Introduction to R for modelling

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In this practical, we will first see some important concepts for programming in R. The second section is the actual practical to run some basic population models in R using these concepts.

I. Some important concepts for programming in R

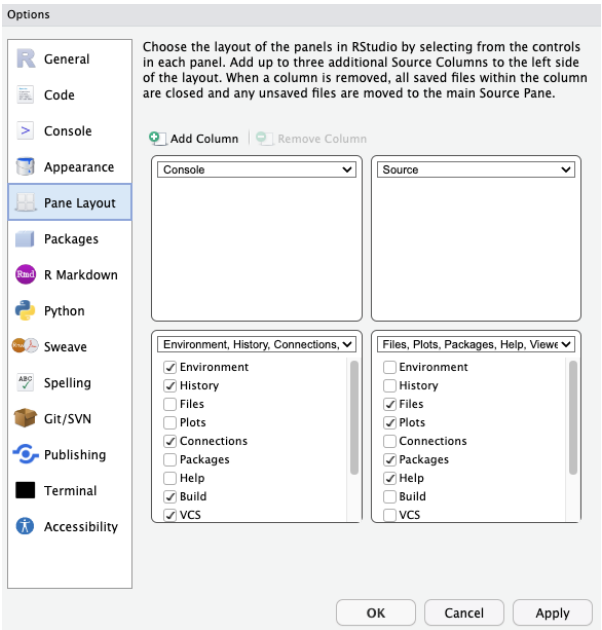
Here we will see some basic but important concepts in R. If you have experience in R, you may already know some (or all) of them, but go through this practical to make sure the results correspond to what you would expect, and to refresh some concepts.

R vs RStudio

It is important to understand the different between the two. R is a programming language. It is the most used language for statistical computing in ecology these days. RStudio is and Integrated Development Environment (IDE), that helps you code in R, by offering a convenient interface, and organise your work. RStudio is a wonderful tool, but R is what does the job. This is why you should cite R (and its version), not RStudio, in a report or paper – you could have achieved the exact same result with another IDE, but the version of R may affect your result.

The different elements of RStudio

RStudio is typically divided into four panels: the Console panel, the Source panel, the Environment etc. panel, and the Files etc. panel. Many early users do not know you can arrange the panels in the order you want in the options. It comes down to one's preferences, but I find the following layout convenient:



Source panel

The source panel is where you write your scripts and functions (see below), to be stored on your computer for later. You can also display variables in the Source panel, either by double-clicking on them in the Environment (see below), or by typing `View(variable_name)`.

Console panel

The console panel is where the outputs of the scripts from your Source panel will be displayed after being executed. You can also directly type lines of code in the Console panel, but they will not be saved to an R file.

Environmental etc. panel

“Environment” shows all the variables that have been created (see section “Variable types” below).

“History” shows previous command lines executed or typed in the Console (up to a certain point in time).

You can check the “Tutorial” panel for more R tutorials.

We don’t need the “Connections” panel.

Files etc. panel

“Files” shows the files in your workspace (see below).

“Plots” is used to display graphs. It is used by default, but you can create an external window with the command `window()` under Windows, and the command `quartz()` under MacOS.

“Packages” shows the packages you have installed on your computed (see section R Packages below for more details).

“Help” displays the help files for functions from R packages. You can access help files with the command ?name_of_function.

Don’t bother with “Viewer” or “Presentation” for now.

Working directory

The working directory is the folder from which you will work. By default, your code will try to access or create files in this folder, unless you specify a specific path. If you open an R file by double-clicking on it, by default, the working directory will be set to the folder in which the file is located. You can change this from the “Session > Set working directory”

Scripts and functions

A script is a piece of code that you can execute directly. In a script, you create variables and parameters in the workspace, and you can directly visualize them by accessing them with their names. E.g.:

```
x <- 1.5
```

The symbol <- stands for “assign”. The code above assigns the value 1.5 to the variable or parameter `x`, which you can now see in your workspace. This is equivalent to writing:

```
1.5 -> x
```

But this is confusing, so better avoiding it. Also, note that

```
x = 1.5
```

does the same thing, but in practice, it is a better practice to use `<-`. Your code will be clearer, more consistent, and easily readable by others. We will see below when to use the “=” sign.

