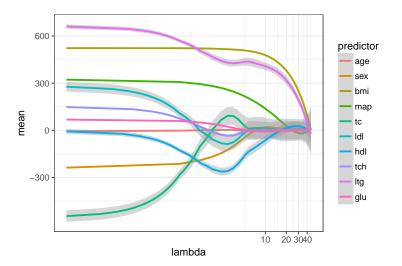
Compute the regularization paths for all subsets, removing one individual at once

```
paths <- parallel::mclapply(1:n, function(i) {
    glmnet(x[-i, ], y[-i], lambda = lasso$lambda)$beta
}, mc.cores = 4)</pre>
```

Computing the envelop around the average regularization path with Reduce

mean.path <- Reduce("+", paths)/n

A Reduce example: "jacknifing" a lasso solution path II II



Outline

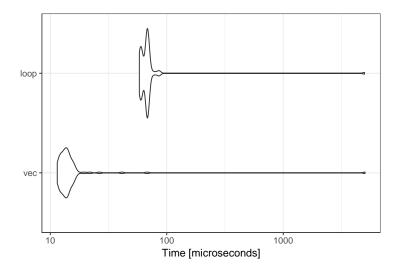
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Vectorize any algebraic operation I

```
Example: compute \exp(x) = \sum_{k=0}^n \frac{x^k}{k!} ## the good way \exp_{\text{vec}} < -\text{function}(\mathbf{x}, \mathbf{n}) { res < -\text{sum}(\mathbf{x}^{\circ}(0:\mathbf{n})/\mathbf{c}(1,\text{cumprod}(1:\mathbf{n}))) res } ## the sad/bad/less readable way \exp_{\text{loop}} < -\text{function}(\mathbf{x}, \mathbf{n}) { res < -1 for (k in 1:n) res < -\text{res} + 2^{\circ} \mathbf{k}/\text{factorial}(\mathbf{k}) res }
```

autoplot(microbenchmark(vec = exp vec(2, 100), loop = exp loop(2, 100)))

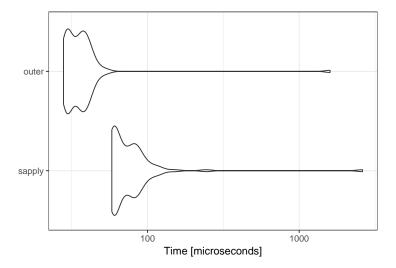
Vectorize any algebraic operation II



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

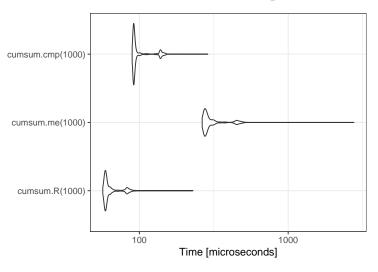


Compile your functions with base::compiler |

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

```
cumsum.R <- function(n) {</pre>
  x \leftarrow rnorm(n)
  cumsum(x)
cumsum.me <- function(n) {</pre>
  x \leftarrow rnorm(n)
  res <- 0
  for (i in 1:length(x))
    res <- res + x[i]
  res
cumsum.cmp <- compiler::cmpfun(cumsum.me)</pre>
autoplot(
  microbenchmark(
    cumsum.R(1000),
    cumsum.me(1000),
    cumsum.cmp(1000),
    times=1000)
```

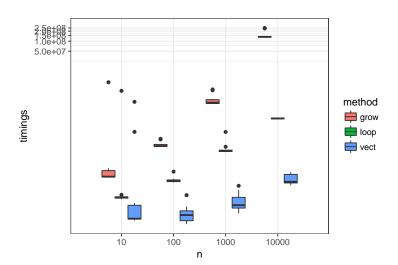
Compile your functions with base::compiler II



→ 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}</pre>
```

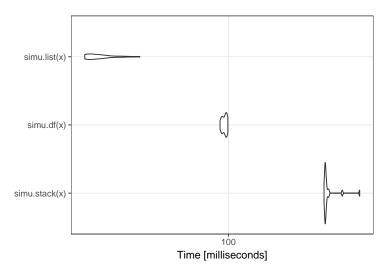


Do not stack objects I

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,])) )</pre>
  return(out)
simu.df <- function(x) {
  out <- data.frame(mean = numeric(n), sd = numeric(n))</pre>
  for (i in 1:n)
    out[i, ] \leftarrow 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,])))</pre>
  out <- data.frame(do.call(rbind, my.list))</pre>
  colnames(out) <- c("mean"."sd")</pre>
  return(out)
n \leftarrow 1000; p \leftarrow 10; x \leftarrow matrix(rnorm(n*p), n, p)
autoplot(microbenchmark(simu.stack(x), simu.df(x), simu.list(x), times=20))
```

