R/RStudio Introductory Workshop by University of San Diego

January 22, 2022

The following link shows what each quadrant in the RStudio IDE represents: https://www.leonshpaner.com/teaching/post/rstudio/

Let's talk about RStudio first. Let's start with the basics of R.

General/Console Operations

In R, we can simply type commands in the console window and hit "enter." This is how they are executed. For example, R can be used as a calculator.

```
2 + 2

## [1] 4

3 * 3

## [1] 9

sqrt(9)

## [1] 3

log10(100)

## [1] 2
```

What is a string?

A string is simply any open alpha/alphanumeric text characters surrounded by either single quotation marks or double quotation marks, with no preference assigned for either single or double quotation marks, with a print statement being called prior to the strings. For example,

```
print('This is a string.')

## [1] "This is a string."

print( "This is also a string123.")

## [1] "This is also a string123."
```

Determining and setting the current working directory

The importance of determining and setting the working directory cannot be stressed enough. Obtain the path to the working directory by running the getwd() function. Set the working directory by running the setwd("...") function, filling the parentheses inside with the correct path.

getwd() setwd()

Installing Packages

install.packages('factoextra')

For example,

To install a package or library, simply type in install.packages('package_name). For the following exercises, let us ensure that we have installed the following packages:

```
# psychological library as extension for statistical tools
install.packages('psych')
# for reading rect. data (i.e., 'csv', 'tsv', and 'fwf')
install.packages("readr")
# additional library for summarizing data
install.packages('summarytools')
# classification and regression training (modeling)
install.packages('caret')
# other miscellaneous function
install.packages('e1071')
# for classification and decision trees
install.packages('rpart')
# for plotting classification and decision trees
install.packages('rpart.plot')
# methods for cluster analysis
install.packages("cluster")
# clustering algorithms & visualization
```

To read the documentation for any given library, simply put a "?" before the library name and press "enter."

```
library(summarytools) # load the library first
# ?summarytools # then view the documentation
```

This will open the documentation in the 'Files, Plots, Packages. Help, Viewer' pane.

Source Pane (Workspace) Scripting

Creating objects:

```
<-: assignment in R. Shortcut: "Alt + -" on Windows or "Option + -" on Mac.
```

```
var1 \leftarrow c(0, 1, 2, 3)
```

Differences between "=" and "<-"

Whereas "=" sign can also be used for assignment in R, it is best suited for specifying field equivalents (i.e., number of rows, columns, etc.). For example, let us take the following dataframe with 4 rows and 3 columns. Here, we specify A=4 and B=3 as follows:

```
dataframe_1 <- c(A = 4, B = 3)
dataframe_1</pre>
```

```
## A B
## 4 3
```

If we specify $A \leftarrow 4$, and $B \leftarrow 3$ instead, A and B will effectively evaluate to those respective values as opposed to listing them in those respective columns. Let us take a look:

```
## [1] 4 3
```

Import data from flat .csv file

Assuming that your file is located in the same working directory that you have specified at the onset of this tutorial/workshop, make an assignment to a new variable (i.e., ex_csv) and call read.csv() in the following generalized format

For Windows users:

```
ex csv 1 <- read.csv(choose.files(), header = T, quote = "")
```

```
# for macOS users
# example1.6 = read.csv(file.choose(), header = T, quote = "'")
```

The choose.files(), file.choose() function calls, respectively. allow the user to locate the file on their local drive, regardless of the working directory. That being said, there is more than one way to read in a .csv file. It does not have to exist on the local machine. If the file exists on the cloud, the path (link) can be parsed into the read.csv() function call as a string.

Now, let us print what is contained in var 1

```
print(var1)
```

```
## [1] 0 1 2 3
```

or we can simply call var1

var1

```
## [1] 0 1 2 3
```

Let us assign a variable to our earlier calculation and call the variable.

```
two <- 2+2
two
```

```
## [1] 4
```

Any object (variable, vector, matrix, etc.) that is created is stored in the R workspace. From time to time, it is best practice to clear certain unused elements from the workspace so that it does not congest the memory.

```
rm(two)
```

When we proceed to type in two, we will see that there is an error, confirming that the variable has been removed from the workspace.

There are 4 main data types in R: numeric, character, factor, and logical. There are data classes. Numeric variables includes integers and decimals.

```
num <- 12.6
num
```

```
## [1] 12.6
```

Character (includes characters and strings):

```
char <- "Male"
char</pre>
```

```
## [1] "Male"
```

Factor (ordinal/categorical data)"

```
gender <- as.factor(char)
gender</pre>
```

```
## [1] Male
## Levels: Male
```

Logical()

```
TRUE

## [1] TRUE

FALSE

## [1] FALSE

T # abbreviation also works for Boolean object

## [1] TRUE

F

## [1] FALSE

TRUE * 7

## [1] 7

FALSE * 7
```

Data Structures

What is a variable?

A variable is a container for storing a data value, exhibited as a reference to "to an object in memory which means that whenever a variable is assigned # to an instance, it gets mapped to that instance. A variable in R can store a vector, a group of vectors or a combination of many R objects" (GeeksforGeeks, 2020).

There are 3 most important data structures in R: vector, matrix, and dataframe.

Vector: the most basic type of data structure within R; contains a series of values of the same data class. It is a "sequence of data elements" (Thakur, 2018).

Matrix: a 2-dimensional version of a vector. Instead of only having a single row/list of data, we have rows and columns of data of the same data class.

Dataframe: the most important data structure for data science. Think of dataframe as loads of vectors pasted together as columns. Columns in a dataframe can be of different data class, but values within the same column must be the same data class.

The c() function is to R what concatenate() is to excel. For example,

```
vector_1 <- c(2,3,5)
vector_1</pre>
```

[1] 2 3 5

Similarly, a vector of logical values will contain the following.

```
vector_2 <- c(TRUE, FALSE, TRUE, FALSE, FALSE)
vector_2</pre>
```

[1] TRUE FALSE TRUE FALSE FALSE

To determine the number of members inside any given vector, we apply the length() function call on the vector as follows:

```
length(c(TRUE, FALSE, TRUE, FALSE, FALSE))
```

[1] 5

or, since we already assigned this to a data frame named vector_2, we can simply call length of vector_2 as follows:

```
length(vector 2)
```

[1] 5

Let's say for example, that we want to access the third element of vector_1. We can do so as follows:

```
vector_1[3]
```

[1] 5

What if we want to access all elements within the dataframe except for the first one? To this end, we use the "-" symbol as follows:

```
vector_1[-1]
```

[1] 3 5

Let us create a longer arbitrary vector so we can illustrate some further examples.

```
vector_3 <- c(1,3,5,7,9,20,2,8,10,35,76,89,207)
```

To access the first, fifth, and ninth elements of this dataframe. To this end, we can do the following:

```
vector_3[c(1,5,9)]
```

[1] 1 9 10

To access all elements within a specified range, specify the exact range using the ":" separator as follows:

```
vector_3[3:11]
```

```
## [1] 5 7 9 20 2 8 10 35 76
```

Let us create a mock dataframe for five fictitious individuals representing different ages, and departments at a research facility.

