MTH3045: Statistical Computing

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Challenges I

 Go to Challenges I of the week 3 lecture 1 challenges at https://byoungman.github.io/MTH3045/challenges

Good practice: useful tips to remember when coding I

- Use scripts: don't type in the Console
 - when programming in R, work from scripts or RMarkdown documents
- Use functions for repeated calculations
 - if you're using a piece of code more than once, it should probably be formulated as a function
- Avoid repeating lines of code
 - if you're copying and pasting code, think about whether this can be avoided
 - here's an example of 'the bad'

```
n <- 5
x <- matrix(0, nrow = n, ncol = 4)
x[, 1] <- rnorm(n, 0, 1.0)
x[, 2] <- rnorm(n, 0, 1.5)
x[, 3] <- rnorm(n, 0, 2.0)
x[, 4] <- rnorm(n, 0, 3.0)</pre>
```

Good practice: useful tips to remember when coding II

• Here's an example of something better, given n and x above

```
sds <- c(1.0, 1.5, 2.0, 3.0)
for (i in 1:4) {
   x[, i] <- rnorm(n, 0, sds[i])
}</pre>
```

- An improvement would be to swap for (i in 1:4) with for (i in 1:length(sds)) or for (i in 1:ncol(x)), as then we're not relying on remembering the length of sds or equivalently the number of columns of x
- Even more tidily, we could use either of the following:

```
x1 <- sapply(sds, rnorm, n = n, mean = 0)
x2 <- sapply(sds, function(z) rnorm(n, 0, z))</pre>
```

- For x1 we've relied on knowing the order of the arguments to rnorm(), and by fixing its first and second arguments, n and mean, R knows that the first argument that we're supplying to sapply() should be sd, its third argument, i.e. rnorm()'s first free argument
 - This approach relies on good knowledge of a function's arguments

Write with style I

- In R we use the <- symbol to assign an object to a name
 - the left-hand side of the <- symbol is the name we're giving the object, and the right-hand side is the code that defines the object
 - Wickham (2019, sec. 5.1.2) states: 'Variable and function names should be lowercase. Use an underscore to separate words within a name.' Particularly usefully, Wickham (2019, sec. 5.1.2) also states: 'Strive for names that are concise and meaningful (this is not easy!)'
 - it is not easy, but worth aiming towards, especially if you're re-using an object multiple times

Write with style II

- Spacing is particularly useful for helping the appearance of code
- For example, the two lines of code

```
x1 <- sapply(sds, rnorm, n = n, mean = 0)
x1<-sapply(sds,rnorm,n=n,mean=0)</pre>
```

will both make the same object x1, but, I hope you'll agree, the first line is easier to read

- In general, spacing should be used either side of <-, mathematical operators (e.g. =, +, *), and control flows (e.g. if (...) not if(...)), and after commas
- Spacing can also be used to align arguments, such as

```
x \leftarrow list(a = c(1, 2, 3, 4, 5, 6),

b = c(7, 8, 9, 10, 11, 12))
```

which can sometimes make code more readable

Comment your code I

- What a line of code does might be self-explanatory, but might not
- When it's not, add comments to explain what it does
 - this is particularly useful at the start of a function, when what a function does and its arguments can be stated

```
fn <- function(x, y, z) {
# function to compute (x + y) * z element-wise
# x, y and z can be compatible scalars, vectors, matrices or arrays
# returns a scalar, vector, matrix or array
# (depending on class of x, y and z)
xplusy <- x + y
xplusy * z
}
fn(2, 3, 4)</pre>
```

[1] 20

 In the above we could – and should – have just done (x + y) * z on one line, but we'll find the formulation above useful for later

Comment your code II

- Commenting code is essential if you're sharing code
- You will be sharing code in MTH3045 to submit assignments
- Marks will be given for sensible commenting, and may also be given if comments make clear your intentions, even if the code itself contains errors
- Commenting is one of those things when coding that can take a bit of discipline
 - it's almost always more exciting, for example, to produce a working function as quickly as possible, than to take a bit longer and also comment that function
 - I tend to think there's a balance between when to comment and when to code, and might delay commenting until a function is finished
- Always comment code while it's fresh in your mind