Do not stack objects II



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

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

```
func.one <- function(n) {return(rnorm(n,0,1))}
func.two <- function(n) {return(rpois(n,1))}

n <- 1000
system.time(replicate(100, func.one(n)))

## user system elapsed
## 0.012 0.000 0.011
system.time(replicate(100, func.two(n)))</pre>
## user system elapsed
```

0.000

##

0.008

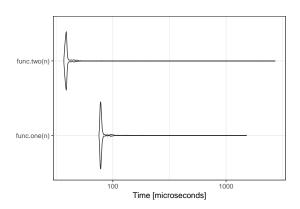
0.010

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)</pre>
```



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) {</pre>
  require (MASS)
  ## draw data
  x <- matrix(rnorm(n*p),n,p)
  v <- rnorm(n)
  ## center/scale
  xs <- scale(x)
  vs \leftarrow v - mean(v)
  ## 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)
summarvRprof("profiling.out")$bv.self</pre>
```

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

```
##
                     self.time self.pct total.time total.pct
## "La.svd"
                          1.20
                                 68.57
                                            1.20
                                                    68.57
## "aperm.default"
                          0.15 8.57
                                            0.15 8.57
                         0.15 8.57
  "is finite"
                                            0.15
                                                   8.57
  "na.omit.data.frame"
                         0.10 5.71
                                            0.10
                                                     5.71
## "lapply"
                         0.05 2.86
                                            1.75 100.00
## "arrav"
                         0.05
                                  2.86
                                            0.05
                                                     2.86
## "rnorm"
                          0.05
                                  2.86
                                            0.05
                                                     2.86
```

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

Profile your code with base Rprof II

##		total.time	-		self.pct
##	"lapply"	1.75	100.00	0.05	2.86
##	"block_exec"	1.75	100.00	0.00	0.00
##	"call_block"	1.75	100.00	0.00	0.00
##	"evaluate"	1.75	100.00	0.00	0.00
##	"evaluate_call"	1.75	100.00	0.00	0.00
##	"evaluate::evaluate"	1.75	100.00	0.00	0.00
##	"FUN"	1.75	100.00	0.00	0.00
##	"in_dir"	1.75	100.00	0.00	0.00
##	"knit"	1.75	100.00	0.00	0.00
##	"knitr::knit"	1.75	100.00	0.00	0.00
##	"process_file"	1.75	100.00	0.00	0.00
##	"process_group"	1.75	100.00	0.00	0.00
##	"process_group.block"	1.75	100.00	0.00	0.00
##	"rmarkdown::render"	1.75	100.00	0.00	0.00
##	"withCallingHandlers"	1.75	100.00	0.00	0.00
##	"eval"	1.70	97.14	0.00	0.00
##	"handle"	1.70	97.14	0.00	0.00
##	"my_func"	1.70	97.14	0.00	0.00
##	"timing_fn"	1.70	97.14	0.00	0.00
##	"withVisible"	1.70	97.14	0.00	0.00
##	"lm.ridge"	1.45	82.86	0.00	0.00
##	"svd"	1.35	77.14	0.00	0.00
##	"La.svd"	1.20	68.57	1.20	68.57
##	"aperm"	0.20	11.43	0.00	0.00
##	"scale"	0.20	11.43	0.00	0.00
##	"scale.default"	0.20	11.43	0.00	0.00

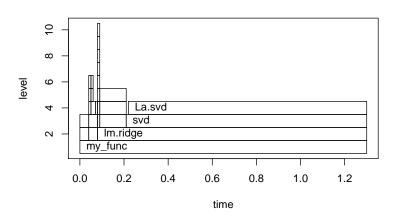
Profile your code with base Rprof III

##	"aperm.default"	0.15	8.57	0.15	8.57
##	"is.finite"	0.15	8.57	0.15	8.57
##	"apply"	0.15	8.57	0.00	0.00
##	"na.omit.data.frame"	0.10	5.71	0.10	5.71
##	"eval.parent"	0.10	5.71	0.00	0.00
##	".External2"	0.10	5.71	0.00	0.00
##	"model.frame.default"	0.10	5.71	0.00	0.00
##	"na.omit"	0.10	5.71	0.00	0.00
##	"stats::model.frame"	0.10	5.71	0.00	0.00
##	"array"	0.05	2.86	0.05	2.86
##	"rnorm"	0.05	2.86	0.05	2.86
##	"handle_output"	0.05	2.86	0.00	0.00
##	"matrix"	0.05	2.86	0.00	0.00
##	"par"	0.05	2.86	0.00	0.00
##	"plot_snapshot"	0.05	2.86	0.00	0.00
##	"sweep"	0.05	2.86	0.00	0.00
##	"unlist"	0.05	2.86	0.00	0.00
##	"w\$get_new"	0.05	2.86	0.00	0.00

