CMDA--3654

Homework 9

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Due as a .pdf upload

Problem 1: [50 pts] k-means clustering

Consider the Hotdog dataset shown in hotdogs.csv. Load in the data but ignore the first column as we'll pretend we know nothing other than the Sodium and Calorie content of the hotdogs.

a. Carry out K-means clustering with 2, 3, 4, 5 clusters. Don't forget to scaled the data first using:

```
#Loading libraries and reading csv file
library(cluster)
library(tidyverse)
hotdogs<-read.csv("/Users/eduardosalvador/Desktop/FINAL\ Spring\ Semester\ 2021/CMDA\ /Assignments/HW9/hotdogs
hotdogs.scaled <- scale(hotdogs [, 2:3])
#Using kmeans function to get kmean for 2,3,4,5 clusters
kmeans2<-kmeans(hotdogs.scaled,centers=2,nstart = 25)
kmeans2
kmeans3<-kmeans(hotdogs.scaled,centers=3,nstart = 25)
kmeans3
kmeans4<-kmeans (hotdogs.scaled,centers=4,nstart = 25)
kmeans4
kmeans5<-kmeans (hotdogs.scaled,centers=5,nstart = 25)
kmeans5</pre>
```

b. Plot the clusters from part (a) using ggplot() and assigning different colors and plot characters to the clusters found using kmeans().

Hint: If km.result <- kmeans(....), then the cluster assignments are in km.result\$cluster, then simply add this to a new data.frame:

```
#Converting to scaled and dataframe
hotdogs2.scaled <- cbind(hotdogs.scaled, "cluster" = as.factor(kmeans2$cluster))
hotdogs2_df <-data.frame(hotdogs2.scaled)
hotdogs3.scaled <- cbind(hotdogs.scaled, "cluster" = as.factor(kmeans3$cluster))
hotdogs3_df<-data.frame(hotdogs3.scaled)
hotdogs4.scaled <- cbind(hotdogs.scaled, "cluster" = as.factor(kmeans4$cluster))
hotdogs4 df<-data.frame(hotdogs4.scaled)</pre>
hotdogs5.scaled <- cbind(hotdogs.scaled, "cluster" = as.factor(kmeans5$cluster))
hotdogs5_df<-data.frame(hotdogs5.scaled)
#Creating ggplot for kmean cluster 2
ggplot(hotdogs2_df,aes(x=Sodium,y=Calories,color=cluster))+theme_bw()+geom_point()
#Creating ggplot for kmean cluster 3
ggplot(hotdogs3_df,aes(x=Sodium,y=Calories,color=cluster))+theme_bw()+geom_point()
#Creating ggplot for kmean cluster 4
ggplot(hotdogs4_df,aes(x=Sodium,y=Calories,color=cluster))+theme_bw()+geom_point()
#Creating ggplot for kmean cluster 5
ggplot(hotdogs5_df,aes(x=Sodium,y=Calories,color=cluster))+theme_bw()+geom_point()
```

and then use ggplot() accordingly to make the plot.

c. Install and earble the following R libraries: cluster, NbClust, factoextra. Then use the fviz_cluster() function to vizualize the clusters you made in part (a). Here is an example of how to use it.

```
library(ggplot2)
library(factoextra)
library(cluster)
library(NbClust)
fviz_cluster(kmeans2, data = hotdogs2.scaled)
fviz_cluster(kmeans3, data = hotdogs3.scaled)
fviz_cluster(kmeans4, data = hotdogs4.scaled)
fviz_cluster(kmeans5, data = hotdogs5.scaled)
```

Determining the optimal number of clusters.

Recall that the basic idea behind partitioning methods, such as k-means clustering, is to define clusters such that the total within-cluster variation or total within-cluster sum of squares is minimized: That is,

$$minimize\left(\sum_{i=1}^{k}W(C_{k})\right)$$

There are a number of methods that we can use to determine the optimal number of clusters that should be used. One such method is called the Elbow Method which plots the total within-cluster sum of squares versus number of clusters.

We can obtain the total within-cluster sum of squares using km.result\$tot.withinss.

The elbow method suggest that you find the "elbow" of this plot, where the total within-cluster sum of squares essentially stops reducing signficantly as the number of clusters grows.

Thankfully I can save you from this the long way by telling you about a function that can do this automatically.

d. Use the function fviz_nbclust(hotdogs.scaled, kmeans, method = "wss") to produce a plot using the Elbow method. Using this plot, determine how many clusters you think should be used.

```
#Using function to produce a plot using the Elbow method
#fviz_nbclust(hotdogs2.scaled, kmeans, method = "wss")
#For some reason it didn't let me knit using fviz_nbclust function but. plot did come out
#I believe I should use 4 clusters since the line after 4 becomes increasingly similar.
```

Discussion: There are other methods for determining the optimal number of clusters that are more sophisticated such as the average silhouette method and the gap statistic method, but these are beyond the scope of this course.

