# Building reproducible analytical pipelines with the R programming language

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# **Preface**

This is a Quarto book.

To learn more about Quarto books visit https://quarto.org/docs/books.

# 1 Introduction

This book will teach how to structure your projects in such a way as to make them reproducible.

I think we should also explain that this book presents one way of doing things, and that it is by no means the only, canonic way, of solving the problems we will be talking about.

# 1.1 Prerequisites

You should be comfortable with the R programming language. This book will assume that you have been using R for some projects already, and want to improve not only your knowledge of the language itself, but also how to successfully manage complex projects.

# 1.2 What is reproducibility?

# 1.3 Are there different types of reproducibility?

Reproducibility is on a continuum.

# 2 Functional programming

This chapter will teach you the fundamentals of functional programming. Functional programming might sound scary, but we will focus on only a handful of concepts that are quite accessible while providing many benefits. Using these functional programming concepts will make your code more reliable, easier to test, document, share, and ultimately rerun.

#### 2.1 Introduction

You are very likely already familiar with some aspects of functional program. Let's start by discussing the two central elements of functional programming: functions and lists.

There are several ways that you can structure a program, called programming paradigms. Functional programming is a paradigm that relies exclusively on the evaluation of functions to achieve the desired end result. If you have already written your own functions in the past, what follows will not be very new. But in order to write a good functional program, the functions that you write and evaluate have to have certain properties. Before discussing these properties, let's start by with *state*.

#### 2.1.1 The state of your program

Let's suppose that you start a fresh R session, and immediately run this next line:

```
ls()
```

If you did not modify any of R's configuration files that get automatically loaded on startup, you should see the following:

```
character(0)
```

Let's suppose that now you load some data:

```
data(mtcars)
```

and define a variable a:

```
a <- 1
```

Running ls() now shows the following:

```
[1] "a" "mtcars"
```

You have just altered the state of your program. You can think of the *state* as a box that holds everything that gets defined by the user and is accessible at any time. Let's now define a simple function that prints a sentence:

```
f <- function(name) {
  print(paste0(name, " likes lasagna"))
}

f("Bruno")</pre>
```

and here's the output:

```
[1] "Bruno likes lasagna"
```

Let's run ls() again:

```
[1] "a" "f" "mtcars"
```

Function f() is now listed there as well. This function has two nice properties:

- For a given input, it always returns exactly the same output. So f("Bruno") will always return "Bruno likes lasagna".
- This function does not change the state of your program, by adding new objects every time it's run.

#### 2.1.2 Predictable functions

Let's now define another function called g(), that does not have the same properties as f(). First, let's define a function that does not always return the same output given a particular input:

```
g <- function(name){
  food <- sample(c("lasagna", "cassoulet", "feijoada"), 1)
  print(paste0(name, " likes ", food))
}</pre>
```

For the same input, "Bruno", this function now produces (potentially) a different output:

```
g("Bruno")
[1] "Bruno likes lasagna"

g("Bruno")
[1] "Bruno likes feijoada"
```

And now let's consider function h() that modifies the state of the program:

```
h <- function(name){
  food <- sample(c("lasagna", "cassoulet", "feijoada"), 1)

if(exists("food_list")){
  food_list <<- append(food_list, food)
} else {
  food_list <<- append(list(), food)
}

print(paste0(name, " likes ", food))
}</pre>
```

This function uses the <<- operator. This operator saves definitions that are made inside the body of functions in the global environment. Before calling this function, run ls() again. You should see the same objects as before, plus the new functions we've defined:

```
[1] "a" "f" "g" "h" "mtcars"
```

Let's now run h() once:

```
h("Bruno")
[1] "Bruno likes feijoada"
```

And now ls() again:

Running h() did two things: it printed the message, but also created a variable called "food list" in the global environment with the following contents:

```
food_list
```

```
[[1]]
[1] "feijoada"

Let's run h() again:
  h("Bruno")
  [1] "Bruno likes cassoulet"
```

and let's check the contents of "food list":

```
food_list

[[1]]
[1] "feijoada"

[[2]]
[1] "cassoulet"
```

If you keep running h(), this list will continue growing. Let me just say that I hesitated showing you this; this is because if you didn't know <<-, you might find the example above useful. But while useful, it is quite dangerous as well. Generally, we want to avoid using functions that change the state as much as possible because these function are unpredictable, especially if randomness is involved. It is much safer to define h() like this instead:

```
h <- function(name, food_list = list()){
  food <- sample(c("lasagna", "cassoulet", "feijoada"), 1)
  food_list <- append(food_list, food)
  print(pasteO(name, " likes ", food))
  food_list
}</pre>
```

The difference now is that we made **food\_list** the second argument of the function. Also, we defined it as being optional by writing:

```
food_list = list()
```

This means that if we omit this argument, the empty list will get used by default. This avoids the users having to manually specify it.

We can call it like this:

```
food_list <- h("Bruno", food_list) # since food_list is already defined, we don't need to

[1] "Bruno likes feijoada"</pre>
```

We save the output back to food\_list. Let's now check its contents:

```
food_list

[[1]]
[1] "feijoada"

[[2]]
[1] "cassoulet"

[[3]]
[1] "feijoada"
```

The only thing that we need now to deal with is the fact that the food gets chosen randomly. I'm going to show you the simple way of dealing with this, but later in this chapter we are going to use the {withr} package for situations like this. Let's redefine h() one last time:

```
h <- function(name, food_list = list(), seed = 123){

# We set the seed, making sure that we get the same selection of food for a given seed
    set.seed(seed)
    food <- sample(c("lasagna", "cassoulet", "feijoada"), 1)

# We now need to unset the seed, because if we don't, guess what, the seed will stay set
    set.seed(NULL)

food_list <- append(food_list, food)

print(paste0(name, " likes ", food))

food_list
}</pre>
```

Let's now call h() several times with its default arguments:

```
h("Bruno")

[1] "Bruno likes feijoada"
[[1]]
[1] "feijoada"

h("Bruno")

[1] "Bruno likes feijoada"
[[1]]
[1] "feijoada"

h("Bruno")

[1] "Bruno likes feijoada"
[[1]]
[1] "feijoada"
```

As you can see, every time this function runs, it now produces the same result. Users can change the seed to have this function produce, consistently, another result.

## 2.1.3 Referentially transparent and pure functions

A referentially transparent function is a function that does not use any variable that is not also one of its inputs. For example, the following function:

```
bad <- function(x){
   x + y
}</pre>
```

is not referentially transparent, because y is not one of the functions inputs. What happens if you run bad() is that bad() needs to look for y. Because y is not one of its inputs, bad() then looks for it in the global environment. If y is defined there, it then gets used. Defining and using such functions must be avoided at all costs, because these functions are unpredictable. For example:

```
y <- 10
bad <- function(x){
    x + y</pre>
```

```
} bad(5)
```

This will return 15. But if y <- 45 then bad(5) would this time around return 50. It is much safer, and easier to make y an explicit input of the function instead of having to keep track of y's value:

```
good <- function(x, y){
  x + y
}</pre>
```

good() is a referentially transparent function; it is much safer than bad(). good() is also a pure function, because it's a function that does not interact in any way with the global environment. It does not write anything to the global environment, nor requires anything from the global environment. Function h() from the previous section was not pure, because it created an object and wrote it to the global environment (the food\_list object). Turns out that pure functions are thus necessarily referentially transparent.

So the first lesson in your functional programming journey that you have to remember is to only use pure functions.

## 2.2 Writing good functions

#### 2.2.1 Functions are first class objects

In a functional programming language, functions are first class objects. Contrary to what the name implies, this means that functions, especially the ones you define yourself, are nothing special. A function is an object like any other, and can thus be manipulated as such. Think of anything that you can do with any object in R, and you can do the same thing with a function. For example, let's consider the +() function. It takes two numeric objects and returns their sum:

```
1 + 5.3

[1] 6.3

# or alternatively: `+`(1, 5.3)
```

You can replace the numbers by functions that return numbers:

```
sqrt(1) + log(5.3)
```

#### [1] 2.667707

It's also possible to define a function that explicitely takes another function as an input:

```
h <- function(number, f){
  f(number)
}</pre>
```

You can call then use h() as a wrapper for f():

```
h(4, sqrt)
```

[1] 2

```
h(10, log10)
```

#### [1] 1

Because h() takes another function as an argument, h() is called a higher-order function.

If you don't know how many arguments f(), the function you're wrapping, has, you can use the ...:

```
h <- function(number, f, ...){
  f(number, ...)
}</pre>
```

... are simply a placeholder for any potential additional argument that f() might have:

```
h(c(1, 2, NA, 3), mean, na.rm = TRUE)
```

[1] 2

```
h(c(1, 2, NA, 3), mean, na.rm = FALSE)
```

[1] NA

na.rm is an argument of mean(). As the developer of h(), I don't necessarily know what f() might be, or maybe I know f() and know all its arguments, but don't want to have to rewrite them all to make them arguments of h(), so I can use ... instead. The following is also possible:

```
w <- function(...){
paste0("First argument: ", ..1, ", second argument: ", ..2, ", last argument: ", ..3)
}
w(1, 2, 3)</pre>
```

[1] "First argument: 1, second argument: 2, last argument: 3"

If you want to learn more about ..., type ?dots in an R console.