##		Name	Age	Experience	Position
##	1	Jack	47	7	Economist
##	2	Kathy	41	5	Director of Operations
##	3	Latesha	23	9	Human Resources
##	4	Brandon	55	3	Admin. Assistant
##	5	Alexa	36	11	Data Scientist
##	6	${\tt Jonathan}$	54	6	Admin. Assistant
##	7	Joshua	48	8	Account Manager
##	8	Emily	23	9	Account Manager
##	9	Matthew	22	5	Attorney
##	10	Anthony	27	2	Paralegal
##	11	Margaret	37	1	Data Analyst
##	12	Natalie	43	4	Research Assistant

Let us examine the structure of the dataframe.

```
str(df)
```

```
## 'data.frame': 12 obs. of 4 variables:
## $ Name : chr "Jack" "Kathy" "Latesha" "Brandon" ...
## $ Age : num   47 41 23 55 36 54 48 23 22 27 ...
## $ Experience: num   7 5 9 3 11 6 8 9 5 2 ...
## $ Position : chr "Economist" "Director of Operations" "Human Resources" "Admin. Assistant" ...
```

Let us examine the dimensions of the dataframe (number of rows and columns, respectively).

```
dim(df)
```

[1] 12 4

Sorting Data

Let us say that now we want to sort this dataframe in order of age (youngest to oldest).

```
df_age <- df[order(Age),]
df_age</pre>
```

```
##
          Name Age Experience
                                              Position
## 9
       Matthew
                22
                             5
                                               Attorney
       Latesha
## 3
                             9
                                       Human Resources
## 8
                 23
                             9
                                       Account Manager
         Emily
## 10
       Anthony
                 27
                             2
                                             Paralegal
## 5
         Alexa
                36
                            11
                                        Data Scientist
                                          Data Analyst
## 11 Margaret
                37
                             1
## 2
         Kathy
                41
                             5 Director of Operations
## 12
       Natalie
                43
                             4
                                    Research Assistant
                             7
## 1
          Jack
                47
                                             Economist
## 7
        Joshua
                48
                             8
                                       Account Manager
                             6
## 6
      Jonathan
                 54
                                      Admin. Assistant
       Brandon
                              3
                                      Admin. Assistant
```

Now, if we want to sort experience by descending order while keeping age sorted according to previous specifications, we can do the following:

```
df_age_exp <- df[order(Age, Experience),]
df_age_exp</pre>
```

```
##
          Name Age Experience
                                              Position
## 9
       Matthew
                22
                                              Attorney
## 3
       Latesha
                23
                             9
                                       Human Resources
## 8
         Emily
                23
                             9
                                       Account Manager
                             2
## 10
       Anthony
                27
                                             Paralegal
## 5
         Alexa
                36
                            11
                                        Data Scientist
## 11 Margaret
                37
                                          Data Analyst
                             1
## 2
                             5 Director of Operations
         Kathy
                41
## 12
       Natalie
                43
                             4
                                   Research Assistant
## 1
          Jack
                47
                             7
                                             Economist
## 7
                             8
        Joshua
                48
                                       Account Manager
## 6
      Jonathan 54
                             6
                                      Admin. Assistant
                                      Admin. Assistant
## 4
       Brandon
               55
                             3
```

Handling #NA values

NA (not available) refers to missing values. What if our dataset has missing values? How should we handle this scenario? For example, age has some missing values.

```
##
        Name_2 Age_2 Experience_2
                                                Position_2
## 1
          Jack
                                                 Economist
                  47
                                 7
## 2
         Kathy
                  NA
                                 5 Director of Operations
## 3
       Latesha
                  23
                                 9
                                           Human Resources
## 4
       Brandon
                  55
                                 3
                                          Admin. Assistant
## 5
                                            Data Scientist
         Alexa
                  36
                                11
      Jonathan
## 6
                  54
                                 6
                                          Admin. Assistant
## 7
        Joshua
                  48
                                 8
                                           Account Manager
## 8
         Emily
                  NA
                                 9
                                           Account Manager
                                 5
## 9
       Matthew
                  22
                                                  Attorney
## 10
       Anthony
                  27
                                 2
                                                 Paralegal
## 11 Margaret
                  37
                                              Data Analyst
                                 1
## 12
      Natalie
                   43
                                 4
                                        Research Assistant
```

Inspecting #NA values

```
is.na(df_2) # returns a Boolean matrix (True or False)
```

```
##
         Name_2 Age_2 Experience_2 Position_2
##
   [1,] FALSE FALSE
                             FALSE
                                        FALSE
   [2,] FALSE TRUE
                             FALSE
                                        FALSE
##
##
   [3,] FALSE FALSE
                             FALSE
                                        FALSE
   [4,] FALSE FALSE
                             FALSE
                                        FALSE
   [5,] FALSE FALSE
##
                             FALSE
                                        FALSE
   [6,]
         FALSE FALSE
##
                             FALSE
                                        FALSE
##
   [7,]
         FALSE FALSE
                                        FALSE
                             FALSE
   [8,]
        FALSE TRUE
                             FALSE
                                        FALSE
##
   [9,]
         FALSE FALSE
                             FALSE
                                        FALSE
## [10,]
         FALSE FALSE
                             FALSE
                                        FALSE
## [11,]
         FALSE FALSE
                             FALSE
                                        FALSE
## [12,] FALSE FALSE
                             FALSE
                                        FALSE
```

```
sum(is.na(df_2)) # sums up all of the NA values in the dataframe
```

[1] 2

```
df_2[!complete.cases(df_2),] # we can provide a list of rows with missing data
```

```
## Name_2 Age_2 Experience_2 Position_2
## 2 Kathy NA 5 Director of Operations
## 8 Emily NA 9 Account Manager
```

We can delete the rows with missing values by making an na.omit() function call in the following manner:

```
df_2_na_omit <- na.omit(df_2)
df_2_na_omit</pre>
```

```
## Name_2 Age_2 Experience_2 Position_2
## 1 Jack 47 7 Economist
```

```
## 3
       Latesha
                   23
                                       Human Resources
## 4
       Brandon
                   55
                                 3
                                      Admin. Assistant
                                        Data Scientist
## 5
         Alexa
                   36
                                 11
## 6
      Jonathan
                                 6
                                      Admin. Assistant
                   54
## 7
        Joshua
                   48
                                 8
                                       Account Manager
## 9
       Matthew
                   22
                                 5
                                              Attorney
       Anthony
                                 2
                                             Paralegal
## 10
                   27
## 11 Margaret
                   37
                                 1
                                          Data Analyst
## 12
       Natalie
                   43
                                 4 Research Assistant
```

Or we can use complete.cases() to subset only those rows that do not have missing values:

df_2[complete.cases(df_2),]

```
##
        Name_2 Age_2 Experience_2
                                            Position_2
          Jack
## 1
                  47
                                 7
                                             Economist
## 3
                                      Human Resources
       Latesha
                                 9
                  23
## 4
       Brandon
                  55
                                 3
                                      Admin. Assistant
## 5
         Alexa
                  36
                                11
                                        Data Scientist
## 6
      Jonathan
                  54
                                 6
                                      Admin. Assistant
## 7
                                 8
        Joshua
                  48
                                       Account Manager
## 9
       Matthew
                  22
                                 5
                                              Attorney
                                 2
## 10 Anthony
                  27
                                             Paralegal
## 11 Margaret
                  37
                                 1
                                          Data Analyst
      Natalie
## 12
                  43
                                 4 Research Assistant
```

What if we receive a dataframe that, at a cursory glance, warehouses numerical values where we see numbers, but when running additional operations on the dataframe, we discover that we cannot conduct numerical exercises with columns that appear to have numbers. This is exactly why it is of utmost importance for us to always inspect the structure of the dataframe using the str() function call. Here is an example of the same dataframe with altered data types.

