FML_Hierarchical Clustering

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Load Data Set and Libraries #First, we will load all of the packages needed for this task. “ISLR”, “caret”, “dplyr”, “tidyverse”, “factoextra”, “ggplot2”, “proxy”, “NbClust”, “ppclust”, “dendextend”, “cluster”, and “tinytex” will be loaded for this problem.

```
library(cluster)
library(ISLR)
library(caret)
```

```
## Loading required package: ggplot2
```

```
## Warning: package 'ggplot2' was built under R version 4.3.2
```

```
## Loading required package: lattice
```

```
## Warning: package 'lattice' was built under R version 4.3.2
```

```
library(dplyr)
```

```
##
## Attaching package: 'dplyr'
```

```
## The following objects are masked from 'package:stats':
##
##     filter, lag
```

```
## The following objects are masked from 'package:base':
##
##     intersect, setdiff, setequal, union
```

```
library(tidyverse)
```

```
## ── Attaching core tidyverse packages ──────────────────────── tidyverse 2.0.0 ──
## ✔ forcats   1.0.0     ✔ stringr   1.5.0
## ✔ lubridate 1.9.3     ✔ tibble    3.2.1
## ✔ purrr     1.0.2     ✔ tidyr     1.3.0
## ✔ readr     2.1.4
```

```
## ── Conflicts ────────────────────────────────────────── tidyverse_conflicts() ──
## ✖ dplyr::filter() masks stats::filter()
## ✖ dplyr::lag()    masks stats::lag()
## ✖ purrr::lift()   masks caret::lift()
## ℹ Use the conflicted package (<http://conflicted.r-lib.org/>) to force all conflicts to become errors
```

```
library(factoextra)
```

```
## Welcome! Want to learn more? See two factoextra-related books at https://goo.gl/ve3WBa
```

```
library(ggplot2)
library(proxy)
```

```
##
## Attaching package: 'proxy'
##
## The following objects are masked from 'package:stats':
##
##     as.dist, dist
##
## The following object is masked from 'package:base':
##
##     as.matrix
```

```
library(NbClust)
library(ppclust)
```

```
## Warning: package 'ppclust' was built under R version 4.3.2
```

```
library(dendextend)
```

```
## Warning: package 'dendextend' was built under R version 4.3.2
```

```
##
## ---------------------
## Welcome to dendextend version 1.17.1
## Type citation('dendextend') for how to cite the package.
##
## Type browseVignettes(package = 'dendextend') for the package vignette.
## The github page is: https://github.com/talgalili/dendextend/
##
## Suggestions and bug-reports can be submitted at: https://github.com/talgalili/dendextend/issues
## You may ask questions at stackoverflow, use the r and dendextend tags:
##   https://stackoverflow.com/questions/tagged/dendextend
##
##  To suppress this message use:  suppressPackageStartupMessages(library(dendextend))
## ---------------------
##
##
## Attaching package: 'dendextend'
##
## The following object is masked from 'package:stats':
##
##     cutree
```

```
library(tinytex)
```

```
## Warning: package 'tinytex' was built under R version 4.3.2
```

#The “cereal” data set will then be imported into the RStudio environment.

```
# Import data set from BlackBoard into the RStudio environment

cereal <- read.csv("D:/Cereals.csv")
```

Review Data Structure #A summary of the data set will be displayed for inspection.Examine the first few rows of the data set

```
head(cereal)
```

```
##                         name mfr type calories protein fat sodium fiber carbo
## 1                 100%_Bran   N    C       70       4   1    130  10.0   5.0
## 2         100%_Natural_Bran   Q    C      120       3   5     15   2.0   8.0
## 3                  All-Bran   K    C       70       4   1    260   9.0   7.0
## 4 All-Bran_with_Extra_Fiber   K    C       50       4   0    140  14.0   8.0
## 5            Almond_Delight   R    C      110       2   2    200   1.0  14.0
## 6   Apple_Cinnamon_Cheerios   G    C      110       2   2    180   1.5  10.5
##   sugars potass vitamins shelf weight cups   rating
## 1      6    280       25     3      1 0.33 68.40297
## 2      8    135        0     3      1 1.00 33.98368
## 3      5    320       25     3      1 0.33 59.42551
## 4      0    330       25     3      1 0.50 93.70491
## 5      8     NA       25     3      1 0.75 34.38484
## 6     10     70       25     1      1 0.75 29.50954
```

```
# Look into the data set's structure.
str(cereal)
```

```
## 'data.frame':    77 obs. of  16 variables:
##  $ name    : chr  "100%_Bran" "100%_Natural_Bran" "All-Bran" "All-Bran_with_Extra_Fiber" ...
##  $ mfr     : chr  "N" "Q" "K" "K" ...
##  $ type    : chr  "C" "C" "C" "C" ...
##  $ calories: int  70 120 70 50 110 110 110 130 90 90 ...
##  $ protein : int  4 3 4 4 2 2 2 3 2 3 ...
##  $ fat     : int  1 5 1 0 2 2 0 2 1 0 ...
##  $ sodium  : int  130 15 260 140 200 180 125 210 200 210 ...
##  $ fiber   : num  10 2 9 14 1 1.5 1 2 4 5 ...
##  $ carbo   : num  5 8 7 8 14 10.5 11 18 15 13 ...
##  $ sugars  : int  6 8 5 0 8 10 14 8 6 5 ...
##  $ potass  : int  280 135 320 330 NA 70 30 100 125 190 ...
##  $ vitamins: int  25 0 25 25 25 25 25 25 25 25 ...
##  $ shelf   : int  3 3 3 3 3 1 2 3 1 3 ...
##  $ weight  : num  1 1 1 1 1 1 1 1.33 1 1 ...
##  $ cups    : num  0.33 1 0.33 0.5 0.75 0.75 1 0.75 0.67 0.67 ...
##  $ rating  : num  68.4 34 59.4 93.7 34.4 ...
```

```
# Investigate the summary of the data set
summary(cereal)
```

```
##      name               mfr                type             calories    
##  Length:77          Length:77          Length:77          Min.   : 50.0  
##  Class :character   Class :character   Class :character   1st Qu.:100.0  
##  Mode  :character   Mode  :character   Mode  :character   Median :110.0  
##                                                           Mean   :106.9  
##                                                           3rd Qu.:110.0  
##                                                           Max.   :160.0  
##                                                                          
##     protein           fat            sodium          fiber       
##  Min.   :1.000   Min.   :0.000   Min.   :  0.0   Min.   : 0.000  
##  1st Qu.:2.000   1st Qu.:0.000   1st Qu.:130.0   1st Qu.: 1.000  
##  Median :3.000   Median :1.000   Median :180.0   Median : 2.000  
##  Mean   :2.545   Mean   :1.013   Mean   :159.7   Mean   : 2.152  
##  3rd Qu.:3.000   3rd Qu.:2.000   3rd Qu.:210.0   3rd Qu.: 3.000  
##  Max.   :6.000   Max.   :5.000   Max.   :320.0   Max.   :14.000  
##                                                                  
##      carbo          sugars           potass          vitamins     
##  Min.   : 5.0   Min.   : 0.000   Min.   : 15.00   Min.   :  0.00  
##  1st Qu.:12.0   1st Qu.: 3.000   1st Qu.: 42.50   1st Qu.: 25.00  
##  Median :14.5   Median : 7.000   Median : 90.00   Median : 25.00  
##  Mean   :14.8   Mean   : 7.026   Mean   : 98.67   Mean   : 28.25  
##  3rd Qu.:17.0   3rd Qu.:11.000   3rd Qu.:120.00   3rd Qu.: 25.00  
##  Max.   :23.0   Max.   :15.000   Max.   :330.00   Max.   :100.00  
##  NA's   :1      NA's   :1        NA's   :2                        
##      shelf           weight          cups           rating     
##  Min.   :1.000   Min.   :0.50   Min.   :0.250   Min.   :18.04  
##  1st Qu.:1.000   1st Qu.:1.00   1st Qu.:0.670   1st Qu.:33.17  
##  Median :2.000   Median :1.00   Median :0.750   Median :40.40  
##  Mean   :2.208   Mean   :1.03   Mean   :0.821   Mean   :42.67  
##  3rd Qu.:3.000   3rd Qu.:1.00   3rd Qu.:1.000   3rd Qu.:50.83  
##  Max.   :3.000   Max.   :1.50   Max.   :1.500   Max.   :93.70  
## 
```

```
#Data Preprocessing
#The data will be scaled prior to removing the NA(Null) values from the data set.
# Create duplicate of data set for preprocessing

cereal_scaled <- cereal
# Scale the data set prior to placing it into a clustering algorithm
cereal_scaled[ , c(4:16)] <- scale(cereal[ , c(4:16)])
# Remove NA values from data set
cereal_preprocessed <- na.omit(cereal_scaled)

# Review the scaled data set with NA's removed
head(cereal_preprocessed)
```

```
##                         name mfr type   calories    protein         fat
## 1                  100%_Bran   N    C -1.8929836  1.3286071 -0.01290349
## 2          100%_Natural_Bran   Q    C  0.6732089  0.4151897  3.96137277
## 3                   All-Bran   K    C -1.8929836  1.3286071 -0.01290349
## 4 All-Bran_with_Extra_Fiber   K    C -2.9194605  1.3286071 -1.00647256
## 6   Apple_Cinnamon_Cheerios   G    C  0.1599704 -0.4982277  0.98066557
## 7                Apple_Jacks   K    C  0.1599704 -0.4982277 -1.00647256
##       sodium       fiber      carbo     sugars     potass   vitamins      shelf
## 1 -0.3539844  3.29284661 -2.5087829 -0.2343906  2.5753685 -0.1453172  0.9515734
## 2 -1.7257708 -0.06375361 -1.7409943  0.2223705  0.5160205 -1.2642598  0.9515734
## 3  1.1967306  2.87327158 -1.9969238 -0.4627711  3.1434645 -0.1453172  0.9515734
## 4 -0.2346986  4.97114672 -1.7409943 -1.6046739  3.2854885 -0.1453172  0.9515734
## 6  0.2424445 -0.27354112 -1.1011705  0.6791317 -0.4071355 -0.1453172 -1.4507595
## 7 -0.4136273 -0.48332864 -0.9732057  1.5926539 -0.9752315 -0.1453172 -0.2495930
##       weight       cups     rating
## 1 -0.1967771 -2.1100340  1.8321876
## 2 -0.1967771  0.7690100 -0.6180571
## 3 -0.1967771 -2.1100340  1.1930986
## 4 -0.1967771 -1.3795303  3.6333849
## 6 -0.1967771 -0.3052601 -0.9365625
## 7 -0.1967771  0.7690100 -0.6756899
```

