University of BRISTOL

How to write an efficient script

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23 June 2022

Introduction

This session will cover;

- Identifying bottlenecks
- The `apply` family
- Parallelizing a script
- High performance computing

Identifying bottlenecks: `system.time()`

```
system.time({
  n <- 1000
  r <- numeric(n)
  for(i in 1:n) {
    x <- rnorm(n)
    r[i] <- mean(x)
  }
})
##    user  system elapsed
##    0.11    0.02    0.13
```

`user` is the time taken to excute the code, `system` is time for the system to open and close files, and `elapsed` is the stopwatch time, i.e. total time code took from start to finish.

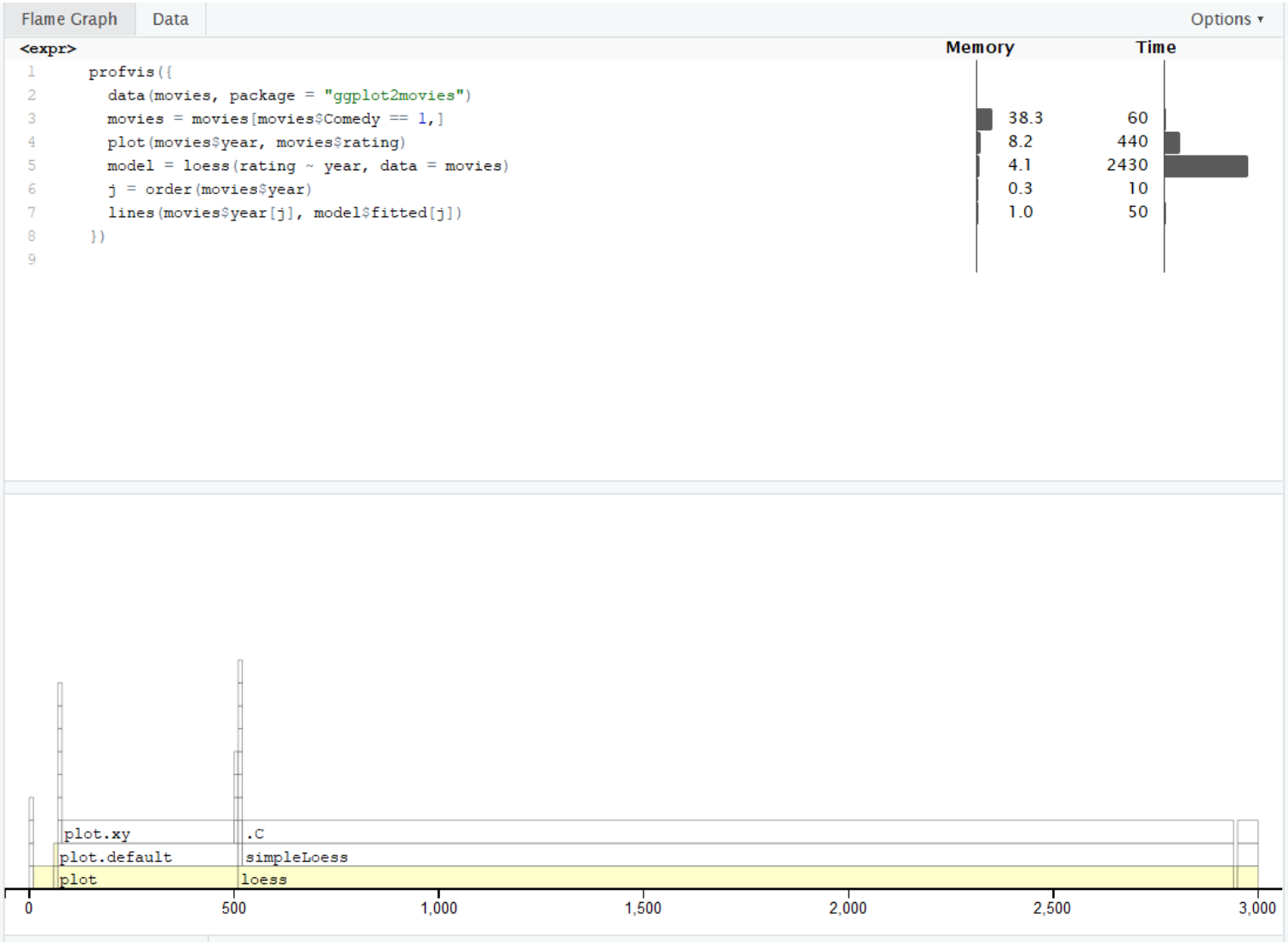
Identifying bottlenecks: The R Profiler

```
library(profvis)
library(bench)
library(ggplot2movies)

profvis({
  data(movies, package = "ggplot2movies")
  movies = movies[movies$Comedy == 1,]
  plot(movies$year, movies$rating)
  model = loess(rating ~ year, data = movies)
  j = order(movies$year)
  lines(movies$year[j], model$fitted[j])
})
```