Because functions are nothing special, you can also write functions that return functions. As an illustration, we'll be writing a function that converts warnings to errors. This can be quite useful if you want your functions to fail early, which often makes debuging easier. For example, try running this:

```
sqrt(-5)
```

Warning in sqrt(-5): NaNs produced

[1] NaN

This only raises a warning and returns NaN (Not a Number). This can be quite dangerous, especially when working non-interactively, which is what we will be doing a lot later on. It is much better if a pipeline fails early due to an error, than dragging an NaN value. This also happens with log():

```
sqrt(-10)
```

Warning in sqrt(-10): NaNs produced

[1] NaN

So it could be useful to redefine this functions to raise an error instead, for example like this:

```
strict_sqrt <- function(x){
  if(x <= 0) stop("x is negative")
  sqrt(x)
}</pre>
```

This function now throws an error for negative x:

```
strict_sqrt(-10)
```

```
Error in strict_sqrt(-10) : x is negative
```

However, it can be quite tedious to redefine every function that we need in our pipeline. This is where a function factory is useful. We can define a function that takes a function as an argument, converts any warning thrown by that function into an error, and returns the new function. For example it could look like this:

```
strictly <- function(f){
  function(...){
    tryCatch({
      f(...)
    },
    warning = function(warning)stop("Can't do that chief"))
  }
}</pre>
```

This function makes use of tryCatch() which catches warnings raised by an expression (in this example the expression is f(...)) and then raises an error insead with the stop() function. It is now possible to define new functions like this:

```
s_sqrt <- strictly(sqrt)
s_sqrt(-4)</pre>
```

Error in value[[3L]](cond) : Can't do that chief

```
s_log <- strictly(log)</pre>
```

```
s_log(-4)
```

```
Error in value[[3L]](cond) : Can't do that chief
```

Functions that return functions are called *functions factories* and they're incredibly useful. I use this so much that I've written a package, available on CRAN, called {chronicler}, that does this:

```
s_sqrt <- chronicler::record(sqrt)

result <- s_sqrt(-4)

result

NOK! Value computed unsuccessfully:
-----
Nothing

-----
This is an object of type `chronicle`.
Retrieve the value of this object with pick(.c, "value").
To read the log of this object, call read_log(.c).</pre>
```

Because the expression above resulted in an error, Nothing is returned. Nothing is a special value defined in the {maybe} package (check it out, very interesting package!). We can then even read the log to see what went wrong:

```
chronicler::read_log(result)
```

- [1] "Complete log:"
- [2] "NOK! sqrt() ran unsuccessfully with following exception: NaNs produced at 2023-01-28 10
- [3] "Total running time: 0.00107216835021973 secs"

The {purrr} package also comes with function factories that you might find useful ({possibly}, {safely} and {quietly}).

#### 2.2.2 Optional arguments

It is possible to make function arguments optional, by using NULL. For example:

```
g <- function(x, y = NULL){
  if(is.null(y)){
    print("optional argument y is NULL")
    x
  } else {
    if(y == 5) print("y is present"); x+y
  }
}</pre>
```

Calling g(10) prints the message "Optional argument y is NULL", and returns 10. Calling g(10, 5) however, prints "y is present" and returns 15. It is also possible to use missing():

```
g <- function(x, y){
  if(missing(y)){
    print("optional argument y is missing")
    x
} else {
  if(y == 5) print("y is present"); x+y
}</pre>
```

I however prefer the first approach, because it is clearer which arguments are optional, which is not the case with the second approach, where you need to read the body of the function.

#### 2.2.3 Safe functions

It is important that your functions are safe and predictable. You should avoid writing functions that behave like nchar(), a base R function. Let's see why this function is not safe:

```
nchar("10000000")
```

[1] 8

It returns the expected result of 8. But what if I remove the quotes?

```
nchar(10000000)
```

[1] 5

What is going on here? I'll give you a hint: simply type 10000000 in the console:

#### [1] 1e+07

10000000 gets represented as 1e+07 by R. This number in scientific notation gets then converted into the character "1e+07" by nchar(), and this conversion happens silently. nchar() then counts the number of characters, and *correctly* returns 5. The problem is that it doesn't make sense to provide a number to a function that expects a character. This function should have returned an error message, or at the very least raised a warning that the number got converted into a character. Here is how you could rewrite nchar() to make it safer:

This function now returns an error message if the input is not a character:

```
nchar2(10000000)
```

Error in nchar2(10000000): x should be of type 'character', but is of type 'integer' instead

#### 2.2.4 Recursive functions

You may have noticed that in the last lines of nchar2(), that nchar2() calls itself. A function that calls itself in its own body is called a recursive function. It is sometimes easier to write down a function in its recursive form than in an iterative form. The most common example is the factorial function. However, there is an issue with recursive functions (in the R programming language, other programming languages may not have the same problem, like Haskell):

while it is sometimes easier to write down a function using a recursive algorithm than an iterative algorithm, like for the factorial function, recursive functions in R are quite slow. Let's take a look at two definitions of the factorial function, one recursive, the other iterative:

```
fact_iter <- function(n){
    result = 1
    for(i in 1:n){
        result = result * i
        i = i + 1
    }
    result
}

fact_recur <- function(n){
    if(n == 0 || n == 1){
        result = 1
    } else {
        n * fact_recur(n-1)
    }
}</pre>
```

Using the {microbenchmark} package we can benchmark the code:

```
microbenchmark::microbenchmark(
  fact_recur(50),
  fact_iter(50)
)
```

#### Unit: microseconds

```
expr min lq mean median uq max neval fact_recur(50) 21.501 21.701 23.82701 21.901 22.0515 68.902 100 fact_iter(50) 2.000 2.101 2.74599 2.201 2.3510 21.000 100
```

We see that the recursive factorial function is 10 times slower then the iterative version. In this particular example it doesn't make much of a difference, because the functions only take microseconds to run. But if you're working with more complex functions, this is a problem. If you want to keep using the recursive function and not switch to an iterative algorithm, there are workarounds. The first is called *trampolining*. I won't go into details, but if you're interested, there is an R package that allows you to use trampolining with R, aptly called *trampoline*. Another solution is using the *memoise* package.

#### 2.2.5 Anonymous functions

It is possible to define a function and not give it a name. For example:

```
function(x)(x+1)(10)
```

Since R version 4.1, there is even a shorthand notation for an onymous functions:

```
(\(x)(x+1))(10)
```

Because we don't name them, we cannot reuse them. So why is this useful? Anonymous functions are useful when you need to apply a function somewhere inside a pipe once, and don't want to define a function just for this. This will become clearer once we learn about lists, but before that, let's philosophize a bit.

#### 2.2.6 The Unix philosophy applied to R

This is the Unix philosophy: Write programs that do one thing and do it well. Write programs to work together. Write programs to handle text streams, because that is a universal interface.

Doug McIlroy, in A Quarter Century of Unix<sup>1</sup>

We can take inspiration from the Unix philosophy and rewrite it like this for our purposes:

Write functions that do one thing and do it well. Write functions that work together. Write functions that handle lists, because that is a universal interface.

Strive for writing simple functions that only perform one task. Don't hesitate to split a big function into smaller ones. Small functions that only perform one task are easier to maintain, test, document and debug. These smaller functions can then be chained using the |> operator. In other words, it is preferable to have something like:

where a is for example a path to a data set, and where f(), g() and h() successively read, clean, and plot the data, than having something like:

big\_function(a)

 $<sup>^{1}</sup>$ https://stackoverflow.com/a/68690065/1298051

that does all the steps above in one go.

This idea of splitting the problem into smaller chunks, each chunk in turn split into even smaller units that can be handled by functions and then the results of these function combined into a final output is called composability.

The advantage of splitting big\_function() into f(), g() and h() is that you can tackle big problems one bite at a time, and also reusing these smaller functions in other projects is much easier. So what's important is that you can make small functions work together by sharing a common interface. The list is usually a good candidate for this.

## 2.3 Lists: a powerful data-structure

Lists are the second important ingredient of functional programming. In the R philosophy inspired from UNIX, I stated that *lists are an universal interface* in R, so our functions should handle lists. This of course depends on what it is your doing. If you need functions to handle numbers, then there's little value in placing these numbers inside lists. But in practice, you will very likely manipulate objects that are more complex than numbers, and this is where lists come into play.

#### 2.3.1 Lists all the way down

Lists are extremely flexible, and most very complex objects classes that you manipulate are actually lists, but just fancier. For example, a data frame is a list:

```
data(mtcars)
  typeof(mtcars)

[1] "list"

A fitted model is a list:
  my_model <- lm(hp ~ mpg, data = mtcars)
  typeof(my_model)

[1] "list"

A ggplot is a list:</pre>
```

```
library(ggplot2)

my_plot <- ggplot(data = mtcars) +
    geom_line(aes(y = hp, x = mpg))

typeof(my_plot)

[1] "list"</pre>
```

It's lists all the way down, and it's not a coincidence. It's because, as stated, lists are very powerful. So it's important to know what you can do with lists.

