Programming for Data Science

Functions in R language

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Function in R

- We have already used several examples of functions:

  mean(x) sd(x) ggplot(data, ...) lm(y $\sim$ x, ...) ....

- Functions are typically written if we need to compute the same thing for several data sets;

- Functions have a **name** and a **list of arguments** or **input objects**. For example, the argument to the function mean() is the vector x;

- Functions can also have a list of **output objects** returned when the function is terminated;

- A function must be written and loaded into R before it can be used.

A simple function in R

- A simple function can be constructed as follows:

```
function_name=function(arg1,arg2,...){
command1
command2
output
}
```

- You can define a function name;
- The function keyword specified that you are writing a function;
- Inside () you can outline the input objects;
- The commands occur inside {};
- The name of whatever output you want goes at the **end of the function**;
- Comments lines are denoted by #.

A simple function in R

- An example:

```
mysum=function(x,y){
 x + y
}
```

- This function is called mysum;
- It has two input arguments, called x,y.
- Whatever values are passed for x and y their sum will be computed and the result visualizes on the screen.
- The function must be loaded into R before being called.

A simple function in R

How to execute a new function:

- Write the function in a text editor;
- Copy the function in the R console.
  Type `ls()` into the console: the function now appears;
- Call the function using:

```
> mysum(3, 4)
[1]7
> mysum(y = 3, x = 4)
[1]7
> mysum(y = c(3, 6), x = c(4, 4))
[1]7 6
```

- Store the result into a variable sumXY:

```
> sumxy = mysum(3, 4)
```

How to load a function from a file

- Command source() is used to read the file and execute/load the commands in the same sequence given in the file.

  source(file,echo ...)

  file : character string giving the pathname of the file;

  echo : if TRUE, each expression is printed after parsing, before evaluation.

How to load a function from a file

- Command source() is used to read the file and execute/load the commands in the same sequence given in the file.
- Use a text editor to save the following function in the file "myfun1.r":

```
myfun=function(x,y,p){
 k = (x + y) * p
 return(k)
}
```

- Use command source() to load the function from the file:

```
> source("myfun1.r")
```

A simple function in R

- An example:

```
myfun=function(x,y,p){
 k = (x + y) * p
 return(k)
}
```

- Function myfun has 3 arguments;

- The command return specifies what the function returns, here the value of k;

```
> myfun(3, 4, 7)
```

```
> res = myfun(3, 4, 7)
```

result is stored in res

A more complex function in R

- The following function returns several values in the form of a list:

```
myfun1=function(x){
 the.mean = mean(x)
 the.sd = sd(x)
 the.min = min(x)
 the.max = max(x)
 return (list(mean = the.mean, stand.dev = the.sd,
 minimum = the.min, maximum = the.max))
}
```

A more complex function in R

- how to call myfun1:

```
> x = rnorm(10)

> res = myfun1(x)

> res

res
$mean
[1]0.29713
$stand.dev
[1]1.019685
$minimum
[1] − 1.725289
$maximum
[1]2.373015
```

Argument Matching in R

How does R know to match arguments?

Argument matching is done in a few different ways:

- The arguments are matched by their positions. The first supplied argument is matched to the first formal argument and so on.

  $> myfun(3, 4, 7)$ **x=3, y=4 and p=7**

- The arguments are matched by name. A named argument is matched to the formal argument with the same name:

  $> myfun(y = 4, x = 3, p = 7)$ **x=3, y=4 and p=7**

- Name matching happens first, then positional matching is used for any unmatched arguments.

Argument Matching in R

- Default values for some/all arguments can be specified:

```
myfun=function(x,y,p=10){
 k = (x + y) * p
 return(k)
}
```

- If a value for the argument *p* is not specified in the function call, a value of 10 is used.

```
> l = myfun(3, 4)
> l
[1]70
```

- If a value for *p* is specified, that value is used.

```
> l = myfun(3, 4, 2)
> l
[1]14
```

Exercises on functions

1. Write a function that when passed a number, returns the number squared, the number cubed, and the square root of the number;
2. Write a function that when passed a numeric vector, prints the value of the mean and standard deviation to the screen (Hint: use the cat() function in R.) and creates a histogram of the data;

Exercises on function

- Write a function that when passed a number, returns the number squared, the number cubed, and the square root of the number;

```
myfun2=function(x){
 squared = x * x
 cubed = x * x * x
 root = sqrt(x)
 return (list(squared, cube, root))
}
```

