Intro to R ENVX3003

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1 Introduction

This is an introduction to R, written for ENVX3003. This work is based on earlier documents from the author and co workers (in particular, Dasapta Erwin Irawan from ITBandung, Thomas Bishop and Floris van Ogtrop) and it also builds on many of the introduction to R literature on CRAN and elsewhere on the internet.

This course is not a complete introduction, and more in depth knowledge on R and the use of R can be gained from many courses on-line and by basic practice.

This course covers three main elements: reading in files, manipulating data and doing some plotting. It particularly uses the package tidyverse and Rstudio. More detail on how to use tidyverse is on this website.

We hope that this introduction offers sufficient depth to at least get you started with R and maybe later explore this in more depth yourself.

2 R as a modelling environment

The origins of R are in statistics, so this is what R does best. However, over time, it has proven to be a flexible language that can also be used quite effectively for programming and data science.

The key power of R is in using "scripts" and "notebooks" or "rmarkdown" files which are ways to record and document the code you are generating. In this course we will focus on using rmarkdown and notebooks.

2.1 R and R Studio

2.1.1 Base R vs IDE

If R is the machine under the hood, then R Studio (and in this case Ed Saturn notebooks) would be the dashboard, steering wheel, as well as the gas and brake paddles. People frequently refer to R as base R and things like R Studio is an Integrated Development Environment (IDE).

Are there other IDEs than R Studio? The answer is Yes. You could check out R Commander. Another interesting project is or Microsoft R Open, which offers a multithreaded version of R.

2.1.2 Running R online

Can we run R online? The answer is also Yes. R Studio offers a paid cloud service. You could try R fiddle for a limited range of code of package installation, CoCalc/Sage Math Cloud, Jupyter, and Code Ocean.

2.1.3 R is cross platform

R and R Studio are cross platform. So you could use R on all major operating systems (OS): Windows, Mac or Linux, so it's OK if you work with another person who doesn't use the same OS as you do. You just have to make sure that all parties have the same data and the same packages installed in the system, and the same code to run.

2.1.4 R components

In R, as in any other programming language, the two main components are the data and the codes. Using both, you could start an analysis and produce plots and tables as outputs. However in order to do some of the analyses, we will need packages. Packages are collections of functions that we can use in R.

The good thing about R is, there are base functions, that is commands that are included in the base R installation. This commands are progressing as you install newer versions of R. It's getting better and easier through time. But, because R is open source, users can develop their own scripts and functions or sets of functions. Sets of functions can be grouped as a package. So you would need to install the package first and load the package, before using the command or function inside that package. You would only need to install the package only once.

Generally we install a package from CRAN server using this basic code. Here packageName is the name of the package that you would like to install.

```
install.packages("packageName") # case sensitive and you need quotes
library(packageName) # to load the package, case sensitive
```

2.1.5 Navigation

If you use R Studio, you can see four panels (clock-wise): A *script* panel on top right, Environment, Files/folder/plots/packages, and console. You write your lines of code in the script panel and then, click the *run* button (or select code and press CTRL+ENTER, or CMD+ENTER) to run and observe the progress of your code in the console panel. Find out in the console, if your code is running well or has a problem (error messages), or just a warning. Then you could see all the *objects* and loaded data components that relate to your code in the Environment panel.

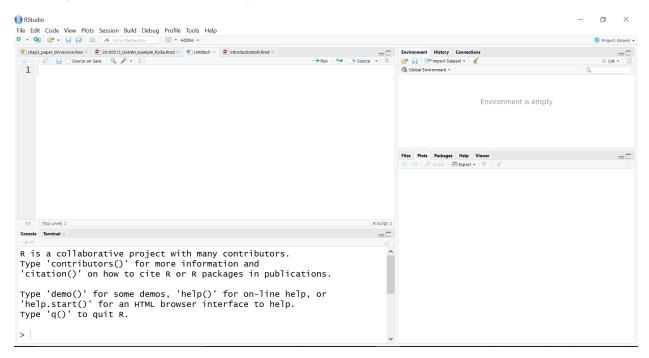


Figure 1: Four panels in R Studio

3 Working folder structure

In R and in any other command line-based application, you would need to tell the program what your current folder location is and what the location of any data is. This is one of the most important steps in the process and many of the errors generated relate to not correctly define the directory. Usually we use the following folder structure:

- main project folder
- data: put your data here
- code or scripts: put your code here
- output: put your plots and tables here

However often we work with scripts, data, outputs in one folder, but use it as a process or intermediate folder. We usually sort out the components at the final stage of our work.

3.1 The working directory

Generally R works from a "working directory". This is the directory on disk where it expects to find files or write files to. You can set this in Rstudio via the menu item "Session" -> "Set working directory", but you

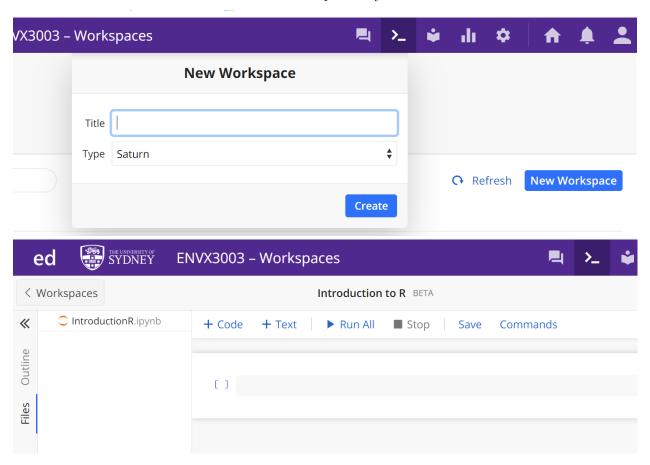
can also set this using code in your script. Setting the working directory is useful when you want to access data in files on your computer or the network.