Debugging I

- When we write code in R, we don't always get it right first time
- The errors or, more commonly, *bugs* in our code may not be straightforward to spot
- We call identifying bugs debugging
- We want an efficient strategy to identify bugs so that we can fix them
- Let's assume that our bug lies within a function somewhere
 - we've tried to run the function, and it's failed
 - I tend to go through the following sequence of events
- 1. Read the error message R has returned, if any. From this we may be able to deduce where the bug in our code is
- 2. If 1. fails, inspect the code and hope to spot the bug (if there's any hope of spotting it); otherwise
- 3. Use some of $R\sp{'}s$ functions to help us debug our function

Debugging II

- Somewhere within our function, something must not be as we expect
- We can inspect what's inside a function with debug()
 - I prefer debugonce(), which inspects a function once, as opposed to every time
- Suppose we want to debug fn() above
 - we simply issue

```
debugonce(fn)
fn(2, 3, 4)
```

in the Console, and then we'll end up inside the function

- So if we type x in the Console, R will print 2
- It will also be showing the line of code that it's about to execute, which will be xplusy <- x + y
- If we hit Enter then R will run the line of code
- If we then type xplusy in the Console R will print 5

Debugging III

- Debugging lets us sequentially go through each line of a function
- When debugging, R will also throw up an error once we try and execute the line of code where the bug is
- This approach to debugging can help us find the offending line of code, and then we may want to debug again up to that line, in order to find what the problem is
- When our function has many lines of code, and we know the bug to be near the end, we may want to choose from which point of the function our debugging starts
- We can do this with browser()

Challenges II

 Go to Challenges II of the week 3 lecture 1 challenges at https://byoungman.github.io/MTH3045/challenges Week 3 lecture 2

Big Data

- You may have heard of the term Big Data
- Essentially this means lots of data

"The definition of big data is data that contains greater variety, arriving in increasing volumes and with more velocity. This is also known as the three Vs.

Put simply, big data is larger, more complex data sets, especially from new data sources."

-- (https://www.oracle.com/uk/big-data/what-is-big-data/)

 The more data we attempt to fit a statistical model to, the more flops involved, and, in general, the longer it takes to fit and the more memory it needs. Typically we should try and use all the *useful* data that we can. If data aren't useful, we shouldn't use them.

Profiling I

- Profiling is the analysis of computer code, typically of its time taken or memory used
- Let's consider a matrix-based update to fn(), which we'll call fn2(), and computes (A + B)C for matrices A, B and C

```
fn2 <- function(x, y, z) {
# function to compute (x + y) %*% z
# x, y and z are matrices with compatible dimensions
# returns a matrix
xplusy <- x + y
xplusy %*% z
}
n <- 5e2
p <- 1e4
A <- matrix(runif(n * p), n, p)
B <- matrix(runif(n * p), n, p)
C <- matrix(runif(n * p), p, n)</pre>
```

Profiling II

- We can profile with Rprof()
 - ... but there are plenty of other options
- Here we'll ask it to write what it's currently doing to file profile.txt every 0.00001 seconds
 - note that Rprof (NULL) ends the profiling

```
Rprof('profile.txt', interval = 1e-5)
D <- fn2(A, B, C)
Rprof(NULL)</pre>
```

Profiling III

• Here's what's in profile.txt

```
## sample.interval=10
## "+" "fn2"
## "%*%" "fn2"
```

Profiling IV

- profile.txt is two-column output as there are at most two functions active
- The second column is the first function to be called and then the second is any subsequent functions
- From the first column, we see that after 0.00001 seconds R is evaluating function +, i.e. matrix addition
 - for the next 17 0.00001-second intervals R is evaluating function %*%,
 i.e. matrix multiplication
- The second column tells us that R is evaluating fn2 throughout
- For $n \times p$ matrices, matrix addition requires np additions, whereas matrix multiplication requires p multiplications and p-1 additions, each repeated np times
- Considering only the dominant terms, we write the computational complexity of matrix multiplication as $O(np^2)$ whereas that of matrix addition is O(np), which uses so-called 'big-O' notation¹

¹big-O notation − Consider functions f() and g(). We write f(x) = O(g(x)) if and only if there exist constants N and C such that $|f(x)| \le C|g(x)| \, \forall \, x > N$. Put simply, this means that f() does not grow faster than g().