Exercises on function

- Write a function that when passed a numeric vector, prints the value of the mean and standard deviation to the screen (Hint: use the cat() function in R.) and creates a histogram of the data;

```
myfun3=function(x,file="hist.png"){
 cat(x,": standard deviation is",sd(x),"\n")
 cat(x,": mean is",mean(x),"\n")
 library(ggplot2)
 ggplot(data.frame(x),aes(x))+geom_histogram()
}
```

if Statement

- **Conditional execution:** the if statement has the form:

  ```
  if (condition){
    expr1
  }
  else {
    expr2
  }
  ```

  Condition is evaluated and returns a logical value (i.e. TRUE or FALSE.)
  If the condition is evaluated **TRUE**, *expr*$_1$ is executed , otherwise *expr*$_2$ is executed.

- Logical operators $\&\&, ||, ==, != , >, <, >=, <=$ are used as the conditions in the if statement.

if Statement: a simple example

- The following function gives a demonstration of the use of if ... else:

```
checkMyfunction=function(number){
 if(number! = 1) {
  cat(number, "is not one \n")
 }
 else {
  cat(number, "is one \n")
 }
}
```

```
> checkMyfunction(1)
1 is one
> checkMyfunction(2)
2 is not one
```

if Statement: a second simple example

- The following function gives a demonstration of the use of && :

```
checkBetween=function(number){
 if((number >= 1)&&(number <= 10)) {
  cat(number,"is between one and ten \n")
 }
 else {
  cat(number,"isn't between one and ten \n")
 }
}
```

```
> checkBetween(2)
1 is between one and ten
> checkMyfunction(12)
12 isn't between one and ten
```

Nested if Statements

- The following function gives a demonstration of the use of if ... else if ... else:

```
checkNum=function(number){
 if(number == 0) {
  cat(number,"is zero \n")
 }
 else if(number < 0) {
  cat(number,"is negative \n")
 }
 else{
  cat(number,"is positive \n")
 }
}
```

For loop

- To loop/iterate through a certain number of repetitions a for loop is used. Its syntax is:

```
for (condition){
 command_1
 command_2
 .....
}
```

A simple example of a for loop:

```
MyLoop=function(x){
 cumsum = rep(0, length(x))
 if(!(is.numeric(x))) {
  cat(x,"must be numeric \n")
  return(cumsum)
 }
 cumsum[1] = x[1]
 for(i in 2 : length(x))
  cumsum[i] = cumsum[i-1] + x[i]
 return(cumsum)
}
```

For loop

- You can nest loops. In this cases indenting the code can be useful.

```
for (condition_1){
 command_1
 command_2
 for(condition_2){
  command_1
  command_2
 }
}
```

- for loops and multiply nested for loops are generally avoided when possible in R because they can be quite slow.

For loop

- Compare using function system.time() the function MyLoop()

```
MyLoop=function(x){
 cumsum = rep(0, length(x))
 if(!(is.numeric(x))) {
  cat(x,"must be numeric \n")
  return(cumsum)
 }
 cumsum[1] = x[1]
 for(i in 2 : length(x))
  cumsum[i] = cumsum[i-1] + x[i]
 return(cumsum)
}
```

and cumsum(). They have a different execution time.

```
> x = rnorm(1000000)
> system.time(cumsum(x))
> system.time(MyLoop(x))
```

While loop

- While loop can be used if the number of iterations required is not known beforehand;
- For example, if loop must continue until a certain condition is met.
- Its syntax is:

```
while (condition){
 command_1
 command_2
 .....
}
```

The loop continues while condition $==$ TRUE.

While loop

- A simple example of a while loop:

```
MyLoop1=function(x){
  cumsum = rep(0, length(x))
  if(!(is.numeric(x))) {
    cat(x,"must be numeric \n")
    return(cumsum)
  }
  cumsum[1] = x[1]
  i = 2
  while(i <= length(x)){
    cumsum[i] = cumsum[i-1] + x[i]
    i = i + 1
  }
  return(cumsum)
}
```

next, break, statements

- The next statement can be used to discontinue one particular iteration of any loop. Useful if you want a loop to continue even if an error is found (error checking);
- The break statement completely terminates a loop. Useful if you want a loop to end if an error is found.

```
MyLogNext=function(x){
 for(i in 1 : length(x)){
  if(x[i] <= 0) {
   next
  }
  x[i] = log(x[i])
 }
 return(x)
}
```

```
MyLogNext1=function(x){
 for(i in 1 : length(x)){
  if(x[i] <= 0) {
   break
  }
  x[i] = log(x[i])
 }
 return(x)
}
```

next, break, statements

- The next statement can be used to discontinue one particular iteration of any loop. Useful if you want a loop to continue even if an error is found (error checking);