You can write a script and save it as an R file in the Source panel.

A function is a suite of instructions that will be applied to some input variables using some parameter values. A function to compute a product between two values can be written as:

```
my.function <- function(x=0,y=0){
     z <- x*y
     return(z)
}
```

`x`, `y` and `z` are variables, but, contrary to a script, they are not stored in the workspace. They only exist during the time the function is executed. `x` and `y` are the input variables. `z` is the output variable, created within the function. You need to execute this code to load the function and be able to call it. It will then appear in your Environment.

A function can be written inside an R script. For large projects with many functions, it is often good practice to write your functions in a dedicated R file. In this case, you can load your functions by typing:

```
Source(“file_containing_functions.R”)
```

But in the following we will just write functions in our script.

You can then call the function as follows:

```
my.value <- my.function(x=2,y=3)
```

This is where the symbol "=" is typically used in R: to assign a value to an input of a function.

Here a default value of 0 has been assigned to `x` and `y`. In that case, even if I do not assign a value to `x` or `y` when calling the function (I have assigned the values 2 and 3 above), a product will be computed.

Execute the code:

```
my.value <- my.function(x=2)
```

What happens?

But you could also define the function as:

```
my.function <- function(x,y){
     z <- x*y
     return(z)
}
```

What happens when you type:

```
my.value <- my.function(x=2,y=3)
```

and

```
my.value <- my.function(x=2)
```

R packages

There are many functions already built in R that you can call. You will use them a lot in this course. Some functions are included in the base version of R, but many are included in packages. A package is simply a suite of functions that are used to perform some tasks for a given application (they also sometimes contain datasets).

You can install a package going through "Tools" → "Install packages", which will execute the function `install.packages()` (that you can call directly in the console). For example, the `vegan` package is installed with the code:

```
install.packages("vegan")
```

You then load all the functions and datasets it contains with the code:

```
library("vegan")
```

Variable types in R

Vectors

There are many classes of variables in R. The most commons are suites of values that can be `numeric()`, `character()`, etc. (we discussed these different types in the last practical). These suites of values (we will call them vectors from now on), are created with the function `c()`, that stands for "concatenate". E.g.:

```
x <- c(1,3,5)
y <- c("a","b","c")
```

You can also create a suite of numbers with an increment of 1:

```
x <- 1:5
```

Matrix and Array

A two-dimensional vector is a matrix. It is created with function `matrix()`. E.g.:

```
X <- matrix(0,nrow=2,ncol=3)
```

For more than 2 dimensions, use an array. E.g.:

```
X <- array(0,dim=c(2,3,5))
```

Data frame

A data frame is similar to a matrix, in the sense it is visualized in two dimensions, but each column corresponds to a variable, and can therefore have a different type. A matrix is an object of its own and all its elements must be of the same type!

```
my.data <- data.frame(x=1:5,y=c("a", "b", "c", "d", "e"))
```

Finally, a list is a suite of elements that can be completely different from each other. They can be data frames, matrices, vectors or different sizes, etc.

```
my.list <- list(x=x,X=X,my.data=my.data)
```

The two most important functions in R: for loops and if conditions

A `for` loop is a way to iterate through a suite of elements (typically numbers, but they can be anything, including a series of words). For example, we can add numbers 1 to 10 by writing:

```
x <- 0
for(i in 1:10){
     x <- x + i
```

```
}
```

Or we can create words as:

```
y <- c("a","b","c")
z <- character(3) ##we create a vector of characters of size 3 but with no values in it
ii <- 0
for(i in y){
     ii <- ii+1
     z[ii] <- paste(i,i)
}
```

An `if` condition is a function that will lead to execute some lines of codes only if a condition is met. For example, we can call `if()` within a `for()` loop as follows:

```
x <- 0
for(i in 1:10){
     x <- x + i
     if(x==10){
          print(x)
     }
}
```

Some other important functions

There are two types of programming languages: compiled and interpreted. A compiled language (e.g. C or C++) compile some code to create an executable file. Every time you make a modification, you need to recompile the whole code to execute it.

An interpreted language is more versatile, as it can execute all or even part of the code you want, and you can therefore check the effects of your modifications as you go easily. The drawback is that they are slower than compiled languages. This is especially true for for loops.