Profiling V

 Instead of trying to interpret the output of Rprof(), R's summaryRprof() function will do that for us

```
summaryRprof('profile.txt')
## $by.self
## [1] self.time self.pct total.time total.pct
## <0 rows> (or 0-length row.names)
##
## $by.total
##
        total.time total.pct self.time self.pct
## "fn2"
                      100.00
                 0
                                    0.00
## "%*%"
                     94.44
                                    0 94.44
  "+"
                      5.56
                                         5.56
##
## $sample.interval
## [1] 1e-05
##
## $sampling.time
## [1] 0.00018
```

by working out the percentage of information in the Rprof() output attributable to each unique line of output

Profiling VI

- Profiling can be useful for finding bottlenecks in our code, i.e. lines that heavily contribute to the overall computational expense (e.g. time or memory) of the code
- If we find a bottleneck and it's unbearably slow and we think there's scope to reduce or eliminate it without disproportionate effort, then we might consider changing our code to make it more efficient
- We'll focus on efficiency in terms of times taken for commands to execute

Bechmarking I

- Suppose that we've put together some code, which we consider to be the benchmark that we want to improve on
- Comparison against a benchmark is called benchmarking
- One of the simplest ways to benchmark in R is with system.time(), which we saw in the first lecture
- Suppose we've got the following line in our code, based on matrix A above
 a_sum <- apply(A, 1, sum)
- The following tells us how long it takes to execute

system.time(a_sum <- apply(A, 1, sum))</pre>

```
## user system elapsed
```

```
## user system elapsed
## 0.037 0.036 0.074
```

Bechmarking II

The following tells us how long it takes to execute

```
system.time(a_sum <- apply(A, 1, sum))</pre>
```

```
## user system elapsed
## 0.053 0.021 0.074
```

- This gives us three timings
 - the last, elapsed, tells us how long our code has taken to execute in seconds
 - then user and system partition this total time into so-called 'user time' and 'system time'
 - their definitions are operating system dependent, but this information from the R help file for proc.time() gives as idea. "The 'user time' is the CPU time charged for the execution of user instructions of the calling process. The 'system time' is the CPU time charged for execution by the system on behalf of the calling process."
 - we'll just consider elapsed time for MTH3045

Bechmarking III

For benchmarking in R we'll consider

```
microbenchmark::microbenchmark()
```

- This notation refers to function microbenchmark() within the microbenchmark package
 - which we can use with microbenchmark::microbenchmark()
 - or just microbenchmark() if we've loaded the package, i.e. run library(microbenchmark)
- I'll use the :: notation for any functions that aren't loaded when R starts

```
library(microbenchmark)
microbenchmark(
   apply(A, 1, sum),
   rowSums(A)
)
```

```
## Unit: milliseconds
##
                          min
                                      lq
                                                      median
                                              mean
                                                                      uq
    apply(A. 1, sum) 70.257099 71.962001 96.272880 115.308210 116.412565
##
##
         rowSums(A) 6.793745 6.905797 6.975179
                                                    6.969879
                                                               7.038577
##
          max neval cld
##
    123.644415 100
      7.212714
               100
##
```

Bechmarking IV

- The microbenchmark::microbenchmark() function is particularly handy because it automatically chooses its units, which here is milliseconds
- For functions that take longer to execute it might, e.g., choose seconds
- The output of microbenchmark::microbenchmark() includes neval, the number of evaluations it's used for each function
 - from these, the range and quartiles are calculated
- If we compare medians, we note that the rowSums() approach is about an order magnitude faster than the apply() approach
- Note that for either approach, timings differ between evaluations, even though they're doing the same calculation and getting the same answer
- On this occasion the minimum and maximum times are between two and three factors different
- Note that we could also use benchmark::rbenchmark() for benchmarking, which gives similar details to system.time()
- For MTH3045, I'll use microbenchmark::microbenchmark(), because I find its output more useful

Challenges I

 Go to Challenges I of the week 3 lecture 2 challenges at https://byoungman.github.io/MTH3045/challenges