Notice how Age is now expressed as a character data type, whereas Experience still shows as a numeric datatype.

```
str(df_3,
    strict.width = 'wrap')
```

```
## 'data.frame': 12 obs. of 4 variables:
## $ Name_3 : chr "Jack" "Kathy" "Latesha" "Brandon" ...
## $ Age_3 : chr "47" "41" "23" "55" ...
## $ Experience_3: num 7 5 9 3 11 6 8 9 5 2 ...
## $ Position_3 : chr "Economist" "Director of Operations" "Human Resources"
## "Admin. Assistant" ...
```

Let us convert Age back to numeric using the as.numeric() function, and re-examine the dataframe.

```
df_3$Age_3 <- as.numeric(df_3$Age_3)
str(df_3, strict.width = 'wrap')

## 'data.frame': 12 obs. of 4 variables:
## $ Name_3 : chr "Jack" "Kathy" "Latesha" "Brandon" ...
## $ Age_3 : num 47 41 23 55 36 54 48 23 22 27 ...
## $ Experience_3: num 7 5 9 3 11 6 8 9 5 2 ...
## $ Position_3 : chr "Economist" "Director of Operations" "Human Resources"
## "Admin. Assistant" ...</pre>
```

We can also convert experience from numeric to character/categorical data as follows:

```
options(width = 60)
df_3$Experience_3 <- as.character(df_3$Experience_3)
str(df_3, width = 60, strict.width = 'wrap')

## 'data.frame': 12 obs. of 4 variables:
## $ Name_3 : chr "Jack" "Kathy" "Latesha" "Brandon" ...
## $ Age_3 : num 47 41 23 55 36 54 48 23 22 27 ...
## $ Experience_3: chr "7" "5" "9" "3" ...
## $ Position_3 : chr "Economist" "Director of Operations"
## "Human Resources" "Admin. Assistant" ...</pre>
```

Basic Statistics

Setting the seed

First, let us discuss the importance of setting a seed. Setting a seed to a specific yet arbitrary value in R ensures the reproducibility of results. It is always best practice to use the same assigned seed throughout the entire experiment. Setting the seed to this arbitrary number (of any length) will guarantee exactly the same output across all R sessions and users, respectively.

Let us create a new data frame of numbers 1 - 100.

```
mystats <- c(1:100)
```

and go over the basic statistical functions

```
mean(mystats) # mean of the vector
```

```
## [1] 50.5
```

```
median(mystats) # median of the vector
## [1] 50.5
min(mystats) # minimum of the vector
## [1] 1
max(mystats) # maximum of the vector
## [1] 100
range(mystats) # range of the vector
## [1]
         1 100
sum(mystats) # sum of the vector
## [1] 5050
sd(mystats) # standard deviation of the vector
## [1] 29.01149
class(mystats) # return data class of the vector
## [1] "integer"
length(mystats) \# the length of the vector
## [1] 100
# summary of the dataset
summary(mystats)
##
      Min. 1st Qu. Median
                               Mean 3rd Qu.
                                               Max.
      1.00
                     50.50
##
             25.75
                              50.50
                                      75.25 100.00
To use an installed library, we must open that library with the following library() function call
library(psych)
```

For example, the psych library uses the describe() function call to give us an alternate perspective int the summary statistics of the data.

```
describe(mystats)
##
       n mean
             sd median trimmed mad min max range
     1 100 50.5 29.01 50.5
                    50.5 37.06
                            1 100
   skew kurtosis se
## X1
       -1.24 2.9
    Ω
library(summarytools)
dfSummary(mystats, plain.ascii = FALSE,
     style = 'grid',
     graph.magnif = 0.85,
     varnumbers = FALSE,
     valid.col = FALSE,
     tmp.img.dir = "/tmp",
     method='pandoc')
## ### Data Frame Summary
## #### mystats
## **Dimensions:** 100 x 1
## **Duplicates:** 0
##
## | Variable | Stats / Values | Freqs (% of Valid) | Graph
(0.0\%)
## |
       | 1 < 50.5 < 100\
                                    1
                                                       Τ
                       | IQR (CV) : 49.5 (0.6) |
```

Simulating a Normal Distribution

Now, We will use the rnorm() function to simulate a vector of 100 random normally distributed data with a mean of 50, and a standard deviation of 10.

```
set.seed(222) # set.seed() for reproducibility
norm_vals <- rnorm(n = 100, mean = 50, sd = 10)
norm_vals</pre>
```

```
##
     [1] 64.87757 49.98108 63.81021 46.19786 51.84136 47.53104 37.84439 65.61405
     [9] 54.27310 37.98976 60.52458 36.94936 43.07392 56.02649 48.02247 38.14125
##
##
    [17] 29.94487 50.07510 55.19490 42.53705 57.26455 57.13657 43.49937 64.98696
    [25] 35.64172 28.38682 53.95220 46.05166 46.90242 63.30827 41.82571 56.75893
##
    [33] 47.84519 48.85350 47.97735 54.06493 56.56772 51.06191 48.15603 59.46034
##
##
    [41] 52.02387 54.95101 44.30645 61.19294 72.09078 53.17183 40.64703 58.13662
    [49] 46.24635 53.33100 55.94415 55.20868 40.47956 37.72315 47.97593 60.59120
##
    [57] 53.81779 62.39694 53.16777 39.56622 38.51764 62.31145 57.89215 57.48845
   [65] 50.57476 58.42951 51.99859 64.51171 45.39840 22.25533 50.56489 49.38629
##
    [73] 38.18032 24.70833 58.13577 52.62389 49.37494 56.71735 50.27176 55.35603
##
   [81] 56.89548 38.00871 37.60845 52.13186 35.42848 48.74239 55.44208 57.20830
##
   [89] 34.28810 60.97272 46.67537 56.16393 55.08799 66.86555 53.79547 52.35471
   [97] 54.24988 38.15064 43.56390 50.52614
```

Plots

Stem-and-leaf

Let's make a Simple stem-and-leaf plot. Here, we call the stem() function as follows:

```
stem(norm_vals)
```

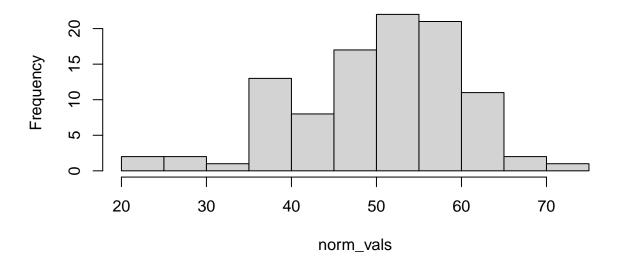
```
##
     The decimal point is 1 digit(s) to the right of the |
##
##
##
     2 | 2
     2 | 58
##
     3 | 04
##
##
     3 | 567888888889
##
     4 | 001233344
     4 | 5666778888889999
##
         0001111222223333444444
##
##
     5 | 555555666777777788889
##
     6 | 11112234
     6 | 55567
##
##
     7 | 2
```

We can plot a histogram of these norm_vals in order to inspect their distribution from a purely graphical standpoint. R uses the built-in hist() function to accomplish this task. Let us now plot the histogram.