This is why you should try to use built-in functions or matrix operations when possible, to make your code faster. A set of functions that can be used to avoid calling for loops are `apply()`, `lapply()`, and `sapply()`.

Fonction	Arguments	Objective	Input	Output
apply	apply(x, MARGIN, FUN)	Apply a function to the rows or columns or both	Data frame, matrix or array	vector, matrix, array
lapply	lapply(X, FUN)	Apply a function to all the elements of the input	List, vector or data frame	list
sapply	sapply(X, FUN)	Apply a function to all the elements of the input	List, vector or data frame	vector or matrix

apply() applies function FUN to input x on dimensions MARGIN, and returns an element of the same type as x.

If I create a matrix and want to sum the elements of its column (i.e. dimension 2), I can type:

```
m1 <- matrix(1:10,nrow=5, ncol=6)
m1
a.m1 <- apply(m1, 2, sum)
a.m1
```

`lapply()` applies function FUN to input list X, and returns a list.

```
species <- c("DOG","CAT","EAGLE","ADER")
species_lower <-lapply(species, tolower)
str(species_lower)
```

You can use function `unlist()` to turn movies_lower into a vector.

`sapply()` applies function FUN to input list X, and returns a vector.

```
dt <- cars ## this is a dataset that is included with base R
lmn_cars <- lapply(dt, min)
smn_cars <- sapply(dt, min)
dt
lmn_cars
smn_cars
```

II. Introduction to modelling with R

Note: In the following, we will use for loops because they are easier to understand, but see the optional questions at the end of the document.

Now that we know some basics in R, let's make our first simple population models. We will use a density-dependent logistic growth, using discrete and continuous models:

$$P(t+1) = r\left(1 - \frac{P(t)}{K}\right)P(t) + P(t) \qquad \text{Eq.1}$$

$$\frac{dP}{dt} = r\left(1 - \frac{P}{K}\right)P \qquad \text{Eq. 2}$$

Discrete model (logistic map)

We will first execute a series of commands to get you through the logic of the process, before actually implementing the model with a "for" loop:

- Initialise a numeric vector P of size 500 for the population, using the function numeric()
- Set the first value of P (i.e P[1]) to 10 individuals. This is your population at time t=0, i.e. your initial population size.
- Set the parameters r and K to 0.1 and 100
- Using Equation 1 above, compute P[2], the population at time t=1, from P[1].
- Using Equation 1 above, compute P[3], the population at time t=2, from P[2].
- Using Equation 1 above, compute P[4], the population at time t=3, from P[3].

Obviously if we want to simulate 500 time steps, we will not write 500 lines of code Instead, we will use a "for" loop:

- Set a for loop for 499 time steps (from 2 to 500).
- Within the for loop, use the same equation you used to compute P[2], P[3] and P[4], but this time, instead of specifying the index by an actual value, you will use the variable you iterate in the for loop.

Plot the output using the `plot()` function, with time on the x axis and population size on the y axis. Note that you can play with the options `xlim`, `ylim` and `log` in plot to improve the plot (see ?plot). Experiment.

Plot also P(t+1) vs P(t).

You can make two plots:

- one in which you only plot the points (this is the default setting when calling `plot()`
- one in which you plot it as a continuous line: `plot(…, type = "l")`

You can also plot both in one plot, using the function `lines()` after calling plot. Check the help file for `lines()` to see what it does.

We will also use the function `lines()` to add a curve showing the whole possible set of [P(t),P(t+1)] combinations. The equivalent to draw points is `points()`. We cannot exactly show the whole possible set of [P(t),P(t+1)] combinations, but we can compute a large number of these combinations and plot the output. To do so, we simply need to compute Equation 1 for many values of P(t):

```
Pt <- seq(0,150,0.1) # that creates a vector from 0 to 150
with an increment of 0.1
Ptt <- r*(1-Pt/K)*Pt+Pt
lines(Pt, Ptt, col = "blue")
lines(c(1,150), c(1,150), col = "red") # that draws the
diagonal, as we saw in the lecture, to show the equilibrium
```

Change the values of P(0), r and K. What do you observe? In particular, increase the value of r until you see more complex population behaviour, until reaching a chaotic behaviour. Does it change anything for the plot showing P(t+1) vs P(t)?