Output

Outputs a tab called “Profile1”;



The apply family

are faster and safer than loops. We will cover

- apply()
- lapply()
- sapply()

but there are also others,

- vapply()
- mapply()
- rapply()
- tapply()

apply()

```
str(apply)
## function (X, MARGIN, FUN, ..., simplify = TRUE)
```

`X` is the input, `MARGIN` should be row (1) or column (2), or both (c(1,2)), `FUN` is the function. Depending what the input is, it can return a vector, list, matrix or array.

apply() example

```
data_fun<-matrix(c(1:4,1:4,1:4,1:4),4,4)
data_fun
##      [,1] [,2] [,3] [,4]
## [1,]    1    1    1    1
## [2,]    2    2    2    2
## [3,]    3    3    3    3
## [4,]    4    4    4    4

apply(data_fun,2,sum)
## [1] 10 10 10 10

apply(data_fun,2,mean)
## [1] 2.5 2.5 2.5 2.5
```

apply() example with function

```
data_fun<-matrix(c(1:4,1:4,1:4,1:4),4,4)
data_fun
##      [,1] [,2] [,3] [,4]
## [1,]    1    1    1    1
## [2,]    2    2    2    2
## [3,]    3    3    3    3
## [4,]    4    4    4    4

apply(data_fun, 1:2, function(x) x/2)
##      [,1] [,2] [,3] [,4]
## [1,]  0.5  0.5  0.5  0.5
## [2,]  1.0  1.0  1.0  1.0
## [3,]  1.5  1.5  1.5  1.5
## [4,]  2.0  2.0  2.0  2.0
```

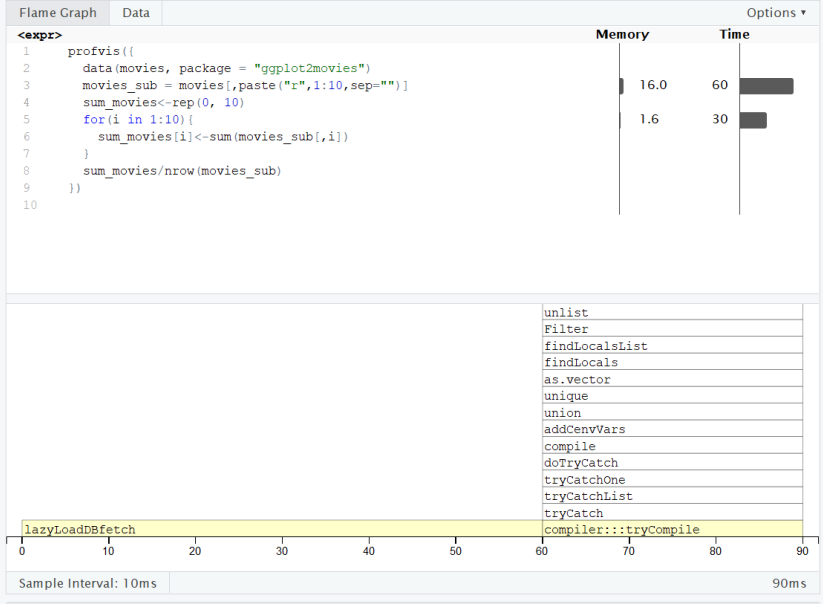
apply vs loops

```
# Using for loop
profvis({
  data(movies, package = "ggplot2movies")
  movies_sub = movies[,paste("r",1:10,sep="")]
  sum_movies<-rep(0, 10)
  for(i in 1:10){
    sum_movies[i]<-sum(movies_sub[,i])
  }
  sum_movies/nrow(movies_sub)
})
```

apply vs loops

```
# Using `apply()` function;
profvis({
  data(movies, package = "ggplot2movies")
  movies_sub = movies[,paste("r",1:10,sep="")]
  apply(movies_sub, 2, mean)
})
```

apply vs loops



Inputs matters

Previous examples used matrices how about data frame?

```
data_df<-data.frame(1:4,1:4,1:4,1:4)
str(data_df)
## 'data.frame':    4 obs. of  4 variables:
##  $ X1.4  : int  1 2 3 4
##  $ X1.4.1: int  1 2 3 4
##  $ X1.4.2: int  1 2 3 4
##  $ X1.4.3: int  1 2 3 4

apply(data_df, 2, mean)
##   X1.4 X1.4.1 X1.4.2 X1.4.3
##    2.5    2.5    2.5    2.5
```