#After pre-processing and scaling the data, the total number of observations went from 77 to 74. Therefore, there were only 3 records with an “NA” value

Assignment Task A #“Apply hierarchical clustering to the data using Euclidean distance to the normalized measurements. Use Agnes to compare the clustering from single linkage, complete linkage, average linkage, and Ward. Choose the best method.”

#Single Linkage:

Create the dissimilarity matrix for the numeric values in the data set via Euclidean distance measurements

```
cereal_d_euclidean <- dist(cereal_preprocessed[ , c(4:16)], method ="euclidean")
```

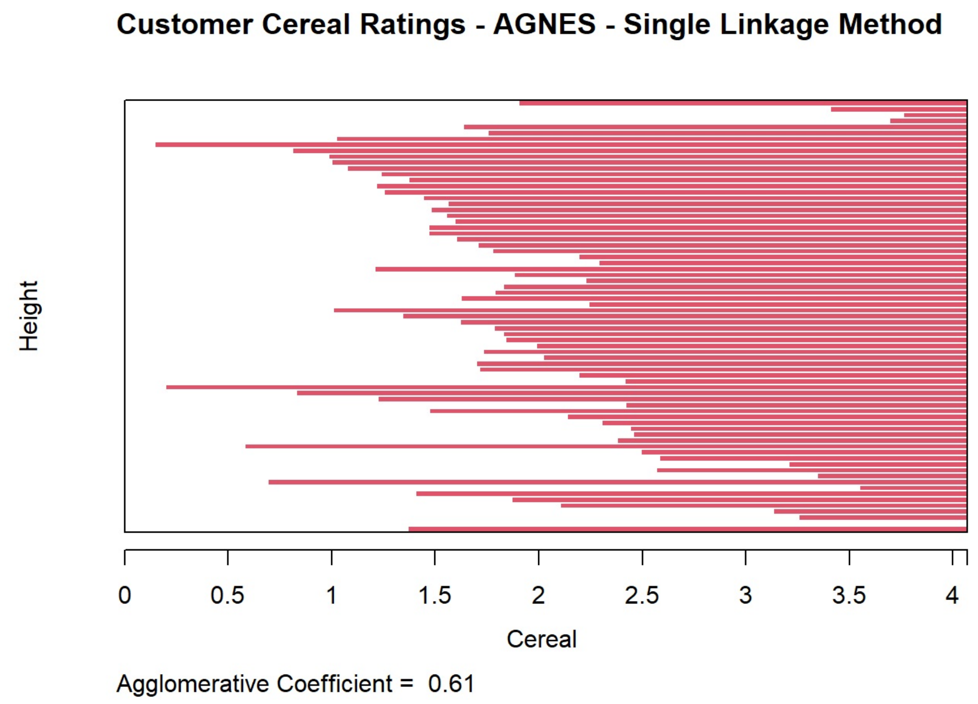
```
# Perform hierarchical clustering via the single linkage method

ag_hc_single <-agnes(cereal_d_euclidean, method = "single")
```