The basic function to use is setwd("path/to/file"). The thing to note is that in the path description you have to use "forward /" rather than the standard windows "backward".

However, if you are using an Rmarkdown file, you are generally discouraged to use "setwd", but here we can use another command which is part of the knitr package

3.2 Saturn notebooks in Edstem

Saturn notebooks are a special version of Jupyter notebooks that allow collaboration between students and staff. The notebooks can be created in the workspaces of your Ed environment



A Saturn notebook allows you to put in blocks of text or code. The workspace is directly linked to the notebook and files can be uploaded by right clicking in the files space on the left.

3.3 Rmarkdown notebooks in Rstudio

Rmarkdown notebooks in Rstudio are very similar to notebooks in Ed (in fact you can also open up a notebook in Rstudio). The nice thing about Rmarkdown is that you can also "publish" the notebook as an html file (webpage) or even as a word file or pdf file. In fact, this practical handout was written in R markdown. We will stick with html for the practical.

A new notebook can be opened from the file menu in R studio:

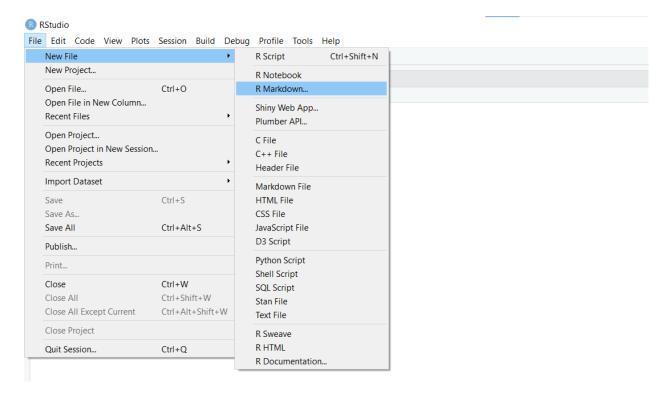


Figure 2: Create a new Rmarkdown notebook

and you have to give a title and your name (but you can change this later) which are inserted into the 'yaml header':

The Rmarkdown notebook comes with some example code below the 'yaml header' which you can delete if you want. Similar to the Ed Saturn notebooks you can write text and use code blocks. Use "CTRL-I" to insert a new code block in the notebook.

3.3.0.1 Exercise

• Can you check your working folder/directory and what's inside it?

in R:

```
getwd() # this tells you your current working directory dir() # this gives you a list of the files in your current working directory ?setwd # this give you the help file on how to set your working directory in code
```

in Rmarkdown you can use opts_knit\$set(root.dir ="path/to/files") to set your working directory.

```
knitr::opts_knit$set(root.dir = "c:/users/rver4657/Desktop") ## windows users
knitr::opts_knit$set(root.dir = "~/Desktop") ## Mac users
dir() # this gives you a list of the files in your current working directory
```

New R Markdown					
Document	Title:	Untitled			
Presentation	Author:	Willem Vervoort			
® Shiny	Date:	2022-07-27			
From Template	From Template Use current date when rendering document Default Output Format:				
 HTML Recommended format for authoring (you can switch to PE or Word output anytime). 					
	PDF PDF output requires TeX (MiKTeX on Windows, Ma 2013+ on OS X, TeX Live 2013+ on Linux).				
	_	Word documents requires an installation of MS ibre/Open Office on Linux).			
Create Empty Document		OK Cancel			

Figure 3: Name for new Rmarkdown notebook

4 BASIC R

4.1 R as a calculator

In its most basic form, R is a calculator

```
3*5

## [1] 15

50/100 + 0.1

## [1] 0.6

10 - 20

## [1] -10
```

4.2 Objects in R

The basic structure of R is based on objects, which are named. **R** is case sensitive, so keep this in mind. The main object we will use here is a *dataframe* or its modern variant the *tibble* in the package tidyverse.

All objects in R exist in the local R memory. So if you have a datafile, the first thing to do is to load it on your memory as an object that can be seen in the Environment panel. Thus, whatever you do with the object will not change your file, unless you save the object as a file.

As convention, R uses "<-" to assign a value (or another object) to an object. You may find "=" works just the same, but we don't recommend it, because you also use "=" with different meaning in the command and parameter setting.

```
# assign
x <- 5
y <- 2
```

You can call up what is stored in the object (inspect) again by just typing its name:

```
x
```

[1] 5

These objects will show up in the "Environment" window in Rstudio, or you can use ls() in the console to list the objects. The function c() can be used to stick things together into a vector. Redo the below commands in your own script.

```
# a vector
x <- c(1,2,5,7,8,15,3,12,11,19)
# another vector
y <- 1:10
# you have now two objects
ls()</pre>
```

```
## [1] "x" "y"
```

```
# you can add, multiply or subtract
z \leftarrow x + y
            4 8 11 13 21 10 20 20 29
zz <- x * y
    Γ17
                 15
                      28
                          40
                              90
                                  21
                                      96
                                          99 190
zzz <- x - y
7.7.7.
##
                      3
   <-0.5*x^2 - 3*x + 2
foo
##
    [1]
         -0.5
               -2.0
                      -0.5
                              5.5
                                  10.0
                                        69.5 -2.5
                                                     38.0 29.5 125.5
```

• How many objects are now in your environment?

5 STATISTICAL ANALYSIS AND DATA MANIPULATION

Now it's time to look a bit further. In particular, we might be interested in how we might manipulate data so we can perform some analyses to answer our research or practical problem. There are, of course, base R commands to do the job, but because of the growth in use and the popularity, you might find it easier to use the tidyverse package. This package is actually a combo of several packages originally written by the same author, but now expanded by mutiple authors. There is also a nice link to this on-line book R for Data science, which is good for background information and to expand your knowledge.