Inputs matters

```
data_df$Day<-as.factor(1:4)
str(data_df)
## 'data.frame':    4 obs. of  5 variables:
##  $ X1.4  : int  1 2 3 4
##  $ X1.4.1: int  1 2 3 4
##  $ X1.4.2: int  1 2 3 4
##  $ X1.4.3: int  1 2 3 4
##  $ Day   : Factor w/ 4 levels "1","2","3","4": 1 2 3 4

apply(data_df, 2, mean)
##   X1.4 X1.4.1 X1.4.2 X1.4.3    Day
##     NA     NA     NA     NA     NA
```

. . . options

. . . within the function have multiple options but the most option is to use for handling missing data

```
data_miss<-matrix(c(1:4,c(1:3,NA),1:4,1:4),4,4)
data_miss
##      [,1] [,2] [,3] [,4]
## [1,]    1    1    1    1
## [2,]    2    2    2    2
## [3,]    3    3    3    3
## [4,]    4   NA    4    4

apply(data_miss, 2, mean)
## [1] 2.5  NA 2.5 2.5
apply(data_miss, 2, mean, na.rm=T)
## [1] 2.5 2.0 2.5 2.5
```

lapply()

```
str(lapply)
## function (X, FUN, ...)
```

`X` is the input, `FUN` is the function. Only returns list object.

lapply() example

```
list_fun<-list(a = 1:5, b = 10:15, c = 21:25)
list_fun
## $a
## [1] 1 2 3 4 5
##
## $b
## [1] 10 11 12 13 14 15
##
## $c
## [1] 21 22 23 24 25
```

lapply() example

```
lapply(list_fun,sum)
## $a
## [1] 15
##
## $b
## [1] 75
##
## $c
## [1] 115
```

lapply() example

```
lapply(list_fun,mean)
## $a
## [1] 3
##
## $b
## [1] 12.5
##
## $c
## [1] 23
```

lapply() example with function

```
lapply(list_fun, function(x) x/2)
## $a
## [1] 0.5 1.0 1.5 2.0 2.5
##
## $b
## [1] 5.0 5.5 6.0 6.5 7.0 7.5
##
## $c
## [1] 10.5 11.0 11.5 12.0 12.5
```

lapply() example with vectors

```
Random<-c("these", "are", "random", "example")
lapply(Random, nchar)
## [[1]]
## [1] 5
##
## [[2]]
## [1] 3
##
## [[3]]
## [1] 6
##
## [[4]]
## [1] 7
```

sapply()

This is a simplified form of `lapply()`

```
str(sapply)
## function (X, FUN, ..., simplify = TRUE, USE.NAMES = TRU
```

`X` is the input, `FUN` is the function. If `simplify` is changed to `F` then it becomes `lapply()` and returns only list object. Otherwise it also outputs vector, matrix, array or list.

sapply() example

```
list_fun<-list(a = 1:5, b = 10:15, c = 21:25)
list_fun
## $a
## [1] 1 2 3 4 5
##
## $b
## [1] 10 11 12 13 14 15
##
## $c
## [1] 21 22 23 24 25

sapply(list_fun,sum)
##   a   b   c
##  15  75 115
```

sapply() example

```
list_fun<-list(a = 1:5, b = 10:15, c = 21:25)
list_fun
## $a
## [1] 1 2 3 4 5
##
## $b
## [1] 10 11 12 13 14 15
##
## $c
## [1] 21 22 23 24 25

sapply(list_fun,mean)
##    a    b    c
##  3.0 12.5 23.0
```

sapply() example

```
sapply(list_fun, function(x) x/2)
## $a
## [1] 0.5 1.0 1.5 2.0 2.5
##
## $b
## [1] 5.0 5.5 6.0 6.5 7.0 7.5
##
## $c
## [1] 10.5 11.0 11.5 12.0 12.5
```

Notice that this is given as a list rather than a vector, this is because each element have different lengths

Others

`vapply()`

similar to `sapply` but offers a third argument which sets a template for the output.

`mapply()`

multivariate version to `sapply` function, but it applies functions to the argument one by one.

