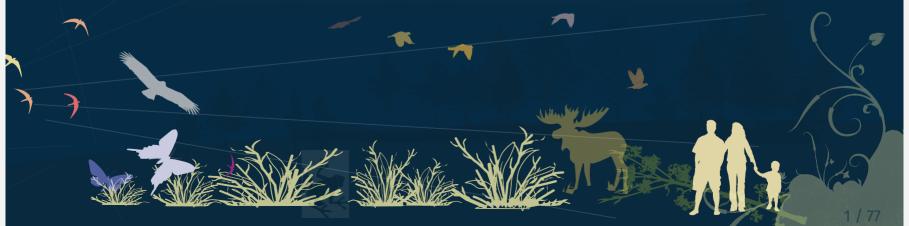


Workshop 5: Programming in R

QCBS R Workshop Series

Québec Centre for Biodiversity Science



About this workshop



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Outline

- 1. Learning what is control flow
- 2. Writing your first functions in R
- 3. Speeding up your code
- 4. Useful R packages for biologists

Review

Objects

Vectors

Numeric vectors

```
num.vector ← c(1, 4, 3, 98, 32, -76, -4)

num.vector

# [1] 1 4 3 98 32 -76 -4
```

Data frames

vectors

```
siteID \leftarrow c("A1.01", "A1.02", "B1.01", "B1.02")
  soil pH \leftarrow c(5.6, 7.3, 4.1, 6.0)
  num.sp \leftarrow c(17, 23, 15, 7)
  treatment ← c("Fert", "Fert", "No_fert", "No_fert")
We then combine them using the function data.frame
  my.first.df ← data.frame(siteID, soil pH, num.sp, treatment)
  my.first.df
# siteID soil_pH num.sp treatment
# 1 A1.01 5.6 17 Fert
# 2 A1.02 7.3 23 Fert
# 3 B1.01 4.1 15 No_fert
# 4 B1.02 6.0 7 No_fert
```

Lists

```
my.first.list ← list(siteID, soil_pH, num.sp, treatment)
  my.first.list
# [[1]]
# [1] "A1.01" "A1.02" "B1.01" "B1.02"
#
# [[2]]
# [1] 5.6 7.3 4.1 6.0
#
# [[3]]
# [1] 17 23 15 7
#
# [[4]]
# [1] "Fert" "Fert" "No_fert" "No_fert"
```

Control flow

Control flow

Program flow control can be simply defined as the order in which a program is executed.

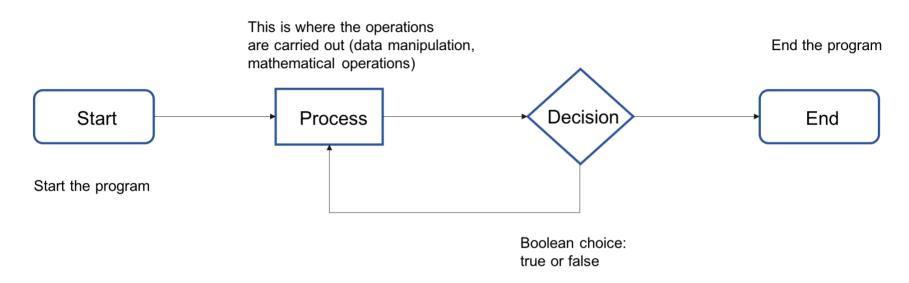
Why is it advantageous to have structured programs?

- It decreases the complexity and time of the task at hand;
- This logical structure also means that the code has increased clarity;
- It also means that many programmers can work on one program.

This means increased productivity

Control flow

Flowcharts can be used to plan programs and represent their structure



Representing structure

The two basic building blocks of codes are the following:

Selection

Program's execution determined by statements

```
if
if else
```

Iteration

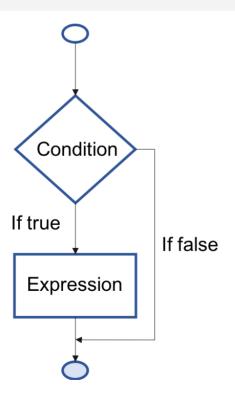
Repetition, where the statement will **loop** until a criteria is met

```
for while repeat
```