#### 2.3.2 Lists can hold many things

If you write a function that needs to return many objects, the only solution is to place them inside a list. For example, consider this function:

```
sqrt_newton <- function(a, init = 1, eps = 0.01, steps = 1){
    stopifnot(a >= 0)
    while(abs(init**2 - a) > eps){
        init <- 1/2 *(init + a/init)
        steps <- steps + 1
    }
    list(
        "result" = init,
        "steps" = steps
    )
}</pre>
```

This function returns the square root of a number using Newton's algorithm, as well as the number of steps, or iterations, it took to reach the solution:

```
result_list <- sqrt_newton(1600)
result_list

$result
[1] 40

$steps
[1] 10</pre>
```

It is quite common to instead print the number of steps to the console instead of returning them. But the issue with a function that prints something to the console instead of returning it, is that such a function is not pure, as it changes something outside of its scope. It is preferable to instead make the function pure by returning everything inside a neat list. It is then possible to separately save these objects if needed:

```
result <- result_list$result
result_steps <- result_list$steps</pre>
```

Or you could define functions that know how to deal with the list:

```
f <- function(result_list){
    list(
        "result" = result_list$result * 10,
        "steps" = result_list$steps + 1
      )
}

f(result_list)

$result
[1] 400

$steps
[1] 11</pre>
```

It all depends on what you want to do. But it is usually better to keep everything neatly inside a list.

Lists can also hold objects of differen types:

```
list(
   "a" = head(mtcars),
   "b" = ~lm(y ~ x)
)
```

\$a

```
mpg cyl disp hp drat wt qsec vs am gear carb
Mazda RX4 21.0 6 160 110 3.90 2.620 16.46 0 1 4 4
Mazda RX4 Wag 21.0 6 160 110 3.90 2.875 17.02 0 1 4 4
```

```
Datsun 710
                  22.8
                          4 108 93 3.85 2.320 18.61
                                                                      1
Hornet 4 Drive
                  21.4
                             258 110 3.08 3.215 19.44
                                                                3
                          6
                                                        1
                                                                      1
                             360 175 3.15 3.440 17.02
Hornet Sportabout 18.7
                          8
                                                        0
                                                           0
                                                                3
                                                                      2
Valiant
                   18.1
                          6
                             225 105 2.76 3.460 20.22 1 0
                                                                3
                                                                      1
$b
\sim lm(y \sim x)
```

The list above has two elements, the first is the head of the mtcars data frame, the second is a formula object. Lists can even hold other lists:

```
list(
   "a" = head(mtcars),
   "b" = list(
      "c" = sqrt,
      "d" = my_plot # Remember this ggplot object from before?
   )
)
```

#### \$a

```
qsec vs am gear carb
                  mpg cyl disp hp drat
                                            wt
Mazda RX4
                  21.0
                            160 110 3.90 2.620 16.46
Mazda RX4 Wag
                  21.0
                            160 110 3.90 2.875 17.02
                                                         1
                                                                   4
Datsun 710
                  22.8
                         4
                            108 93 3.85 2.320 18.61
                                                         1
                                                              4
                                                                   1
Hornet 4 Drive
                  21.4
                            258 110 3.08 3.215 19.44
                                                              3
                         6
                                                      1
                                                         0
                                                                   1
Hornet Sportabout 18.7
                         8
                            360 175 3.15 3.440 17.02 0
                                                         0
                                                              3
                                                                   2
                            225 105 2.76 3.460 20.22 1 0
Valiant
                  18.1
                         6
                                                              3
                                                                   1
```

```
$b
$b$c
function (x) .Primitive("sqrt")
```

\$b\$d



Use this to your advantage.

#### 2.3.3 Lists as the cure to loops

Loops are incredibly useful, and you are likely familiar with them. The problem with loops is that they are a concept from iterative programming, not functional programming, and this is a problem because loops rely on changing the state of your program to function. For example, let's suppose that you wish to use a for-loop to compute the sum of the first 100 integers:

```
result <- 0
for (i in 1:100){
   result <- result + i
}
print(result)</pre>
```

#### [1] 5050

If you run ls() now, you should see that there's a variable i in your global environment. This could cause issues further down in your pipeline if you need to re-use i. Also, writing loops is, in my opinion, quite error prone. But how can we avoid using loops? For looping in a

functional programming language, we need to use higher-order functions and lists. A reminder: a higher-order function is a function that takes another function as an argument. Looping is a task like any other, so we can write a function that does the looping for us. We will call it looping(), which will take a function as an argument, as well as list. The list will serve as the container to hold our numbers:

```
looping <- function(a list, a func, init = NULL, ...){</pre>
  # If the user does not provide an `init` value, set the head of the list as the initial
  if(is.null(init)){
    init <- a_list[[1]]</pre>
    a_list <- tail(a_list, -1)
  }
  # Separate the head from the tail of the list and apply the function to the initial value
  head_list = a_list[[1]]
  tail_list = tail(a_list, -1)
  init = a_func(init, head_list, ...)
  # Check if we're done: if there is still some tail, rerun the whole thing until there's
  if(length(tail_list) != 0){
    looping(tail_list, a_func, init, ...)
  }
  else {
    init
  }
}
```

Now, this might seem much more complicated than a for loop. However, now that we have abstracted the loop away inside a function, we can keep reusing this function:

```
looping(as.list(seq(1:100)), `+`)
```

[1] 5050

Of course, because this is so useful, looping() actually ships with R, and is called Reduce():

```
Reduce(`+`, seq(1:100)) # the order of the arguments is `function` then `list` for `Reduce
```

[1] 5050

But this is not the only way that we can loop. We can also write a loop that applies a function to each element of a list, instead of operating on the whole list:

```
result <- as.list(seq(1:5))
for (i in seq_along(result)){
    result[[i]] <- sqrt(result[[i]])
}

print(result)

[[1]]
[1] 1

[[2]]
[1] 1.414214

[[3]]
[1] 1.732051

[[4]]
[1] 2</pre>
```

Here again, we have to pollute the global environment by first creating a vessel for our results, and then apply the function at each index. We can abstract this process away in a function:

```
applying <- function(a_list, a_func, ...){
   head_list = a_list[[1]]
   tail_list = tail(a_list, -1)
   result = a_func(head_list, ...)

# Check if we're done: if there is still some tail, rerun the whole thing until there's if(length(tail_list) != 0){
      append(result, applying(tail_list, a_func, ...))
   }
   else {
      result
   }
}</pre>
```

}

Once again this might seem complicated, and I would agree. Abstraction is complex. But once we have it, we can focus on the task at hand, instead of having to always tell the computer what we want:

```
applying(as.list(seq(1:5)), sqrt)
[1] 1.000000 1.414214 1.732051 2.000000 2.236068
```

Of course, R ships with its own, much more efficient, implementation of this function:

```
lapply(list(seq(1:5)), sqrt)

[[1]]
[1] 1.000000 1.414214 1.732051 2.000000 2.236068
```

In other programming languages, lapply() is often called map(). The {purrr} packages ships with other such useful higher-order functions that abstract loops away. For example, there's the function called map2(), that maps a function of two arguments to each element of two atomic vectors or lists, two at a time:

```
library(purrr)

map2(
    .x = seq(1:5),
    .y = seq(1:5),
    .f = `+`
    )

[[1]]
[1] 2

[[2]]
[1] 4

[[3]]
[1] 6
```

```
[[4]]
[1] 8
[[5]]
[1] 10
```

If you have more than two lists, you can use pmap() instead.

#### 2.3.4 Data frames

As mentioned in the introduction of this section, data frames are a special type of list of atomic vectors. This means that just as I can use lapply() to compute the square root of the elements of an atomic vector, as in the previous example, I can also operate on all the columns of a data frame. For example, it is possible to determine the class of every variable like this:

```
lapply(iris, class)

$Sepal.Length
[1] "numeric"

$Sepal.Width
[1] "numeric"

$Petal.Length
[1] "numeric"

$Petal.Width
[1] "numeric"

$Species
[1] "factor"
```

Unlike a list however, the elements of a data frame must be of the same length. Data frames remain very flexible however, and using what we have learned until now, it is possible to use the data frame as a structure for all our computations. For example, suppose that we have a data frame that contains data on unemployment for the different subnational divisions of the Grand-Duchy of Luxembourg, the country the author of this book hails from. Let's suppose that I want to generate several plots, per subnational division and per year. Typically, we would use a loop for this, but we can use what we've learned here, as well as some functions from the {dplyr}, {purrr}, {ggplot2} and {tidyr} packages. I will be downloading data

that I made available inside a package, but instead of installing the package, we will dowload the .rda file (which is the file format of packaged data) and then load that data into our R session:

```
# Create a temporary file
  unemp_path <- tempfile(fileext = ".rda")</pre>
  # Download the data and save it to the path of the temporary file
  download.file("https://github.com/b-rodrigues/myPackage/raw/main/data/unemp.rda", destfile
  # Load the data. The data is now available as 'unemp'
  load(unemp_path)
Let's load the required packages and take a look at the data:
  library(dplyr)
Attaching package: 'dplyr'
The following objects are masked from 'package:stats':
    filter, lag
The following objects are masked from 'package:base':
    intersect, setdiff, setequal, union
  library(purrr)
  library(ggplot2)
  library(tidyr)
  glimpse(unemp)
Rows: 472
Columns: 9
                                <dbl> 2013, 2013, 2013, 2013, 2013, 2013, 2013,~
$ year
                                <chr> "Luxembourg", "Capellen", "Dippach", "Gar~
$ place_name
                                <chr> "Country", "Canton", "Commune", "Commune"~
$ level
$ total_employed_population
                                <dbl> 223407, 17802, 1703, 844, 1431, 4094, 214~
```

Column names are self-descriptive, but the level column needs some explanations. The country of Luxembourg is divided into *Cantons*, and these *Cantons* themselves into *Communes*.