- The break statement completely terminates a loop. Useful if you want a loop to end if an error is found.

```
MyLogNext=function(x){
 for(i in seq_along(x)){
  if(x[i] <= 0) {
   next
  }
  x[i] = log(x[i])
 }
 return(x)
}
```

```
MyLogNext1=function(x){
 for(i in seq_along(x)){
  if(x[i] <= 0) {
   break
  }
  x[i] = log(x[i])
 }
 return(x)
}
```

Exercises on loops and functions

- Create a function find_value(), which takes as input a number b and a vector m, and returns first occurrence of b in m;
- Create a function find_all_value(), which takes as input a number b and a matrix m, and returns all the occurrences of b in m;
- Create a function translate(), which takes as input a numeric vector c and returns a string vector f such that $f[i] = "P"$ iff $c[i] > 0$ otherwise $f[i] = "N"$.

Exercises on loops and functions

- Create a function find_value(), which takes as input a number *b* and a vector *m*, and returns first occurrence of *b* in *m*;

```
find_value=function(b,m){
 if(length(m) < 2) {
  cat("m size must be greater 1 \n")
  return(-1)
 }
 ind = 1
 while(ind <= length(m)){
  if(m[ind] == b)
    return(ind)
  ind = ind + 1
 }
 return(-1)
}
```

Exercises on loops and functions

- Create a function find_all_value(), which takes as input a number *b* and a matrix *m*, and returns all the occurrences of *b* in *m*;

```
find_all_value=function(b,m){
 f = NULL
 for(row in 1 : dim(m)[1]){
  for(col in 1 : dim(m)[2]){
   if(m[row, col] == b)
   if(length(f) == 0)
     f = list(c(row, col))
   else
     f = list(f, c(row, col))
  }
 }
 return(f)
}
```

Exercises on loops and functions

- Create a function translate(), which takes as input a numeric vector c and returns a string vector f such that $f[i] = "P"$ iff $c[i] > 0$ otherwise $f[i] = "N"$.

```
translate=function(m){
 f = NULL
 if(!(is.numeric(x))) {
  cat(x,"must be numeric \n")
  return(f)
 }
 for(ind in 1 : length(m)){
  if(m[ind] > 0)
     f = c(f,"P")
  else
     f = c(f,"N")
 }
 return(f)
}
```

How to replace a for loop with apply functions

There are three basic ways to loop over a vector:

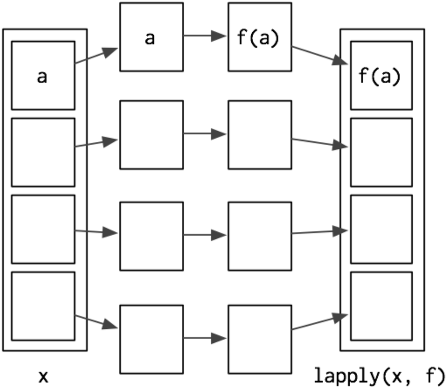
- loop over the elements: `for (x in xs)`
- loop over the numeric indices: `for (i in seq_along(xs))`
- loop over the names: `for (nm in names(xs))`

that can be implemented using **lapplay/(sapply)**:

- `lapply(xs, function(x) {})`
- `lapply(seq_along(xs), function(i) {})`
- `lapply(names(xs), function(nm) {})`

How to replace a for loop with apply functions

The *lapply()* function takes a function, applies it to each element of the input, and returns the results in the form of a list.



How to replace a for loop with apply functions

An example showing the conversion:

```
NormalLoop=function(x){
 for(i in 1 : length(x)){
  if(x[i] <= 0) {
    x[i] = abs(x[i])
  }
  else
    x[i] = log(x[i])
 }
 return(x)
}
```

⇔ **?**

How to replace a for loop with apply functions

An example showing the conversion:

```
NormalLoop=function(x){
 for(i in 1 : length(x)){
  if(x[i] <= 0) {
    x[i] = abs(x[i])
  }
  else
    x[i] = log(x[i])
 }
 return(x)
}
```

$\Longleftrightarrow$

```
lapply(x, function(x){
  if(x <= 0) {
    x = abs(x)
  }
  else
    x = log(x)
})
```