Decision making

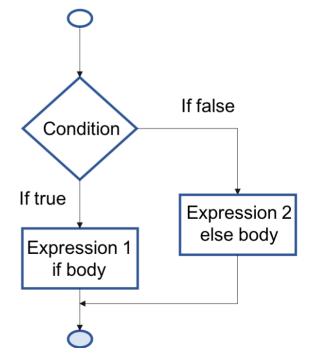
if statement

```
if(condition) {
  expression
}
```



if else statement

```
if(condition) {
   expression 1
} else {
   expression 2
}
```



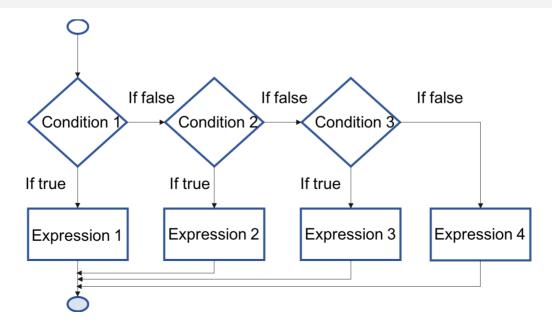
What if you want to test more than one condition?

- if and if else test a single condition
- You can also use ifelse function to:
 - test a vector of conditions;
 - apply a function only under certain conditions.

```
a \leftarrow 1:10
ifelse(a > 5, "yes", "no")
a \leftarrow (-4):5
sqrt(ifelse(a \geqslant 0, a, NA))
```

Nested if else statement

```
if (test_expression1) {
  statement1
} else if (test_expression2) {
  statement2
} else if (test_expression3) {
  statement3
} else {
  statement4
}
```



Challenge 1



```
Paws ← "cat"
Scruffy ← "dog"
Sassy ← "cat"
animals ← c(Paws, Scruffy, Sassy)
```

- 1. Use an [if] statement to print "meow" if Paws is a "cat".
- 2. Use an if else statement to print "woof" if you supply an object that is a "dog" and "meow" if it is not. Try it out with Paws and Scruffy.
- 3. Use the [ifelse function to display "woof" for [animals that are dogs and "meow" for [animals that are cats.

Challenge 1 - Solution



1- Use an [if] statement to print "meow" if Paws is a "cat".

```
if(Paws = 'cat') {
  print("meow")
}
# [1] "meow"
```

2- Use an if else statement to print "woof" if you supply an object that is a "dog" and "meow" if it is not. Try it out with Paws and Scruffy.

```
x = Paws
# x = Scruffy
if(x == 'cat') {
   print("meow")
} else {
   print("woof")
}
# [1] "meow"
```

Challenge 1 - Solution



3- Use the ifelse function to display "woof" for animals that are dogs and "meow" for animals that are cats.

```
animals ← c(Paws, Scruffy, Sassy)

ifelse(animals = 'dog', "woof", "meow")
# [1] "meow" "woof" "meow"
```

Or

```
for(val in 1:3) {
   if(animals[val] = 'cat') {
      print("meow")
   }else if(animals[val] = 'dog') {
      print("woof")
   }else print("what?")
}
# [1] "meow"
# [1] "meow"
# [1] "meow"
```

Beware of R's expression parsing!

Use curly brackets {} so that R knows to expect more input. Try:

```
if (2+2) = 4 print("Arithmetic works.")
else print("Houston, we have a problem.")
```

This doesn't work because R evaluates the first line and doesn't know that you are going to use an else statement

Instead use:

```
if (2+2 = 4) {
  print("Arithmetic works.")
} else {
  print("Houston, we have a problem.")
}
# [1] "Arithmetic works."
```

Remember the logical operators

Command	Meaning
	equal to
\neq	not x
<	less than
\leq	less than or equal to
>	greater than
\geqslant	greater than or equal to
хву	x AND y
x y	x OR y
<pre>isTRUE(x)</pre>	test if X is true

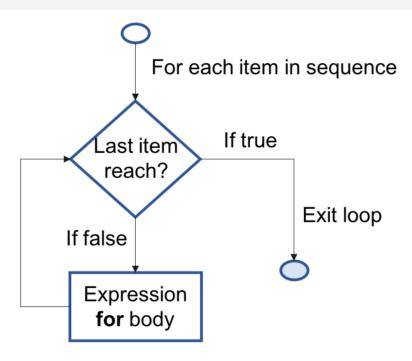
Iteration

Every time some operations have to be repeated, a loop may come in handy Loops are good for:

- doing something for every element of an object
- doing something until the processed data runs out
- doing something for every file in a folder
- doing something that can fail, until it succeeds
- iterating a calculation until it converges

A for loop works in the following way:

```
for(val in sequence) {
  statement
  }
```



The letter i can be replaced with any variable name and the sequence can be almost anything, even a list of vectors.

```
# Try the commands below and see what happens:
for (a in c("Hello", "R", "Programmers")) {
  print(a)
for (z in 1:30) {
  a \leftarrow rnorm(n = 1, mean = 5, sd = 2)
  print(a)
elements \leftarrow list(1:3, 4:10)
for (element in elements) {
  print(element)
```

In the example below, R would evaluate the expression 5 times:

```
for(i in 1:5) {
  expression
}
```

In the example, every instance of m is being replaced by each number between 1:10, until it reaches the last element of the sequence.

```
for(m in 1:10) {
   print(m*2)
}
```

```
# [1] 2  # [1] 12

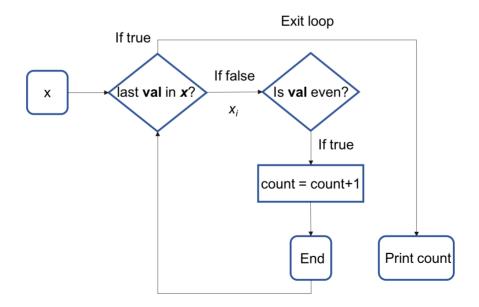
# [1] 4  # [1] 14

# [1] 6  # [1] 16

# [1] 8  # [1] 18

# [1] 10  # [1] 20
```

```
x \( \sigma \cdot \cdot (2,5,3,9,6) \)
count \( \sigma \cdot 0 \)
for (val in x) {
   if(val %% 2 = 0) {
      count = count+1
    }
}
print(count)
```



For loops are often used to loop over a dataset. We will use loops to perform functions on the CO2 dataset which is built in R.

```
data(CO2) # This loads the built in dataset

for (i in 1:length(CO2[,1])) { # for each row in the CO2 dataset
    print(CO2$conc[i]) # print the CO2 concentration
}

for (i in 1:length(CO2[,1])) { # for each row in the CO2 dataset
    if(CO2$Type[i] = "Quebec") { # if the type is "Quebec"
        print(CO2$conc[i]) # print the CO2 concentration
        }
}
```

Tip 1. To loop over the number of rows of a data frame, we can use the function (nrow())

```
for (i in 1:nrow(CO2)) { # for each row in the CO2 dataset
  print(CO2$conc[i]) # print the CO2 concentration
}
```

Tip 2. If we want to perform operations on the elements of one column, we can directly iterate over it

```
for (p in CO2$conc) { # for each element of the column "conc" of the CO2
  print(p) # print the p-th element
}
```

The expression within the loop can be almost anything and is usually a compound statement containing many commands.

```
for (i in 4:5) { # for i in 4 to 5
  print(colnames(CO2)[i])
  print(mean(CO2[,i])) # print the mean of that column from the CO2 datas
}
```

Output:

```
# [1] "conc"
# [1] 435
# [1] "uptake"
# [1] 27.2131
```

for loops within for loops

In some cases, you may want to use nested loops to accomplish a task. When using nested loops, it is important to use different variables as counters for each of your loops. Here we used i and n:

```
for (i in 1:3) {
   for (n in 1:3) {
     print (i*n)
   }
}
```

```
# Output
# [1] 1
# [1] 2
# [1] 3
# [1] 4
# [1] 6
# [1] 3
# [1] 6
# [1] 9
```

Getting good: using the apply() family

R disposes of the apply() function family, which consists of vectorized functions that aim at minimizing your need to explicitly create loops.

apply() can be used to apply functions to a matrix.

```
(height \leftarrow matrix(c(1:10, 21:30), nrow = 5, ncol = 4))

# [,1] [,2] [,3] [,4]

# [1,] 1 6 21 26

# [2,] 2 7 22 27

# [3,] 3 8 23 28

# [4,] 4 9 24 29

# [5,] 5 10 25 30
```

lapply()

[lapply()] applies a function to every element of a [list].