Histograms

```
hist(norm_vals)
```

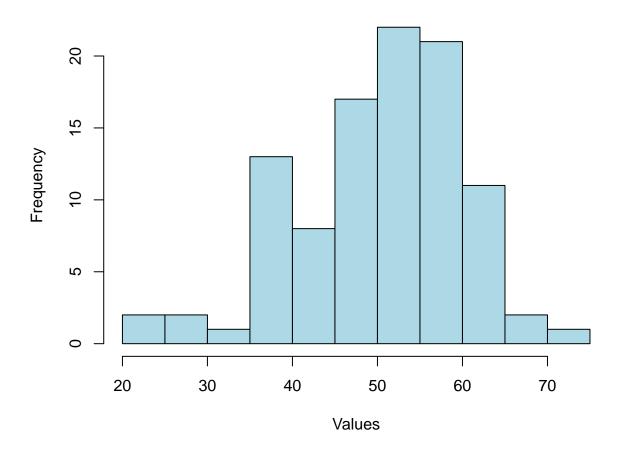
Histogram of norm_vals



Our title, x-axis, and y-axis labels are given to us by default. However, let us say that we want to change all of them to our desired specifications. To this end, we can parse in and control the following parameters:

```
hist(norm_vals,
    col = 'lightblue', # specify the color
    xlab = 'Values', # specify the x-axis label
    ylab = 'Frequency', # specify the y-axis label
    main = 'Histogram of Simulated Data', # specify the new title
)
```

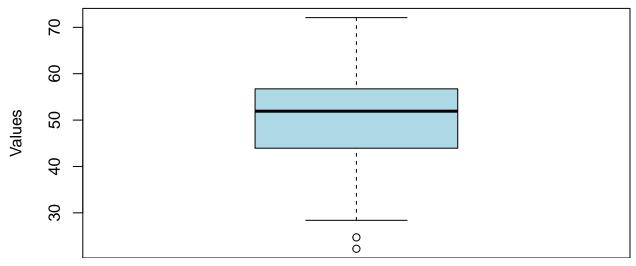
Histogram of Simulated Data



Boxplots

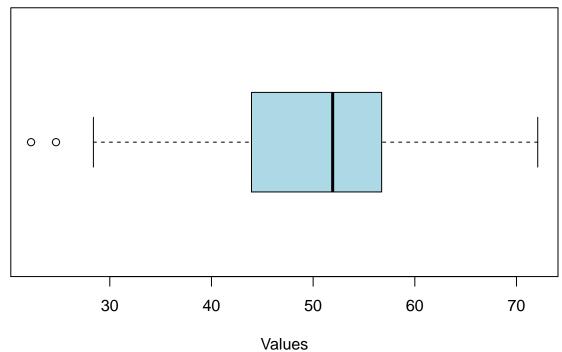
Similarly, we can make a boxplot in base R using the boxplot() function call as follows:





Now, let us pivot the boxplot by parsing in the horizontal = TRUE parameter:

Boxplot of Simulated Data

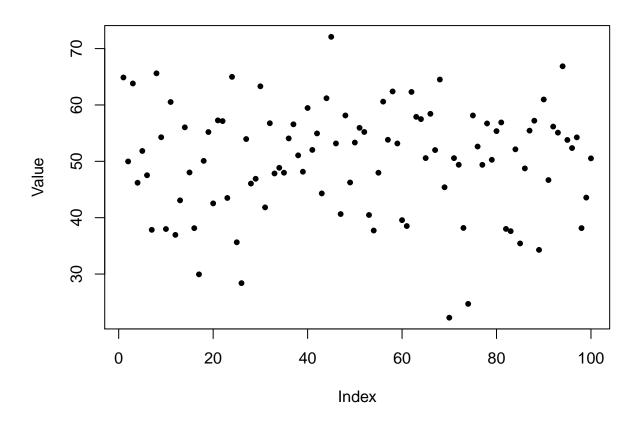


Scatter Plots

To make a simple scatter plot, we will simply call the plot() function on the same dataframe as follows:

```
plot(norm_vals,
    main = 'Scatter Plot of Simulated Data',
    pch = 20, # plot character - in this case default (circle)
    xlab = 'Index',
    ylab = 'Value')
```

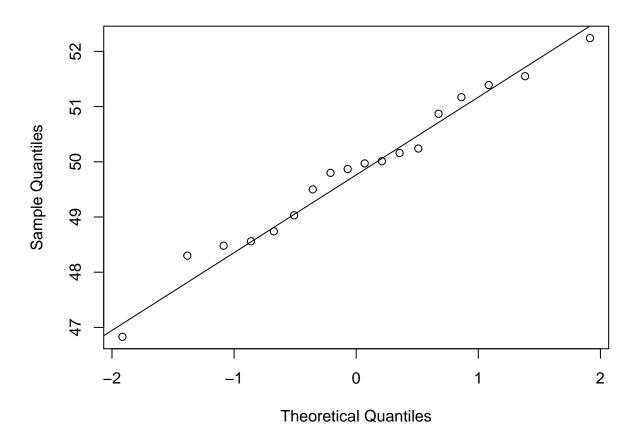
Scatter Plot of Simulated Data



Quantile-Quantile Plot

Let us create a vector for the next example data and generate a normal quantile plot.

Normal Q-Q Plot



Skewness and Box-Cox Transformation

[1] -0.497993

From statistics, let us recall that if the mean is greater than the median, the distribution will be positively skewed. Conversely, if the median is greater than the mean, or the mean is less than the median, the distribution will be negatively skewed. Let us examine the exact skewness of our distribution.

```
# Applying Box-Cox Transformation on skewed variable
library(caret)
trans <- preProcess(data.frame(norm_vals), method=c("BoxCox"))
trans

## Created from 100 samples and 1 variables
##
## Pre-processing:
## - Box-Cox transformation (1)
## - ignored (0)
##
## Lambda estimates for Box-Cox transformation:
## 1.8</pre>
```

Basic Modeling

Linear Regression

Let us set up an example dataset for the following modeling endeavors.

```
# independent variables (x's):

# X1

Hydrogen <- c(.18,.20,.21,.21,.21,.22,.23,.23,.24,.24,.25,.28,.30,.37,.31,.90,.81,.41,.74,.42,.37,.49,.07,.94,.47,.35,.83,.61,.30,.61,.54)

# X2

Oxygen <- c(.55,.77,.40,.45,.62,.78,.24,.47,.15,.70,.99,.62,.55,.88,.49,.36,.55,.42,.39,.74,.50,.17,.18,.94,.97,.29,.85,.17,.33,.29,.85)

# X3

Nitrogen <- c(.35,.48,.31,.75,.32,.56,.06,.46,.79,.88,.66,.04,.44,.61,.15,.48,.23,.90,.26,.41,.76,.30,.56,.73,.10,.01,.05,.34,.27,.42,.83)

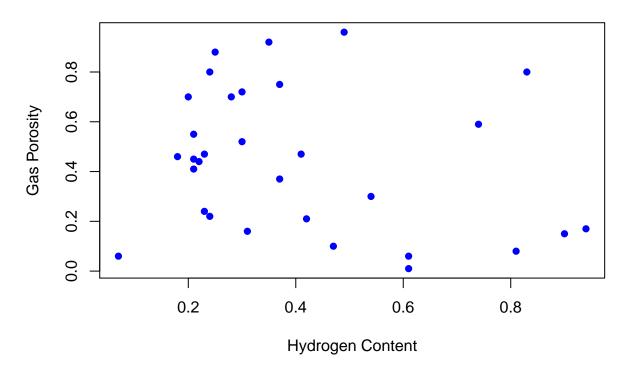
# there is always one dependent variable (target, response, y)

Gas_Porosity <- c(.46,.70,.41,.45,.55,.44,.24,.47,.22,.80,.88,.70,.72,.75,.16,.15,.08,.47,.59,.21,.37,.96,.06,.17,.10,.92,.80,.06,.52,.01,.3)
```

Simple Linear Regression

Prior to partaking in linear regression, it is best practice to examine correlation from a strictly visual perspective visa vie scatterplot as follows:

Scatter Plot - Gas Porosity vs. Hydrogen Content



Now, let's find the correlation coefficient, r.

```
r1 <- cor(Hydrogen, Gas_Porosity)
r1</pre>
```

[1] -0.2424314

Now we can set-up the linear model between one independent variable and one dependent variable.

```
simple_linear_mod <- data.frame(Hydrogen, Gas_Porosity)</pre>
```

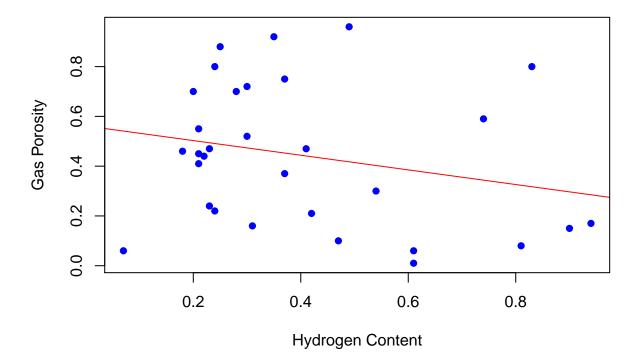
By the correlation coefficient r you will see that there exists a relatively moderate (positive) relationship. Let us now build a simple linear model from this dataframe.

```
lm_model1 <- lm(Gas_Porosity ~ Hydrogen, data = simple_linear_mod)
summary(lm_model1)</pre>
```

```
##
## Coefficients:
##
              Estimate Std. Error t value Pr(>|t|)
                            0.1018
                                     5.516 6.06e-06 ***
                0.5616
## (Intercept)
## Hydrogen
                -0.2943
                            0.2187
                                   -1.346
##
## Signif. codes:
                  0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
## Residual standard error: 0.2807 on 29 degrees of freedom
## Multiple R-squared: 0.05877,
                                    Adjusted R-squared:
## F-statistic: 1.811 on 1 and 29 DF, p-value: 0.1888
```

Notice how the p-value for hydrogen content is 0.189, which lacks statistical significance when compared to the alpha value of 0.05 (at the 95% confidence level). Moreover, the R-Squared value of .05877 suggests that roughly 6% of the variance for gas propensity is explained by hydrogen content.

Scatter Plot – Gas Porosity vs. Hydrogen Content



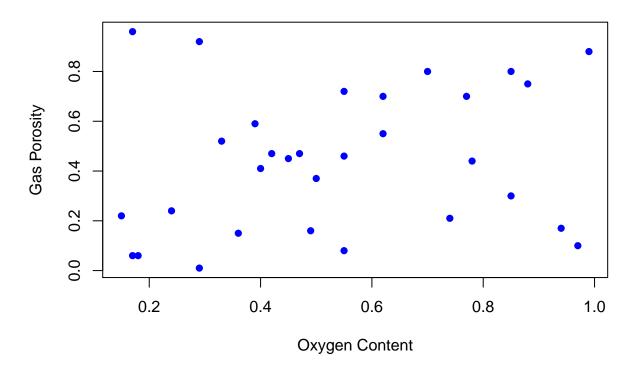
Multiple Linear Regression

To account for all independent (x) variables in the model, let us set up the model in a dataframe:

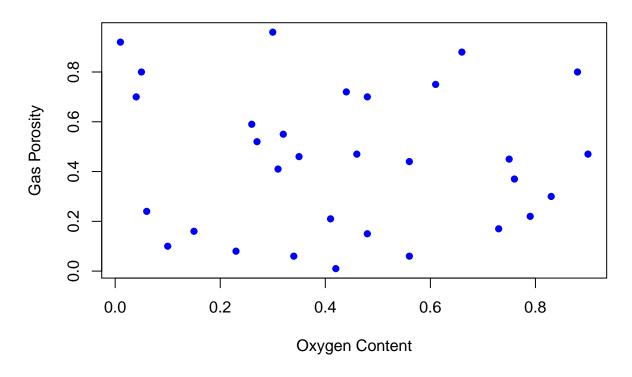
```
multiple_linear_mod <- data.frame(Hydrogen, Oxygen, Nitrogen, Gas_Porosity)</pre>
```

We can make additional scatter plots:

Scatter Plot - Gas Porosity vs. Oxygen Content



Scatter Plot - Gas Porosity vs. Oxygen Content



and lastly, we can build a multiple linear model from these 3 independent variables:

```
##
## lm(formula = Gas_Porosity ~ Hydrogen + Oxygen + Nitrogen, data = multiple_linear_mod)
## Residuals:
##
       Min
                  1Q
                       Median
                                    3Q
                                            Max
  -0.49593 -0.18800 -0.02835 0.17512
##
## Coefficients:
               Estimate Std. Error t value Pr(>|t|)
##
## (Intercept)
                 0.4853
                            0.1605
                                     3.024
                                           0.00542 **
                -0.3536
                            0.2210
                                    -1.600
                                           0.12122
## Hydrogen
## Oxygen
                 0.2998
                            0.2036
                                     1.473
                                           0.15241
## Nitrogen
                            0.1970
                                   -0.708
                -0.1395
                                           0.48496
## Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
## Residual standard error: 0.2788 on 27 degrees of freedom
## Multiple R-squared: 0.1352, Adjusted R-squared: 0.03906
## F-statistic: 1.407 on 3 and 27 DF, p-value: 0.2624
```

Logistic Regression

Whereas in linear regression, it is necessary to have a quantitative and continuous target variable, logistic regression is part of the generalized linear model series that has a categorical (often binary) target (outcome) variable. For example, let us say we want to predict grades for mathematics courses taught at a university.

So, we have the following example dataset:

At this juncture, we cannot build a model with categorical values until and unless they are binarized using the ifelse() function call as follows. A passing score will be designated by a 1, and failing score with a respectively.

```
math_outcome <- ifelse(pass_fail=='P', 1, 0)
math_outcome</pre>
```

```
## 'data.frame': 31 obs. of 5 variables:
## $ calculus1 : num 56 80 10 8 20 90 38 42 57 58 ...
## $ calculus2 : num 83 98 50 16 70 31 90 48 67 78 ...
## $ linear_alg : num 87 90 85 57 30 78 75 69 83 85 ...
## $ pass_fail : chr "P" "F" "P" "F" ...
## $ math_outcome: num 1 0 1 0 1 1 1 1 0 1 ...
```

We can also specify glm instead of just lm as in linear regression example:

```
lm_model3 <- glm(math_outcome ~ calculus1 +</pre>
                                calculus2 +
                                linear_alg,
                 family = binomial(),
                 data = logistic_model)
summary(lm_model3)
##
## Call:
## glm(formula = math_outcome ~ calculus1 + calculus2 + linear_alg,
       family = binomial(), data = logistic_model)
##
## Deviance Residuals:
       Min
                 1Q
                     Median
                                   3Q
                                           Max
## -1.8114 0.5365
                      0.6425
                                         0.8988
                               0.7439
##
## Coefficients:
                Estimate Std. Error z value Pr(>|z|)
## (Intercept) 1.132509
                           1.278396
                                      0.886
                                                0.376
                                                0.518
## calculus1
               -0.010621
                           0.016416
                                     -0.647
                                      0.347
                                                0.728
## calculus2
                0.006131
                           0.017653
## linear_alg
                0.004902
                           0.014960
                                      0.328
                                                0.743
##
## (Dispersion parameter for binomial family taken to be 1)
##
       Null deviance: 33.118 on 30
                                     degrees of freedom
## Residual deviance: 32.589 on 27 degrees of freedom
## AIC: 40.589
## Number of Fisher Scoring iterations: 4
```

Decision Trees

\$ disp: num 160 160 108 258 360 ...