Problem 2: [50 pts] Hierarchical Clustering.

Consider the mtcars dataset.

a. Using Euclidean distance as the dissimilarity measure, perform hierarchical clustering on the data, with (i) Complete Linkage, (ii) Average Linkage, and (iii) Single Linkage. Don't forget that you need to scale the data and compute the distances before using the hclust() function.

```
#Scaling mt cars data
mtcars.scaled<-scale(mtcars)
#Get distance mtcars
dist.mtcars<-dist(mtcars.scaled)

#Performing hierarchical clustering with Complete Linkage
complete.mtcars<-hclust(dist.mtcars)

#Performing hierarchical clustering with Average Linkage
average.mtcars<-hclust(dist.mtcars,method = "average")

#Performing hierarchical clustering with Single Linkage
single.mtcars<-hclust(dist.mtcars,method = "single")</pre>
```

b. For all three methods in (a), cut the hierarchical clustering tree at 4 clusters and report the two-way table of the car name and the cluster it belongs to.

```
#Cutting the complete linkage tree at 4 clusters
complete.cut<-cutree(complete.mtcars,4)
#Reporting two-way table of the car name and the cluster
complete.table<-table(rownames(mtcars),complete.cut)

#Cutting the average linkage tree at 4 clusters
average.cut<-cutree(average.mtcars,4)
#Reporting two-way table of the car name and the cluster
average.table<-table(rownames(mtcars),average.cut)

#Cutting the single linkage tree at 4 clusters
single.cut<-cutree(single.mtcars,4)
#Reporting two-way table of the car name and the cluster
single.table<-table(rownames(mtcars),single.cut)

#Displaying tables
complete.table</pre>
```

	complete.cut			
	1	2	3	4
AMC Javelin	0	0	0	1
${\tt Cadillac\ Fleetwood}$	0	0	0	1
Camaro Z28	0	0	0	1
Chrysler Imperial	0	0	0	1
Datsun 710	0	1	0	0
Dodge Challenger	0	0	0	1
Duster 360	0	0	0	1
Ferrari Dino	1	0	0	0
Fiat 128	0	1	0	0
Fiat X1-9	0	1	0	0
Ford Pantera L	1	0	0	0

Honda Civic	0	1	0	0
Hornet 4 Drive	0	0	1	0
Hornet Sportabout	0	0	0	1
Lincoln Continental	0	0	0	1
Lotus Europa	0	1	0	0
Maserati Bora	1	0	0	0
Mazda RX4	1	0	0	0
Mazda RX4 Wag	1	0	0	0
Merc 230	0	0	1	0
Merc 240D	0	0	1	0
Merc 280	0	0	1	0
Merc 280C	0	0	1	0
Merc 450SE	0	0	0	1
Merc 450SL	0	0	0	1
Merc 450SLC	0	0	0	1
Pontiac Firebird	0	0	0	1
Porsche 914-2	0	1	0	0
Toyota Corolla	0	1	0	0
Toyota Corona	0	0	1	0
Valiant	0	0	1	0
Volvo 142E	0	1	0	0

average.table

	ave	average.cut		
	1	2	3	4
AMC Javelin	0	0	1	0
Cadillac Fleetwood	0	0	1	0
Camaro Z28	0	0	1	0
Chrysler Imperial	0	0	1	0
Datsun 710	1	0	0	0
Dodge Challenger	0	0	1	0
Duster 360	0	0	1	0
Ferrari Dino	1	0	0	0
Fiat 128	1	0	0	0
Fiat X1-9	1	0	0	0
Ford Pantera L	0	0	0	1
Honda Civic	1	0	0	0
Hornet 4 Drive	0	1	0	0
Hornet Sportabout	0	0	1	0
Lincoln Continental	. 0	0	1	0
Lotus Europa	1	0	0	0
Maserati Bora	0	0	0	1
Mazda RX4	1	0	0	0
Mazda RX4 Wag	1	0	0	0
Merc 230	0	1	0	0
Merc 240D	0	1	0	0
Merc 280	0	1	0	0
Merc 280C	0	1	0	0
Merc 450SE	0	0	1	0
Merc 450SL	0	0	1	0
Merc 450SLC	0	0	1	0
Pontiac Firebird	0	0	1	0
Porsche 914-2	1	0	0	0
Toyota Corolla	1	0	0	0
Toyota Corona	0	1	0	0
Valiant	0	1	0	0
Volvo 142E	1	0	0	0