You should know that the word *Luxembourg* can refer to the country, the canton or the commune of Luxembourg. Now let's suppose that I want a separate plot for the three communes of Luxembourg, Esch-sur-Alzette and Wiltz. Instead of creating three separate data frames and feeding them to the same ggplot code, I can instead take advantage of the fact that data frames are lists, and are thus quite flexible. Let's start with filtering:

```
filtered unemp <- unemp %>%
    filter(
      level == "Commune",
      place_name %in% c("Luxembourg", "Esch-sur-Alzette", "Wiltz")
  glimpse(filtered_unemp)
Rows: 12
Columns: 9
                               <dbl> 2013, 2013, 2013, 2014, 2014, 2014, 2015,~
$ year
$ place_name
                               <chr> "Esch-sur-Alzette", "Luxembourg", "Wiltz"~
                               <chr> "Commune", "Commune", "Commune", "Commune"
$ level
$ total_employed_population
                               <dbl> 12725, 39513, 2344, 13155, 40768, 2377, 1~
                               <dbl> 12031, 35531, 2149, 12452, 36661, 2192, 1~
$ of which wage earners
$ of_which_non_wage_earners
                               <dbl> 694, 3982, 195, 703, 4107, 185, 710, 4140~
                               <dbl> 2054, 3855, 318, 1997, 3836, 315, 2031, 3~
$ unemployed
$ active_population
                               <dbl> 14779, 43368, 2662, 15152, 44604, 2692, 1~
$ unemployment_rate_in_percent <dbl> 13.898099, 8.889043, 11.945905, 13.179778~
```

We are now going to use the fact that data frames are lists, and that lists can hold any type of object. For example, remember this list from before where one of the elements is a data frame, and the second one a formula:

```
list(
   "a" = head(mtcars),
   "b" = ~lm(y ~ x)
```

)

```
$a
```

```
hp drat
                    mpg cyl disp
                                               wt
                                                   qsec vs am gear carb
Mazda RX4
                   21.0
                              160 110 3.90 2.620 16.46
                                                                   4
                                                                        4
                                                          0
                                                             1
Mazda RX4 Wag
                   21.0
                              160 110 3.90 2.875 17.02
                                                                   4
                                                                        4
                                                             1
                                   93 3.85 2.320 18.61
Datsun 710
                   22.8
                                                             1
                                                                   4
                                                                        1
Hornet 4 Drive
                   21.4
                              258 110 3.08 3.215 19.44
                                                                   3
                                                                        1
                           6
                              360 175 3.15 3.440 17.02
                                                                   3
                                                                        2
Hornet Sportabout 18.7
                              225 105 2.76 3.460 20.22
Valiant
                   18.1
                                                                   3
                                                                        1
```

```
$b
~lm(y ~ x)
```

{dplyr} comes with a function called group\_nest() which groups the data frame by a variable (such that the next computations will be performed group-wise) and then nests the other columns into a smaller data frame. Let's try it and see what happens:

```
nested_unemp <- filtered_unemp %>%
group_nest(place_name)
```

Let's see how this looks like:

```
nested_unemp
```

nested\_unemp is a new data frame of 3 rows, one per commune ("Esch-sur-Alzette", "Lux-embourg", "Wiltz"), and of two columns, one for the names of the communes, and the other contains every other variable inside a smaller data frame. So this is a data frame that has one column where each element of that column is itself a data frame. Such a column is called a list-column. This is essentially a list of lists.

Let's now think about this for a moment. If the column titled data is a list of data frames, it should be possible to use a function like map() or lapply() to apply a function on each of these data frames. Remember that map() or lapply() require a list of elements of whatever

type and a function that accepts objects of this type as input. So this means that we could apply a function that plots the data to each element of the column titled data. Since each element of this column is a data frame, this functions needs a data frame as an input. As a first, simple, example to illustrate this, let's suppose that we want to determine the number of rows of each data frame. This is how we would do it:

The new column, titled **nrows** is a list of integers. We can simplify it by converting it directly to an atomic vector of integers by using map\_int() instead of map():

Let's try for a more complex example now. What if we want to filter rows? (The simplest way would of course to filter the rows we need before nesting the data frame). We need to apply the function filter() where its first argument is a data frame and the second argument is a predicate:

```
1 Esch-sur-Alzette [4 x 8] <tibble [1 x 8] > 2 Luxembourg [4 x 8] <tibble [1 x 8] > 3 Wiltz [4 x 8] <tibble [1 x 8] >
```

In this case here, we need to use an anonymous function. This is because filter() has two arguments, and we need to make clear what it is we are mapping over and what argument stays fixed; we are mapping over, or iterating if you will, data frames, but the predicate stays fixed.

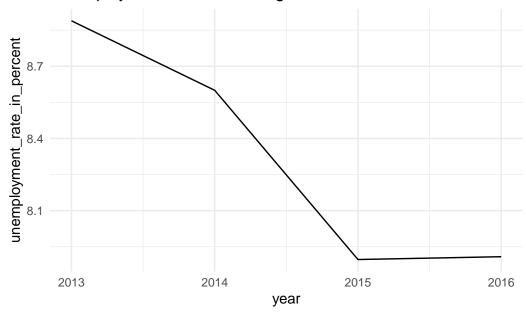
We are now ready to plot our data. The best way to continue is to first get the function right by creating one plot for one single commune. Let's select the dataset for the commune of Luxembourg:

```
lux_data <- nested_unemp %>%
  filter(place_name == "Luxembourg") %>%
  unnest(data)
```

To plot this data, we can now write the required ggplot2() code:

```
ggplot(data = lux_data) +
  theme_minimal() +
  geom_line(
   aes(year, unemployment_rate_in_percent, group = 1)
  ) +
  labs(title = "Unemployment in Luxembourg")
```

## Unemployment in Luxembourg



To turn the lines of code above into a function, you need to think about how many arguments that function would have. There is an obvious one, the data itself (in the snippet above, the data is the lux\_data object). Another one that is less obvious is in the title:

```
labs(title = "Unemployment in Luxembourg")

$title
[1] "Unemployment in Luxembourg"

attr(,"class")
[1] "labels"
```

Ideally, we would want that title to change, depending on the data set. So we could write the function like so:

```
make_plot <- function(x, y){
    ggplot(data = x) +
    theme_minimal() +
    geom_line(
        aes(year, unemployment_rate_in_percent, group = 1)
        ) +</pre>
```

```
labs(title = paste("Unemployment in", y))
}
```

Let's try it on our data:

```
make_plot(lux_data, "Luxembourg")
```

# Unemployment in Luxembourg



Ok, so now, we simply need to apply this function to our nested data frame:

1	Esch-sur-Alzette	[4	X	8]	<gg></gg>
2	Luxembourg	[4	x	8]	<gg></gg>
3	Wiltz	[4	x	8]	<gg></gg>

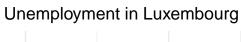
If you look at the plots column, you see that it is a list of gg objects: these are our plots. Let's take a look at them:

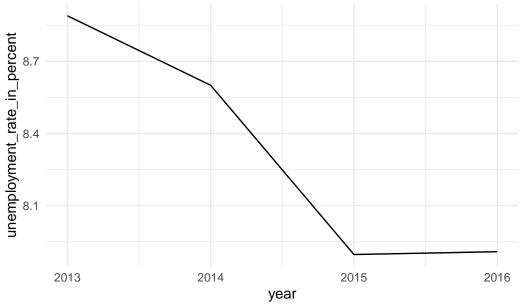
nested\_unemp\$plots

#### [[1]]



[[2]]





# [[3]]

# Unemployment in Wiltz 12.1 12.0 11.0 11.8 2013 2014 2015 2016

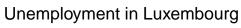
We could also have used an anonymous function:

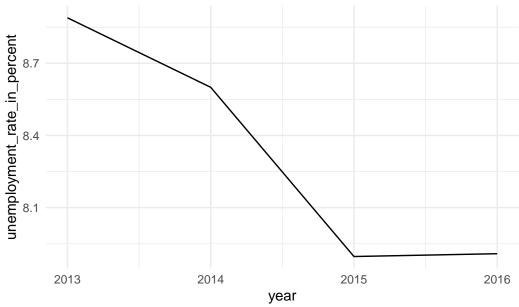
[[1]]

#### Unemployment in Esch-sur-Alzette



[[2]]





# [[3]]

# Unemployment in Wiltz 12.1 12.0 11.0 11.0 2013 2014 2015 2016

This column-list based workflow is extremely powerful and I highly advise you to take the required time to master it.

#### 2.4 Functional programming in R

Up until now we focused more on concepts than on specificities of the R programming language when it comes to functional programming. In the section, we will be focusing entirely on R-specific capabilities and packages for functional programming.

#### 2.4.1 Base capabilities

R is a functional programming language, as already stated, and as such it comes with many functions out of the box to write functional code. We have already discussed lapply() and Reduce(). You should know that depending on what you want to achieve, there are other functions that are similar to lapply(): apply(), sapply(), vapply(), mapply() and tapply(). There's also Map() which is a wrapper around mapply(). Each function performs the same basic task of applying a function over all the elements of a list or list-like structure, but it can be hard to keep them apart. This is why {purrr}, which we will discuss in the next section, is quite an interesting alternative to base R's offering.

Another one of the quintessential functional programming functions (alongside Reduce() and Map()) that ships with R is Filter(). If you know dplyr::filter() you should be familiar with the concept of filtering rows of a data frame where the elements of one particular column satisfy a predicate. Filter() works the same way, but focusing on lists instead of data frame:

The call above only returns the elements where is.character() evaluates to TRUE.

Another useful function is Negate() which is a function factory that takes a boolean function as an input and returns the opposite boolean function. As an illustration, suppose that in the example above we wanted to get everything but the character:

There are some other functions like this that you might want to check out: type ?Negate in console to read more about them.