\$ hp : num 110 110 93 110 175 105 245 62 95 123 ...

Decision trees are valuable supplementary methods for tracing consequential outcomes diagrammatically.

We can plot the trajectory of the outcome using the rpart() function of the library(rpart) and library(rpart.plot), respectively.

```
library(rpart)
library(rpart.plot)
```

In favor of a larger dataset to illustrate the structure, function, and overall efficacy of decision trees in R, we will rely on the built-in mtcars dataset.

```
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 ...
```

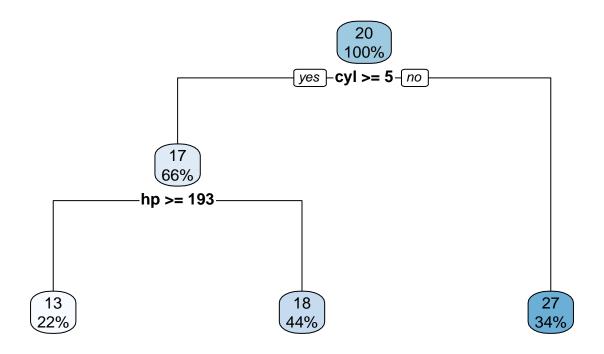
```
## $ drat: num 3.9 3.9 3.85 3.08 3.15 2.76 3.21 3.69 3.92 3.92 ...
## $ wt : num 2.62 2.88 2.32 3.21 3.44 ...
## $ qsec: num 16.5 17 18.6 19.4 17 ...
## $ vs : num 0 0 1 1 0 1 0 1 1 1 ...
## $ am : num 1 1 1 0 0 0 0 0 0 0 ...
## $ gear: num 4 4 4 3 3 3 3 3 4 4 4 ...
## $ carb: num 4 4 1 1 2 1 4 2 2 4 ...
```

mtcars

```
mpg cyl disp hp drat
                                                 wt qsec vs am gear carb
                      21.0
## Mazda RX4
                              6 160.0 110 3.90 2.620 16.46
## Mazda RX4 Wag
                              6 160.0 110 3.90 2.875 17.02
                      21.0
                      22.8
## Datsun 710
                             4 108.0 93 3.85 2.320 18.61
                                                                         1
                                                            1
                              6 258.0 110 3.08 3.215 19.44
## Hornet 4 Drive
                      21.4
                                                            1
                                                               0
                                                                         1
                      18.7
                             8 360.0 175 3.15 3.440 17.02
                                                                   3
                                                                         2
## Hornet Sportabout
                                                               0
## Valiant
                      18.1
                              6 225.0 105 2.76 3.460 20.22
                                                               0
                                                            1
                                                                         1
## Duster 360
                      14.3
                             8 360.0 245 3.21 3.570 15.84
                                                            0
                                                               0
                                                                   3
## Merc 240D
                      24.4
                              4 146.7
                                      62 3.69 3.190 20.00
                                                                   4
                                                                         2
                                                            1
                                                              0
## Merc 230
                      22.8
                              4 140.8 95 3.92 3.150 22.90
## Merc 280
                      19.2
                              6 167.6 123 3.92 3.440 18.30
                                                              0
                                                                         4
## Merc 280C
                      17.8
                              6 167.6 123 3.92 3.440 18.90
                                                               0
                                                                   4
                                                                         4
## Merc 450SE
                      16.4
                             8 275.8 180 3.07 4.070 17.40
                                                                   3
                                                                         3
                                                            0
                                                              0
## Merc 450SL
                      17.3
                             8 275.8 180 3.07 3.730 17.60
                                                              0
## Merc 450SLC
                      15.2
                             8 275.8 180 3.07 3.780 18.00
                                                            0
                                                              Ω
                                                                   3
                                                                         3
## Cadillac Fleetwood 10.4
                             8 472.0 205 2.93 5.250 17.98
                                                            0
                                                               0
                                                                   3
                                                                         4
## Lincoln Continental 10.4
                             8 460.0 215 3.00 5.424 17.82
                                                                   3
                                                                         4
                                                              Ω
                             8 440.0 230 3.23 5.345 17.42
## Chrysler Imperial 14.7
## Fiat 128
                              4 78.7 66 4.08 2.200 19.47
                                                                   4
                      32.4
                                                            1
                                                              1
                                                                         1
## Honda Civic
                      30.4
                                75.7 52 4.93 1.615 18.52
                                                            1
                                                                   4
                                                                         2
                      33.9
                                                                   4
## Toyota Corolla
                             4 71.1 65 4.22 1.835 19.90
                                                              1
                                                                         1
## Toyota Corona
                      21.5
                              4 120.1 97 3.70 2.465 20.01
                                                                         1
## Dodge Challenger
                      15.5
                              8 318.0 150 2.76 3.520 16.87
                                                            0
                                                                   3
                                                                         2
                                                              0
## AMC Javelin
                      15.2
                              8 304.0 150 3.15 3.435 17.30
                                                            0
                                                               0
                                                                   3
                                                                         2
## Camaro Z28
                      13.3
                             8 350.0 245 3.73 3.840 15.41
                                                                   3
                                                                         4
## Pontiac Firebird
                      19.2
                             8 400.0 175 3.08 3.845 17.05
                                                                   3
                                                                         2
                                                            0
                                                              0
## Fiat X1-9
                      27.3
                             4 79.0 66 4.08 1.935 18.90
                                                            1
                                                                   4
                                                                         1
## Porsche 914-2
                      26.0
                             4 120.3 91 4.43 2.140 16.70
                                                            0
                                                                   5
                                                                         2
                                                              1
                                                                   5
                                                                         2
## Lotus Europa
                      30.4
                             4 95.1 113 3.77 1.513 16.90
## Ford Pantera L
                             8 351.0 264 4.22 3.170 14.50 0 1
                                                                   5
                                                                         4
                      15.8
                              6 145.0 175 3.62 2.770 15.50
## Ferrari Dino
                      19.7
                                                            0 1
                                                                   5
                                                                         6
                             8 301.0 335 3.54 3.570 14.60
                                                                   5
                                                                        8
## Maserati Bora
                      15.0
                                                            Λ
                                                             1
## Volvo 142E
                      21.4
                              4 121.0 109 4.11 2.780 18.60 1 1
                                                                         2
```

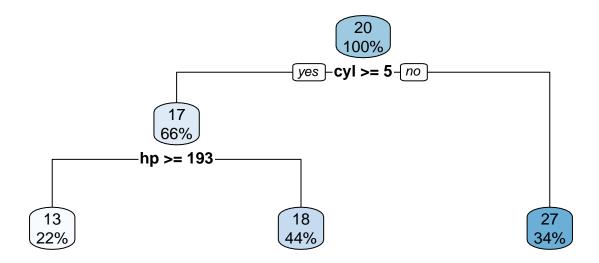
So we introduce the model as follows:

Cars: Classification Tree



Passing in a `type=1,2,3,4, or 5` value changes the appearance of the tree
rpart.plot(tree_model, main = 'Cars: Classification Tree', type=2)

Cars: Classification Tree



Basic Modeling with Cross-Validation in R

We use cross-validation as a "a statistical approach for determining how well the results of a statistical investigation generalize to a different data set" (finnstats, 2021). The library(caret) will help us in this endeavor.