5.1 Packages to use

As highlighted, much of the power in R comes from the fact that it is open source and this means many people write new code and share this code. The formal way to do this is via "packages", which, once checked and endorsed by the R community, appear in the CRAN repository as a **package**.

In this introduction we want to use some of the features in the package tidyverse. This package includes a series of other useful packages that you might need.

There are two components to using packages. The first is to make sure that the package is installed, for which we can use the functions install.packages(). Note that the name of the package is a *string* so needs to between quotes "".

Within the Edstem environment, we have made sure that those packages are installed, so you don't need to separately install those packages.

```
install.packages("tidyverse")
```

If the package is installed in your personal library, you will need to load the package in R using require() or library(). There are subtle differences between these two functions, but they are currently not that important. Check the help files.

```
require(tidyverse)
```

5.1.1 Optional Exercise

• Can you load (and maybe first install) the package lubridate? This package is great for manipulating dates and times and works well with tidyverse.

5.2 A dataframe in tidyverse

A dataframe is a bit more complex. It is essentially a list, but presented as a table. Here is a simple demonstration of its power. We are using tibble() from tidyverse, which is a funny name, but is very similar to data.frame() in base R.

```
## # A tibble: 6 x 2
##
     City
                Rain mm
##
     <chr>>
                  <dbl>
## 1 Montevideo
                    950
## 2 New York
                    1174
## 3 Amsterdam
                    838
## 4 Sydney
                    1215
## 5 Moscow
                    707
## 6 Hong Kong
                    2400
```

As you can see a data frame (in this case a tibble) can mix character columns (City) and numeric columns (Rain_mm). Here I used c() to generate vectors of numbers of characters which I put in the columns. In addition, the columns have names, which you can access using colnames() or names:

```
colnames(Rainfall)
## [1] "City" "Rain_mm"

## [1] "City" "Rain mm"
```

Once you have a data frame or tibble, you can access parts of the dataframe or manipulate the dataframe. Such as finding a column

```
# call a column
Rainfall$City
                                                 "Sydney"
## [1] "Montevideo" "New York"
                                   "Amsterdam"
                                                               "Moscow"
## [6] "Hong Kong"
Rainfall["City"]
## # A tibble: 6 x 1
##
     City
##
     <chr>>
## 1 Montevideo
## 2 New York
## 3 Amsterdam
## 4 Sydney
## 5 Moscow
## 6 Hong Kong
# or
Rainfall[,1]
## # A tibble: 6 x 1
##
     City
##
     <chr>>
## 1 Montevideo
## 2 New York
## 3 Amsterdam
## 4 Sydney
## 5 Moscow
## 6 Hong Kong
Sub-setting rows is slightly different, you can still use numbers
# see the first two rows
Rainfall[1:2,]
## # A tibble: 2 x 2
##
     City
             Rain_mm
     <chr>
                   <dbl>
## 1 Montevideo
                     950
## 2 New York
                    1174
5.2.1 filter()
But, because this is a tibble, we can use the power of tidyverse and the function filter to find rows
```

Rainfall %>%

filter(City=="Montevideo")

OK, what is that %>% thing?? It is a further little symbol (apart from assign <-) in R that you need to know. It means "then".

So to read the above code in words, it says:

• Take the Rainfall data, then, find the row where City equals "Montevideo"

Let's expand this idea and show another filter:

Here I did two things, I did the filter using a comparison (and got multiple rows) and I "assigned" the result to a new object lots.

5.2.2 select()

Similar to filter, we can extract columns using select. So repeating the above example:

```
# call a column
Rainfall %>%
select(City)
```

```
## # A tibble: 6 x 1
## City
## <chr>
## 1 Montevideo
## 2 New York
## 3 Amsterdam
## 4 Sydney
## 5 Moscow
## 6 Hong Kong
```

5.2.3 Exercise

Using the above examples, can you do the following?

- Extract the column with the rainfall values?
- Extract the row with the annual rainfall at Amsterdam and assign to an object?
- Create an object with cities that have rainfall below 1500 mm?

5.3 Reading data from different sources

There are a multitude of functions to read data from the disk into the R memory, I will demonstrate only one here, but more are given in the tidyverse book

Because a lot of data is stored in comma delimited txt files (such as Excel exports), using read_csv() is a good standard option.

Here I am reading in some monthly data from the Concordia station in the Uruguay river in Argentina. This data was originally downloaded from the Global River Discharge Database

```
UR_flow <- read_csv("Data/UruguayRiver_ConcordiaSt.csv")

##

## -- Column specification ------
## cols(
## Year = col_double(),
## Month = col_double(),
## Flow = col_double()</pre>
```

```
# check the first few lines (6 by default)
UR_flow
```

```
## # A tibble: 132 x 3
##
       Year Month Flow
##
      <dbl> <dbl> <dbl>
##
    1 1969
                   7888
                1
##
    2 1969
                2
                   5951
##
    3 1969
                3
                   4296
##
    4
       1969
                4
                   4173
##
   5
       1969
                5
                   4539
##
   6
      1969
                6
                   4857
    7
                7
                   4018
##
       1969
##
    8
       1969
                8
                   3110
##
   9
       1969
                9
                   2541
       1969
               10
                   2822
## # ... with 122 more rows
```

)

Previously you would have to save a specific program's data file, say in xls in to a pure text file such as csv or txt. However, there are now many packages that allow you to read a dataset directly from its binary format. There are many packages to do such task, readxl package is one of them. You could google your way to the most convenient package to use.

5.3.1 Exercise

• Can you read in the file: "Parana_CorrientesSt.csv" (supplied) from your data directory?