Before continuing with R packages that extend R's functional programming capabilities it's also important to stress that just as R is a functional programming language, it is also an object oriented language. In fact, R is what John Chambers called a functional OOP language (Chambers (2014)). We won't delve too much into what this means (read Wickham (2019) for this), but as a short discussion, consider the print() function. Depending on what type of object the user gives it, it seems as if somehow print() knows what to do with it:

```
print(5)

[1] 5

print(head(mtcars))
```

```
qsec vs am gear carb
                   mpg cyl disp hp drat
                                              wt
Mazda RX4
                   21.0
                             160 110 3.90 2.620 16.46
                                                            1
Mazda RX4 Wag
                  21.0
                             160 110 3.90 2.875 17.02
                                                           1
                                                                 4
                                                                      4
Datsun 710
                   22.8
                                  93 3.85 2.320 18.61
                                                                 4
                                                        1
                                                           1
                                                                      1
Hornet 4 Drive
                  21.4
                             258 110 3.08 3.215 19.44
                                                                 3
                                                        1
                                                                      1
Hornet Sportabout 18.7
                          8
                             360 175 3.15 3.440 17.02
                                                           0
                                                                 3
                                                                      2
                                                        0
                                                                 3
Valiant
                   18.1
                             225 105 2.76 3.460 20.22
                                                                      1
```

```
print(str(mtcars))

'data.frame': 32 obs. of 11 variables:
$ mpg : num 21 21 22.8 21.4 18.7 18.1 14.3 24.4 22.8 19.2 ...
$ cyl : num 6 6 4 6 8 6 8 4 4 6 ...
```

```
$ disp: num 160 160 108 258 360 ...
$ hp : num 110 110 93 110 175 105 245 62 95 123 ...
$ drat: num 3.9 3.9 3.85 3.08 3.15 2.76 3.21 3.69 3.92 3.92 ...
$ wt : num 2.62 2.88 2.32 3.21 3.44 ...
$ qsec: num 16.5 17 18.6 19.4 17 ...
$ vs : num 0 0 1 1 0 1 0 1 1 1 ...
$ am : num 1 1 1 0 0 0 0 0 0 0 ...
$ gear: num 4 4 4 3 3 3 3 4 4 4 ...
$ carb: num 4 4 1 1 2 1 4 2 2 4 ...

NULL
```

The way this works, is essentially a mixture of functional and object oriented programming, so functional OOP. Let's take a closer look at the source code of print() by simply typing print without brackets, into a console:

```
print
```

```
function (x, ...)
UseMethod("print")
<bytecode: 0x55cf8e1b89e0>
<environment: namespace:base>
```

Quite unexpectedly, the source code of print() is one line long and is just UseMethod("print"). So all print() does is use a generic method called "print". If your text editor has autocompletion enabled, you might see that there are actually quite a lot of print() functions. For example, type print.data.frame into a console:

```
}
    else {
        if (is.null(max))
            max <- getOption("max.print", 99999L)</pre>
        if (!is.finite(max))
            stop("invalid 'max' / getOption(\"max.print\"): ",
        omit <- (n0 <- max%/%length(x)) < n
        m <- as.matrix(format.data.frame(if (omit)</pre>
            x[seq_len(n0), drop = FALSE]
        else x, digits = digits, na.encode = FALSE))
        if (!isTRUE(row.names))
            dimnames(m)[[1L]] <- if (isFALSE(row.names))</pre>
                rep.int("", if (omit)
                  n0
                else n)
            else row.names
        print(m, ..., quote = quote, right = right, max = max)
        if (omit)
            cat(" [ reached 'max' / getOption(\"max.print\") -- omitted",
                n - n0, "rows ]\n")
    invisible(x)
}
<bytecode: 0x55cf8fe21e28>
<environment: namespace:base>
```

This is the print function for data.frame objects. So what print() does is look at the class of its argument x, and then look for the right print function. In more traditional OOP languages, users would type something like:

```
mtcars.print()
```

In these languages, objects encapsulate method (the equivalent of our functions), so if mtcars is a data frame, it encapsulates a print() method that then does the printing. R is different, because classes and methods are kept separate. If a package developer creates a new class of object, then the developer also must implement the required methods. For example in the {chronicler} package, the chronicler class is defined and a print.chronicler() function is defined to print these objects.

All of this to say that if you want to extend R by writing packages, learning some OOP essentials is also important. But for data analysis, functional programming does the job perfectly. To learn more about R's different OOP systems (yes, R can do OOP in diffirent

ways and the one I sketched here is the simplest, but probably the most used as well, one), take a look at Wickham (2019).

#### 2.4.2 purrr

The {purrr} package, developed by Posit, contains many functions to make functional programming with R more smooth. In the previous section, we discussed the apply() family of function; they all do a very similar thing, which is looping over a list and applying a function to the elements of the list, but it is not quite easy to remember which one does what. Also, for some of these functions like apply(), the list comes first, and then the function, but in the case of mapply(), the function comes first. Another issue with these functions is that it is not always easy to know what type the output is going to be. List? Atomic vector? Something else?

{purrr} solves this issue by offering the map() family of functions, which behave in a very consistent way. The basic function is called map() and we've already used it:

```
map(seq(1:5), sqrt)

[[1]]
[1] 1

[[2]]
[1] 1.414214

[[3]]
[1] 1.732051

[[4]]
[1] 2

[[5]]
[1] 2.236068
```

But there are many interesting variants:

```
map_dbl(seq(1:5), sqrt)
[1] 1.000000 1.414214 1.732051 2.000000 2.236068
```

map\_dbl() coerces the output to an atomic vector of doubles instead of a list of doubles. Then there's:

```
map_chr(letters, toupper)

[1] "A" "B" "C" "D" "E" "F" "G" "H" "I" "J" "K" "L" "M" "N" "O" "P" "Q" "R" "S"

[20] "T" "U" "V" "W" "X" "Y" "Z"
```

for when the output needs to be an atomic vector of characters.

There are many others, so take a look at the document with ?map. There's also walk() which is used if you're only interested in the side-effect of the function (for example if the function takes paths as input and saves something to disk).

{purrr} also has functions to replace Reduce(), simply called reduce() and accumulate(), and there are many, many other useful functions. Read through the documentation of the package and take the time to learn about all it has to offer.

#### 2.4.3 withr

{withr} is a powerful package that makes it easy to "purify" functions that behave in a way that can cause problems. Remember the function from the introduction that randomly gave out a recipe Bruno liked? Here it is again:

```
h <- function(name, food_list = list()){
  food <- sample(c("lasagna", "cassoulet", "feijoada"), 1)
  food_list <- append(food_list, food)
  print(paste0(name, " likes ", food))
  food_list
}</pre>
```

Because this function returns results that are not consistent for a fixed input, this function is not referentially transparent. So we improved the function like this:

```
h2 <- function(name, food_list = list(), seed = 123){

# We set the seed, making sure that we get the same selection of food for a given seed set.seed(seed)</pre>
```

```
food <- sample(c("lasagna", "cassoulet", "feijoada"), 1)

# We now need to unset the seed, because if we don't, guess what, the seed will stay set
set.seed(NULL)

food_list <- append(food_list, food)

print(pasteO(name, " likes ", food))

food_list
}</pre>
```

The problem with this approach is that we need to modify our function. We can instead use withr::with\_seed() to achieve the same effect:

Before we downloaded a dataset and loaded it into memory; we did so by first created a temporary file, then downloading it and then loading it. Suppose that instead of loading this

data into our session, we simply wanted to test whether the link was still working. We wouldn't want to keep the loaded data in our session, so to avoid having to delete it again manually, we could use with\_tempfile():

```
withr::with_tempfile("unemp", {
   download.file("https://github.com/b-rodrigues/myPackage/raw/main/data/unemp.rda", destfi
   load(unemp)
   nrow(unemp)
  }
)
```

Warning in unlink(mget(new, envir = env), recursive = TRUE): expanded path length 35189 would list(year = c(2013, 2013,

[1] 472

The data got downloaded, and then loaded, and then we computed the number of rows of the data, without touching the global environment, or state, of our current session.

Just like for {purrr}, {withr} has many useful functions which I encourage you to familiarize yourself with.

#### 2.5 Conclusion

If there is only one thing that you should remember from this chapter, it would be pure functions. This is in my opinion not very difficult to do and comes with many benefits. But, avoiding loops and replacing them with higher-order functions (lapply(), Reduce(), purrr::map() – and its variants –) also pays off. While this chapter stresses the advantages of functional programming, you should not forget that R is not a pure, and solely, functional programming language and that other paradigms, like object oriented programming, are also available to you, and if your goal is to master the language (instead of "just" using it to solve data analysis problems), then you also need to know about R's OOP capabilities.

# 3 Version control

What Miles said on the matter:

There are still a lot of people that find git intimidating and still potential for some things to go badly for a project if git is used in the wrong way. I once had a colleague who assured me they knew how to use git proceed to use a repo like their personal dropbox folder. Perhaps the details of git usage can be basically waved away, but some detail about good git workflow could be incorporated. For example: The branching model to use. IMHO trunk-based development works much better than gitflow for analysis teams. Version number discipline. Why you always bump the version number when making changes to your packages. Why keeping commits small and confined to just one target at a time if possible is useful when tracing problems with a pipeline.