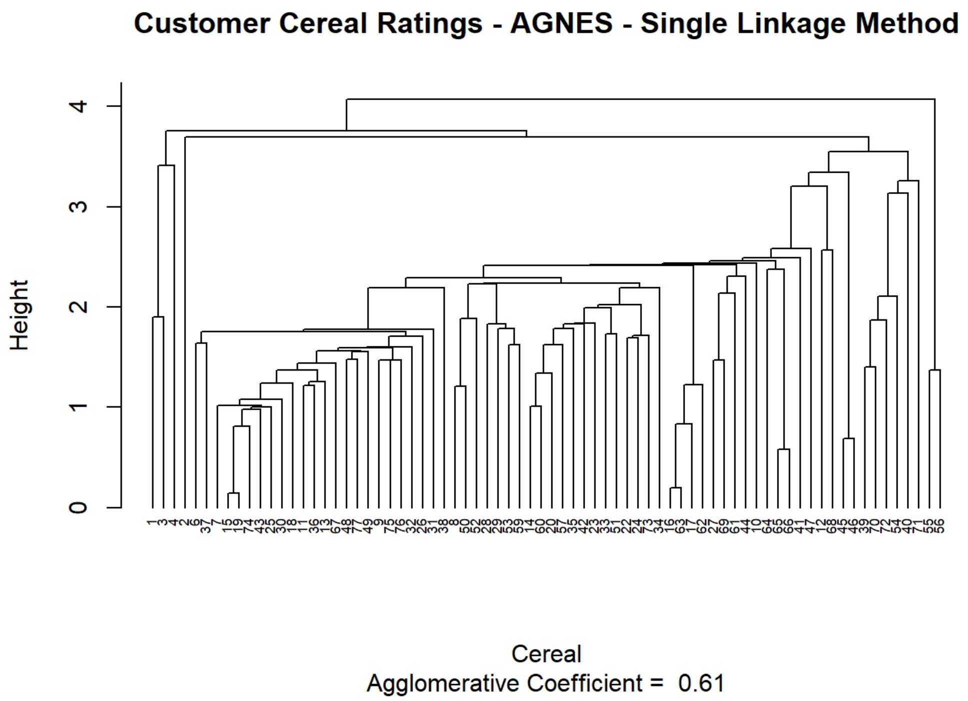
```
# Plot the results of the different methods

plot(ag_hc_single,
     main = "Customer Cereal Ratings - AGNES - Single Linkage Method",
     xlab = "Cereal",
     ylab = "Height",
     cex.axis = 1,
     cex = 0.55,
 hang = -1)
```

```
## Warning in plot.window(xlim, ylim, log = log, ...): "hang" is not a graphical
## parameter
```

```
## Warning in title(main = main, sub = sub, xlab = xlab, ylab = ylab, ...): "hang"
## is not a graphical parameter
```

```
## Warning in axis(1, at = at.vals, labels = lab.vals, ...): "hang" is not a
## graphical parameter
```





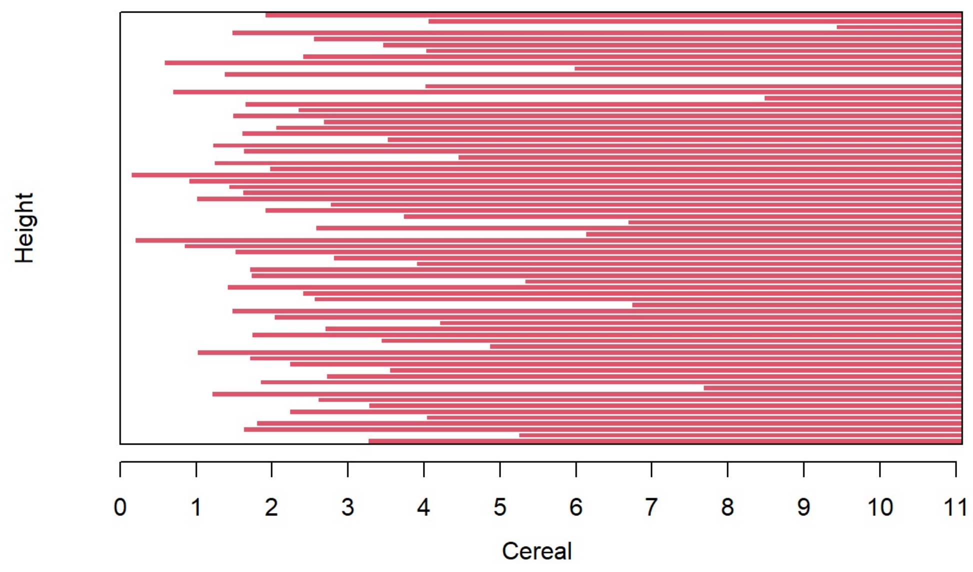
```
#Complete Linkage:
# Perform hierarchical clustering via the complete linkage method
ag_hc_complete <- agnes(cereal_d_euclidean, method = "complete")
# Plot the results of the different methods
plot(ag_hc_complete,
 main = "Customer Cereal Ratings - AGNES - Complete Linkage Method",
 xlab = "Cereal",
 ylab = "Height",
 cex.axis = 1,
 cex = 0.55,
 hang = -1)
```

```
## Warning in plot.window(xlim, ylim, log = log, ...): "hang" is not a graphical
## parameter
```

```
## Warning in title(main = main, sub = sub, xlab = xlab, ylab = ylab, ...): "hang"
## is not a graphical parameter
```

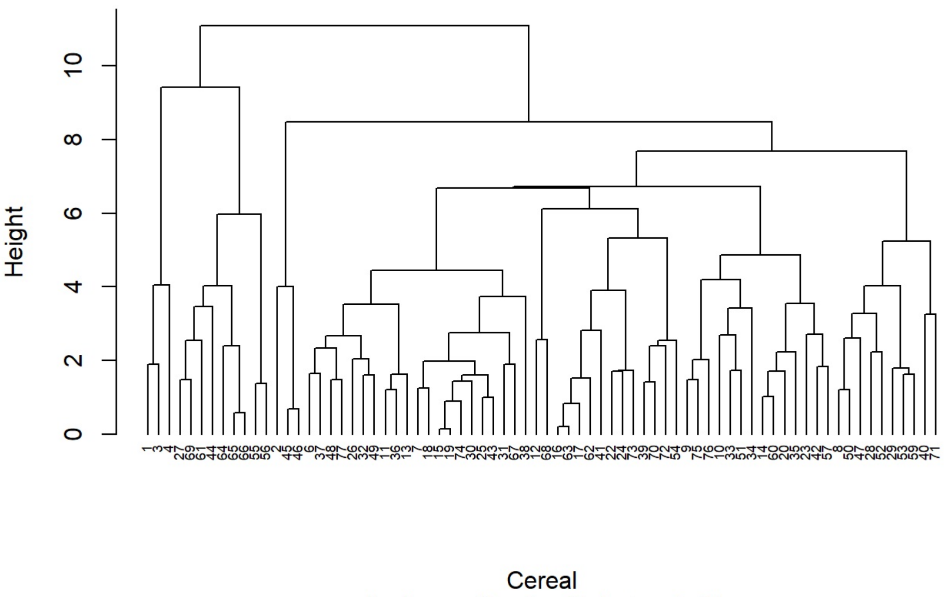
```
## Warning in axis(1, at = at.vals, labels = lab.vals, ...): "hang" is not a
## graphical parameter
```