`rapply()`

Similar to `lapply` but you can specify the structure of the output

`tapply()`

applies a function to numeric data distributed across various categories.

Parallelizing a script: when

When to parallelize?

“its important to evaluate the computational efficiency of requests, and work to ensure that additional compute resources brought to bear will pay off in terms of increased work being done.”

Parallelizing a script: how

When parallelizing jobs, one can:

- Use the multiple cores on a local computer through `mclapply`
- Use multiple processors on local (and remote) machines using `makeCluster` and `clusterApply` (Note this approach, one has to manually copy data and code to each cluster member using `clusterExport`. This is extra work, but sometimes gaining access to a large cluster is worth it.)

Parallel package: mclapply

```
library(parallel)
library(MASS)

starts <- rep(100, 40)
fx <- function(nstart) kmeans(Boston, 4, nstart=nstart)
numCores <- detectCores()
numCores
## [1] 8

system.time(
  results <- lapply(starts, fx)
)
##    user  system elapsed
##    1.12    0.21    1.33
```

Parallel package: mclapply

```
system.time(
  results <- mclapply(starts, fx, mc.cores = numCores)
)

##    user  system elapsed
##   0.801   0.178   0.367
```

foreach package: %do% and %dopar%

```
for (i in 1:3) {
  print(sqrt(i))
}
## [1] 1
## [1] 1.414214
## [1] 1.732051
```

In `foreach` package %do% evaluates the expression sequentially,

```
library(foreach)
foreach (i=1:3, .combine=c) %do% {
  sqrt(i)
}
## [1] 1.000000 1.414214 1.732051
```

foreach package with doParallel

while %dopar% evaluates it in parallel, but %dopar% has to work with doParallel package

```
library(foreach)
library(doParallel)
```

Use multicore, set to the number of our cores

```
registerDoParallel(numCores)
foreach (i=1:3, .combine=c) %dopar% { sqrt(i) }
## [1] 1.000000 1.414214 1.732051
```

%do%

Using the iris data set to do a parallel bootstrap from the doParallel vignette

```
x <- iris[which(iris[,5] != "setosa"), c(1,5)]
trials <- 10000

system.time({
  r <- foreach(icount(trials), .combine=rbind) %do% {
    ind <- sample(100, 100, replace=TRUE)
    result1 <- glm(x[ind,2]~x[ind,1],
                   family=binomial(logit))
    coefficients(result1)
  }
})
##    user  system elapsed
##   21.36    0.46   21.82
```

%dopar%

```
system.time({
  r <- foreach(icount(trials), .combine=rbind) %dopar% {
    ind <- sample(100, 100, replace=TRUE)
    result1 <- glm(x[ind,2]~x[ind,1],
                   family=binomial(logit))
    coefficients(result1)
  }
})
##    user  system elapsed
##    4.42    0.80    9.11
```

Outputs

To simplify output, foreach has the .combine parameter that can simplify return values

```
# Default: Return a list
foreach (i=1:3) %dopar% { sqrt(i) }
## [[1]]
## [1] 1
##
## [[2]]
## [1] 1.414214
##
## [[3]]
## [1] 1.732051
```

Outputs

```
# Return a vector
foreach (i=1:3, .combine=c) %dopar% { sqrt(i) }
## [1] 1.000000 1.414214 1.732051

# Return a data frame
foreach (i=1:3, .combine=rbind) %dopar% { sqrt(i) }
##                [,1]
## result.1 1.000000
## result.2 1.414214
## result.3 1.732051
```

Further tips parallel computing

- To clear up and stop parallel use;

```
stopImplicitCluster()
```

- To set the cluster seed if you want reproducible results, don't use use `set.seed()`, use `clusterSetRNGStream()` instead

High performance computing

When all else fails running your script on a high powered server:

BlueCrystal Phase 4

```
#!/bin/bash

#SBATCH --job-name=job_name
#SBATCH --output=job_name
#SBATCH --error=job_name
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=16
#SBATCH --time=2:0:0

module load languages/r/4.1.0

R CMD BATCH /your_dir/your_Rscript.R
```

Check your shell script!