5.4 More on data manipulation (using tidyverse)

5.4.1 Important commands

Based on the above, and building on this, the following list are the most used commands in tidyverse:

- select() select columns
- filter() filter rows
- arrange() re-order or arrange rows (row sorting)
- mutate() create new columns
- summarise() summarise values
- group_by() allows for group operations in the "split-apply-combine" concept

5.4.1.1 mutate, arrange and select Here is a short demonstration for mutate, select and arrange using the Rainfall data:

mutate and select to add columns, select columns and rearrange columns

```
# I can add a column of countries
Rainfall_new <- Rainfall %>%
   mutate(country = c("UY", "US", "NL", "AU", "RU", "CN")) %>%
   # and maybe a column of the average monthly rainfall
   mutate(M_rain = Rain_mm/12)

# You can use select to reorder the columns and put country to the front
Rainfall_new <- Rainfall_new %>%
   select(country, everything())

# And if you would like to drop the M_rain column you can use
Rainfall_new %>%
   select(-M_rain)
```

```
## # A tibble: 6 x 3
##
     country City
                        Rain_mm
     <chr>
                          <dbl>
##
            <chr>
## 1 UY
             Montevideo
                            950
## 2 US
            New York
                           1174
## 3 NL
            Amsterdam
                           838
## 4 AU
             Sydney
                           1215
## 5 RU
             Moscow
                            707
## 6 CN
             Hong Kong
                           2400
```

arrange to sort rows, and add desc() to do this in decreasing order

```
Rainfall_new %>%
  arrange(desc(Rain_mm))
```

```
## 3 US
             New York
                            1174
                                    97.8
## 4 UY
             Montevideo
                             950
                                    79.2
## 5 NL
             Amsterdam
                             838
                                    69.8
## 6 RU
                             707
                                    58.9
             Moscow
```

5.4.1.2 summarise and group_by Another useful function is summarise(), which allows you to apply a function over a data frame and particular across different factors. In tidyverse this is often combined with the function group_by to define how you would like to summarise.

Here is an example of summing the Uruguay river flow by year. Note that putting brackets around the statement makes it print out the result.

```
# aggregate to annual flow
(annual_flow <- UR_flow %>% #then
group_by(Year=Year) %>% #then
summarise(Sumflow = sum(Flow)))
```

```
## # A tibble: 11 x 2
##
       Year Sumflow
##
      <dbl>
              <dbl>
       1969
##
    1
              53753
##
    2
       1970
              52130
##
    3 1971
              66648
##
    4 1972
              99562
##
    5
       1973
             103070
##
    6 1974
              47130
##
    7
       1975
               68075
##
    8
      1976
              53500
##
    9
       1977
              73650
## 10
       1978
              41700
## 11
       1979
               61047
```

If you just wanted the overall mean and standard deviation of monthly flow, you could also ask for (and note how we drop group_by):

```
## # A tibble: 1 x 2

## Meanflow SdFlow

## <dbl> <dbl>

## 1 5457. 3492.
```

5.4.2 Exercise

• Can you calculate the standard deviation of the monthly flow by year using summarise()?

5.5 Different data set for practice

Let's open a water quality data set in csv format.

Here we will introduce some groundwater chemical data from Semarang in Indonesia, kindly supplied by Dasapta Erwin Irawan from ITB

```
chemdata <- read_csv("data/semarang_chem.csv")</pre>
```

```
##
## -- Column specification ---------
## cols(
    .default = col_double(),
##
    ID = col character(),
##
##
    Area = col_character(),
##
    UTM_zone = col_character(),
    Aq = col_character(),
##
    Fac = col_character()
##
## )
## i Use `spec()` for the full column specifications.
```

chemdata

```
## # A tibble: 58 x 24
                     Year
##
      ID
             Area
                            Lat Long UTM_east UTM_north UTM_zone Depth
                                                                           WL Elev
##
      <chr> <chr>
                    <dbl> <dbl> <dbl>
                                         <dbl>
                                                   <dbl> <chr>
                                                                  <dbl> <dbl> <dbl>
##
   1 SB_185 PT. N~
                     1992 -6.96
                                 110.
                                        439936
                                                 9230800 49M
                                                                      96 23.4
   2 SB_273 PT. I~ 1992 -6.98
                                        438500
                                                                      94 14.4
##
                                 110.
                                                 9228100 49M
                                                                                  20
   3 SB_283 Obs. ~ 1992 -6.96
                                 110.
                                        435500
                                                 9230150 49M
                                                                    150 15.2
                                                                                   2
   4 SB_271 PT. S~ 1992 -6.98
                                        424150
##
                                                 9228400 49M
                                                                     65 31.5
                                                                                  25
                                 110.
   5 SB_270 Dolog~ 1992 -6.97
                                 110.
                                        421950
                                                 9229400 49M
                                                                     NA 19.8
                                                                                  20
##
   6 SB_278 Hotel~ 1992 -6.99
                                 110.
                                        436950
                                                 9226950 49M
                                                                     86 7.86
                                                                                  5
   7 SB_325 PT Wa~ 1992 -6.99
                                        427950
                                                 9226950 49M
                                                                     76 44.6
                                                                                  72
                                 110.
  8 SB_190 PT. G~
                                                                                   4
##
                    1992 -6.98
                                        436900
                                                 9228050 49M
                                                                     NA 22.1
                                 110.
## 9 SB 256 Tamba~ 1992 -6.98
                                        429800
                                                                                   2
                                 110.
                                                 9228600 49M
                                                                     NA
                                                                         4.64
## 10 SB 206 Tamba~ 1992 -6.95
                                110.
                                        423100
                                                 9231700 49M
                                                                      80 11.6
                                                                                   1
## # ... with 48 more rows, and 13 more variables: TDS <dbl>, ph <dbl>, EC <dbl>,
      K <dbl>, Ca <dbl>, Mg <dbl>, Na <dbl>, SO4 <dbl>, Cl <dbl>, HCO3 <dbl>,
      Bal <dbl>, Aq <chr>, Fac <chr>
```