Compiled code with Rcpp I

- We've seen that vectorised functions can simplify our code (and later we'll see that they can bring considerable gains in computation time)
- Suppose, though, that we want a vectorised function, but that it doesn't exist for our purposes
- We could write a function in C or FORTRAN and call in from R
- However, using Rcpp is much more convenient
- Rcpp is an R package that efficiently and tidily links R and C++

Compiled code with Rcpp II

 Let's consider a simple example of a function to calculate the sum of a vector

```
sum_R <- function(x) {
# function to calculate sum of a vector
# x is a vector
# returns a scalar
out <- 0
for (i in 1:length(x))
  out <- out + x[i]
out
}</pre>
```

Obviously, we should use sum(), but if it wasn't available to us, then the
above would be an alternative

Compiled code with Rcpp III

 Consider the following C++ function, which I've got stored as sum_Rcpp.cpp, so that the contents of the .cpp file are as below

```
#include <RcppArmadillo.h>
// [[Rcpp::depends(RcppArmadillo)]]

// [[Rcpp::export]]
double sum_Rcpp(arma::vec x) {
  double out = 0.0;
  int n = x.size();
  for (int i = 0; i++; i < n) {
    out += x[i];
  }
  return out;
}</pre>
```

Compiled code with Rcpp IV

- We won't go into great detail on Rcpp in MTH3045. The purpose of this section is to raise awareness of its existence, should you ever need it
- In the above .cpp file:
 - #include <RcppArmadillo.h> and \\
 [[Rcpp::depends(RcppArmadillo)]] point to the RcppArmadillo
 library;
 - // [[Rcpp::export]] makes a function that is visible to R;
 - double sum_Rcpp(arma::vec x) { specifies that our function returns a
 double, i.e. a single value of double-precision, is called sum_Rcpp, and that
 its one argument is a vector, hence arma::vec, which we're calling x;
 - double out = 0.0; forms the double that will be returned, and sets its initial value to 0.0;
 - int n = x.size(); finds the length of x and stores it as an integer called n;
 - for (int i = 0; i++; i < n) { initiates a loop: we've called our index i and specified that it's an integer; then we've specified that it goes up by one each time with i++, and stops at n 1 with i < n. (Note here that indices in C++ start at zero, whereas they start at one in R.)
 - We then update out at each iteration by adding x[i]. (Note that out += ... is equivalent to out = out +)
 - We then close the loop, and specify what we return.

Compiled code with Rcpp V

- An important difference between R and C++ code is that for the latter we're specifying what's an integer and what's a double
- Then Rcpp::sourceCpp() checks that what we've specified is okay
- By not specifying these normally in R, time is needed to interpret the code
- We avoid these overheads with C++ code
- The trade-off is that C++ code usually takes a bit longer to write, because we need to think about the form of our data, whereas R can handle most of this for us
- To use the cpp function in R, we compile it with Rcpp::sourceCpp()
- We're also going to load RcppArmadillo, which gives access to the excellent Armadillo C++ library for linear algebra and scientific computing, more details of which can be found at http://arma.sourceforge.net/docs.html.

Compiled code with Rcpp VI

• We can then perform a quick benchmark on what we've done.

```
library(RcppArmadillo)
Rcpp::sourceCpp('sum_Rcpp.cpp')
x <- runif(le3)
microbenchmark::microbenchmark(
   sum_R(x),
   sum_Rcpp(x),
   sum(x)
)</pre>
```

```
## Unit: nanoseconds
##
                 min
                          lq
                                 mean median
                                                  ua
                                                        max neval cld
          expr
       sum R(x) 25078 25397.5 45620.39 25840.0 26052 1986123
##
                                                               100
                                                                     h
##
    sum Rcpp(x) 1564 1740.5
                              7811.21 1810.5
                                                1891
                                                      581179
                                                               100
                                                                    ab
                 827
##
         sum(x)
                       840.0
                               899.41
                                        866.5
                                                904
                                                        2085
                                                               100
                                                                   а
```

 We see that sum_Rcpp() is typically at least an order of magnitude faster than sum_R(). However, it's still slower than sum(), because it's one of R's functions that's heavily optimised for efficiency. It's great that we have such efficiency at our disposal.

