

CW4

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Problem 2: Practical (20 marks)

```
library(readr)
moons_data <- read_csv("C:/Users/tanwe/OneDrive/Documents/Stats_Machine_Learning/CW4/moons.csv")

## Rows: 300 Columns: 2
## -- Column specification -----
## Delimiter: ","
## dbl (2): X, Y
##
## i Use 'spec()' to retrieve the full column specification for this data.
## i Specify the column types or set 'show_col_types = FALSE' to quiet this message.

colnames(moons_data)

## [1] "X" "Y"

head(moons_data)

## # A tibble: 6 x 2
##       X       Y
##   <dbl> <dbl>
## 1 -0.277  0.474
## 2 -1.11  -0.627
## 3  1.23  -0.0580
## 4  0.601  0.0766
## 5 -0.246  0.317
## 6 -0.408  0.287
```

- (i) **{10 marks}** Load in `$ moons.csv $`, and use the native `$ kmeans $` function in *R* to cluster the data into $K = \{2, 3, 4, 5\}$ components, according to each of the following loss functions :

```
#Loading necessary libraries
library(ggplot2)
library(gridExtra)
```

```
## Warning: package 'gridExtra' was built under R version 4.4.3
```

```

set.seed(420)

#Define K values
K_values <- c(2,3,4,5)

#Seperate Data
X_1 <- moons_data[,1]

#List to store plots
plots_list <- list()

#Loooping through each value
for (k in K_values){
  #Apply K-Means Clustering Algorithm
  result <- kmeans(X_1, centers=k, nstart=50)

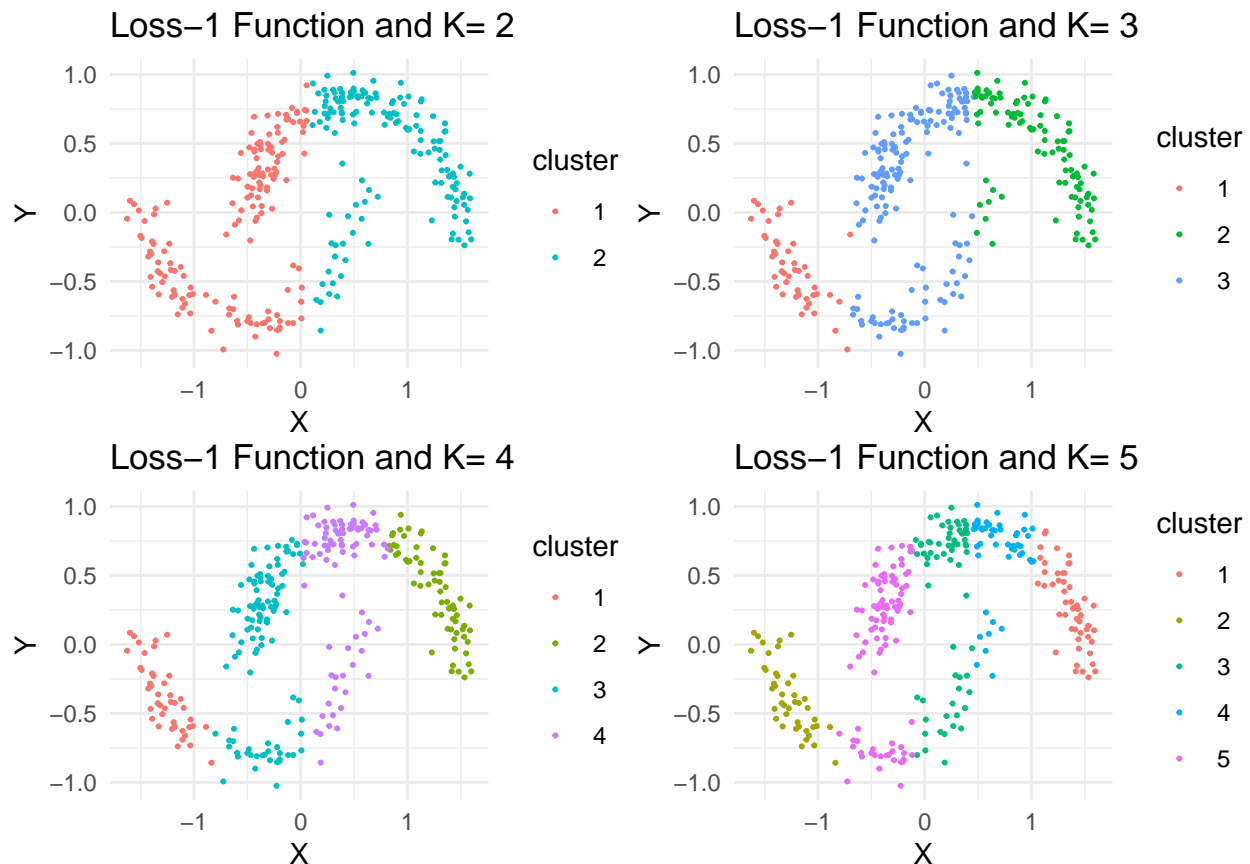
  #Store cluster assignments
  moons_data$cluster <- as.factor(result$cluster)

  #Scatter Plot for each K-value
  plot <- ggplot(moons_data, aes(x= X, y= Y, color=cluster))+
    geom_point(size=0.4) +
    ggtitle(paste("Loss-1 Function and K=",k)) +
    labs(x = "X", y= "Y") +
    theme_minimal() +
    theme(plot.margin = margin(1, 1, 1, 1, "pt"))

  #Store plot in the list
  plots_list[[length(plots_list) + 1]] <- plot
}

grid.arrange(grobs = plots_list, nrow = 2, ncol = 2, widths = c(3,3), height = c(3,3))