5.5.1 select()

A bit more on select. If you want multiple columns, for example Lat, Long until Depth, you can simply use the select() function.

```
chemdata %>%
  select(Lat, Long:Depth)
```

```
## # A tibble: 58 x 6
## Lat Long UTM_east UTM_north UTM_zone Depth
## <dbl> <dbl> <dbl> <dbl> <chr> ## 1 -6.96 110. 439936 9230800 49M 96
```

```
2 -6.98 110.
                     438500
                               9228100 49M
                                                     94
##
    3 - 6.96
                                                    150
##
             110.
                     435500
                               9230150 49M
                               9228400 49M
##
    4 - 6.98
             110.
                     424150
                                                     65
    5 -6.97
             110.
                     421950
                               9229400 49M
##
                                                     NA
##
    6 - 6.99
             110.
                     436950
                               9226950 49M
                                                     86
    7 -6.99
##
             110.
                     427950
                               9226950 49M
                                                     76
##
    8 - 6.98
             110.
                     436900
                               9228050 49M
                                                     NA
##
    9 -6.98
             110.
                     429800
                               9228600 49M
                                                     NA
## 10 -6.95
             110.
                     423100
                               9231700 49M
                                                     80
## # ... with 48 more rows
```

Or you want multiple columns Lat, Long until Depth, but you don't want UTM_zone. Again, you can use the select() function.

```
chemdata %>%
  select(Lat, Long:Depth, -UTM_zone)
```

```
## # A tibble: 58 x 5
##
        Lat Long UTM east UTM north Depth
##
      <dbl> <dbl>
                      <dbl>
                                 <dbl> <dbl>
    1 -6.96
             110.
                     439936
                               9230800
##
                                           96
    2 -6.98
##
             110.
                     438500
                               9228100
                                           94
    3 - 6.96
             110.
                     435500
                               9230150
                                          150
##
##
    4 -6.98
                                           65
             110.
                     424150
                               9228400
    5 - 6.97
              110.
                     421950
                               9229400
                                           NA
##
    6 - 6.99
             110.
                     436950
                               9226950
                                           86
    7 -6.99
##
             110.
                     427950
                               9226950
                                           76
##
    8 -6.98
             110.
                     436900
                               9228050
                                           NA
##
    9 -6.98
             110.
                     429800
                               9228600
                                           NA
## 10 -6.95
             110.
                     423100
                               9231700
                                           80
## # ... with 48 more rows
```

5.5.2 arrange()

Sorting the data by the Aq (aquifer) and Fac (facies) columns. Use the arrange() function.

```
chemdata %>%
  arrange(Aq, Fac)
```

```
## # A tibble: 58 x 24
##
      ID
              Area
                      Year
                              Lat
                                  Long UTM_east UTM_north UTM_zone Depth
                                                                                    Elev
      <chr>
##
             <chr>>
                     <dbl> <dbl> <dbl>
                                            <dbl>
                                                      <dbl> <chr>
                                                                       <dbl> <dbl> <dbl>
##
    1 SB_271 PT. S~
                      1992 -6.98
                                   110.
                                           424150
                                                    9228400 49M
                                                                          65 31.5
                                                                                       25
    2 SB_270 Dolog~
                                           421950
                                                    9229400 49M
                                                                                       20
##
                      1992 -6.97
                                   110.
                                                                          NA 19.8
##
    3 SB_325 PT Wa~
                      1992 -6.99
                                   110.
                                           427950
                                                    9226950 49M
                                                                          76 44.6
                                                                                       72
                                                                         100 56.6
##
    4 SB_225 PDAM ~
                      1992 -7.00
                                           431850
                                                    9226100 49M
                                                                                       65
                                   110.
    5 SB_92 RS Ka~
                      1992 -6.99
                                           434400
                                                    9227200 49M
                                                                          75 6.8
                                   110.
                                                                                        6
##
    6 SB_112 Hotel~
                      1993 -7.00
                                   110.
                                           435763
                                                    9226415 49M
                                                                         122 25.0
                                                                                       30
    7 SB 215 S. Pa~
                      2003 -7.00
                                           432811
                                                    9225924 49M
                                                                         152
                                                                             5.97
                                                                                       18
##
                                   110.
                                                                                       25
##
    8 SB_33 Es Pr~
                      2003 -6.99
                                   110.
                                           429310
                                                    9227496 49M
                                                                          90 22.5
    9 SB 590 Bukit~
                      2003 -6.99
                                           427050
                                                                          90 23.6
                                                                                       25
                                   110.
                                                    9227750 49M
## 10 SP_341 Obs. ~
                      2003 -6.99
                                   110.
                                           426474
                                                    9227278 49M
                                                                          NA 56.9
                                                                                       40
```

```
## # ... with 48 more rows, and 13 more variables: TDS <dbl>, ph <dbl>, EC <dbl>, ## # K <dbl>, Ca <dbl>, Mg <dbl>, Na <dbl>, SO4 <dbl>, Cl <dbl>, HCO3 <dbl>, ## Bal <dbl>, Aq <chr>>, Fac <chr>>
```

5.5.3 mutate()