Customer Cereal Ratings - AGNES - Complete Linkage Method



Agglomerative Coefficient = 0.84

Customer Cereal Ratings - AGNES - Complete Linkage Method



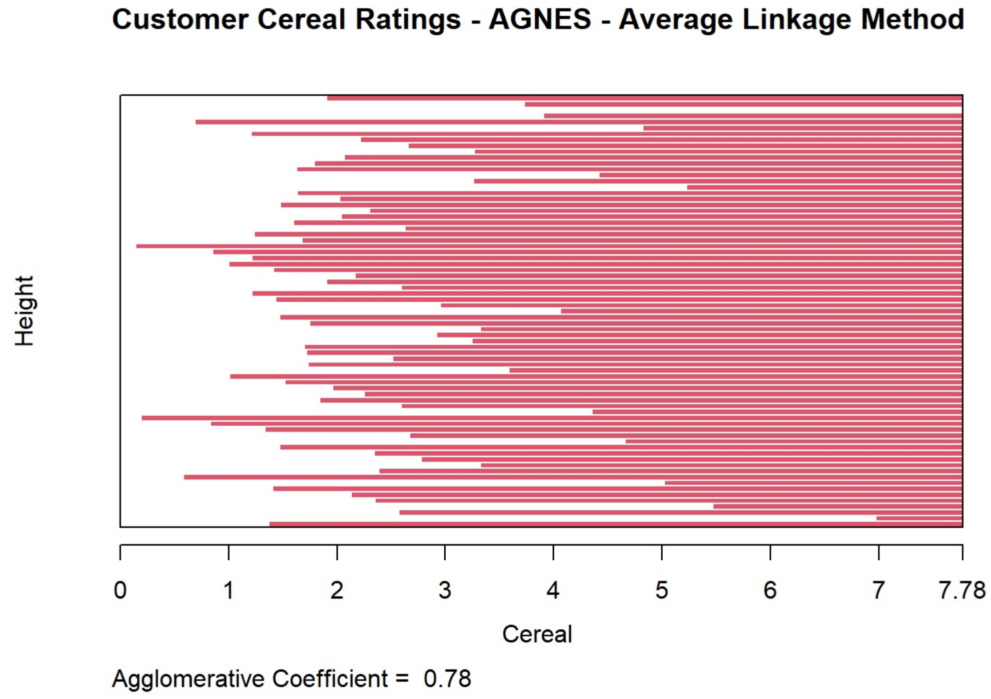
Agglomerative Coefficient = 0.84

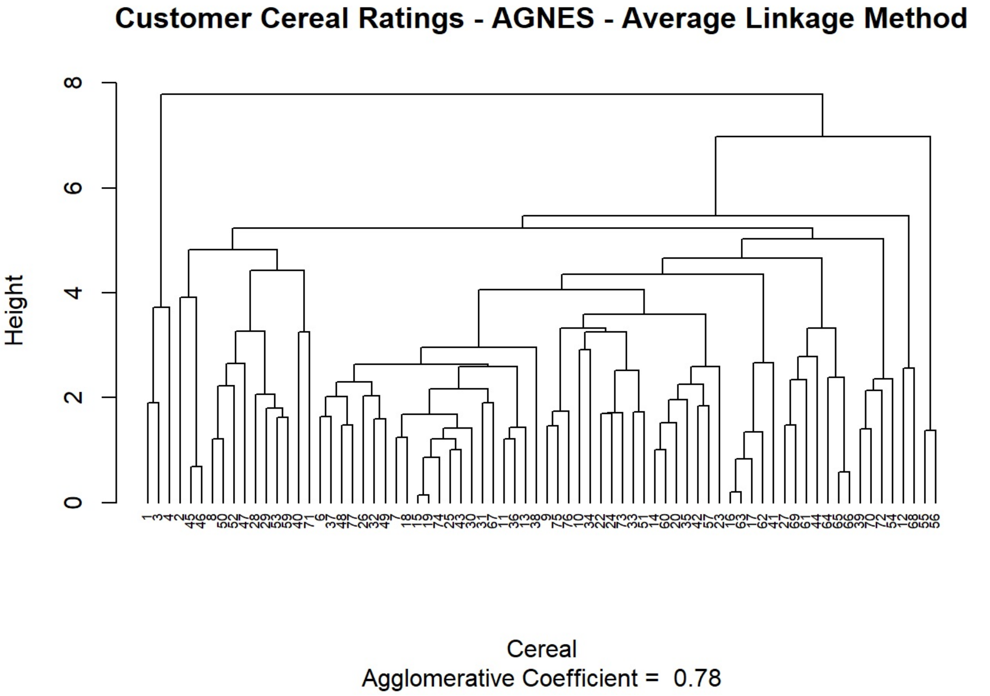
```
#Average Linkage:
# Perform hierarchical clustering via the average linkage method
ag_hc_average <- agnes(cereal_d_euclidean, method = "average")
# Plot the results of the different methods
plot(ag_hc_average,
 main = "Customer Cereal Ratings - AGNES - Average Linkage Method",
 xlab = "Cereal",
 ylab = "Height",
 cex.axis = 1,
 cex = 0.55,
 hang = -1)
```

```
## Warning in plot.window(xlim, ylim, log = log, ...): "hang" is not a graphical
## parameter
```

```
## Warning in title(main = main, sub = sub, xlab = xlab, ylab = ylab, ...): "hang"
## is not a graphical parameter
```

```
## Warning in axis(1, at = at.vals, labels = lab.vals, ...): "hang" is not a
## graphical parameter
```