```



Now, using the Loss-2 Function:

```
#Seperate Data
X_2 <- moons_data[,2]

#List to store plots
plots_list <- list()

#Define K values
K_values <- c(2,3,4,5)

#Looping through each value
for (k in K_values){
  #Apply K-Means Clustering algorithm
  result <- kmeans(X_2, centers=k, nstart=50)

  #Store cluster assignments
  moons_data$cluster <- as.factor(result$cluster)

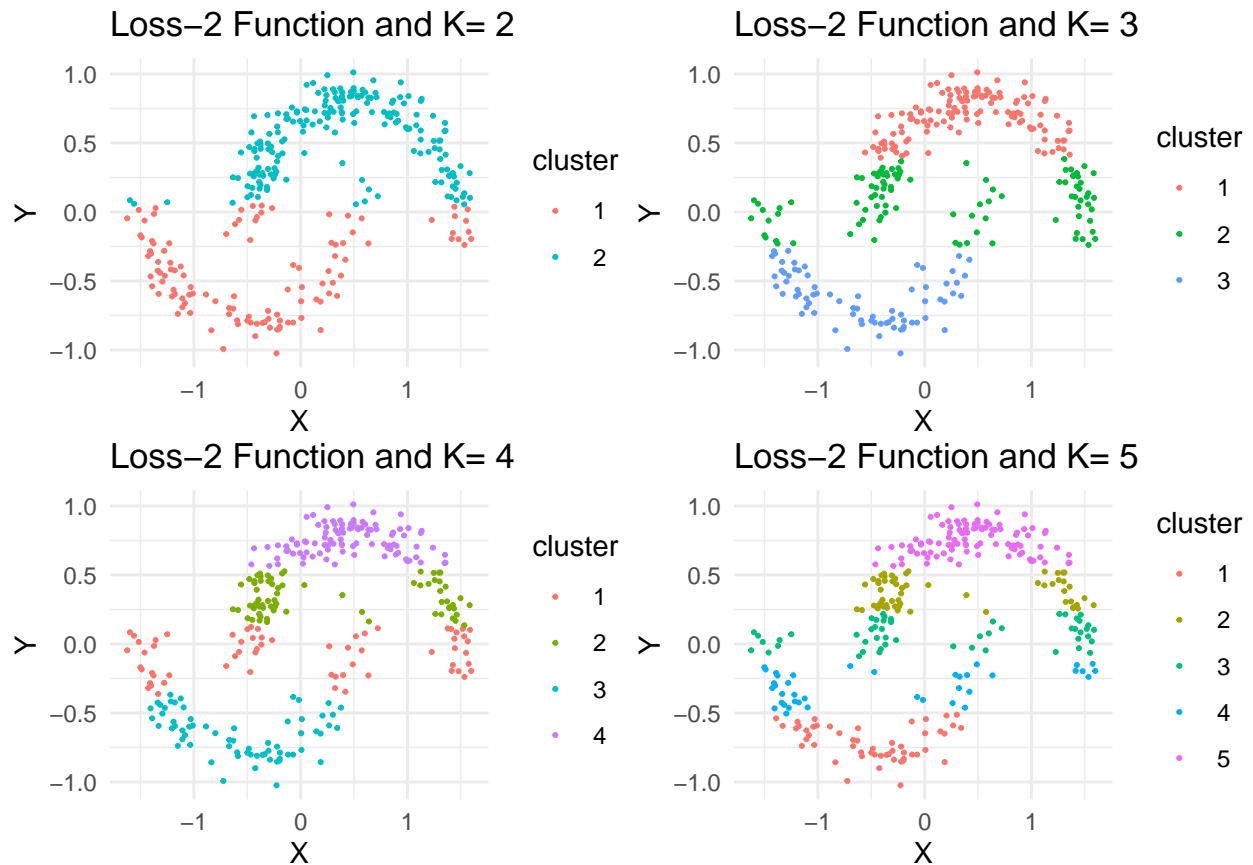
  #Scatter Plot for each K-value
  plot <- ggplot(moons_data, aes(x= X, y= Y, color=cluster))+
    geom_point(size=0.4) +
    ggtitle(paste("Loss-2 Function and K=",k)) +
    labs(x = "X", y= "Y") +
    theme_minimal() +
    theme(plot.margin = margin(1, 1, 1, 1, "pt"))
}
```

```

#Store plot in the list
plots_list[[length(plots_list) + 1]] <- plot
}

grid.arrange(grobs = plots_list, nrow = 2, ncol = 2, widths = c(3,3), height = c(3,3))

```



Now, using the Loss-3 Function, where the full feature vector is utilised:

```

#List to store plots
plots_list <- list()

#Define K values
K_values <- c(2,3,4,5)

#Looping through each value
for (k in K_values){
  #Apply K-Means Clustering Algorithm
  result <- kmeans(moons_data, centers=k, nstart=50)

  #Store cluster assignments
  moons_data$cluster <- as.factor(result$cluster)

  #Scatter Plot for each K-value
  plot <- ggplot(moons_data, aes(x= X, y= Y, color=cluster))+
    geom_point(size=0.4) +