Making new columns, for instance, calculating the ratio between Ca and Na. Use the mutate() function

```
chemdata %>%
  mutate(ratio_Cana = Ca / Na)
```

```
## # A tibble: 58 x 25
                           Lat Long UTM_east UTM_north UTM_zone Depth
##
      ID
            Area
                     Year
##
      <chr> <chr> <dbl> <dbl> <dbl> <dbl>
                                         <dbl>
                                                   <dbl> <chr>
                                                                  <dbl> <dbl> <dbl>
  1 SB 185 PT. N~ 1992 -6.96
                                        439936
                                                 9230800 49M
                                                                     96 23.4
## 2 SB_273 PT. I~ 1992 -6.98
                                110.
                                       438500
                                                 9228100 49M
                                                                     94 14.4
                                                                                 20
## 3 SB_283 Obs. ~
                    1992 -6.96
                                 110.
                                       435500
                                                 9230150 49M
                                                                    150 15.2
                                                                                  2
## 4 SB_271 PT. S~ 1992 -6.98
                                110.
                                       424150
                                                                     65 31.5
                                                                                 25
                                                 9228400 49M
## 5 SB_270 Dolog~ 1992 -6.97
                                       421950
                                                 9229400 49M
                                                                     NA 19.8
                                 110.
                                                                                 20
## 6 SB_278 Hotel~ 1992 -6.99
                                                 9226950 49M
                                                                     86 7.86
                                       436950
                                                                                  5
                                110.
## 7 SB_325 PT Wa~ 1992 -6.99
                                 110.
                                       427950
                                                 9226950 49M
                                                                     76 44.6
                                                                                 72
## 8 SB_190 PT. G~ 1992 -6.98
                                110.
                                       436900
                                                 9228050 49M
                                                                     NA 22.1
                                                                                  4
## 9 SB_256 Tamba~ 1992 -6.98
                                        429800
                                                 9228600 49M
                                                                                  2
                                110.
                                                                     NA 4.64
                                                                     80 11.6
## 10 SB_206 Tamba~ 1992 -6.95 110.
                                        423100
                                                 9231700 49M
                                                                                  1
## # ... with 48 more rows, and 14 more variables: TDS <dbl>, ph <dbl>, EC <dbl>,
## # K <dbl>, Ca <dbl>, Mg <dbl>, Na <dbl>, SO4 <dbl>, Cl <dbl>, HCO3 <dbl>,
      Bal <dbl>, Aq <chr>, Fac <chr>, ratio_Cana <dbl>
```

5.5.4 summarise()

Making a summary from your data. Use summarise() function.

```
## # A tibble: 1 x 4
## mean_TDS max_Cl min_Cl total
## <dbl> <dbl> <dbl> <int>
## 1 1041. 15753. 11.2 58
```

5.5.5 group_by()

Sorting out the data based on certain order. Use group_by() function.

```
min_Cl = min(Cl),
total = n())
```

```
# A tibble: 3 x 5
                        mean_TDS max_Cl min_Cl total
##
##
     <chr>
                            <dbl>
                                   <dbl>
                                           <dbl> <int>
## 1 Damar
                             371.
                                            11.2
                                     70
                                                     14
## 2 Garang
                             445.
                                    146.
                                            19.6
                                                     11
                            1523. 15753.
## 3 Quaternary marine
                                            25
                                                     33
```

5.5.5.1 Exercise

• Can you calculate the mean(Cl) and sd(Na) for the dataset grouped by Fac?

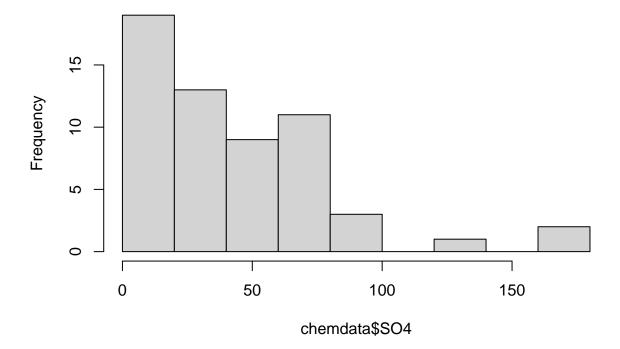
As we have indicated earlier, be sure to check out R for Data Science for more info about tidyverse and its use in data science.

6 PLOTTING

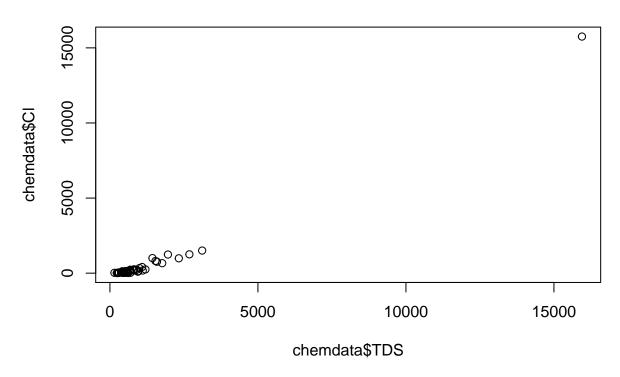
R is good at plotting. There are many ways to create a plot. So you just have to choose which one is the easiest for you. One way is using base R plotting engine. Like these plots.

```
hist(chemdata$S04, main = "histogram of S04")
```

histogram of SO4



scatter plot of TDS and CI

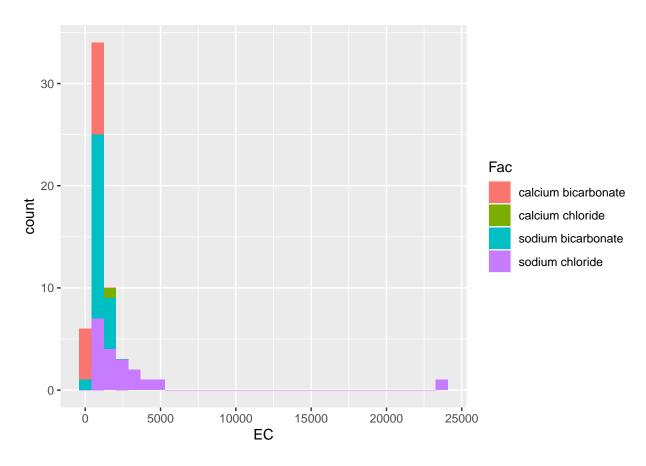


You could always tweak the plot to suits your needs. There are many resources about plotting in R on the web.