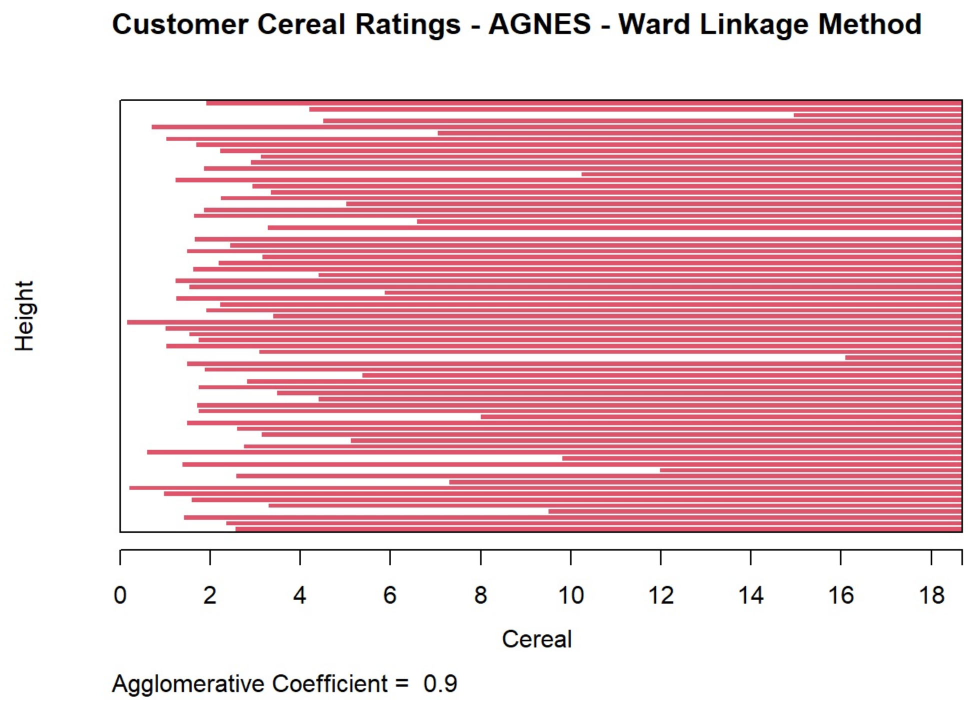


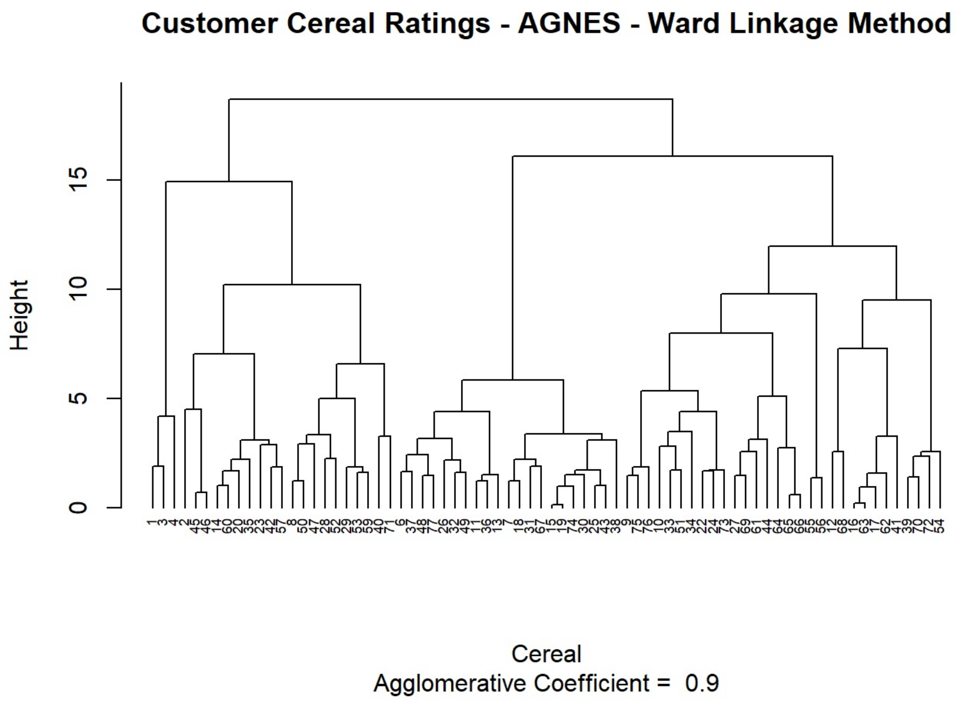
```
#Ward Method:
# Perform hierarchical clustering via the ward linkage method
ag_hc_ward <- agnes(cereal_d_euclidean, method = "ward")
# Plot the results of the different methods
plot(ag_hc_ward,
 main = "Customer Cereal Ratings - AGNES - Ward Linkage Method",
 xlab = "Cereal",
 ylab = "Height",
 cex.axis = 1,
 cex = 0.55,
 hang = -1)
```

```
## Warning in plot.window(xlim, ylim, log = log, ...): "hang" is not a graphical
## parameter
```

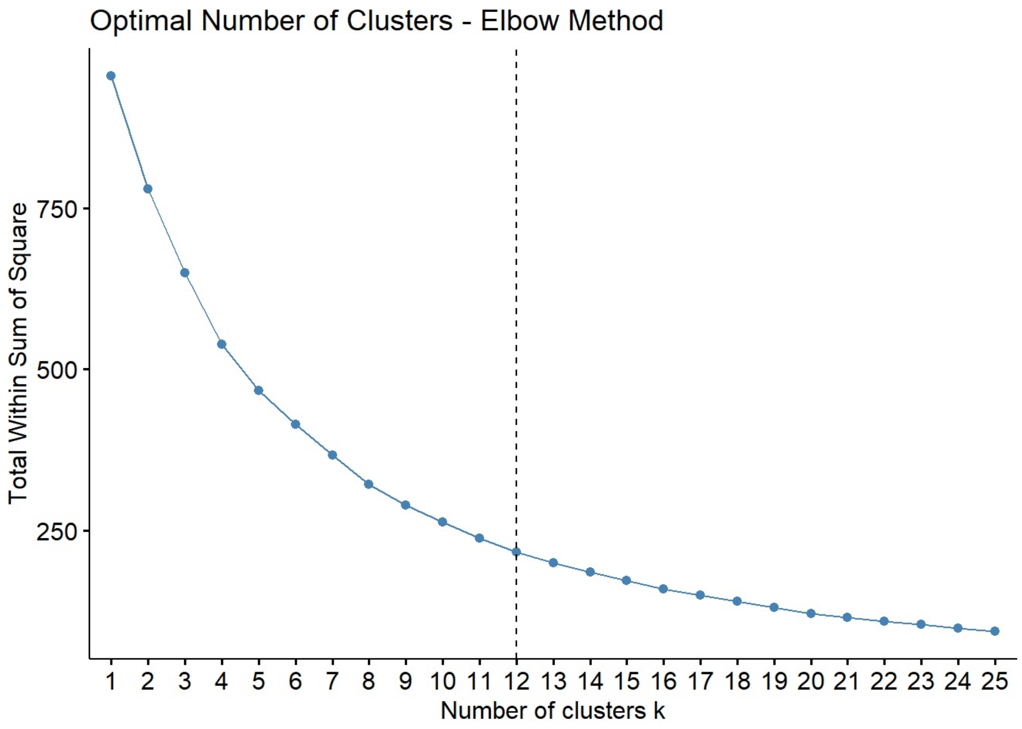
```
## Warning in title(main = main, sub = sub, xlab = xlab, ylab = ylab, ...): "hang"
## is not a graphical parameter
```

```
## Warning in axis(1, at = at.vals, labels = lab.vals, ...): "hang" is not a
## graphical parameter
```