```

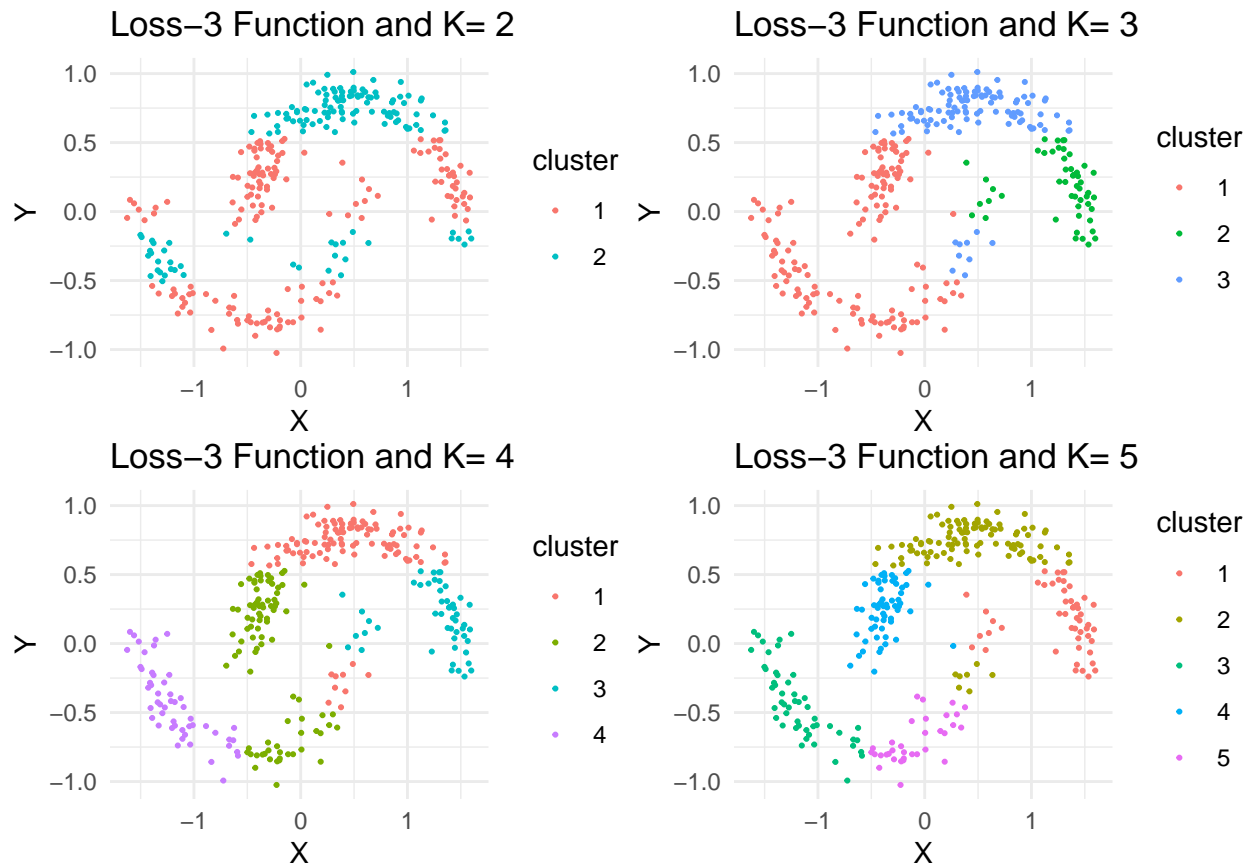
```

ggtitle(paste("Loss-3 Function and K=",k)) +
labs(x = "X", y= "Y") +
theme_minimal() +
theme(plot.margin = margin(1, 1, 1, 1, "pt"))

#Store plot in the list
plots_list[[length(plots_list) + 1]] <- plot
}

grid.arrange(grobs = plots_list, nrow = 2, ncol = 2, widths = c(3,3), heights = c(3,3))

```



Now, we use the last loss function, where there is transformation:

```

#List to store plots
plots_list <- list()

#Define K values
K_values <- c(2,3,4,5)

#Transform Function
transform_to_g <- function(x1,x2) {
  g_x1 <- sqrt((x1 + 1/2)^2 + x2^2)
  g_x2 <- sqrt((x1 - 1/2)^2 + x2^2)
  return(c(g_x1, g_x2))
}