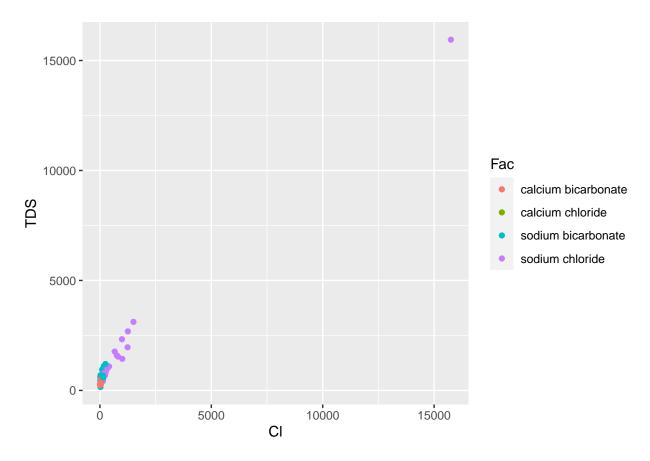
Nicer plots are made with ggplot2 which is the plotting engine from tidyverse. The best book for this is the $\bf R$ Graphics Cookbook

```
chemdata %>%
  ggplot(aes(EC, fill = Fac)) + geom_histogram()
```

`stat_bin()` using `bins = 30`. Pick better value with `binwidth`.



```
chemdata %>%
  ggplot(aes(C1, TDS, colour = Fac)) + geom_point()
```



In the second plot, note how colour is used to identify different facies.

6.1 Exercise

- try to make a plot between Ca vs Na using base R and ggplot2.
- try to make histogram for one parameter that you have in your dataset. Use ggplot2.
- can you tweak it by adding title to the plot and title to all axis. Hint: use ggtitle() and labs().

7 Programming: if else and for loops

Loops are essential in programming. There are a range of different types of loops, but here I will only demonstrate "if else" and "for". I have always been told that all other loops are just derivatives or short cuts.

An "if else" loop allows you to program a switch in the code.

Basically it is used to evaluate an expression if the statement is TRUE and to evaluate another expression if the statement is FALSE:

```
if (comparison) do this, else do that
```

You might call the above line "pseudo code". It is sometimes handy to first write something in pseudo code, basically you want to write in broad language what you want to happen.

You could also use only the "if" part, which means nothing happens if the statement is FALSE.

As an example I want to do: if (a data frame has more than 10 rows) write data frame is LONG, else write data frame is SHORT.

```
#We will first generate the data frame:
x <- UR_flow
# now wrote loop
if (nrow(x) > 10) {
print("the dataframe is LONG")
} else {
print("the dataframe is SHORT")
}
```

[1] "the dataframe is LONG"

There are a few things to note here. I use the statement nrow() to check how many rows the data frame has. I use the statement print() to write something to the screen.

7.0.1 Exercise

• Try generating another data frame x and rerun the program, or change the program to get it to say "the dataframe is short".

R also has an ifelse() command. This is a vectorized version of the if command - which means that it can be used on vectors of data - the command is applied to each element (or value) of the vector in turn. The if command only evaluates single values.

Using the ifelse command will return a vector of values, the same length as the longest argument in the expression.

Wherever possible, it is preferable to use the ifelse command rather than using the if command in combination with a loop - writing the program is more efficient and R evaluates vectorised functions more efficiently than it does loops. Here is an example which changes the program above.

```
x <- UR_flow
# add a column which identifies whether the flow < 5000
x[,4] <- ifelse(x[,3] > 5000, "large", "small")
# this creates a third column
tail(x,10)
```

```
## # A tibble: 10 x 4
##
       Year Month Flow V1
##
      <dbl> <dbl> <dbl> <chr>
       1979
                    1699 small
##
    1
                 3
##
       1979
                 4
                    1650 small
    3
       1979
                    5052 large
##
                 5
                    2619 small
##
       1979
                 6
                 7
##
    5
       1979
                    3776 small
##
    6
       1979
                 8
                    6134 large
    7
##
       1979
                 9
                    3275 small
    8
       1979
                10 15692 large
                11 12244 large
       1979
##
    9
## 10
       1979
                12
                    7380 large
```

I check in the second column of the data frame whether the flows are greater than 5000 or not. I then write in the third column whether they are large or small numbers. A more complex (nested) if else version would be:

```
x[,5] \leftarrow ifelse(x[,3] > 2500,ifelse(x[,3] > 10000, "large", "intermediate"), "small") tail(x,10)
```

```
## # A tibble: 10 x 5
##
       Year Month Flow V1
##
      <dbl> <dbl> <chr> <chr>
##
    1
       1979
                3
                   1699 small small
    2
       1979
                   1650 small small
##
                4
##
    3
       1979
                5
                   5052 large intermediate
##
    4
       1979
                   2619 small intermediate
    5
       1979
                7
                   3776 small intermediate
##
##
    6
       1979
                   6134 large intermediate
##
    7
       1979
                9
                   3275 small intermediate
##
       1979
               10 15692 large large
               11 12244 large large
##
    9
       1979
##
   10
       1979
                   7380 large intermediate
```

You can try out some of your own versions of this

7.1 The "for" loop, getting the program to do something repeatedly

Loops are used to repeat a set of commands. Normally, there will be a variable which changes value in each successive loop through the commands. Reference to this changing value results in differences in output from successive iterations.

The for loop is used when the number of required iterations is known before the loop begins. It is used in the following way: for (name in expression1) {expression2}

- name is the name of the loop variable. Its value changes during each iteration, starting with the first value and ending with the last value in expression1.
- expression is a vector expression (often a sequence, such as 1:10).
- expression 2 is a command or group of commands that are repeatedly evaluated. It usually contains references to name, which result in changes to the value of the expression as the value of name changes.