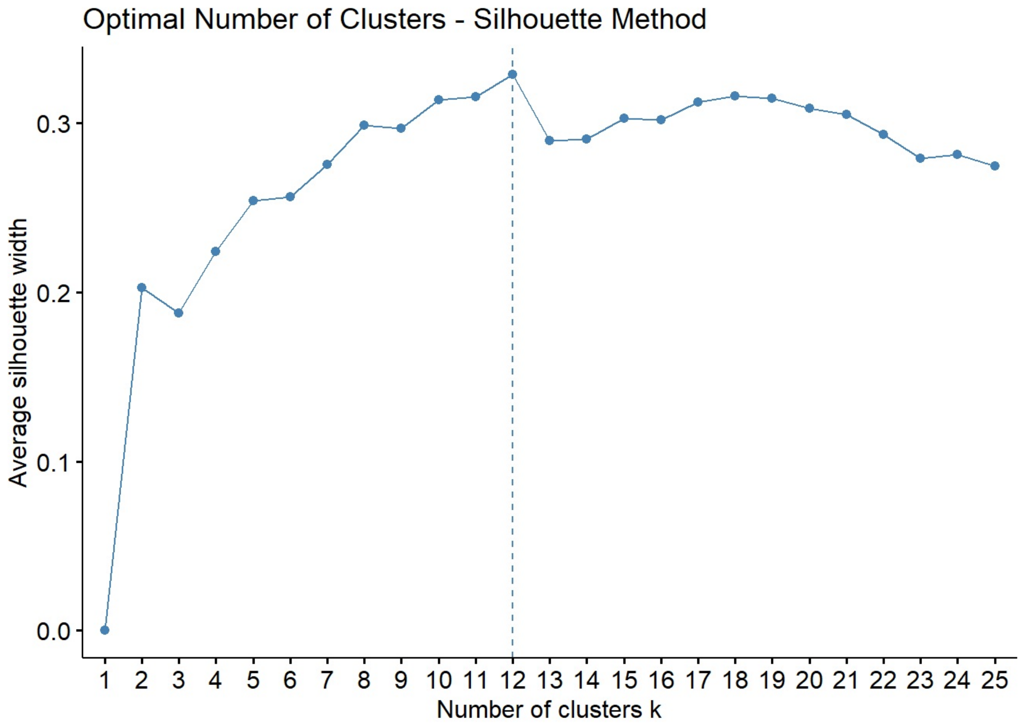




```
#The best clustering method would be based on the agglomerative coefficient that is returned from each method. Th
e close the value is to 1.0, the closer the clustering structure is. Therefore, the method with the value closest
to 1.0 will be chosen.

#Single Linkage: 0.61 #Complete Linkage: 0.84 #Average Linkage: 0.78 #Ward Method: 0.90
#As a result, the Ward method will be chosen as the best clustering model in this problem.

#Assignment Task B

#“How many clusters would you choose?”
#To determine the appropriate number of clusters, we will use the elbow and silhouette methods.
#Elbow Method:
# Determine the optimal number of clusters for the dataset via the Elbow method
fviz_nbclust(cereal_preprocessed[ , c(4:16)], hcut, method = "wss", k.max =
25) +
 labs(title = "Optimal Number of Clusters - Elbow Method") +
 geom_vline(xintercept = 12, linetype = 2)
```



```
#Silhouette Method:
# Determine the optimal number of clusters for the dataset via the silhouette method
fviz_nbclust(cereal_preprocessed[ , c(4:16)],
                               hcut,
                               method = "silhouette",
                               k.max = 25) +
labs(title = "Optimal Number of Clusters - Silhouette Method")
```



```
#Based on the agreement of the silhouette and elbow method, the appropriate number of clusters would be 12 in thi
s case.
#Below we will outline the 12 clusters on the hierarchical tree
# Plot of the Ward hierarchical tree with the 12 clusters outlined for reference
plot(ag_hc_ward,
 main = "AGNES - Ward Linkage Method - 12 Clusters Outlined",
 xlab = "Cereal",
 ylab = "Height",
 cex.axis = 1,
 cex = 0.55,
 hang = -1)
```

```
## Warning in plot.window(xlim, ylim, log = log, ...): "hang" is not a graphical
## parameter
## Warning in title(main = main, sub = sub, xlab = xlab, ylab = ylab, ...): "hang"
## is not a graphical parameter
```

```
## Warning in axis(1, at = at.vals, labels = lab.vals, ...): "hang" is not a
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```
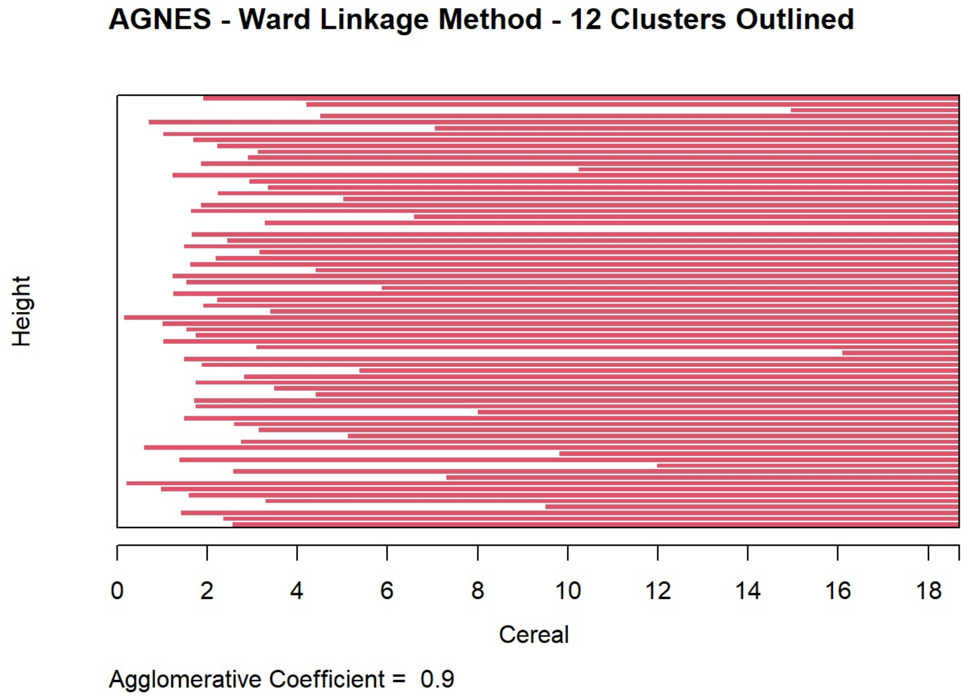
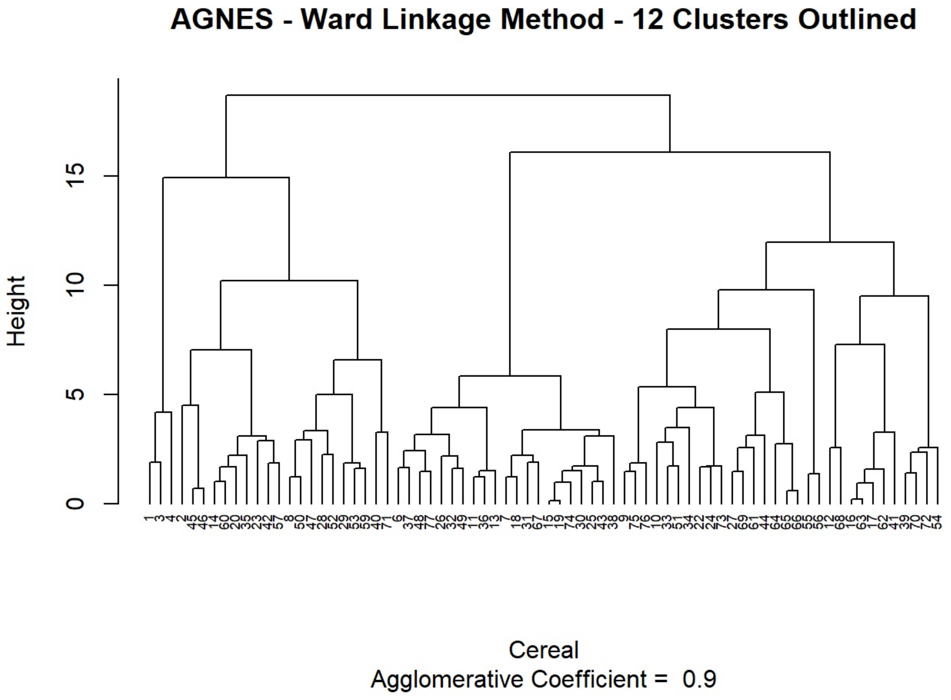





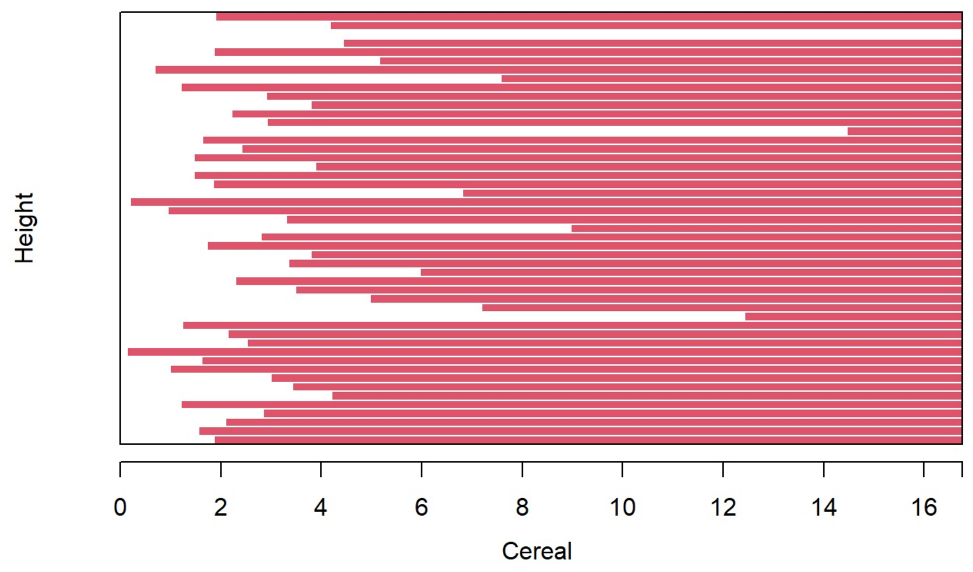
```
#Assignment Task C

#“Comment on the structure of the clusters and on their stability. Hint: To check stability, partition the data and see how well clusters formed based on one part apply to the other part. To do this:

#1. Cluster partition A #2. Use the cluster centroids from A to assign each record in partition B (each record is assigned to the cluster with the closest centroid).