```

```

# Apply the transformation using sapply()
transformed_data <- as.data.frame(t(sapply(1:nrow(moons_data),
                                          function(i) transform_to_g(moons_data[i,1], moons_data[i,2]))))

#Set new column names
colnames(transformed_data) <- c("gx1", "gx2")

#Convert into numeric data
transformed_data$gx1 <- as.numeric(transformed_data$gx1)
transformed_data$gx2 <- as.numeric(transformed_data$gx2)

#Loopping through each value
for (k in K_values){
  #Apply K-Means Clustering Algorithm
  result <- kmeans(transformed_data, centers=k, nstart=50)

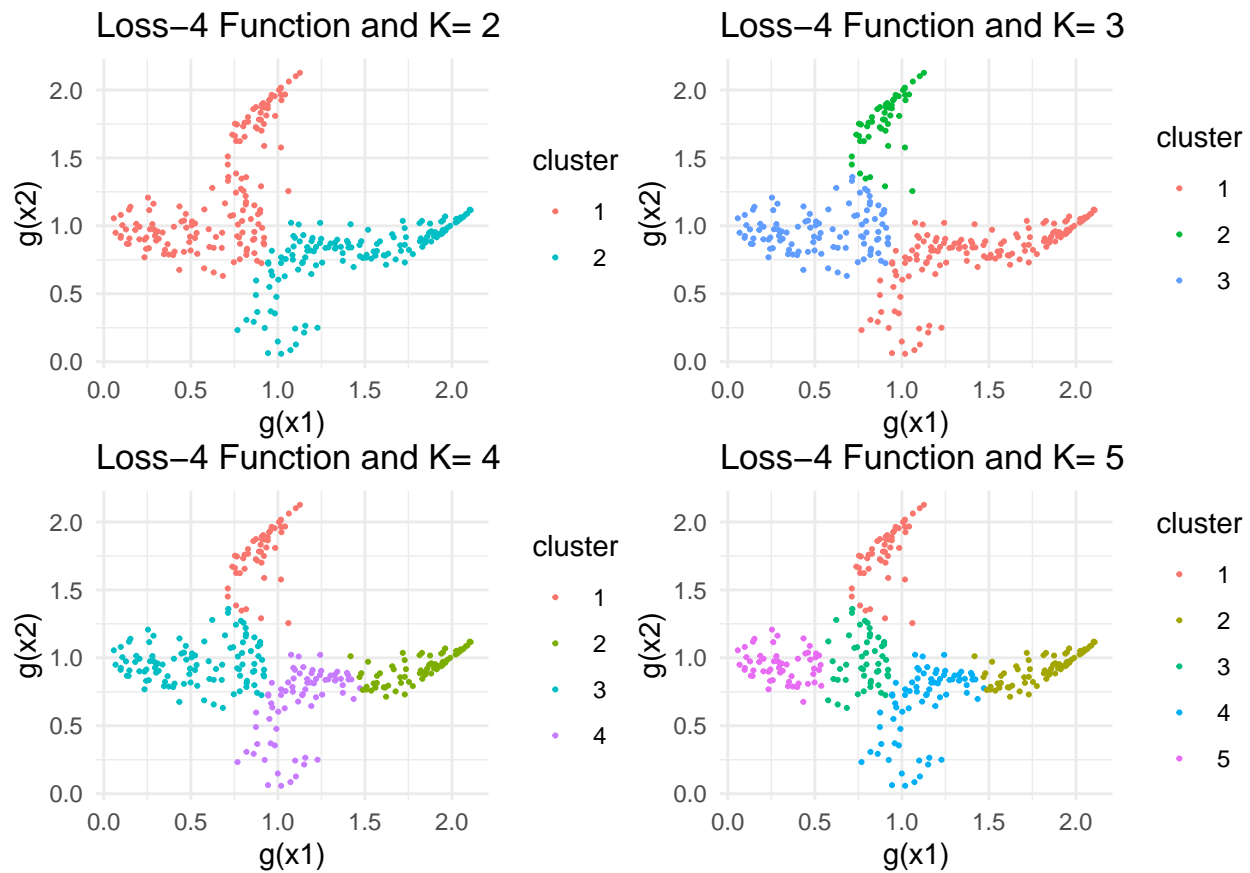
  #Store cluster assignments
  transformed_data$cluster <- as.factor(result$cluster)

  #Scatter Plot for each K-value
  plot <- ggplot(transformed_data, aes(x= gx1, y= gx2, color=cluster))+
    geom_point(size=0.4) +
    ggtitle(paste("Loss-4 Function and K=",k)) +
    labs(x = "g(x1)", y= "g(x2)") +
    theme_minimal() +
    theme(plot.margin = margin(1, 1, 1, 1, "pt"))

  #Store plot in the list
  plots_list[[length(plots_list) + 1]] <- plot
}

grid.arrange(grobs = plots_list, nrow = 2, ncol = 2, widths = c(3,3), heights = c(3,3))