Continuous model

Here we will see how to use a function to find a continuous solution to the logistic growth equation. Start by installing the following packages: `deSolve`, `tidyverse`, and `ggplot2`.

`deSolve` is a package that contains the function `ode()` for solving the differential equation. It applies complex mathematical algorithms to do so, that you do not need to understand in detail at this stage.

`tidyverse` contains some useful functions to manipulate data.

`ggplot2` makes beautiful graphs (you will see these in more details in the data visualization lecture in the Professional skills course).

Access the help file for the `ode()` function. We can see we need to define four parameters: `y`, `times`, `func`, `parms` (we don't need to look at the other parameters at this stage, we will just use the default values).

- `y` – the initial (state) values for the ODE system, a vector. If y has a name attribute, the names will be used to label the output matrix.

Here there is only one variable with an initial value: `P`. We will therefore define:

```
state <- c(P=10)
```

- `times` – time sequence for which output is wanted; the first value of times must be the initial time.

Let's simulate 500 time steps, and get values for every 0.1 interval:

```
times <- seq(0,100,by=0.01)
```

- `parms` – parameters passed to func.

These are the parameters r and K. We will store them in a vector:

```
parameters <- c(r=0.1, K=1000)
```

- `func` – either an R-function that computes the values of the derivatives in the ODE system (the model definition) at time t, or a character string giving the name of a compiled function in a dynamically loaded shared library.

  If `func` is an R-function, it must be defined as: `func <- function(t, y, parms,...)`. `t` is the current time point in the integration, `y` is the current estimate of the variables in the ODE system. If the initial values `y` has a names attribute, the names will be available inside `func`. `parms` is a vector or list of parameters; … (optional) are any other arguments passed to the function.

  The return value of `func` should be a list, whose first element is a vector containing the derivatives of y with respect to time, and whose next elements are global values that are required at each point in times. The derivatives must be specified in the same order as the state variables y.

`func` is a bit more complicated to define, but basically it is just an R function that implements the differential equation above:

```
LG <- function(t,state,parameters){ ##logistic grown function, that takes a set of parameter values, initial conditions and a time sequence
  with(as.list(c(state, parameters)),{ ##"with" is a function that allows us to use the variable names directly - it looks for r, K and P in state and parameters

    dP <- r*(1-P/K)*P ##this is our logistic equation governing the rate of change of P

    return(list(dP)) ## return the rate of change - it needs to be a list
  }) # end with(as.list ...
}
```

From there, we just need to call function ode with these four elements:

```
out <- ode(y=state, times = times, func = LG, parms = parameters)
```

Look at `out` in your workspace. What kind of element is it?

Some functions create elements that are in a specific format (here it is a `deSolve` object). This format is useful when calling other functions from the same package, but sometimes quite annoying for plotting the results. We therefore need to convert it to a more convenient data frame:

```
out.df <- data.frame(out)
```

We can now plot the output:

```
plot(out.df,type="l")
```

or if you want something fancier using ggplot:

```
ggplot(data = out.df)+
  geom_line(mapping=aes(x=time,y=P),color="blue") +
  geom_hline(yintercept=0,color="darkgrey") +
  geom_vline(xintercept=0,color="darkgrey") +
  labs(x = "Time", y = "P")
```

Change the values of P(0), r and K. What do you observe this time?

Model calibration

We have implemented a population model following a logistic growth. This is all good and interesting, and it can be used to examine some theoretical behaviour (such as chaotic behaviours), but we may want to apply it to some real data, and estimate the values of parameters `r` and `K` for a population, as well as the initial conditions `P(t=0)`. This is called model calibration. Here we will see a simple way to do it, for some data I have generated with a model (instead of real data, so that I know the real values of `r` and `K`!).

Here is the code I used (without the parameter values 😉). Can you see how it differs from the code you wrote for the discrete model, and why I made this modification?

```
tmax <- 300
x <- numeric(tmax+1)
for(i in 2:(tmax+1)){
  x[i] <- r*x[i-1]*(1-x[i-1]/K)+x[i-1]+rnorm(1,0,x[i-1]/100)
}
```

<u>Get the data</u>

Read the file “pop_LG_simul_noise_small.csv” and store the values in a data frame. Plot and look at the values.