Train_Test_Split

```
set.seed(222) # for reproducibility
dt <- sort(sample(nrow(mtcars), nrow(mtcars)*.75))</pre>
train cars <-mtcars[dt,]</pre>
test_cars <-mtcars[-dt,]</pre>
# check size dimensions of respective partitions
n_train <- nrow(train_cars)[1]</pre>
n_test <- nrow(test_cars)[1]</pre>
train_size = n_train/(n_train+n_test)
test_size = n_test/(n_train+n_test)
cat('\n Train Size:', train_size,
    '\n Test Size:', test_size)
##
##
    Train Size: 0.75
    Test Size: 0.25
Let us bring in a generalized linear model for this illustration.
cars_model <- glm(mpg ~., data = mtcars)</pre>
cars_predictions <- predict(cars_model, test_cars)</pre>
# computing model performance metrics
data.frame(R2 = R2(cars_predictions, test_cars$mpg),
           RMSE = RMSE(cars_predictions, test_cars$mpg),
           MAE = MAE(cars_predictions, test_cars$mpg))
```

```
## R2 RMSE MAE
## 1 0.9149732 1.72719 1.400446
```

In order to use the trainControl() function for cross-validation, we will bring in the library(caret).

```
library(caret)
```

```
## Generalized Linear Model
##
## 32 samples
## 10 predictors
## No pre-processing
## Resampling: Cross-Validated (5 fold)
## Summary of sample sizes: 24, 26, 25, 26, 27
## Resampling results:
##
##
     RMSE
              Rsquared
                          MAE
                         2.587204
##
     3.12627
              0.8167969
```

K-Means Clustering

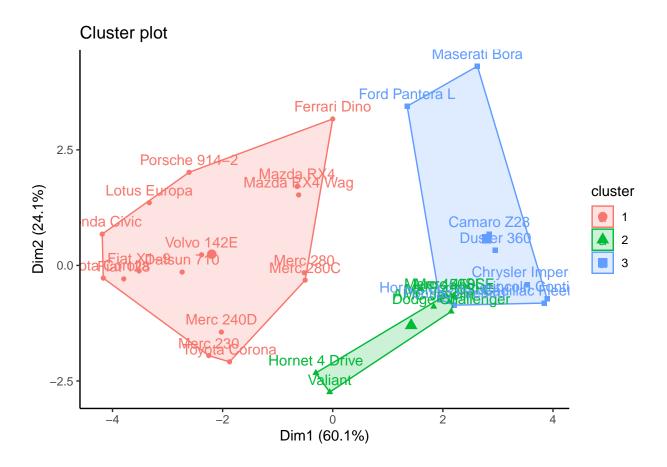
A cluster is a collection of observations. We want to group these observations based on the most similar attributes. We use distance measures to measure similarity between clusters.

This is one of the most widely-used unsupervised learning techniques that groups "similar data points together and discover underlying patterns. To achieve this objective, K-means looks for a fixed number (k) of clusters in a dataset" (Garbade, 2018).

```
## K-means clustering with 3 clusters of sizes 16, 7, 9
## Cluster means:
##
                   cyl
                            disp
                                       hp
                                               drat
          mpg
                                                          wt
                                                                 asec
                                                                              VS
## 1 24.50000 4.625000 122.2937 96.8750 4.002500 2.518000 18.54312 0.7500000
## 2 17.01429 7.428571 276.0571 150.7143 2.994286 3.601429 18.11857 0.2857143
## 3 14.64444 8.000000 388.2222 232.1111 3.343333 4.161556 16.40444 0.0000000
                   gear
##
            am
## 1 0.6875000 4.125000 2.437500
## 2 0.0000000 3.000000 2.142857
## 3 0.2222222 3.444444 4.000000
##
##
  Clustering vector:
##
             Mazda RX4
                              Mazda RX4 Wag
                                                      Datsun 710
                                                                       Hornet 4 Drive
##
                      1
##
     Hornet Sportabout
                                    Valiant
                                                      Duster 360
                                                                            Merc 240D
##
                                                               3
##
              Merc 230
                                   Merc 280
                                                       Merc 280C
                                                                           Merc 450SE
##
                      1
##
            Merc 450SL
                                Merc 450SLC
                                             Cadillac Fleetwood Lincoln Continental
##
                                          2
                      2
```

```
Chrysler Imperial
                                    Fiat 128
                                                      Honda Civic
                                                                        Toyota Corolla
##
##
         Toyota Corona
                                                      AMC Javelin
##
                           Dodge Challenger
                                                                            Camaro Z28
##
                                                                                     3
      Pontiac Firebird
##
                                  Fiat X1-9
                                                   Porsche 914-2
                                                                          Lotus Europa
##
##
        Ford Pantera L
                               Ferrari Dino
                                                   Maserati Bora
                                                                            Volvo 142E
##
##
   Within cluster sum of squares by cluster:
##
   [1] 32838.00 11846.09 46659.32
    (between_SS / total_SS = 85.3 %)
##
##
##
  Available components:
##
## [1] "cluster"
                       "centers"
                                       "totss"
                                                       "withinss"
                                                                       "tot.withinss"
   [6] "betweenss"
                       "size"
                                       "iter"
                                                       "ifault"
```

Now let's visualize the cluster using the fviz_cluster() function from the factoextra library.



But what is the appropriate number of clusters that we should generate? Can we do better with more clusters?

```
# total sum of squares
kmeans_cars$totss

## [1] 623387.5

# between sum of squares
kmeans_cars$betweenss

## [1] 532044.1

# within sum of squares
kmeans_cars$withinss

## [1] 32838.00 11846.09 46659.32

# ratio for between sum of squares/ total sum of squares
kmeans_cars$betweenss/kmeans_cars$totss

## [1] 0.8534725
```

Let's create a numeric vector populated with zeroes and ten spots long.

```
wss <- numeric(10)
```

Can we do better? Let's run k-means from 1:10 clusters.

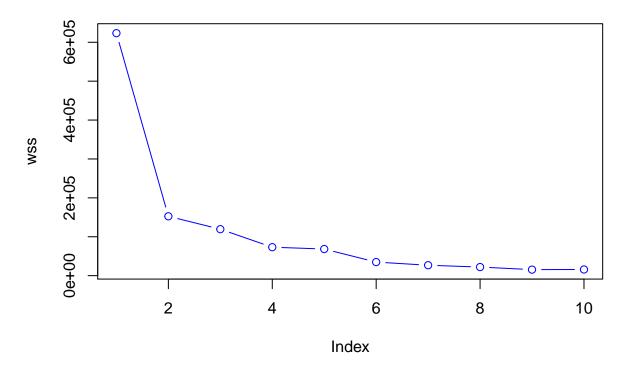
This will effectively measure the homogeneity of the clusters as the number of clusters increases.

Now let us use a basic for-loop to run through k-means 10 times. K-means is iterated through each of these 10 clusters as follows:

Basic Elbow Method

Now let's plot these within sum of squares using the elbow method, which is one of the most commonly used approaches for finding the optimal k.

Elbow Method for K-Means



Once we start to add clusters, the within sum of squares is reduced. Thus, the incremental reduction in within sum of squares is getting progressively smaller. We see that after approximately k = 3, each of the new clusters is not separating the data as well.