```



(ii) (5 marks) Write a function `cluster_eval` which, for a given data set X and a range of natural numbers $K_1 \leq K_2$,

- Computes the K -Means clusterings for each $K_1 \leq K \leq K_2$, and
- Given this collection of clusterings, plots the values of the K -Means loss function at the optimal clusterings, as a function of K .

Use your implementation of `cluster_eval` to compare the clusterings which you obtained in Part (i) of this problem. Do you find that you different clusterings agree on what the ‘correct’ number of clusters in this data are?):

```
library(ggplot2)

cluster_eval <- function(data, K1, K2){
  #Create empty numeric vector to store the WCSS
  wcss_value <- numeric(length = K2 - K1 + 1)

  #Loop values from K1 to K2
  for (k in K1:K2){
    #Apply k-means algorithm
    result <- kmeans(data, centers=k, nstart = 50)

    #Store the WCSS
    wcss_value[k - K1 + 1] <- result$tot.withinss
  }
}
```

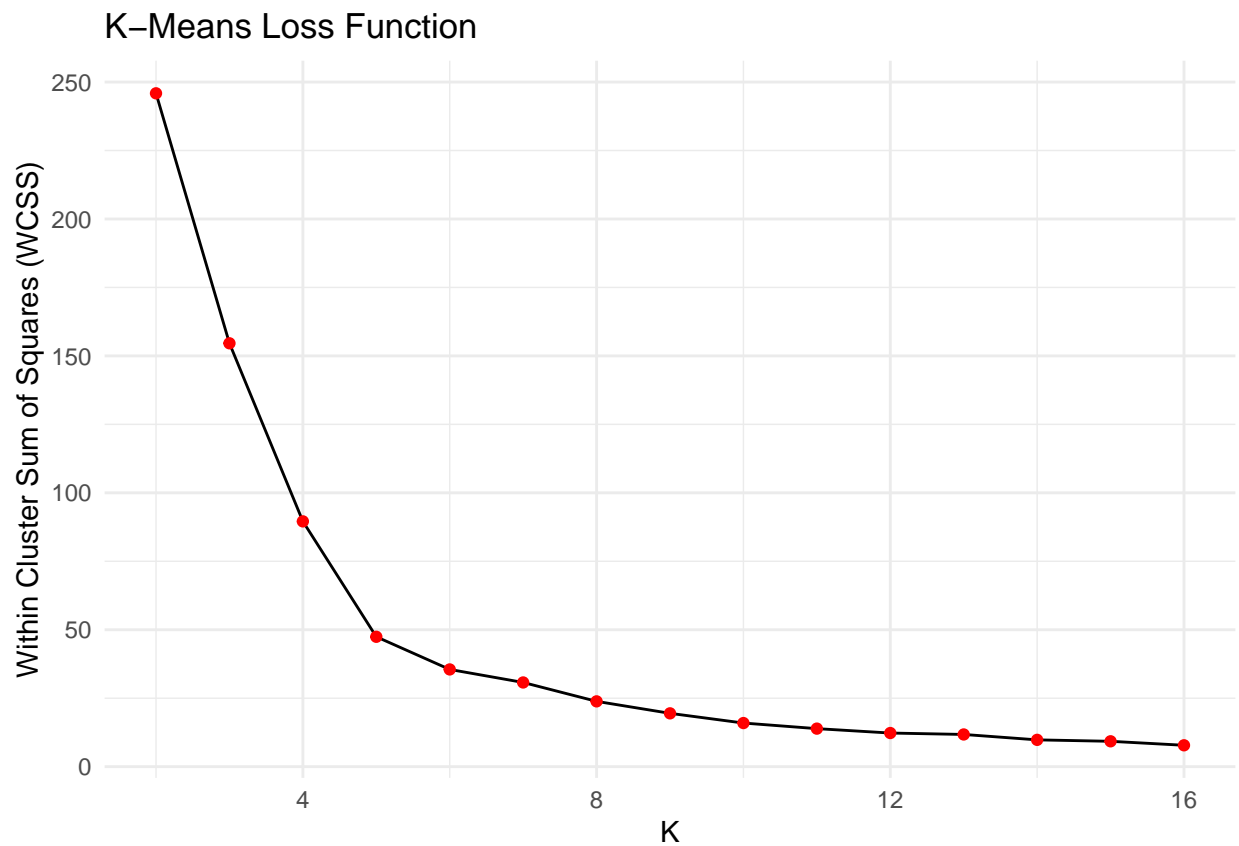
```

wcscs_df <- data.frame(K = K1:K2, WCSS= wcscs_value)

ggplot(wcscs_df, aes(x= K, y= WCSS))+
  geom_line(color="black") +
  geom_point(size=1.5, color="red") +
  ggtitle("K-Means Loss Function") +
  labs(x = "K", y= "Within Cluster Sum of Squares (WCSS)") +
  theme_minimal()
}

#Use cluster_eval function
cluster_eval(moons_data, 2, 16)