Profile your code with profr

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

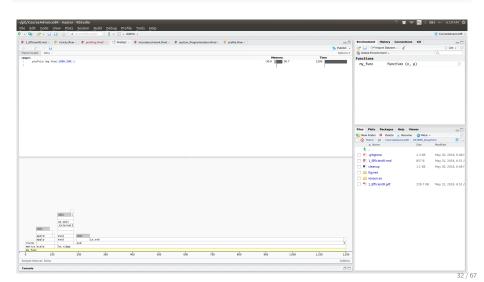
```
library(profr)
profiling <- profr({my_func(1000,500)}, interval = 0.01)
plot(profiling)</pre>
```



Profile your code within R Studiow with profvis

Profvis integrates the profiling to the Rstudio API

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



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Parallel computing

Usual Roadmap

- f 0 Start up and intialize M 'worker' processes
- Send data required for each task to the workers
- $oldsymbol{3}$ Split the task into M roughly equally-sized chunks and send them (including the R code needed) to the workers
- 4 Wait for all the workers to complete their tasks, and ask them for their results
- **5** Repeat steps (2–4) for any further tasks
- 6 Shut down the worker processes

Socketing vs Forking

Two approaches achieving the same goal

The socket approach

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

The forking approach

- copies the entire current version of R and moves it to a new core
- several processes acheive the same task resulting in different outputs
- → Forking is only possible on Unix systems (Linux, Mac OS)

Parallel computing with parallel

Package parallel

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

Check your computer

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

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

 \leadsto parallel features both socketing (parLapply) and forking (mclapply)

Forking approach with parallel::mclapply

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

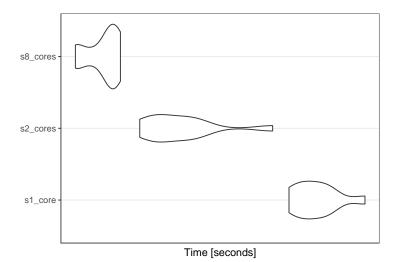
Example: estimates the test error from ridge regression

```
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)))
}</pre>
```

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

```
## err sd
## [1,] 13.05205 18.83241
## [2,] 11.55134 16.13871
## [3,] 14.30768 18.50712
```

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



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</pre>
```

```
## [,1] [,2] [,3] [,4] [,5] [,6] [,7]
## err 13.49596 8.664762 11.92576 16.50807 11.66757 11.9488 10.24255
## sd 17.35077 12.70468 17.35847 22.63689 15.63746 16.89484 15.01289
## [,8]
## err 10.59383
## sd 14.29349
```

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)
```

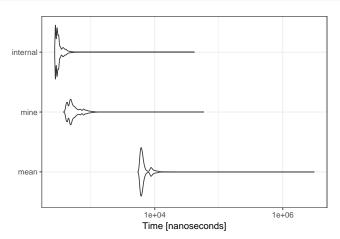
```
## [,1] [,2] [,3] [,4] [,5] [,6] [,7]
## err 13.30902 9.801744 10.50707 11.04491 10.75684 11.29892 15.66317
## sd 19.76283 14.13212 14.63621 15.87187 13.71803 15.57207 21.81625
## [,8]
## err 11.09748
## sd 14.70388
```

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Internal function are faster

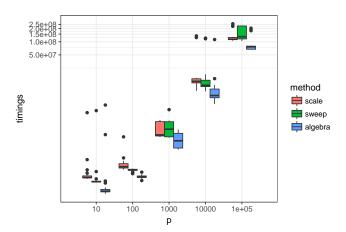
Function defined internally are sometimes incredibly faster (written in C), but cannot by called in packages submitted to CRAN.



Mind some algebra

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

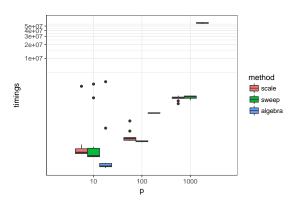
```
center1 <- function(x) return(scale(x, colMeans(x), FALSE))
center2 <- function(x) return(sweep(x, 2, colMeans(x), "-", check.margin = FALSE))
center3 <- function(x) return(x - outer(rep(1, nrow(x)), colMeans(x)) )
seq.p <- 10^(1:5); n <- 100; times <- 20</pre>
```



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</pre>
```



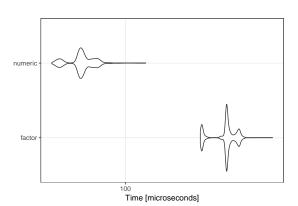
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Factor conversion are slow (nlevels)

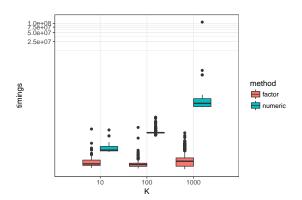
Do not convert large vector to factor if you need to perform just one operation on it.