As we discussed in the introduction to modelling lecture, there are two ways to calibrate a model: directly from data, or by retro-fitting or inverse modelling, i.e. by adjusting the parameter values so that the output of the model fits the data. Ideally, we want to estimate most of parameter values from real data, to avoid overfitting.

Initial conditions `P`(t=0)

How can you get this information from the data? Implement it in R.

Parameter `K`

Can you think of a way to estimate `K` directly from the data? Think of what `K` means in your model (look at the plots you have generated above). It is possible to estimate `K` in one line of code. Implement it in R.

Parameter `r`

Here we will use inverse modelling. The idea is the following: we will run multiple simulations, generating data for different values of `r`. We will then compare the model outputs to the data from the csv file. The `r` value generating the outputs closest to the data should be close to the real one.

First, we need to decide if we want to use all the data, or only part of it. What do you think? What part of the curve has `r` an effect on? Create a variable `tmax` representing the cutoff (the number of data points you will use).

We will then execute the following code I commented it, but take the time to understand what each line of code is doing. Ask if you don't get it.

```
out.df.list <- list() ##create a list in which we will store
the model outputs for the different values of r
i <- 1 ##this is used to keep track of indices for out.df.list
for (r in seq(0.01,1,0.01)){ ##we vary r from 0.01 to 1, by
steps of 0.01. Check ?seq for further details
  parameters <- c(r=r, K=K) ##these are our parameters, as
before
  state <- c(P=pop$P[1]) ##this is our initial population
value, as before
  times <- seq(0,tmax,by=1) ##these are our time steps. This
time, we want one value every time step, to match how the data
was generated
  out <- ode(y=state, times = times, func = LG, parms =
parameters) ##we apply the ode() function, as before
  out.df.list[[i]] <- data.frame(out) ##we store the data
frame in the list out.df.list
  i <- i+1 ##we need to increment i for the previous line of
code
}
```

`out.df.list` is a list containing the data frames with the population values for the different values of `r`. We now need a measure of fit. Here we will simply take the sum of the absolute values of the differences between the simulated and the "real" data points. The "best" `r` value is therefore the one minimising this difference. You can compute it with the following code:

```
fit <- numeric(length(out.df.list))
for(i in 1:length(out.df.list)){
  fit[i] <- sum(abs(out.df.list[[i]]$P-pop$P[1:(tmax+1)]))
}
ind.est <- which.min(fit) ##this is the index of fit which
corresponds to the minimum value in fit
```

In the original mode, I used `r <- 0.2`. We can find the corresponding model outputs with the following line of code:

```
ind.real <- which(seq(0.01,1,0.01)==0.2)
```

Are `ind.est` and `ind.real` the same, or do they differ? By how much? What does it mean? To help you interpret the difference, we can plot both the values generated by the estimated and the real r value with the following code:

```
colors <- c("Estimated"="red","Real"="cyan4")
ggplot()+
  geom_line(mapping=aes(x=0:tmax,y=pop$P[1:(tmax+1)])) +
  geom_line(mapping=aes(x=0:tmax,y=out.df.list[[ind.est]]
$P,color="Estimated")) +
  geom_line(mapping=aes(x=0:tmax,y=out.df.list[[ind.real]]
$P,color="Real")) +
  geom_hline(yintercept=0,color="darkgrey") +
  geom_vline(xintercept=0,color="darkgrey") +
  xlim(0,tmax*1.1) +
  ylim(0,K+100) +
  labs(x = "Time", y = "P",color = "Legend") +
  scale_color_manual(values = colors)
```

Change the value of `tmax`. Does it change anything?

Now, redo all of the above with the data from the csv file named "pop_LG_simul_noise_big.csv", for which I used a noise 10 times as high as before. Does it change your results? How and why?

That was too easy and you have some extra time?

Task 1

Can you rewrite some of your code using apply / lapply / sapply instead of for loops?

Task 2

Try to produce a bifurcation plot from a discrete model output:

- Define the initial conditions
- Execute the model for r of increasing values, for 500 time steps
- For each simulation, store the last 50 poplation values
- Plot the population values (y axis) against the corresponding r values, all in a same graph