# 4 Getting started with your project

In order to build a reproducible pipeline, we will be working together on a project. The project itself will be quite simple and will simply consist is getting some data "trapped" inside a Microsoft Excel Workbook into a data frame, and then creating a plot. The point is not making this plot, engineering the project in such a way that it is:

- Documented;
- Tested;
- Reproducible.

We will start our project like someone with time constraints does, and see how we can reach our goal of having a nice reproducible project as painlessly as possible. There is only one catch; to make the whole process as easy as possible, we will start our analysis by writing a Quarto file, not a standard R script.

What Sébastien said on the matter:

\*There seems to be two way of presenting such a workflow:

What does the complete project looks like at the end and what tools do I need? How do I start working on it?\*

This questions should get answered in the intro?

Refer to https://github.com/b-rodrigues/rap4all/issues/1#issuecomment-1327627267

#### 4.1 Literate programming

In literate programming, we mix code and prose together, in a way that makes it easy for both non-technical users and programmers to understand what is going on. Scripts written this way are also very easy to compile, or render, into a variety of document formats like html and docx. R supports several ways of doing literate programming: Sweave, knitr and Quarto.

Sweave was the first tool available to R (and S) users, and allowed the mixing of R and LaTeX code to create a document. Sweave as was authored by Friedrich Leisch in 2002 and described in his 2002 paper (Leisch (2002)). As Leisch argues, the traditional way of writing a report as part of a statistical data naalysis project uses two separate steps: running the analysis using some software, and then copy and pasting the results into a word processing tool. The problem

with this approach is that much time is wasted copy and pasting things, so experimenting with different layouts is very time consuming. Copy and paste mistakes will also happen (it's not a question of if, but when) and updating reports (for example, when new data comes in) means that someone will have, again, to copy and paste the updated results into a new document.

Sweave provided a way to embed the analysis in the document itself, in this case a LATEX source file, and R code was executed whenever the document was compiled. This gave statisticians considerable time savings when it was time to update a report (or to experiment with different layouts).

The snippet below shows the example from Leisch's paper:

```
\documentclass[a4paper]{article}
\begin{document}

In this example we embed parts of the examples from the \texttt{kruskal.test} help page into a LaTeX document:

<<>>=
data (airquality)
kruskal.test(Ozone ~ Month, data = airquality)
@
which shows that the location parameter of the Ozone
distribution varies significantly from month to month.
Finally we include a boxplot of the data:
\begin{center}
<<fig=TRUE,echo=FALSE>>=
boxplot(Ozone ~ Month, data = airquality)
@
\end{center}
\end{document}
```

Even if you've never seen a LATEX source file, you should be able to figure out what's going on. The first line states what type document of document we're writing. Then comes \begin{document} which tells the compiler where the document starts. Then comes the content. You can see that it's a mixture of plain English with R code defined inside a chunk starting with <>>= and ending with @. Finally, the documents ends with \end{document}. Getting a humand readable PDF from this source is a two-step process: first this source get's converted into a .tex file and then this .tex file into a PDF. Sweave is included with every

R installation since version 1.5.0, and still works to this day. For example, we can test that our Sweave installation works just fine by compiling the example above. This is what the final output looks like:

Let us just state that the fact that it is still possible to compile this example more than 20 years later is an incredible testament to how mature and stable this software is (both R, Sweave, and LATEX). But as impressive as this is, LATEX has a steep learning curve, and Leisch even advocated the use of the Emacs text editor to edit Sweave files, which also has a very steep learning curve (but this is entirely optional; for example we edited and compiled the example on the Rstudio IDE).

The following generation of literate programming tools was provided by a package called {knitr} in 2012. From the perspective of the user, the biggest change from Sweave is that {knitr} is able to use many different formats for the source files. The one that became very likely the most widely used format is a flavour of the Markdown markup language, R Markdown (Rmd). But {knitr} can also run code chunks from other languages, such as Python, Perl, Awk, Haskell, bash and more (Xie (2014)). Since version 1.18, {knitr} uses the {reticulate} package to provide a Python engine for the Rmd format. To illustrate the Rmd format, let's rewrite the example from Leisch's Sweave paper into it:

```
output: pdf_document

In this example we embed parts of the examples from the 
\texttt{kruskal.test} help page into a LaTeX document:

\``{r}
data (airquality)
kruskal.test(Ozone ~ Month, data = airquality)

\``

which shows that the location parameter of the Ozone 
distribution varies significantly from month to month. 
Finally we include a boxplot of the data:

\``{r, echo = FALSE}
boxplot(Ozone ~ Month, data = airquality)

\``
```

This is what the output looks like:

In this example we embed parts of the examples from the kruskal.test help page into a LATEX document:

```
> data (airquality)
> kruskal.test(Ozone ~ Month, data = airquality)
```

Kruskal-Wallis rank sum test

data: Ozone by Month
Kruskal-Wallis chi-squared = 29.267, df = 4, p-value = 6.901e-06

which shows that the location parameter of the Ozone distribution varies significantly from month to month. Finally we include a boxplot of the data:

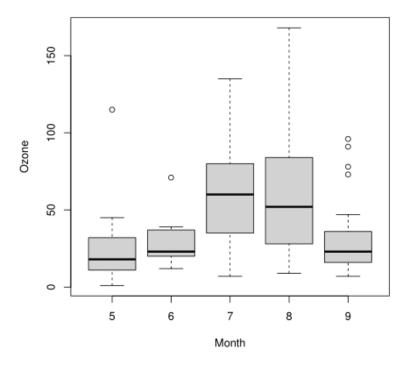


Figure 4.1: More than 20 years later, the output is still the same

In this example we embed parts of the examples from the kruskal.test help page into a  $L^{k}T_{E}X$  document:

```
data (airquality)
kruskal.test(Ozone ~ Month, data = airquality)

##
## Kruskal-Wallis rank sum test
##
## data: Ozone by Month
## Kruskal-Wallis chi-squared = 29.267, df = 4, p-value = 6.901e-06
```

which shows that the location parameter of the Ozone distribution varies significantly from month to month. Finally we include a boxplot of the data:

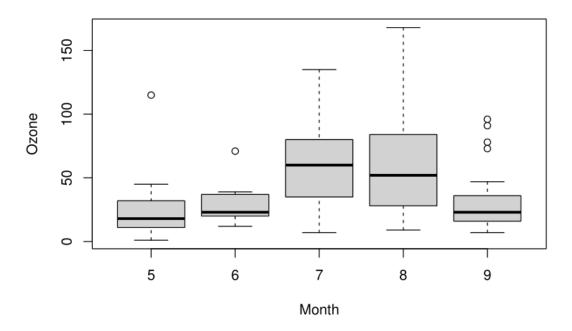


Figure 4.2: It's very close to the Sweave output

Just like in a Sweave document, an Rmd source file also had a header in which authors can define a number of options. Here we only specified that we wanted a pdf document as an output file. We then copy and pasted the contents from the Sweave source, but changed the chunk delimiters from <<>>= and @ to  $\times60\times60$  to start an R chunk and  $\times60\times60\times60$  to end it. Remember; we need to specify the engine in the chunk because  $\{knitr\}$  supports many engines. For example, it is possible to run a bash command by adding this chunk to the source:

```
output: pdf_document

In this example we embed parts of the examples from the 
\texttt{kruskal.test} help page into a LaTeX document:

\(\text{r}\)
data (airquality)
kruskal.test(Ozone ~ Month, data = airquality)

which shows that the location parameter of the Ozone distribution varies significantly from month to month. 
Finally we include a boxplot of the data:

\(\text{r}\), echo = FALSE}
boxplot(Ozone ~ Month, data = airquality)

\(\text{c}\)
\(\text{c}\)
\(\text{bash}\)
pwd
```

(bash's pwd command shows the current working directory). You may have noticed that we also keep two LaTeX commands in the source Rmd, \texttt{} and LaTeX. This is because Rmd files get first converted into LaTeX files and then into a PDF. If you're using RStudio, this document can be compiled by clicking a button or using a keyboard shortcut, but you can also use the rmarkdown::render() function. This function does two things transparently: it first converts the Rmd file into a source LaTeX file, and then converts it into a PDF. It is of course possible to convert the document to a Word document as well however, LaTeX commands will be ignored. Html is another widely used output format.