Additional resources for Chapter 2

- For further details on topics covered in this chapter, consider the following.
 - Positional number systems: Press et al. (2007, sec. 1.1.1) and Monahan (2011, sec. 2.2).
 - Fundamentals of programming in R: W. N. Venables and R Core Team (2021), Wickham (2019, Ch. 2) and Grolemund (2014, Ch. 1-5).
 - Profiling and benchmarking: Wickham (2019, Ch. 22-24) and almost all of Gillespie and Lovelace (2016), especially Section 1.6.
 - R coding style: Various parts of Wickham (2019) and Gillespie and Lovelace (2016).

Bibliography

Week 3 lecture 3



Motivation

- Perhaps surprisingly, much of a computation that we do when fitting a statistical model can be formulated with matrices
- The linear model is a prime example
- In this chapter we'll explore some key aspects of matrices and calculations involving them that are important for statistical computing
- A particularly useful reference for matrices, especially in the context of statistical computing, is the Matrix Cookbook (Petersen and Pedersen (2012)).

Definitions

Matrix properties I

- Consider an $n \times n$ matrix **A** and $n \times p$ matrix **B**
- Let A_{ij} , for $i,j=1,\ldots,n$ denote the (i,j)th element of ${\bf A}$, i.e. in row i and column j
- Assume that A is stored in R as A and B as B

```
A \%*\% B # computes AB for matrices A and B
```

 Definition: A is real if all its elements are real numbers. (We'll only consider real matrices in MTH3045, so 'real' may be taken as given.)

```
!is.complex(A) && is.finite(A) # checks whether a matrix A is real
```

 Definition: The transpose of a matrix, denoted A^T, is given by interchanging the rows and columns of A.

```
t(A) # computes the transpose of a matrix A
```

Matrix properties II

• **Definition**: The **cross product** of matrices **A** and **B** is **A**^T**B**.

```
crossprod(A, B) # computes t(A) %*% B
```

Remark: crossprod(A, B) is more efficient that t(A) %*% B because R recognises that it doesn't need to transpose A and can instead perform a modified matrix multiplication in which the columns of A are multiplied by the columns of B.

```
tcrossprod(A, B) # computes A %*% t(B)
```

 Remark: crossprod(A) is equivalent to crossprod(A, A) and tcrossprod(A) to tcrossprod(A, A).

Matrix properties III

- **Definition**: A matrix is **diagonal** if its values are zero everywhere, except for its diagonal, i.e. $A_{ii} = 0$ for $i \neq j$.
- **Definition**: A matrix is **square** if it has the same numbers of rows and columns.
- **Definition**: The **rank** of **A**, denoted rank(**A**), is the dimension of the vector space generated (or spanned) by its columns. This corresponds to the maximal number of linearly independent columns of **A**. A matrix is of *full rank* if its rank is equal to its number of rows.

Matrix properties IV

The following apply only to square matrices.

• The $n \times n$ identity matrix, denoted \mathbf{I}_n , is diagonal and all its diagonal elements are one.

```
diag(n) # creates the n x n identity matrix for integer n
```

- A is orthogonal if $A^TA = I_n$ and $AA^T = I_n$.
- A is symmetric if $A = A^T$.
- The **trace** of **A**, denoted $tr(\mathbf{A})$, is the sum of its diagonal entries, i.e. $tr(\mathbf{A}) = \sum_{i=1}^{n} A_{ii}$. In R, diag(A) extracts the diagonal elements of A, and so sum(diag(A)) computes the trace of A.

Matrix properties V

- A is invertible is there exists a matrix B such that AB = I_n. Note that B must be n × n.
- The **inverse** of **A**, if it exists, is denoted A^{-1} .

```
solve(A) # computes the inverse of A
```

• A symmetric matrix \mathbf{A} is **positive definite** if $\mathbf{x}^T\mathbf{A}\mathbf{x}>0$ for all non-zero \mathbf{x} , i.e. provided all elements of \mathbf{x} aren't zero. (Changes to the inequality define positive semi-definite (\geq), negative semi-definite (\leq), and negative definite (<) matrices, but in statistical computing it's usually positive definite matrices that we encounter.)