It may be used for other objects like dataframes, lists or vectors.

The output returned is a list (explaining the "l" in lapply) and has the same number of elements as the object passed to it.

```
SimulatedData ← list(
   SimpleSequence = 1:4,
   Norm10 = rnorm(10),
   Norm20 = rnorm(20, 1),
   Norm100 = rnorm(100, 5))

# Apply mean to each element
## of the list
lapply(SimulatedData, mean)
```

```
# $SimpleSequence
# [1] 2.5
#
# $Norm10
# [1] 0.1784198
#
# $Norm20
# [1] 0.8261701
#
# $Norm100
# [1] 5.005759
```

sapply()

```
sapply() is a 'wrapper' function for [lapply()], but returns a simplified
output as a vector, instead of a [list].
```

The output returned is a <u>list</u> (explaining the "l" in <u>lapply</u>) and has the same number of elements as the object passed to it.

mapply()

```
mapply() works as a multivariate version of [sapply()].
```

It will apply a given function to the first element of each argument first, followed by the second element, and so on. For example:

```
lilySeeds ← c(80, 65, 89, 23, 21)
poppySeeds ← c(20, 35, 11, 77, 79)

# Output
mapply(sum, lilySeeds, poppySeeds)
# [1] 100 100 100 100 100
```

tapply()

tapply() is used to apply a function over subsets of a vector.

6

82.63636 122.28571 209.21429

It is primarily used when the dataset contains dataset contains different groups (i.e. levels/factors) and we want to apply a function to each of these groups.

```
head(mtcars)
#
                 mpg cyl disp hp drat wt gsec vs am gear carb
# Mazda RX4
                 21.0 6
                          160 110 3.90 2.620 16.46 0
# Mazda RX4 Wag 21.0 6 160 110 3.90 2.875 17.02 0 1
                             93 3.85 2.320 18.61 1 1
# Datsun 710
           22.8 4
                         258 110 3.08 3.215 19.44 1 0
# Hornet 4 Drive 21.4 6
# Hornet Sportabout 18.7 8
                         360 175 3.15 3.440 17.02 0 0
# Valiant
                 18.1
                         225 105 2.76 3.460 20.22
# get the mean hp by cylinder groups
tapply(mtcars$hp, mtcars$cyl, FUN = mean)
```

Challenge 2



You have realized that your tool for measuring uptake was not calibrated properly at Quebec sites and all measurements are 2 units higher than they should be.

- 1. Use a loop to correct these measurements for all Quebec sites.
- 2. Use a vectorisation-based method to calculate the mean CO2-uptake in both areas.

For this, you will have to load the CO2 dataset using data(CO2), and then use the object CO2.

Challenge 2: Solution



1. Using for and if to correct the measurements:

```
for (i in 1:dim(CO2)[1]) {
   if(CO2$Type[i] = "Quebec") {
      CO2$uptake[i] ← CO2$uptake[i] - 2
   }
}
```

1. Using () to calculate the mean for each group:

```
tapply(CO2$uptake, CO2$Type, mean)
# Quebec Mississippi
# 31.54286 20.88333
```

Modifying iterations

Normally, loops iterate over and over until they finish.

Sometimes you may be interested in breaking this behaviour.

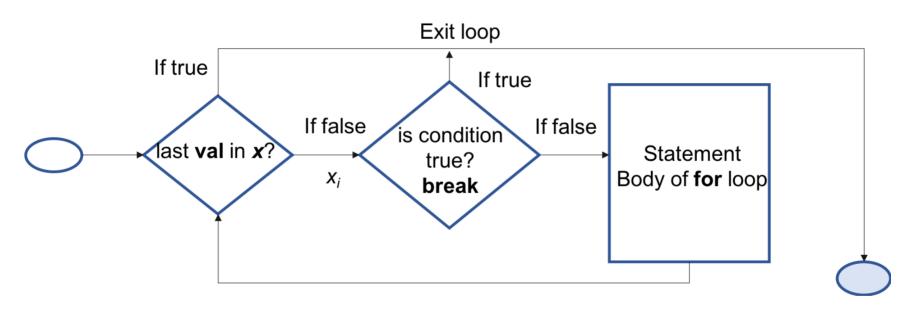
For example, you may want to tell R to stop executing the iteration when it reaches a given element or condition.