You should know that {knitr} makes it possible to author many, many different types of documents. It is possible to write books, blog, package documentation (and even entire packages,

as we shall see later in this book), Powerpoint slides... It is extremely powerful because we can use the same general R Markdown knowledge to build many different outputs:

Finally, the latest in literate programming for R is a new tool developed by Posit, called Quarto. If you're an R user and already know {knitr} and the Rmd format, you should be able to immediately use Quarto. So what's the difference? In practice and for R users not much. There are many things that Quarto is able to do out of the box that you can't, without extensions, do with {knitr}. Quarto has some nice defaults; in fact this book is written in Quarto instead of {knitr} because the default Quarto output looks nicer than the default {knitr} output. However, there may even be things that Quarto can't do at all (at least for now) when compared to {knitr}. So why bother switching? Well, Quarto provides sane defaults and some nice features out of the box, and the cost of switching from the Rmd format to Quarto's Qmd format is basically 0. Also, and this is probably the biggest reason to use Quarto, is that Quarto is not tied to R. Quarto is actually a standalone tool that needs to be installed alongside your R installation, and works completely independently. In fact, you can use Quarto without having R installed at all, as Quarto, just like {knitr} supports many engines. This means that if you're primarily using Python, you can author documents with Quarto. Quarto also supports the Julia programming language and Observable JS, making it possible to include interactive visualisations into an Html document. Let's take a look at how the example from Leisch's paper look as a Qmd file:

```
output: pdf
---

In this example we embed parts of the examples from the \texttt{kruskal.test} help page into a LaTeX document:

'``{r}

data (airquality)

kruskal.test(Ozone ~ Month, data = airquality)

'``

which shows that the location parameter of the Ozone distribution varies significantly from month to month. Finally we include a boxplot of the data:

'``{r, echo = FALSE}

boxplot(Ozone ~ Month, data = airquality)

'``
```

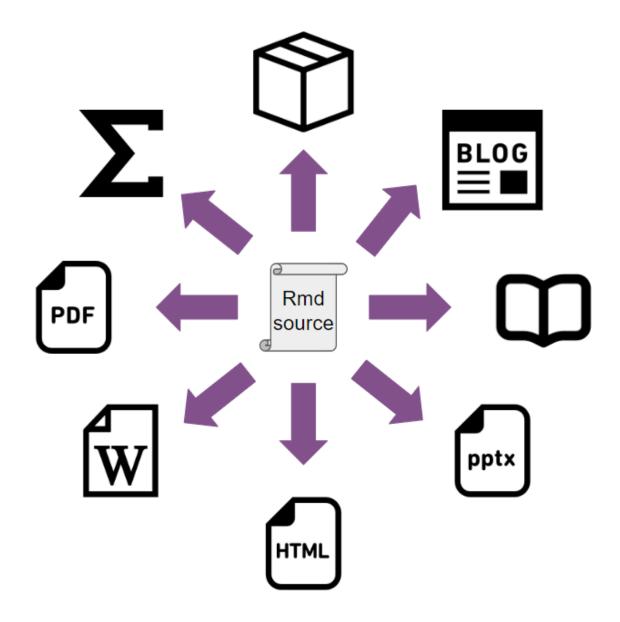


Figure 4.3: One format to rule them all

(I've omitted the bash chunk from before, not because Quarto does not support it, but to keep close to the original example from the paper.)

As you can see, it's exactly the same as the Rmd file from before. The only difference is in the header. In the Rmd file we specified the output format as:

```
---
output: pdf_document
---
whereas in the Qmd file we changed it to:
---
output: pdf
---
```

While Quarto is the latest option in literate programming, it is quite recent, and as such, we feel it might be better to stick with {knitr} and the Rmd format for now, so that's what we're going to use going forward. However, we won't be focused on anything really {knitr} or Rmd specific, so should you want to use Quarto instead, you should be able to follow along without any problems at all, since the Rmd and Qmd formats have so much overlap (but whenever there would be major differences between the two formats, we will highlight them).

#### 4.2 {knitr} basics

This section will be a very small intro. We are going to teach you just enough to get started, and we are going to focus on the Rmd format. There are many resources out there that you can use if you want to dig deeper, for instance the R Markdown website from Posit, or the R Markdown: The Definitive Guide eBook. We will also not assume that you are using the RStudio IDE and give you instead the lower level commands to render documents. If you use RStudio and want to know how to use it effectively to author Rmd documents, you should take a look at Quick Tour page. In fact, this section will basically focus on the same topics, but without focusing on how to use RStudio.

#### 4.2.1 Set up

The first step is to install the {knitr} and the {rmarkdown} packages. Simple type:

```
install.packages("rmarkdown")
```

in an R console. Since {knitr} is required to install {rmarkdown}, this gets installed automatically. If you want to compile PDF documents, you should also have a working LaTeX distribution. You can skip this next part if you're only interested in generating PDF and Word files. For what follows, we will only be rendering Html documents, so no need to install LaTeX (by the way, you do not need a working Word installation to compile document to the docx format). However, if you already have a working LaTeX installation, you shouldn't have to do anything else to generate PDF documents. If you don't have a working LaTeX distribution, then Yihui Xie, the creator of {knitr} created an R package called {tinytex} that makes it extremely easy to install a LaTeX distribution. In fact, this is the way we recommend to install LaTeX even if you're not an R user (it is possible to use the tinytex distribution without R; it's just that the {tinytex} R package provides many functions that makes installing and maintaining it very easy). Simply run these commands in an R console to get started:

```
install.packages("tinytex")
tinytex::install_tinytex()
```

and that's it! If you need to install specific LaTeX packages, then refer to the Maintenance section on tinytex's website. For example, to compile the example from Leisch's article on Sweave discussed previously, we had to install the grfext LaTeX package (as explained by the error output in the console when I tried compiling). So, we simply needed to run the following command to get it:

```
tlmgr_install("grfext")
```

After you've installed {knitr}, {rmarkdown} and, optionally, {tinytex}, simply try to compile the following document:

```
---
output: html_document
---

# Document title

## Section title

### Subsection title
```

```
This is **bold** text. This is *text in italics*.

My favourite programming language for statistics is ~~SAS~~ R.
```

save this document into a file called rmd\_intro.rmd using you're favourite text editor. Then render it into an Html file by running the following command in the R console:

```
rmarkdown::render("path/to/rmd_test.rmd")
```

This should create a file called rmd\_test.html; open it with your web browser and you should see the following:

# Document title

# Section title

#### Subsection title

This is bold text. This is text in italics.

My favourite programming language for statistics is SAS R.

Figure 4.4: It's very close to the Sweave output

Congratulations, you just knitted your first Rmd document!

#### 4.2.2 Markdown ultrabasics

R Markdown is a flavour of Markdown, which means that you should know some Markdown to really take full advantage of R Markdown. The document from before should have already shown you some basics, title, sections and subsections all start with a # and the depth level is determined by the number of #s. For bold text, simply put the words in between \*\* and for italics use only one \*. If you want **bold and italics**, use \*\*\*. The original designer of Markdown did not think that underlining text was important, so there is no *easy* way of doing it unfortunately. For this, you need to use a somewhat hidden feature; without going into

too much technical details, the program that converts Rmd files to the final output format is called Pandoc, and it's possible to use Pandoc instead for this:

```
[This is some underlined text in a R Markdown document] {.underline}
```

This will underline the text between square brackets.<sup>1</sup>

The next step is actually to mix code and prose. As you've seen from Leisch's canonical example, this is quite easily achieved by using R code chunks. The R Markdown example below shows various code chunks alongside some options. For example, a code chunk that use the echo = FALSE option will not appear (but the output of the computation will):

 $<sup>^1</sup> https://stackoverflow.com/a/68690065/1298051$ 

```
The last one runs, but code and output from the code is not shown in the final document.
This is useful for loading libraries and hiding startup messages:

'``{r, include = FALSE}
library(dplyr)
```

If you use RStudio and create a new R Markdown file from the menu, a new R Markdown file is generated for you to fill out. The first R chunk is this one:

```
```{r setup, include=FALSE}
knitr::opts_chunk$set(echo = TRUE)
```

This is an R chunk, named setup and with the option include = FALSE. Naming chunks is optional, but we are going to make use of this later on. What this chunk runs is one line of code that defines a global options to show all chunks by default (which is the default behaviour). You can change TRUE to FALSE if you want to hide every code chunk instead (if you're using Quarto, global options are set differently).

Something else you might have noticed in the previous example, is that we've added some more content in the header:

```
title: "Document title"
output: html_document
date: "2023-01-28"
```

There are several other options available that you can define in the header. Later on, when we'll be building our project together, we will provide some more options (like having a table of contents).

The finish this part on code chunks, you should know about inline code chunks. Take a look at following example:

```
title: "Document title"
output: html_document
date: "2023-01-28"
---

# R code chunks

``{r, echo = FALSE}
data(iris)

The iris dataset has `r nrow(iris)` rows.
```

This quite useful, as it allows to parametrize sentences and paragraphs, and thus avoids needing to copy and paste (and we will go quite far into how to avoid copy and pasting, thanks to parametrized reports, discussed in the next section).

To finish this crash course, you should know that to use footnotes you need to write the following:

```
This sentence has a footnote. [^1]
[^1]: This is the footnote.
```

and that you can write LaTeX formulas as well. For example, add the following into the the example from before and render either a PDF or a html document (don't put the LaTeX formula belowe inside a chunk. This doesn't work for Word output because Word does not support LaTeX equations):

#### 4.3 Keep it DRY

Whatever you're doing, you should keep it DRY - DRY stands for *don't repeat yourself*. Repeating yourself by, say, copy and pasting, leads to errors and makes reading and understanding your code more difficult. This can be avoided by using functions, as we discussed in the previous chapter, but what if you need to write a document that has the following structure:

- A title
- A section
- A table inside this section
- Another section
- Another table inside this section
- Yet another section
- Yet another table inside this section

Is there a way to automate the creation of such a document by taking advantage of the repeating structure? Of course there is. The question is not, is it possible to do X?, but how to do ?.

#### 4.3.1 Generating R Markdown code from code

The example below is a fully working minimal example of this. Copy it inside a document titled something like rmd\_templating.Rmd and render it. You will see that the output contains more sections that defined in the source. This is because we use templating at the end:

```
title: "Templating"
output: html_document
date: "2023-01-27"
---

```{r setup, include=FALSE}
knitr::opts_chunk$set(echo = TRUE)

...

## A function that creates tables