Here is the classic example of a loop

[1] "1969 Year"

```
# Hello world
for (i in 1:5) {
print(paste(i, "hello world"))
## [1] "1 hello world"
## [1] "2 hello world"
## [1] "3 hello world"
## [1] "4 hello world"
## [1] "5 hello world"
Note the use of paste() to combine character vectors.
Here is another simple loop that tells you the first 5 values of the flow data.
for (i in 1:5) {
print(paste(UR_flow$Flow[i], "is the flow (ML/day)"))
## [1] "7888 is the flow (ML/day)"
## [1] "5951 is the flow (ML/day)"
## [1] "4296 is the flow (ML/day)"
## [1] "4173 is the flow (ML/day)"
## [1] "4539 is the flow (ML/day)"
# or more complex:
for (i in 1:5) {
print(paste("in Year", UR_flow$Year[i],"and month",
UR_flow$Month[i],
"the flow is", UR_flow$Flow[i], "(ML/day)"))
}
## [1] "in Year 1969 and month 1 the flow is 7888 (ML/day)"
## [1] "in Year 1969 and month 2 the flow is 5951 (ML/day)"
## [1] "in Year 1969 and month 3 the flow is 4296 (ML/day)"
## [1] "in Year 1969 and month 4 the flow is 4173 (ML/day)"
## [1] "in Year 1969 and month 5 the flow is 4539 (ML/day)"
```

You can also nest loops, that is, embed one loop into another. Here is an example that prints both the year and the flow using the column names in the dataframe.

```
for (i in 1:5) {
  for (j in c(1,3)) {
    print(paste(UR_flow[i,j], colnames(UR_flow)[j]))
  }
}

## [1] "1969 Year"
## [1] "7888 Flow"
```

```
## [1] "5951 Flow"
## [1] "1969 Year"
## [1] "4296 Flow"
## [1] "1969 Year"
## [1] "4173 Flow"
## [1] "1969 Year"
## [1] "4539 Flow"
```

7.1.1 Exercise

• Write another program that includes a loop and a logical test

7.1.2 Comparison and Logical Operators

Comparison operators return a true or false value:

- $\bullet == Equal to$
- > Greater than
- \bullet >= Greater than or equal to
- < Less than
- <= Less than or equal to

Comparison operators can be combined with logical operators to describe more complex conditions.

Logical operators:

- ! Not
- or (used for vectors, with the ifelse command)
- || or (used for single values)
- & and (used for vectors, with the ifelse command)
- && and (used for single values)

7.1.3 Exercise

Write a small program that uses comparison operators and a logical operator.

8 Date and times

This is a small demonstration of the package lubridate, which works well with tidyverse and allows you to convert times and dates with less effort. There is more description about this in this chapter of the tidyverse book.

```
#install.packages("lubridated") do this if you haven't done so.
require(lubridate)
UR_flow_d <- UR_flow %>%
  mutate(Dates = make_datetime(Year, Month))
```

Once we have this zoo data frame, it can be plotted quite easily with the basic plotting package.

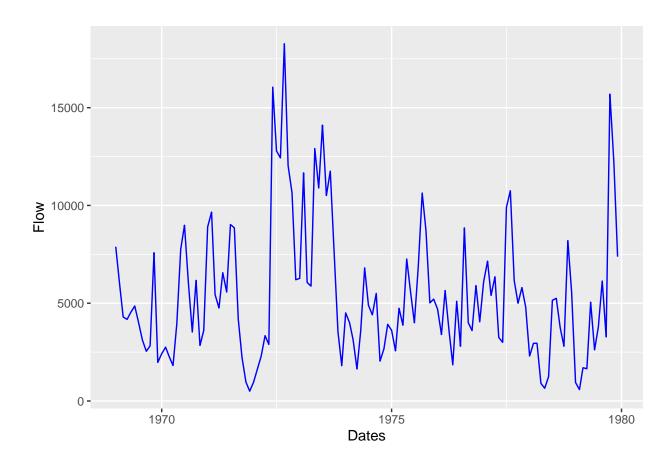


Figure 4: Demonstration of dates in plotting R

9 Writing functions in R

Until now you have used several functions in R that are part of packages or part of "core" R. However, another powerful element in R is the ability to write your own functions. There are two major advantages with writing functions:

- 1. They are easy to test, as they are contained. This is especially true if keep functions short.
- 2. They are short cuts and repeatable and therefore limit the possibility of typos.

Let's go back to the "hello world" example that we used in a loop earlier. We can write the same example in a function.

The first thing to do is to decide which inputs we want the function to use to create the output. In this case I suggest we might want to change how many times the function produces output (which was 5 in the earlier example) and the actual output text, which was "hello world" in the original function.

The basic structure of a function is:

```
NameOfFunction <- function(input1, input2,...) {</pre>
doSomething <- ....
return(doSomething)
Here is the hello world example:
HW <- function(n, outtext) {</pre>
  for (i in 1:n) {
    print(outtext)
  # return("nothing")
}
# test
HW(5, "Hello World")
## [1] "Hello World"
# switch input by naming
HW(outtext = "I can switch the inputs", n = 3)
## [1] "I can switch the inputs"
## [1] "I can switch the inputs"
## [1] "I can switch the inputs"
```

Note that in this case the function produces output as part of its execution rather than returning an actual value (which is why I commented out the return statement). In the first example, you can see that you don't have to name the inputs if you keep the inputs in the same order as the defined function. R assumes that you mean n = 5 and outtext = "Hello world". In the second example I show that you can switch the inpurs if you name them and that the function allows you to choose different inputs.

9.0.1 Exercise

- Can you write a function that calculates $y = a^*x + b$ for different values of x, a and b?
- Make the function return the output using return()

END OF DOCUMENT