#3.Assess how consistent the cluster assignments are compared to the assignments based on all the data”

#All Data Assigned Clusters:

#The assigned clusters for all data sets will be in “cereal_preprocessed_1”:

# Cut the tree into 12 clusters for analysis
ward_clusters_12 <- cutree(ag_hc_ward, k = 12)

# Add the assigned cluster to the preprocessed data set
cereal_preprocessed_1 <- cbind(cluster = ward_clusters_12,
cereal_preprocessed)

#Partition Data:

#To check stability of clusters, the data set will be split into a 70/30 partition. The 70% will be used to create cluster assignments again, and then the remaining 30% will be assigned based on their closest centroid.

# Set the seed for randomized functions
set.seed(982579)

# Split the data into 70% partition A and 30% partition B
cerealIndex <- createDataPartition(cereal_preprocessed$protein, p=0.3, list =F)
cereal_preprocessed_PartitionB <- cereal_preprocessed[cerealIndex, ]
cereal_preprocessed_PartitionA <- cereal_preprocessed[-cerealIndex,]

#Re-Run Clustering with Partitioned Data:

#For the purposes of this task, we will assume the same K value (12) and ward clustering method to determine the stability of the clusters. We will then assign clusters to the nearest points in Partition B (for clusters 1 to 12).

# Create the dissimilarity matrix for the numeric values in the partitioned data set via Euclidean distance measurements
cereal_d_euclidean_A <- dist(cereal_preprocessed_PartitionA[ , c(4:16)],
method = "euclidean")

# Perform hierarchical clustering via the ward linkage method on partitioned data
ag_hc_ward_A <- agnes(cereal_d_euclidean_A, method = "ward")

# Plot the results of the different methods
plot(ag_hc_ward_A,
     main = "Customer Cereal Ratings - Ward Linkage Method - Partition A",
     xlab = "Cereal",
     ylab = "Height",
     cex.axis = 1,
     cex = 0.55,
     hang = -1)
```

```
## Warning in plot.window(xlim, ylim, log = log, ...): "hang" is not a graphical
## parameter
```

```
## Warning in title(main = main, sub = sub, xlab = xlab, ylab = ylab, ...): "hang"
## is not a graphical parameter
```

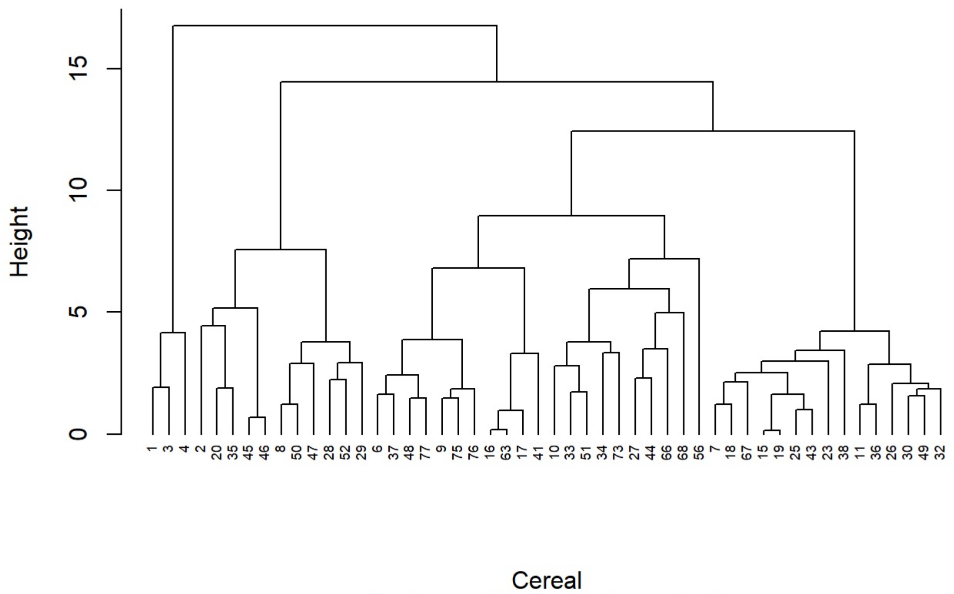
```
## Warning in axis(1, at = at.vals, labels = lab.vals, ...): "hang" is not a
## graphical parameter
```

Customer Cereal Ratings - Ward Linkage Method - Partition A



Agglomerative Coefficient = 0.88

Customer Cereal Ratings - Ward Linkage Method - Partition A



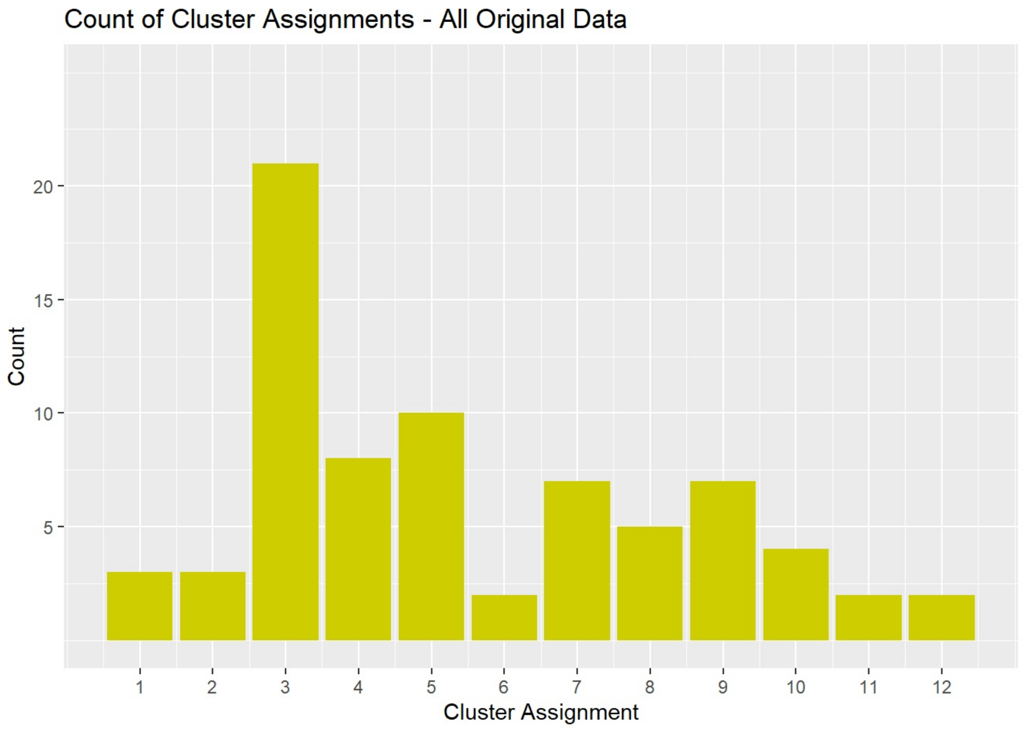
Agglomerative Coefficient = 0.88

```
# Cut the tree into 12 clusters for analysis
ward_clusters_12_A <- cutree(ag_hc_ward_A, k = 12)

# Add the assigned cluster to the preprocessed data set
cereal_preprocessed_A <- cbind(cluster = ward_clusters_12_A,
cereal_preprocessed_PartitionA)

#The centroids for each of the clusters will need to be calculated, so we can find the closest centroid for the d
ata points in partition B.