How to replace a for loop with apply functions

An example showing the conversion:

```
> x = c(−1, 20, 4)
> names(x) = c("o", "p", "o")

 NameLoop=function(x){
  for(i in 1 : length(x)){
   if(names(x)[i] == "o") {
     x[i] = x[i] + 10
   }
   else
     x[i] = x[i] + 100
  }
  return(x)
 }
```

$\Leftrightarrow$ **?**

How to replace a for loop with apply functions

An example showing the conversion:

```
> x = c(−1, 20, 4)
> names(x) = c("o", "p", "o")
```

```
NameLoop=function(x){
 for(i in 1 : length(x)){
  if(names(x)[i] == "o") {
    x[i] = x[i] + 10
  }
  else
    x[i] = x[i] + 100
 }
 return(x)
}
```

⇔

```
lapply(seq_along(x), function(i){
  if(name(x)[i] == "o") {
    x[i] = x[i] + 10
  }
  else
    x[i] = x[i] + 100
})
```

How to replace a nested loops with apply functions

An example showing the conversion:

```
NestedLoop=function(x,y){
 el = rep(FALSE, length(x) * length(y))
 Shared = matrix(el, nrow = length(x))
 for(i in 1 : length(x)){
  for(j in 1 : length(y)){
    if(x[i] == y[j]) {
       Shared[i, j] = TRUE)
    }
  }
 }
 return(Shared)
}
```

$\Leftrightarrow$ **?**

How to replace a nested loops with apply functions

An example showing the conversion:

```
NestedLoop=function(x,y){
 el = rep(FALSE, length(x) ∗ length(y))
 Shared = matrix(el, nrow = length(x))
 for(i in 1 : length(x)){
  for(j in 1 : length(y)){
    if(x[i] == y[j]) {
       Shared[i, j] = TRUE)
    }
  }
 }
 return(Shared)
}
```

⇔

```
sapply(y, function(y){
   sapply(x, function(x){
     if(x == y) {
        return(TRUE)
     }
     else
        return(FALSE)
   })
})
```

In this case a better solution is to use outer product:

```
>outer(x,y,"==")
```

Exercises on loops and functions

- Use **DeSolve** package to solve the following ODE system between 0 to 10.

$$
\begin{aligned}
\frac{dx_1}{dt} &= -3x_1 + 4x_2 + 3.5x_3 \\
\frac{dx_2}{dt} &= +3x_1 - 14.5x_2 \\
\frac{dx_3}{dt} &= +10.5x_2 - 3.5x_3
\end{aligned}
$$

$$
\begin{aligned}
x_1(0) &= 100 \\
x_2(0) &= 10 \\
x_3(0) &= 1.0
\end{aligned}
$$

and plot the evolution of x_1, x_2, x_3 over the time.

Exercises on loops and functions

- Use **deSolve** package to solve the following ODE system between 0 to 10.

$$
\begin{aligned}
\frac{dx_1}{dt} &= -3x_1 + 4x_2 + 3.5x_3 \\
\frac{dx_2}{dt} &= +3x_1 - 14.5x_2 \\
\frac{dx_3}{dt} &= +10.5x_2 - 3.5x_3
\end{aligned}
$$

$$
\begin{aligned}
x_1(0) &= 100 \\
x_2(0) &= 10 \\
x_3(0) &= 1.0
\end{aligned}
$$

and plot the evolution of x_1, x_2, x_3 over the time.

```
> install.packages("deSolve")
> library(deSolve)
>?lsode
```

lsode(y, times, func, ...)

- *y* is the initial (state) values for the ODE system;
- *time* is time sequence for which output is wanted;
- *func* is an R-function that computes the values of the derivatives in the ODE system.

Exercises on loops and functions

- Use **deSolve** package to solve the following ODE system between 0 to 10.

$$\begin{aligned}\frac{dx_1}{dt} &= -3x_1 + 4x_2 + 3.5x_3\\ \frac{dx_2}{dt} &= +3x_1 - 14.5x_2\\ \frac{dx_3}{dt} &= +10.5x_2 - 3.5x_3\end{aligned}$$

$$\begin{aligned}x_1(0) &= 100\\ x_2(0) &= 10\\ x_3(0) &= 1.0\end{aligned}$$

and plot the evolution of x_1, x_2, x_3 over the time.

```
> y = c(100, 10, 1.0)

> times = seq(0, 10, 0.1)

>funODE=function(t, x, parms){
    dx1 = −3∗x[1]+4∗x[2]+3.5∗x[3]
    dx2 = +3 ∗ x[1] − 14.5 ∗ x[2]
    dx3 = +10.5 ∗ x[2] − 3.5 ∗ x[3]
    return(list(c(dx1, dx2, dx3)))
}

>res=lsode(y,times,funODE,parms=0)
>colnames(res)=c("Time","x1","x2","x3")
```