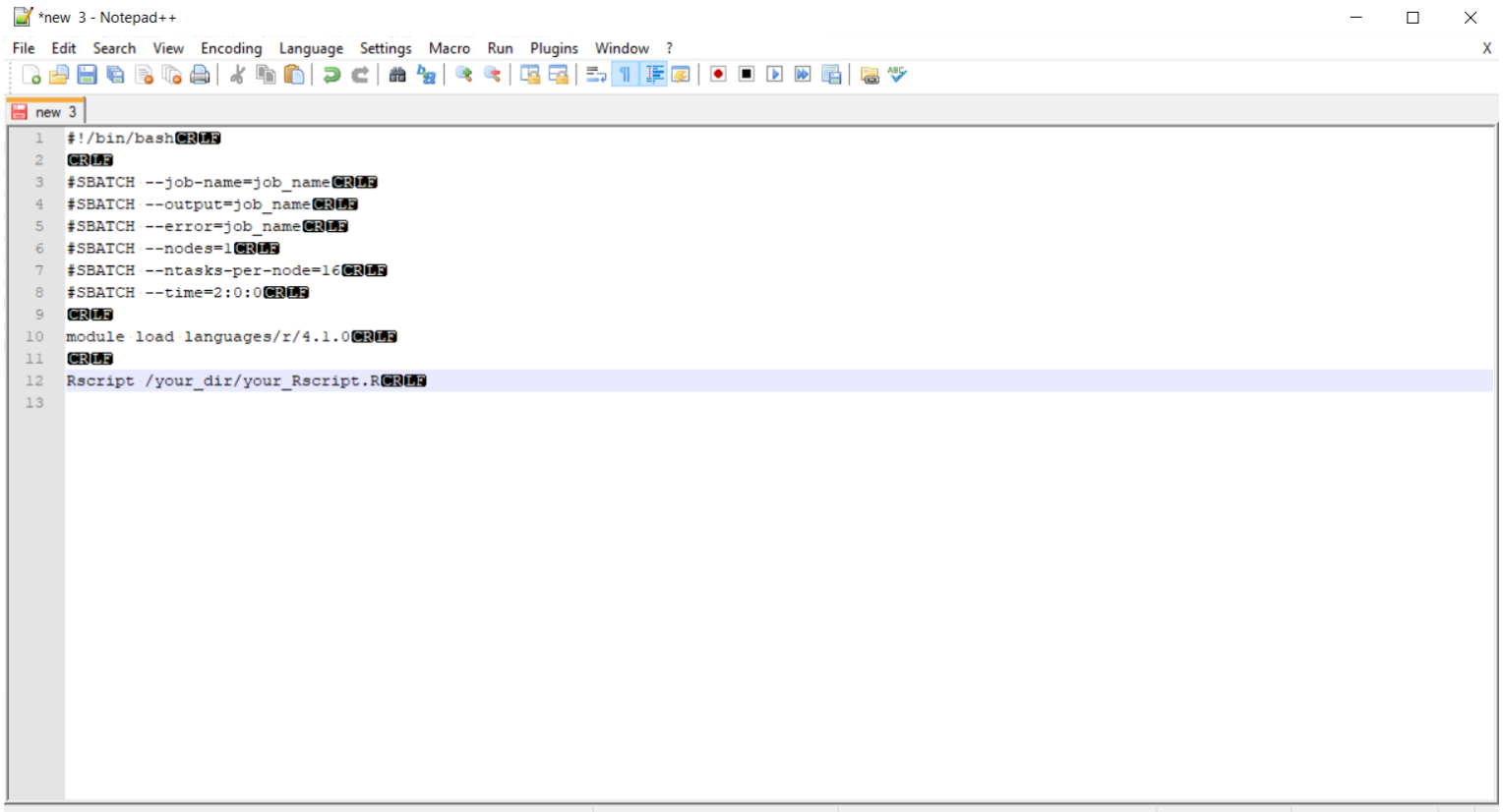
Use **cat -v** command within BlueCrystal, when you write your shell script(.sh) in RStudio or notepad it leaves a bunch of none printable characters like this;

```
#!/bin/bash^M
^M
#SBATCH --job-name=job_name^M
#SBATCH --output=job_name^M
#SBATCH --error=job_name^M
#SBATCH --nodes=1^M
#SBATCH --ntasks-per-node=16^M
#SBATCH --time=2:0:0^M
^M
module load languages/r/4.1.0^M
^M
Rscript /your_dir/your_Rscript.R^M
```

Solution: Check your shell script!