```
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)
)</pre>
```



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

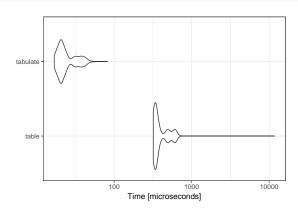
Use factor if you need repeated operations on the same vector.



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)
)</pre>
```



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
```

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] 0.0999999999999999
```

R masks the numerical errors

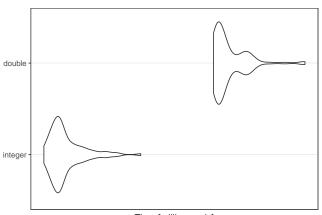
[1] TRUE

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] 0.0999999999999999
Try
all.equal(.1, .3/3)
```

Variable type matters

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



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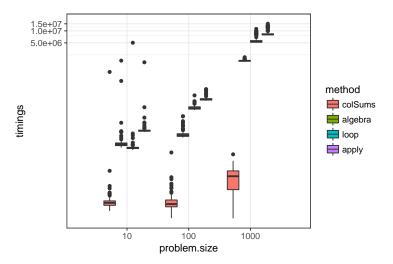
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The row/colSums family I

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
}</pre>
```

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).

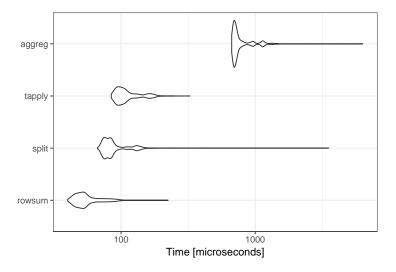
```
vec <- runif(1000)
grp <- sample(1:5, 1000, TRUE)
print(c(rowsum(vec, grp)))</pre>
```

[1] 119.25299 92.34115 90.63687 115.88947 105.82181

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)</pre>
```

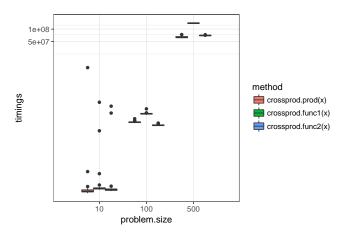
The secret function rowsum II



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))</pre>
```

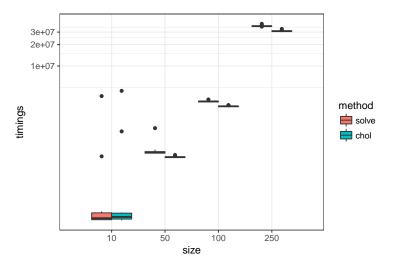


Dedicated function: inverting a PD matrices I

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.
                            = rep(as.character(p),times)))
                    size
```

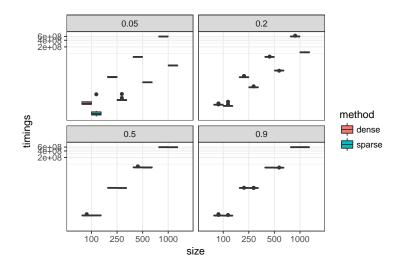
Dedicated function: inverting a PD matrices II



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.)

The Matrix package II



Outline

- ¶ Function, Functionals
- 2 Good and bad practices in R
- Benchmark your code
- 4 Use all your cores when needed
- **5** Tricks
- 6 Remember that R is object oriented
- 7 Mind your vocabulary: R fast built in function

Interfacing C++ with R is really easy I

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

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

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

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

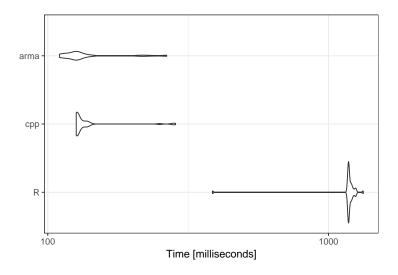
int n = x.size();
  NumericVector res(x);
  res(0) = log(x(0));
  for (int i=1; i<n; i++) {
    res(i) = res(i-1) + log(x(i));
  }
  return(wrap(res));
}')</pre>
```

Interfacing C++ with R is really easy II

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

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

Interfacing C++ with R is really easy III



Interfacing C++ with R is really easy I

Example that couples C+++ algebraic tricks

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

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

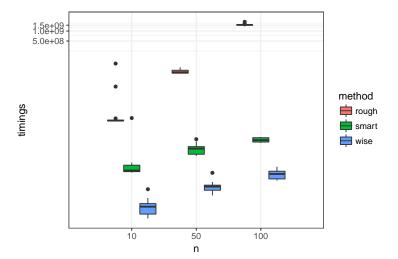
```
library(Matrix); library(inline); library(RcppArmadillo)

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

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

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

Interfacing C++ with R is really easy II



References

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