Example: Hilbert matrix I

- The Hilbert matrix, \mathbf{H}_n , is the $n \times n$ matrix with (i,j)th elements 1/(i+j-1) for $i,j=1,\ldots,n$
- Write a function to form a Hilbert matrix for arbitrary n
- Use this to form H₃ and then check whether the matrix that you have formed is symmetric

Example: Hilbert matrix II

- There are many ways that we could write this function
 - we should, though, avoid a for loop
 - here's one option

```
hilbert <- function(n) {
    # Function to evaluate n by n Hilbert matrix
    # Returns n by n matrix
    # n is an integer
    ind <- 1:n
    1 / (outer(ind, ind, FUN = '+') - 1)
}</pre>
```

Example: Hilbert matrix III

• This gives \mathbf{H}_3 .

```
H <- hilbert(3)
H
```

```
## [,1] [,2] [,3]
## [1,] 1.0000000 0.5000000 0.3333333
## [2,] 0.5000000 0.3333333 0.2500000
## [3,] 0.3333333 0.2500000 0.2000000
```

- A matrix is symmetric if it and its transpose are equal
 - any of the following check for symmetry

```
H - t(H) # should be all zero, i.e. all(H - t(H) == 0)

## [1,] [,2] [,3]

## [1,] 0 0 0

## [2,] 0 0 0

## [3,] 0 0 0

all.equal(H, t(H)) # should be TRUE
```

```
## [1] TRUE
isSymmetric(H) # should be TRUE
## [1] TRUE
```

Challenges I

• Go to Challenges I of the week 3 lecture 3 challenges at

Example: evaluating the multivariate Normal pdf I

- Let $\mathbf{Y} \sim MVN_p(\mu, \mathbf{\Sigma})$ denote a random p-vector with a multivariate Normal (MVN) distribution that has mean vector μ and variance-covariance matrix $\mathbf{\Sigma}$
- Its probability density function (pdf) is then

$$f(\mathbf{y} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{\sqrt{(2\pi)^p |\boldsymbol{\Sigma}|}} \exp\left\{-\frac{1}{2}(\mathbf{y} - \boldsymbol{\mu})^\mathsf{T} \boldsymbol{\Sigma}^{-1} (\mathbf{y} - \boldsymbol{\mu})\right\}$$

- So, note that to compute the MVN pdf, we need to consider both the determinant and inverse of Σ, amongst other calculations
- Write a function dmvn1() to evaluate its pdf in R, and then evaluate $\log f(\mathbf{y} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma})$ for

$$\mathbf{y} = \begin{pmatrix} 0.7 \\ 1.3 \\ 2.6 \end{pmatrix}, \ \boldsymbol{\mu} = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} \text{ and } \mathbf{\Sigma} = \begin{pmatrix} 4 & 2 & 1 \\ 2 & 3 & 2 \\ 1 & 2 & 2 \end{pmatrix}$$

Example: evaluating the multivariate Normal pdf II

• The function dmvn1() below evaluates the multivariate Normal pdf

$$f(\mathbf{y} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{\sqrt{(2\pi)^p |\boldsymbol{\Sigma}|}} \exp \left\{ -\frac{1}{2} (\mathbf{y} - \boldsymbol{\mu})^\mathsf{T} \boldsymbol{\Sigma}^{-1} (\mathbf{y} - \boldsymbol{\mu}) \right\}$$

- Note that above determinant()\$modulus directly calculates
 log(det()), and is usually more reliable, so should be used when possible
- We'll later see that this is a crude attempt

Example: evaluating the multivariate Normal pdf III

• The following create y, μ and Σ as objects y, y and y and y are spectively.

```
y <- c(.7, 1.3, 2.6)

mu <- 1:3

Sigma <- matrix(c(4, 2, 1, 2, 3, 2, 1, 2, 2), 3, 3)
```

• Then we evaluate $\log f(\mathbf{y} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma})$ with

```
## [,1]
## [1,] -3.654535
## attr(,"logarithm")
## [1] TRUE
```

dmvn1(y, mu, Sigma)

- Remark: It's usually much more sensible to work with log-likelihoods, and then if the likelihood itself is actually sought, simply exponentiate the log-likelihood at the end
 - this has been implemented for dmvn1()
 - this will sometimes avoid underflow

Challenges II

 Go to Challenges II of the week 3 lecture 3 challenges at https://byoungman.github.io/MTH3045/challenges

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