You may also want R to jump certain elements when certain conditions are met.

For this, we will introduce break, next and while.

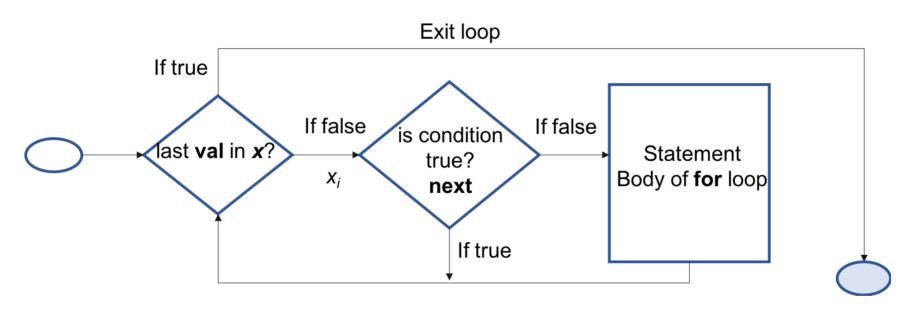
Modifying iterations: break

```
for(val in x) {
  if(condition) { break }
  statement
}
```



Modifying iterations: next

```
for(val in x) {
  if(condition) { next }
  statement
}
```



Modifying iterations: next

Print the CO_2 concentrations for "chilled" treatments and keep count of how many replications were done.

```
count \leftarrow \emptyset
 for (i in 1:nrow(CO2)) {
   if (CO2$Treatment[i] = "nonchilled") next
   # Skip to next iteration if treatment is nonchilled
   count \leftarrow count + 1
   print(CO2$conc[i])
 print(count) # The count and print command were performed 42 times.
# [1] 42
 sum(CO2$Treatment = "nonchilled")
 # [1] 42
```

Modifying iterations: break

This could be equivalently written using a repeat loop and break:

```
count ← 0
i ← 0
repeat {
    i ← i + 1
    if (CO2$Treatment[i] = "nonchilled") next # skip this loop
    count ← count + 1
    print(CO2$conc[i])
    if (i = nrow(CO2)) break # stop looping
    }
print(count)
```

Modifying iterations: while

This could also be written using a while loop:

```
i ← 0
count ← 0
while (i < nrow(CO2))
{
   i ← i + 1
   if (CO2$Treatment[i] = "nonchilled") next # skip this loop
   count ← count + 1
   print(CO2$conc[i])
}
print(count)</pre>
```

Challenge 3



You have realized that your tool for measuring concentration did not work properly.

At Mississippi sites, concentrations less than 300 were measured correctly, but concentrations equal or higher than 300 were overestimated by 20 units!

Your *mission* is to use a loop to correct these measurements for all Mississippi sites.

Tip. Make sure you reload the data so that we are working with the raw data for the rest of the exercise:

data(CO2)

Challenge 3: Solution



```
for (i in 1:nrow(CO2)) {
   if(CO2$Type[i] = "Mississippi") {
      if(CO2$conc[i] < 300) next
      CO2$conc[i] ← CO2$conc[i] - 20
   }
}</pre>
```

Note: We could also have written it in this way, which is more concise and clear:

```
for (i in 1:nrow(CO2)) {
   if(CO2$Type[i] = "Mississippi" & CO2$conc[i] ≥ 300) {
      CO2$conc[i] ← CO2$conc[i] - 20
   }
}
```