Hierarchical Clustering

This is another form of unsupervised learning type of cluster analysis, which takes on a more visual method, working particularly well with smaller samples (i.e., n < 500), such as this mtcars dataset. We start out with as many clusters as observations, and we go through a procedure of combining observations into clusters, and culminating with combining clusters together as a reduction method for the total number of clusters that are present. Moreover, the premise for combining clusters together is a direct result of:

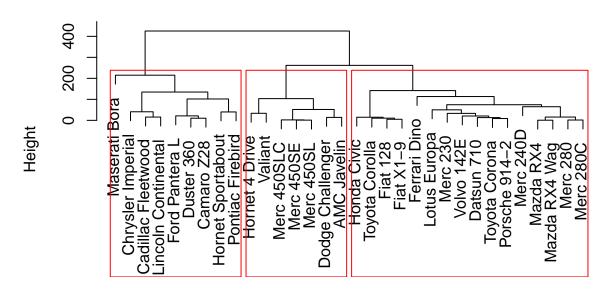
complete linkage - or largest Euclidean distance between clusters.
single linkage - conversely, we look at the observations which are closest together (proximity).
centroid linkage - we can the distance between the centroid of each cluster.
group average (mean) linkage - taking the mean between the pairwise distances of the observations.

Complete linkage is the most traditional approach.

The tree structure that examines this hierarchical structure is called a dendogram.

```
# plot the hierarchical cluster
plot(auto_cluster)
rect.hclust(auto_cluster, k = 3, border = 'red') # visualize cluster borders
```

Cluster Dendrogram



auto_dist hclust (*, "complete")

Our dendogram indicates which observation is within which cluster.

We can cut our tree at let's say 3 clusters, segmenting them out as follows:

```
cut_tree <- cutree(auto_cluster, 3) # each obs. now belongs to cluster 1,2, or 3
mtcars$segment <- cut_tree # segment out the data</pre>
```

Now we can view our segmented data in the workspace window as follows:

```
View(mtcars)
```

Or see it as a dataframe, per usual:

```
print(mtcars)
```

```
##
                                                  wt qsec vs am gear carb segment
                        mpg cyl disp hp drat
## Mazda RX4
                              6 160.0 110 3.90 2.620 16.46
                       21.0
                                                                         4
## Mazda RX4 Wag
                       21.0
                              6 160.0 110 3.90 2.875 17.02
                                                                                 1
## Datsun 710
                       22.8
                              4 108.0 93 3.85 2.320 18.61
                                                                                 1
## Hornet 4 Drive
                              6 258.0 110 3.08 3.215 19.44
                       21.4
```

```
## Hornet Sportabout
                         18.7
                                8 360.0 175 3.15 3.440 17.02
                                                                          3
                                                                               2
                                                                                        3
                                6 225.0 105 2.76 3.460 20.22
                                                                         3
                                                                               1
                                                                                        2
## Valiant
                         18.1
                                                                 1
                                                                    0
## Duster 360
                         14.3
                                8 360.0 245 3.21 3.570 15.84
                                                                          3
                                                                               4
                                                                                        3
## Merc 240D
                         24.4
                                4 146.7
                                          62 3.69 3.190 20.00
                                                                          4
                                                                               2
                                                                                        1
                                                                 1
                                                                    0
## Merc 230
                         22.8
                                4 140.8
                                          95 3.92 3.150 22.90
                                                                 1
                                                                    0
                                                                          4
                                                                               2
                                                                                        1
                                6 167.6 123 3.92 3.440 18.30
                                                                          4
                                                                               4
## Merc 280
                         19.2
                                                                    0
                                                                                        1
                                                                 1
## Merc 280C
                         17.8
                                6 167.6 123 3.92 3.440 18.90
                                                                          4
                                                                               4
                                                                                        1
                                                                                        2
## Merc 450SE
                         16.4
                                8 275.8 180 3.07 4.070 17.40
                                                                 0
                                                                    0
                                                                          3
                                                                               3
## Merc 450SL
                         17.3
                                8 275.8 180 3.07 3.730 17.60
                                                                 0
                                                                    0
                                                                          3
                                                                               3
                                                                                        2
                                                                          3
                                                                                        2
## Merc 450SLC
                         15.2
                                8 275.8 180 3.07 3.780 18.00
                                                                 0
                                                                    0
                                                                               3
## Cadillac Fleetwood
                        10.4
                                8 472.0 205 2.93 5.250 17.98
                                                                 0
                                                                          3
                                                                               4
                                                                                        3
                                                                                        3
                                8 460.0 215 3.00 5.424 17.82
                                                                          3
                                                                               4
## Lincoln Continental 10.4
                                                                 0
                                                                    0
## Chrysler Imperial
                         14.7
                                8 440.0 230 3.23 5.345 17.42
                                                                 0
                                                                    0
                                                                          3
                                                                               4
                                                                                        3
## Fiat 128
                         32.4
                                   78.7
                                          66 4.08 2.200 19.47
                                                                          4
                                                                               1
                                                                                        1
                         30.4
                                                                          4
                                                                               2
## Honda Civic
                                4
                                   75.7
                                          52 4.93 1.615 18.52
                                                                 1
                                                                    1
                                                                                        1
## Toyota Corolla
                         33.9
                                4
                                   71.1
                                          65 4.22 1.835 19.90
                                                                          4
                                                                               1
                                                                                        1
                                                                          3
## Toyota Corona
                         21.5
                                4 120.1
                                          97 3.70 2.465 20.01
                                                                    0
                                                                               1
                                                                                        1
                                                                 1
                                                                                        2
## Dodge Challenger
                         15.5
                                8 318.0 150 2.76 3.520 16.87
                                                                          3
                                                                               2
                                                                         3
                                                                               2
                                                                                        2
## AMC Javelin
                         15.2
                                8 304.0 150 3.15 3.435 17.30
                                                                 0
                                                                    0
                                                                                        3
## Camaro Z28
                         13.3
                                8 350.0 245 3.73 3.840 15.41
                                                                 0
                                                                          3
                                                                               4
## Pontiac Firebird
                         19.2
                                8 400.0 175 3.08 3.845 17.05
                                                                 0
                                                                    0
                                                                         3
                                                                               2
                                                                                        3
## Fiat X1-9
                                  79.0
                                          66 4.08 1.935 18.90
                                                                          4
                         27.3
                                                                               1
                                                                                        1
                                         91 4.43 2.140 16.70
                                                                               2
## Porsche 914-2
                         26.0
                                4 120.3
                                                                 0
                                                                         5
                                                                                        1
                                                                    1
                                   95.1 113 3.77 1.513 16.90
                                                                          5
                                                                               2
## Lotus Europa
                        30.4
                                                                 1
                                                                    1
                                                                                        1
                                                                                        3
## Ford Pantera L
                        15.8
                                8 351.0 264 4.22 3.170 14.50
                                                                    1
                                                                          5
                                                                               4
## Ferrari Dino
                         19.7
                                6 145.0 175 3.62 2.770 15.50
                                                                 0
                                                                    1
                                                                          5
                                                                               6
                                                                                        1
                                8 301.0 335 3.54 3.570 14.60
                                                                          5
                                                                               8
                                                                                        3
## Maserati Bora
                        15.0
                                                                 0
                                                                    1
                                4 121.0 109 4.11 2.780 18.60
                                                                               2
## Volvo 142E
                         21.4
                                                                                        1
```

Sources

finnstats. (2021, October 31). What Does Cross Validation Mean? *R-bloggers*. https://www.r-bloggers.com/2021/10/cross-validation-in-r-with-example/

Garbade, Michael. (2018, September 12). Understanding K-means Clustering in Machine Learning. *Towards Data Science*.

GeeksforGeeks. (2020, April 22). Scope of Variable in R. GeeksforGeeks.

https://www.geeksforgeeks.org/scope-of-variable-in-r/

Shmueli, G., Bruce, P. C., Yahav, I., Patel, N. R., & Lichtendahl Jr., K. C. (2018).

Data mining for business analytics: Concepts, techniques, and applications in R. Wiley.