# Find the centroids for the re-ran Ward hierarchical clustering
ward_Centroids_A <- aggregate(cereal_preprocessed_A[ , 5:17],
list(cereal_preprocessed_A$cluster), mean)
ward_Centroids_A <- data.frame(Cluster = ward_Centroids_A[ , 1], Centroid =
rowMeans(ward_Centroids_A[ , -c(1:4)]))
ward_Centroids_A <- ward_Centroids_A$Centroid

# Calculate Centers of Partition B data set
cereal_preprocessed_PartitionB_centers <-
data.frame(cereal_preprocessed_PartitionB[, 1:3], Center =
rowMeans(cereal_preprocessed_PartitionB[ , 4:16]))

# Calculate the distance between the centers of partition A and the values of partition B
B_to_A_centers <- dist(ward_Centroids_A,
cereal_preprocessed_PartitionB_centers$Center, method = "euclidean")

# Assign the clusters based on the minimum distance to cluster centers
cereal_preprocessed_B <- cbind(cluster =
c(4,8,7,3,5,6,7,11,11,10,8,5,10,1,10,1,4,12,12,7,7,1,4,9),
cereal_preprocessed_PartitionB)

# Combine partitions A and B for comparision to original clusters
cereal_preprocessed_2 <- rbind(cereal_preprocessed_A, cereal_preprocessed_B)
cereal_preprocessed_1 <-
cereal_preprocessed_1[order(cereal_preprocessed_1$name), ]
cereal_preprocessed_2 <-
cereal_preprocessed_2[order(cereal_preprocessed_2$name), ]

#Now that the data has been assigned by both methods (full data and partitioned data), we can compare the number
of matching assignments to see the stability of the clusters.
sum(cereal_preprocessed_1$cluster == cereal_preprocessed_2$cluster)
```

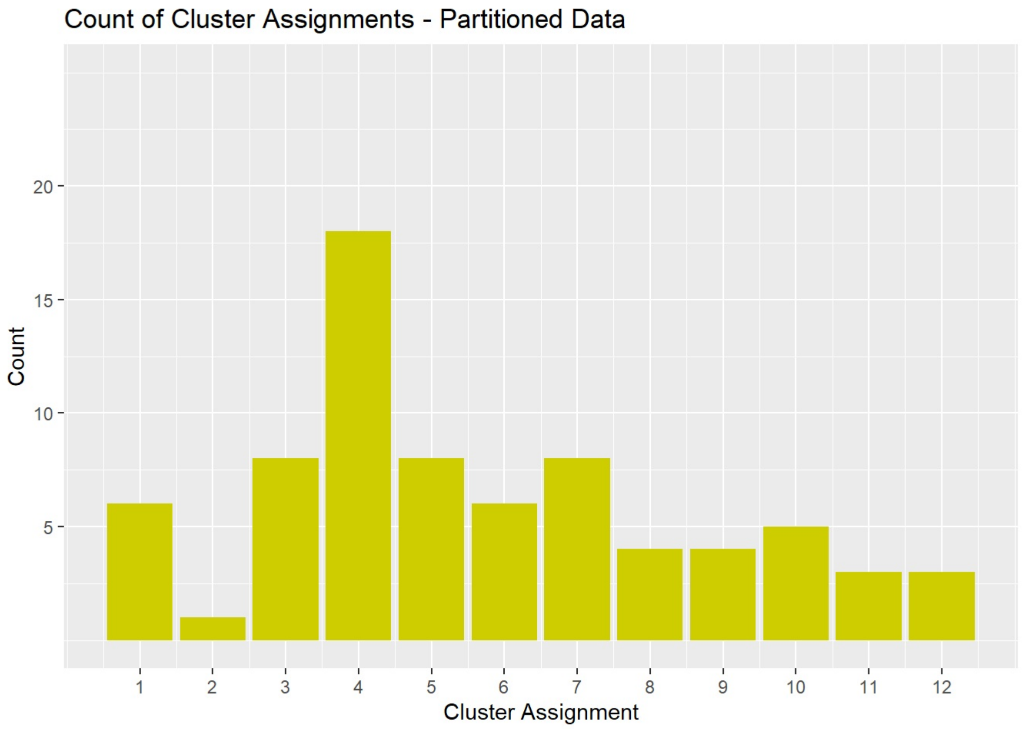
```
## [1] 14
```

```
#From this result, it can be stated that the clusters are not very stable. With 70% of the data available, the re
sulting assignments were only identical for 35 out of the 74 observations. This results in a 47% repeatability of
assignment.

# Visualize the cluster assignments to see any difference between the two

# Plot of original hierarchical clustering algorithm

ggplot(data = cereal_preprocessed_1, aes(cereal_preprocessed_1$cluster)) +
 geom_bar(fill = "yellow3") +
 labs(title="Count of Cluster Assignments - All Original Data") +
 labs(x="Cluster Assignment", y="Count") +
 guides(fill=FALSE) +
 scale_x_continuous(breaks=c(1:12)) +
 scale_y_continuous(breaks=c(5,10,15,20), limits = c(0,25))
```

```
## Warning: The `<scale>` argument of `guides()` cannot be `FALSE`. Use "none" instead as
## of ggplot2 3.3.4.
## This warning is displayed once every 8 hours.
## Call `lifecycle::last_lifecycle_warnings()` to see where this warning was
## generated.
```



```
# Plot of algorithm that was partitioned prior to assigning the remaining data
ggplot(data = cereal_preprocessed_2, aes(cereal_preprocessed_2$cluster)) +
 geom_bar(fill = "yellow3") +
 labs(title="Count of Cluster Assignments - Partitioned Data") +
 labs(x="Cluster Assignment", y="Count") +
 guides(fill=FALSE) +
 scale_x_continuous(breaks=c(1:12)) +
 scale_y_continuous(breaks=c(5,10,15,20), limits = c(0,25))
```



#When we use partitioned data, we can see that Cluster 3 shrinks dramatically. As a result, several of the other clusters grew in size. When the data is partitioned, the clusters appear to be more uniformly spread over the 12 clusters, according to the graphic.

Assignment Task D

#“The elementary public schools would like to choose a set of cereals to include in their daily cafeterias. Every day a different cereal is offered, but all cereals should support a healthy diet. For this goal, you are requested to find a cluster of “healthy cereals.” Should the data be normalized? If not, how should they be used in the cluster analysis?”

#Normalizing the data would be inappropriate in this circumstance. This is due to the fact that the scaling or normalization of cereal nutrition data is dependent on the exact sample of cereal being investigated. As a result, the data set gathered may only include cereals with extremely high sugar content but poor fiber, iron, and other nutritious features. When the data inside the sample set is scaled or normalized, estimating the nutritional value of the cereal for a child becomes impossible. An uneducated observer could believe that a cereal with an iron score of 0.999 provides virtually all of a child’s needed iron; yet, it could just be the best among the worst in the sample set, providing little to no iron.

#As a result, a better way to preprocess the data would be to make it a ratio to a child’s daily prescribed calories, fiber, carbohydrates, and so on. This would allow analysts to make more educated decisions on clusters when reviewing them, while not allowing a few larger variables to trump distance calculations. An analyst might evaluate the cluster averages to calculate what percentage of a student’s daily needed nutrition would come from XX cereal while evaluating the clusters. This would enable the staff to make more educated selections about which “healthy” cereal clusters to select.