Edit a plot using for and if

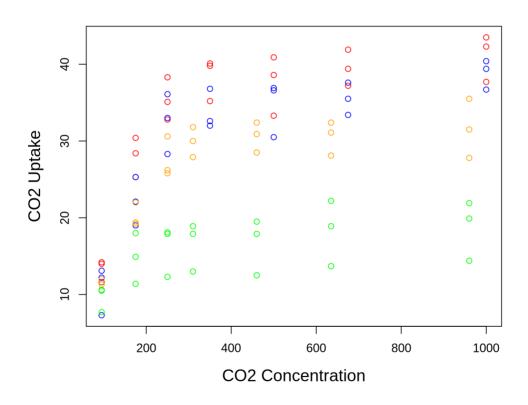
Let's plot **uptake** vs **concentration** with points of different colors according to their type (*Quebec* or *Mississippi*) and **treatment** (*chilled* or *nonchilled*).

```
plot(x = CO2\$conc, y = CO2\$uptake, type = "n", cex.lab=1.4,
     xlab = "CO2 concentration", ylab = "CO2 uptake")
# Type "n" tells R to not actually plot the points.
for (i in 1:length(CO2[,1])) {
  if (CO2$Type[i] = "Quebec" & CO2$Treatment[i] = "nonchilled") {
    points(CO2$conc[i], CO2$uptake[i], col = "red")
  if (CO2$Type[i] = "Quebec" & CO2$Treatment[i] = "chilled") {
    points(CO2$conc[i], CO2$uptake[i], col = "blue")
  if (CO2$Type[i] = "Mississippi" & CO2$Treatment[i] = "nonchilled") {
    points(CO2$conc[i], CO2$uptake[i], col = "orange")
  if (CO2$Type[i] = "Mississippi" & CO2$Treatment[i] = "chilled") {
    points(CO2$conc[i], CO2$uptake[i], col = "green")
```

Challenge 4



Create a plot using for loop and [if]



Challenge 4



Generate a plot showing **concentration versus uptake** where each plant is shown using a different **colour** point.

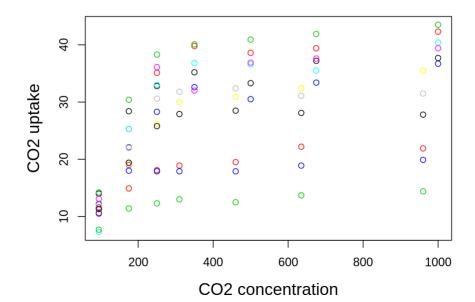
Bonus points for doing it with nested loops!

Steps:

- 1. Create an empty plot
- 2. Create a list of plants (hint: [?unique])
- 3. Fill the plot using for and [if] statements

Challenge 4: Solution





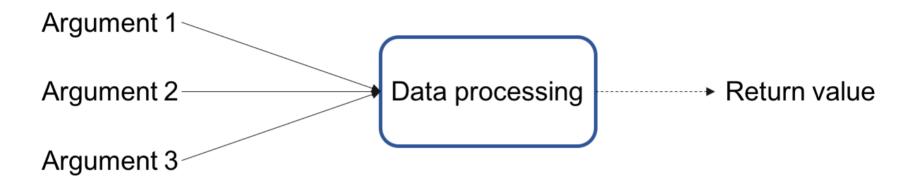
Writing functions

Why write functions?

Much of the heavy lifting in R is done by functions. They are useful for:

- 1. Performing a task repeatedly, but configurably;
- 2. Making your code more readable;
- 3. Make your code easier to modify and maintain;
- 4. Sharing code between different analyses;
- 5. Sharing code with other people;
- 6. Modifying R's built-in functionality.

What is a function?



Syntax of a function

```
function_name 
    function(argument1, argument2, ...) {
    expression ...  # What we want the function to do
    return(value)  # Optional
}
```

Arguments of a function

```
function_name ← function(argument1, argument2, ...) {
  expression ...
  return(value)
}
```

Arguments are the entry values of your function and will have the information your function needs to be able to perform correctly.

A function can have between 0 and an infinity of arguments. See the following example:

```
operations ← function(number1, number2, number3) {
  result ← (number1 + number2) * number3
  print(result)
}
```

```
operations(1, 2, 3) # [1] 9
```

Challenge 5



Using what you learned previously on flow control, create a function print_animal that takes an animal as argument and gives the following results:

```
Scruffy ← "dog"
Paws ← "cat"

print_animal(Scruffy)
# [1] "woof"

print_animal(Paws)
# [1] "meow"
```

Challenge 5: Solution



Default values in a function

Arguments can also be optional and be provided with a default value.

This is useful when using a function with the same settings, but still provides the flexibility to change its values, if needed.