```{r}
create_table <- function(dataset, var){
  table(dataset[var]) |>
```

```
knitr::kable()
}
The function above uses the `table()` function to create frequency tables,
and then this gets passed to the `knitr::kable()` function that produces
a good looking table for our rendered document:
```{r}
create_table(mtcars, "am")
Let' suppose that we want to generate a document that would look like this:
- first a section title, with the name of the variable of interest
- then the table
So it would look like this:
## Frequency table for variable: "am"
```{r}
create_table(mtcars, "am")
We don't want to create these sections for every variable by hand.
Instead, we can define a function that returns the R markdown code required
to create this. This is this function:
```{r}
return_section <- function(dataset, var){</pre>
  a <- knitr::knit_expand(text = c("## Frequency table for variable: {{variable}}}",
                                   create_table(dataset, var)),
                          variable = var)
```

```
cat(a, sep = "\n")
}

This new function, `return_section()` uses `knitr::knit_expand()` to generate
R Markdown code. Words between `{{}}` get replaced by the provided `var` argument
to the function. So when we call `return_section("am")`, `{{variable}}` is replaced
by `"am"`. `"am"` then gets passed down to `create_table()` and the frequency
table gets generated. We can now generate all the section by simply applying
```

```
```{r, results = "asis"}
invisible(lapply(colnames(mtcars), return_section, dataset = mtcars))
```

The last function, named return\_section() uses knitr::knit\_expdand(), which is the one that does the heavy lifting. This section return literal R Markdown code. It returns ## Frequency table for variable: {{variable}} which creates a level 2 section title with the text Frequency table for variable: xxx where the xxx will get replaced by the variabled passed to return\_section(). So calling return\_section(mtcars, "am") will print the following in your console:

```
## Frequency table for variable: am

|am | Freq|

|:--|---:|

|0 | 19|

|1 | 13|
```

our function to a list of column names:

We now simply need to find a clever way to apply this function to each variable in the mtcars dataset. For this, we are going to use lapply() which implements a for loop (you could use purrr::map() just as well for this):

```
invisible(lapply(colnames(mtcars), return_section, dataset = mtcars))
```

This will create, for each variable in mtcars, the same R Markdown code as above. Notice that the R Markdown chunk where the call to lapply() is has the option results = "asis". This is because the function returns literal Markdown code, and we don't want the parser to have to parse it again. We tell the parser "don't worry about this bit of code, it's already good". As you see, the call to lapply() is wrapped inside invisible(). This is because return\_section() does not return anything, it just prints something to the console. No

object is returned. So if you don't wrap the call to lapply() inside invisible(), then a bunch of NULLs will also get printed. To avoid this, use invisible() (and use purrr::walk() rather than purrr::map()).

Click here to see the output.

This is not an easy topic, so take the time to play around with the example above. Try to print a plot instead of a table, try to generate more complex Markdown code, remove the call to invisible() and knit the document and see what happens with the output, replace the call to lapply() with purrr::walk() or purrr::map(). Really take the time to understand what is going on.

#### 4.3.2 Tables in R Markdown documents

Getting tables right in Rmd documents is not always an easy task. There are several packages specifically made just for this task.

In this short section, we want to point you towards two packages that check the following boxes:

- Work the same way regardless of output format we want to knit our document into:
- Work for any type of table: summary tables, regression tables, two-way tables, etc.

Let's start with the simplest type of table, which would be showing the head of a dataset for example. {knitr} comes with the kable() function, but this function generates a very plain looking output. For something publication-worthy, we recommend the {flextable} package, developed by Gohel and Skintzos (2023):

```
library(flextable)
my_table <- head(mtcars)

flextable(my_table) |>
   set_caption(caption = "Head of the mtcars dataset")
```

ge	am	vs	qsec	wt	drat	hp	disp	cyl	mpg
	1	0	16.46	2.620	3.90	110	160	6	21.0
	1	0	17.02	2.875	3.90	110	160	6	21.0
	1	1	18.61	2.320	3.85	93	108	4	22.8
	0	1	19.44	3.215	3.08	110	258	6	21.4
	0	0	17.02	3.440	3.15	175	360	8	18.7

	Model 1	Model 2
(Intercept)	26.585	30.099
	(1.425)	(1.634)
hp	-0.059	-0.068
	(0.008)	(0.010)
am	5.277	, ,
	(1.080)	
Num.Obs.	32	32
R2	0.782	0.602
R2 Adj.	0.767	0.589
AIC	164.0	181.2
BIC	169.9	185.6
Log.Lik.	-78.003	-87.619
RMSE	2.77	3.74

$\operatorname{mpg}$	cyl	disp	hp	drat	wt	qsec	vs	am	g
18.1	6	225	105	2.76	3.460	20.22	1	0	

We won't go into much detail on how {flextable} works, but it is very powerful, and the fact that it works for PDF, Html, Word and Powerpoint outputs is really a massive plus. If you want to learn more about {flextable}, there's a whole, free, ebook on it. {flextable} can create very complicated tables, so really take the time to dig in!

The next package is {modelsummary}, by Arel-Bundock (2022), and this one focuses on regression and summary tables. It is extremely powerful as well, and just like {flextable}, works for any type of output. It is very simple to get started:

Here again, we won't got into much detail, but recommend instead that you read the package's website which has very detailed documentation.

#### 4.3.3 Parametrized reports

# 4.4 Project start

hpi: https://ec.europa.eu/eurostat/databrowser/bookmark/e2758aae-6a88-4684-9f6d-d0946cae3f6b?lang=fr
deflated hpi: https://ec.europa.eu/eurostat/databrowser/view/tipsho10/default/table?lang=en
prix des logements en euros courants: https://data.public.lu/fr/datasets/r/1d20f982-57e1-4ae2-a278-dc78c88c21dc

# 4.5 Your project is done (?)

So here the project is done, but actually it's just an Qmd file that gets compiled, so we would need to explain why this is not enough, and motivate the readers to go the full way: developing packages, using targets, and so on

# 5 Testing your code

#### 5.1 Assertive testing (and defenvise programming?)

The analysis is still in Quarto, so how could the readers of this book test their code? Copying here what Miles wrote on the subject:

'Assertive programming' is a topic that might be missing from the book. I think of it as a kind of dual of unit testing. Unit testing is for more generally applicable packaged code. But when you have functions in your analysis pipeline that operate on a very specific kind of input data, unit testing becomes kind of nonsensical because you're left to dream up endless variations of your input dataset that may never occur. It's a bit easier to flip the effort to validating the assumptions you have about your input and output data, which you can do in the pipeline functions themselves rather than separate unit testing ones. This is nice because it ensures the validation is performed in the pipeline run, and so is backed by the same reproducibility guarantees.

I think at the end of the chapter we should hint at unit testing, but leave it as a subsection of the next chapter that deals with packaging code.

# 6 Packaging your code

In this chapter you're going to learn how to create your own package.

We should make clear that this does not mean publishing the package on CRAN.

#### 6.1 Benefits of packages

#### 6.2 Intro to packge dev

This is where fusen comes into play I guess; so we start from the Qmd file that was written before, containing the functions an the analysis, and see how we can now create a package from it, and use that file as a vignette? Copying here what Sébastien said on the matter

### 6.3 Document your package (?)

I guess fusen makes this process easy and leverages roxygen?

# 6.4 Managing package dependencies (?)

Discuss NAMESPACE and DESCRIPTION and all that. I think it's important to also discuss here how to define dependencies from remotes, not just CRAN.

#### 6.5 Unit testing

This is where I think we should discuss unit testing

#### 6.6 pkgdown

# 7 Build automation

Why build automation: removes cognitive load, is a form of documentation in and of itself, as Miles said

It is possible to communicate a great deal of domain knowledge in code, such that it is illuminating beyond the mere mechanical number crunching. To do this well the author needs to make use of certain styles and structures that produce code that has layers of domain specific abstraction a reader can traverse up and down as they build their understanding of the project. Functional programming style, coupled with a dependency graph as per {targets} are useful tools in this regard.

# 8 Introduction to reproducibility

Since we said in the intro to the book that reproducibility is on a continuum, I think that this chapter should focus on the bare minimum, which would culminate with renv

Then at the end, explain why renv is not enough (does nothing for R itself, nor the environment the code is running on)

# 9 Advanced topics in reproducibility

Now that the readers are familiar with renv, but also its shortcomings, we can go a step further and introduce Docker. I think some primer on the Linux command line could be included here

#### 9.1 First steps with Docker

To write your own Dockerfile, you need some familiarity with the Linux cli, so here's...

#### 9.2 A primer on the Linux command line

# 9.3 Dockrizing your project

# 10 Continuous integration and continuous deployment/delivery

# References

- Arel-Bundock, Vincent. 2022. "modelsummary: Data and Model Summaries in R." *Journal of Statistical Software* 103 (1): 1–23. https://doi.org/10.18637/jss.v103.i01.
- Chambers, John M. 2014. "Object-Oriented Programming, Functional Programming and R." Statistical Science 29 (2): 167–80. https://doi.org/10.1214/13-STS452.
- Gohel, David, and Panagiotis Skintzos. 2023. Flextable: Functions for Tabular Reporting.
- Leisch, Friedrich. 2002. "Sweave: Dynamic Generation of Statistical Reports Using Literate Data Analysis." In *Compstat*, edited by Wolfgang Härdle and Bernd Rönz, 575–80. Physica-Verlag HD.
- Wickham, Hadley. 2019. Advanced r. CRC press.
- Xie, Yihui. 2014. "Knitr: A Comprehensive Tool for Reproducible Research in R." In *Implementing Reproducible Computational Research*, edited by Victoria Stodden, Friedrich Leisch, and Roger D. Peng. Chapman; Hall/CRC. http://www.crcpress.com/product/isbn/9781466561595.