Exercises on loops and functions

- Use **deSolve** package to solve the following ODE system between 0 to 10.

$$\begin{aligned}
\frac{dx_1}{dt} &= -3x_1 + 4x_2 + 3.5x_3 \\
\frac{dx_2}{dt} &= +3x_1 - 14.5x_2 \\
\frac{dx_3}{dt} &= +10.5x_2 - 3.5x_3
\end{aligned}$$

$$\begin{aligned}
x_1(0) &= 100 \\
x_2(0) &= 10 \\
x_3(0) &= 1.0
\end{aligned}$$

and plot the evolution of x_1, x_2, x_3 over the time.

```
>gp=ggplot(data.frame(res),aes(x=Time))

>gp+geom_line(aes(y=x1),color="red")

>gp+geom_line(aes(y=x2),color="blue")

>gp+geom_line(aes(y=x3),color="green")
```

Exercises on loops and functions

- Find α and β which maximize $x_1(t) + x_2(t)$ with $t = 1$.

$$\begin{aligned}
\frac{dx_1}{dt} &= \alpha - x_1 + 4x_2 + \beta x_3 \\
\frac{dx_2}{dt} &= \alpha x_1 - 14.5x_2 \\
\frac{dx_3}{dt} &= +10.5x_2 - \beta x_3
\end{aligned}$$

$$\begin{aligned}
x_1(0) &= 100 \\
x_2(0) &= 10 \\
x_3(0) &= 1.0
\end{aligned}$$

with $10 \leq \alpha, \beta \leq 100$

You can use **GenSA** packages: Generalized Simulated Annealing for Global Optimization. It searches for global minimum of a very complex non-linear objective function with a very large number of optima

Exercises on loops and functions

```
> install.packages("GenSA")
> library(GenSA)
>?GenSA
```

```
GenSA(par, fn, lower, upper, control = list(), ...)
```

- *par* initial vector values for the components to be optimized;
- *fn* is the function to be minimized;
- *lower*, *upper* bounds for components;
- *control* is a list that can be used to control the behavior of the algorithm.

Exercises on loops and functions

```
> p0 = c(20, 20)

> LB = c(10, 10)

> UB = c(100, 100)

> x0 = c(100, 10, 1.0)

>ObjF=function(p){
    Times = seq(from = 0, to = 1, by = 0.1)
    res = lsode(x0, Times, funODE, parm = p)
    last = tail(res, 1)
    fn = -1 * (last[2] + last[3])
    return(fn)
}
```

```
>funODE=function(t, x, parm){
    dx1 = -parm[1] * x[1] + 4 * x[2] + parm[2] * x[3]
    dx2 = +parm[1] * x[1] - 14.5 * x[2]
    dx3 = +10.5 * x[2] - p[2] * x[3]
    return(list(c(dx1, dx2, dx3)))
}
```

```
>k=GenSA(p0,ObjF,LB,UB,control=list(max.time=5))

>k.par

>k.value
```

Exercises on loops and functions

- Find α and β which maximize $x_1(t) + x_2(t)$ with $t = 1$ varying the initial value for the components (i.e. par vector).

$$
\begin{aligned}
\frac{dx_1}{dt} &= \alpha - x_1 + 4x_2 + \beta x_3 \\
\frac{dx_2}{dt} &= \alpha x_1 - 14.5x_2 \\
\frac{dx_3}{dt} &= +10.5x_2 - \beta x_3
\end{aligned}
$$

$$
\begin{aligned}
x_1(0) &= 100 \\
x_2(0) &= 10 \\
x_3(0) &= 1.0
\end{aligned}
$$

with $10 \leq \alpha, \beta \leq 100$

Exercises on loops and functions

```
> LB = c(10, 10)
> UB = c(100, 100)
> x0 = c(100, 10, 1.0)

> y0 = lapply(seq_along(1 : 10), function(i){runif(2, 10, 100)})

> s = lapply(y0, function(y0){
 GenSA(par = y0, fn = ObjF, upper = UB, lower = LB, control = list(max.time = 5), x0 = x0)
})
```