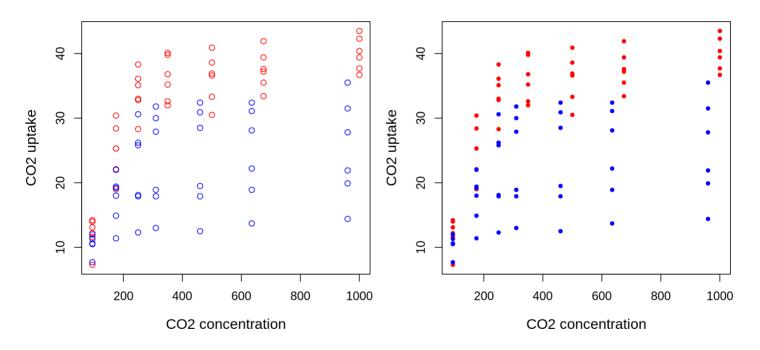
Argument

The special argument ... allows you to pass on arguments to another function used inside your function. Here we use ... to pass on arguments to plot() and points().

```
plot.CO2 ← function(CO2, ...) {
    plot(x=CO2$conc, y=CO2$uptake, type="n", ...)
    for (i in 1:length(CO2[,1])){
        if (CO2$Type[i] = "Quebec") {
            points(CO2$conc[i], CO2$uptake[i], col = "red", type = "p", ...)
        } else if (CO2$Type[i] = "Mississippi") {
            points(CO2$conc[i], CO2$uptake[i], col = "blue", type = "p", ...)
        }
    }
    plot.CO2(CO2, cex.lab=1.2, xlab="CO2 concentration", ylab="CO2 uptake")
    plot.CO2(CO2, cex.lab=1.2, xlab="CO2 concentration", ylab="CO2 uptake", p
```

Argument

The special argument ... allows you to pass on arguments to another function used inside your function. Here we use ... to pass on arguments to plot() and points().



Argument

The special argument ... allows you to input an indefinite number of arguments.

```
sum2 \leftarrow function(...)
  args \leftarrow list(...)
  result \leftarrow 0
  for (i in args) {
    result ← result + i
  return (result)
sum2(2, 3)
# [1] 5
sum2(2, 4, 5, 7688, 1)
# [1] 7700
```

Return values

The last expression evaluated in a function becomes the return value.

```
myfun ← function(x) {
   if (x < 10) {
      0
   } else {
      10
   }
}
myfun(5)
# [1] 0
myfun(15)
# [1] 10</pre>
```

function() itself returns the last evaluated value even without including return() function.

Return values

It can be useful to explicitly return() if the routine should end early, jump out of the function and return a value.

```
simplefun1 ← function(x) {
  if (x<0)
  return(x)
}</pre>
```

Functions can return only a single object (and text). But this is not a limitation because you can return a list containing any number of objects.

```
simplefun2(1,
```

```
# $result
# [1] 3
#
# $x
# [1] 1
#
# $y
# [1] 2
```

Challenge 6



Using what you have just learned on functions and control flow, create a function named bigsum that takes two arguments a and b and:

- 1. Returns 0 if the sum of a and b is strictly less than 50;
- 2. Else, returns the sum of a and b.

Challenge 6: Solution



Answer 1

```
bigsum ← function(a, b) {
   result ← a + b
   if (result < 50) {
      return(0)
   } else {
      return (result)
   }
}</pre>
```

Answer 2

```
bigsum ← function(a, b) {
  result ← a + b
  if (result < 50) {
  0
  } else {
  result
  }
}</pre>
```

It is essential to always keep in mind where your variables are, and whether they are defined and accessible:

- → Variables defined **inside** a function are not accessible outside of it!
- → Variables defined **outside** a function are accessible inside. But it is NEVER a good idea, as your function will not function if the outside variable is erased.

```
var1 ← 3 # var1 is defined outside our function
vartest ← function() {
 a \leftarrow 4 # 'a' is defined inside
  print(a) # print 'a'
  print(var1) # print var1
             # we cannot print 'a' as it exists only inside the function
a
# Error in eval(expr, envir, enclos): object 'a' not found
vartest() # calling vartest() will print a and var1
# [1] 4
# [1] 3
rm(var1) # remove var1
vartest() # calling the function again doesn't work anymore
# [1] 4
# Error in print(var1): object 'var1' not found
```

Mandatory tip. Use arguments then!