```



In this case, we use the entire set of features to be part of the loss function. We can examine the elbow point in the plot ; it looks like the optimal value of K is either 4 or 5. From part (i), depending on the loss function, we can inspect visually what the optimal value of K could be. In my opinion, these are the optimal values of K for each function:

- $Loss^1$: $K=3$
- $Loss^2$: $K= 4$
- $Loss^3$: $K = 4$
- $Loss^4$: $K= 4$

Again, these are completely subjective to each person. Since most of the “correct” cluster number is 4, it agrees with the elbow method that the choice of $K = 4$ is more or less correct.

iii. (5 marks) Load in R’s quakes dataset. This dataset stores information about 1000 seismic events (i.e. earthquakes and similar) which have occurred in the vicinity of the island of Fiji over the past 60 or so years. The first three columns (lat, long, depth) record the geographical location of the event, the fourth (mag) records the strength of the event (as measured on the Richter scale), and the fifth (station) records how many stations documented the event in question.

In the context of this question, we are interested in whether the locations at which these seismic events take place are spatially localised, i.e. if they cluster around specific areas of the island.

- Run a standard K-Means clustering on the full data set for $K = \{2, 3, 4, 5\}$, and plot the outcome, focusing on the `lat` and `long` dimensions.
- Does the clustering which you obtain in this way look spatially reasonable? Propose an alternative approach to obtaining a clustering which is more coherent (still using K-Means).

```
data("quakes")

#List to store plots
plots_list <- list()

#Define K values
K_values <- c(2,3,4,5)

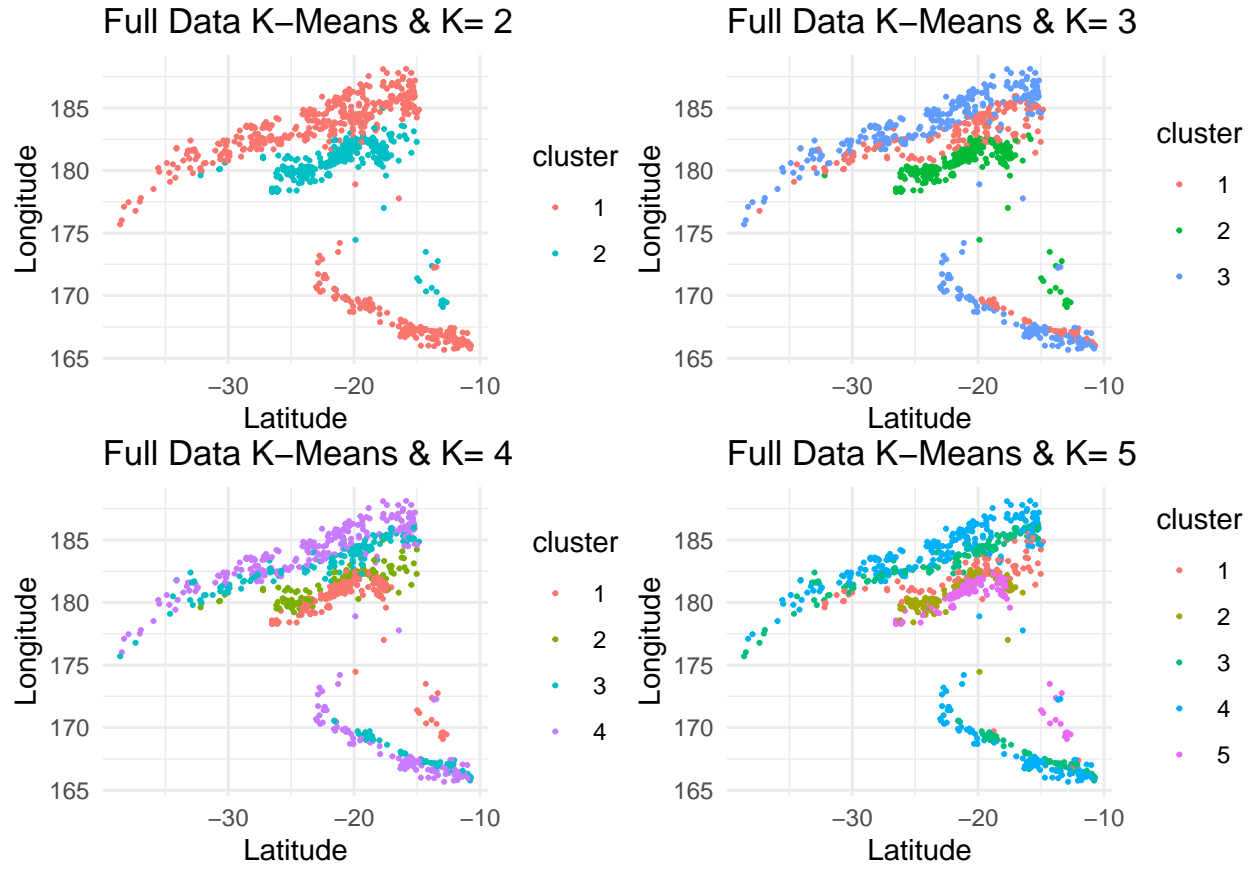
#Looping through each value
for (k in K_values){
  #Apply K-Means Clustering Algorithm
  result <- kmeans(quakes, centers=k, nstart=50)

  #Store cluster assignments
  quakes$cluster <- as.factor(result$cluster)

  #Scatter Plot for each K-value
  plot <- ggplot(quakes, aes(x= lat, y= long, color=cluster))+
    geom_point(size=0.4) +
    ggtitle(paste("Full Data K-Means & K=",k)) +
    labs(x = "Latitude", y= "Longitude") +
    theme_minimal() +
    theme(plot.margin = margin(1, 1, 1, 1, "pt"))

  #Store plot in the list
  plots_list[[length(plots_list) + 1]] <- plot
}

grid.arrange(grobs = plots_list, nrow = 2, ncol = 2, widths = c(3,3), heights = c(3,3))
```



For $K = 2$, the clusters are well separated but there are some overlapping points ; overall, it looks spatially reasonable. As the number of clusters increase, they appear more fragmented and artificially split, especially for $K \in \{4, 5\}$. An alternative approach while still using K-Means will be to normalise selected features which are on a different scale before clustering, as it prevents features with large magnitudes to dominate the learning process. Also, PCA would be another suggestion if the features are highly correlated, but it *may* not be necessary since `quakes` has 5 features which may contain important information.