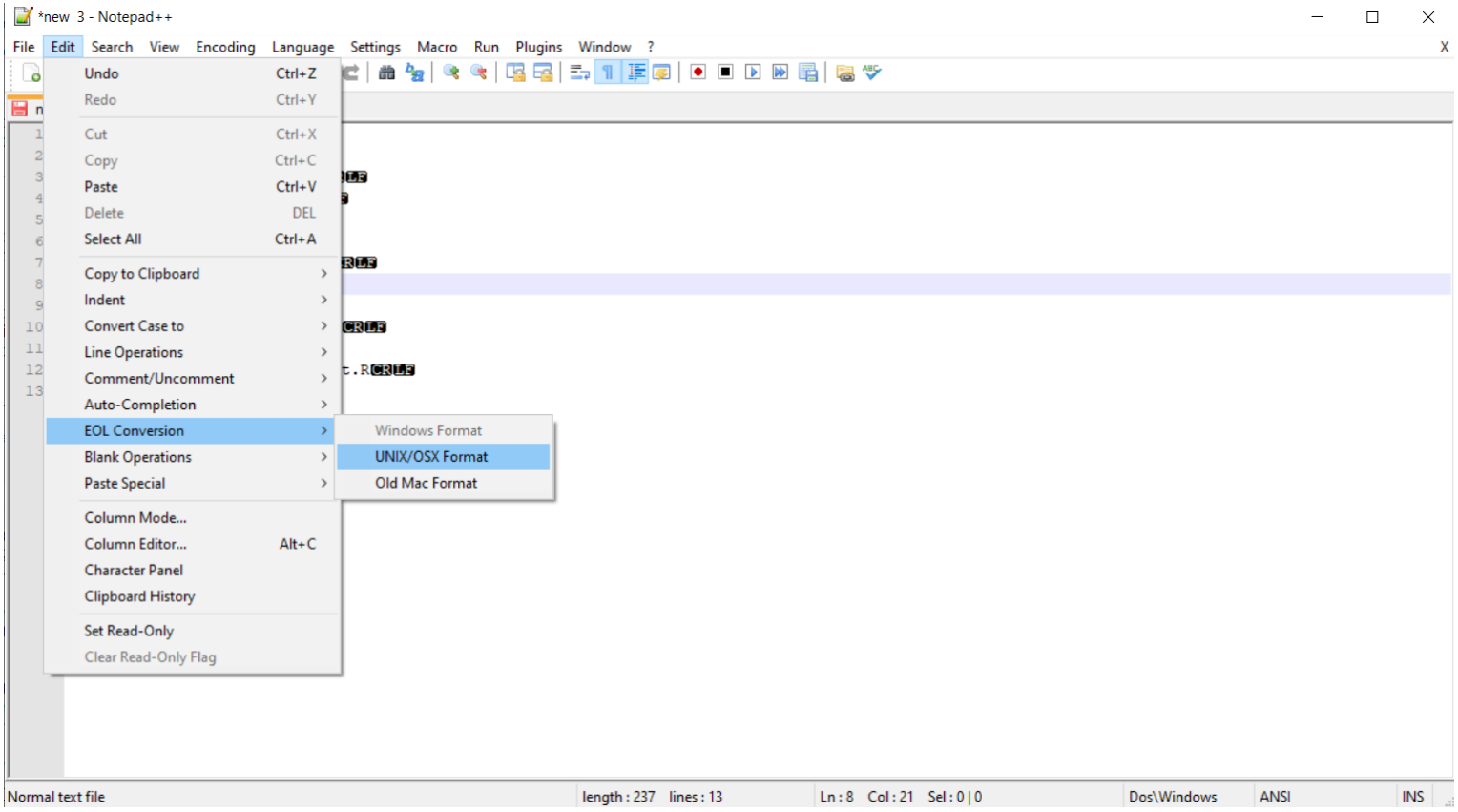
^M is another way of representing CRLF line endings in text files on Windows.

If we open this script in notepad and switch on “Show All Characters”. This shows every line the script ends with CRLF:



Solution 1: Check your shell script!

Shell scripts need LF line endings (as used by Linux, Unix, and macOS). For notepad, you can change to LF line endings by going to “Edit” -> “EOL Conversion” -> “UNIX/OSX Format”.



Solution 2: Check your shell script!

Another solution is use a text editor in BlueCrystal, such nano, emacs or vi (very user friendly editors).

References

Help from HPC https://www.bristol.ac.uk/acrc/high-performance-computing/hpc-documentation-support-and-training/

Top 5 tips for efficient performance by Colin Gillespie https://csgillespie.github.io/efficientR/performance.html#top-5-tips-for-efficient-performance

Quick Intro to Parallel Computing in R by Matt Jones https://nceas.github.io/oss-lessons/parallel-computing-in-r/parallel-computing-in-r.html