Also, inside a function, arguments names will take over other variable names.

```
var1 ← 3  # var1 is defined outside our function
vartest ← function(var1) {
  print(var1) # print var1
}

vartest(8)  # Inside our function var1 is now our argument and takes it
# [1] 8

var1  # var1 still has the same value
# [1] 3
```

Tip. Be very careful when creating variables inside a conditional statement as the variable may never have been created and cause (sometimes imperceptible) errors.

Tip. It is good practice to define variables outside the conditions and then modify their values to avoid any problem

```
a \leftarrow 3
if (a > 5) {
b \leftarrow 2
}
a + b
```

```
# Error: object 'b' not found
```

If you had **b** already assigned in your environment, with a different value, you could have had a **bigger** problem!

No error would have been shown and a + b would have meant another thing!

Good programming practices

Why should I care about programming practices?

- To make your life easier;
- To achieve greater readability and makes sharing and reusing your code a lot less painful;
- To reduce the time you will spend to understand your code.

Pay attention to the next tips!

Keep a clean and nice code

Proper indentation and spacing is the first step to get an easy to read code:

- Use spaces between and after you operators;
- Use consistentely the same assignation operator. ← is often preferred. = is OK, but do not switch all the time between the two;
- Use brackets when using flow control statements:
 - Inside brackets, indent by at least two spaces;
 - Put closing brackets on a separate line, except when preceding an else statement.
- Define each variable on its own line.

Keep a clean and nice code

On the left, code is not spaced. All brackets are in the same line, and it looks "messy".

```
a←4;b=3

if(a<b){

if(a=0)print("a zero")}else{

if(b=0){print("b zero")}else pri
```

Keep a clean and nice code

On the left, code is not spaced. All brackets are in the same line, and it looks "messy". On the right, it looks more organized, no?

```
a←4;b=3

if(a<b){

if(a=0)print("a zero")}else{

if(b=0){print("b zero")}else pri
```

```
a \leftarrow 4
b \leftarrow 3
if(a < b){
  if(a = 0) {
    print("a zero")
} else {
  if(b = 0)
    print("b zero")
  } else {
    print(b)
```

Use functions to simplify your code

Write your own function:

- 1. When portion of the code is repeated more than twice in your script;
- 2. If only a part of the code changes and includes options for different arguments.

This would also reduce the number of potential errors done by copy-pasting, and the time needed to correct them.

Use functions to simplify your code

Let's modify the example from **Challenge #3** and suppose that all CO_2 uptake from Mississipi plants was overestimated by 20 and Quebec underestimated by 50.

We could write this:

```
for (i in 1:length(CO2[,1])) {
   if(CO2$Type[i] = "Mississippi"
        CO2$conc[i] ← CO2$conc[i] -
   }
}
for (i in 1:length(CO2[,1])) {
   if(CO2$Type[i] = "Quebec") {
        CO2$conc[i] ← CO2$conc[i] +
   }
}
```

Or this:

```
recalibrate 
function(CO2, type
for (i in 1:nrow(CO2)) {
   if(CO2$Type[i] = type) {
      CO2$conc[i] 
      CO2$conc[i]
   }
}
return(CO2)
}
```

```
newCO2 ← recalibrate(CO2, "Missi
newCO2 ← recalibrate(newCO2, "Qu
```

Use meaningful names for functions

Same function as before, but with vague names.

```
rc ← function(c, t, b) {
   for (i in 1:nrow(c)) {
     if(c$Type[i] = t) {
      c$uptake[i] ← c$uptake[i]
     }
   }
   return (c)
}
```

What is c and rc?

Whenever possible, avoid using names of existing $\mathbb R$ functions and variables to avoid confusion and conflits.

Use comments

Final tip. Add comment to describe what your code does, how to use its arguments or a detailed step-by-step description of the function.

```
# Recalibrates the CO2 dataset by modifying the CO2 uptake concentration
# by a fixed amount depending on the region of sampling
# Arguments
# CO2: the CO2 dataset
# type: the type ("Mississippi" or "Quebec") that need to be recalibrated
# bias: the amount to add or remove to the concentration uptake
recalibrate ← function(CO2, type, bias) {
  for (i in 1:nrow(CO2)) {
    if(CO2\$Type[i] = type) {
      CO2$uptake[i] \leftarrow CO2$uptake[i] + bias
  return(CO2)
```

Thank you for attending this workshop!