single.table

```
single.cut
                  1 2 3 4
AMC Javelin
             0 1 0 0
Cadillac Fleetwood 0 1 0 0
Camaro Z28 0 1 0 0
Chrysler Imperial 0 1 0 0
Datsun 710
            1 0 0 0
Dodge Challenger 0 1 0 0
Duster 360 0 1 0 0
Ferrari Dino
                1 0 0 0
                 1 0 0 0
Fiat 128
Fiat X1-9 1 0 0 0 Ford Pantera L 0 0 1 0
Honda Civic
                 1 0 0 0
Hornet 4 Drive 1 0 0 0
Hornet Sportabout 0 1 0 0
Lincoln Continental 0 1 0 0
Lotus Europa 1 0 0 0
               0 0 0 1
Maserati Bora
Mazda RX4
                 1 0 0 0
                1 0 0 0
Mazda RX4 Wag
Merc 230
                 1 0 0 0
Merc 240D
                 1 0 0 0
Merc 280
                1 0 0 0
Merc 280C
                 1 0 0 0
Merc 450SE
                0 1 0 0
Merc 450SL 0 1 0 0
Merc 450SLC 0 1 0 0
Pontiac Firebird 0 1 0 0
Porsche 914-2
                 1 0 0 0
Toyota Corolla 1 0 0 0 Toyota Corona 1 0 0 0
Valiant
                 1 0 0 0
             1 0 0 0
Volvo 142E
```

c. We can plot the dendrograms easily enough by doing the following:

```
plot(complete.mtcars, labels = rownames(mtcars),
    main = "Cluster Dendrogram (Complete Linkage)")
```

Where the above would plot the dendrogram for the Complete Linkage case. Provide this plot and repeat the above for the other 2 cases from part (a). Alternatively we can use the following library that makes use of ggplot2, called ggdendro.

```
library(ggplot2)
library(ggdendro)
# Vertical
ggdendrogram(complete.mtcars) + labs(title = "Cluster Dendrogram (Complete Linkage)")
# or horizontal with a different theme
ggdendrogram(complete.mtcars, rotate = T, theme_dendro = F) +
    labs(title = "Cluster Dendrogram (Complete Linkage)")

# Vertical Average Linkage
ggdendrogram(average.mtcars) + labs(title = "Cluster Dendrogram (Average Linkage)")
# or horizontal with a different theme Average Linkage
ggdendrogram(average.mtcars, rotate = T, theme_dendro = F) +
    labs(title = "Cluster Dendrogram (Average Linkage)")
```

```
# Vertical Single Linkage
ggdendrogram(single.mtcars) + labs(title = "Cluster Dendrogram (Single Linkage)")
# or horizontal with a different theme Single Linkage
ggdendrogram(single.mtcars, rotate = T, theme_dendro = F) +
labs(title = "Cluster Dendrogram (Single Linkage)")
```

Some alternative tools for plotting & customizing dendrograms can be found here: http://www.sthda.com/english/wiki/beautiful-dendrogram-visualizations-in-r-5-must-known-methods-unsupervised-machine-learning

Section 5 has some really cool examples of how to colorize clusters, etc.

Another awesome example can be found here: https://www.r-graph-gallery.com/340-custom-your-dendrogram-with-dendextend/

d. Use the elbow method to determine the optimal number of clusters that you should use. This works the same basic way as in problem 1, but the call is slightly different because it needs to use the hcut() function (named without the ()) as an option as seen below.

```
fviz_nbclust(mtcars.scaled, hcut, method = "wss")
```

e. Add colored rectangles around the clusters you have determined in part (d) to the dendrogram in part (c). You can simply run the following line after the plot in (c) if you used the first method (other methods required other functions).

library(dendextend)

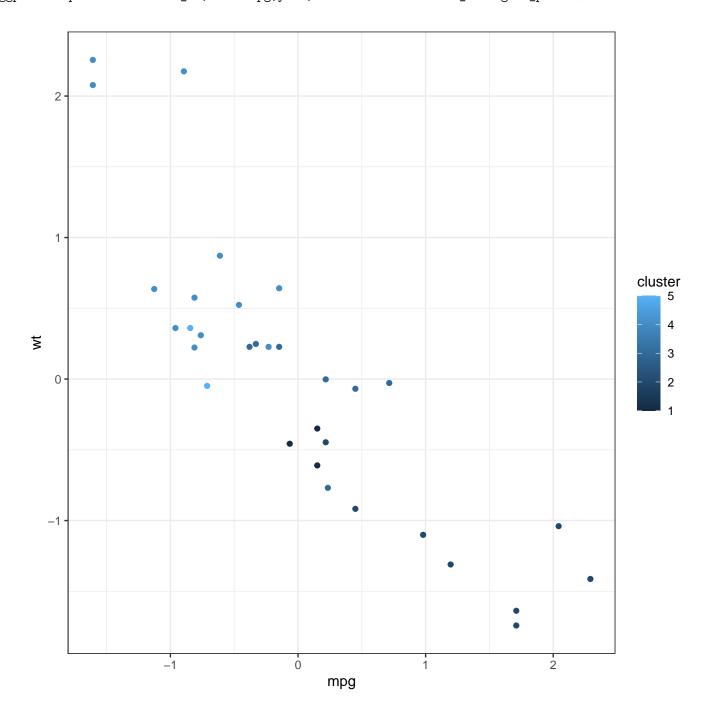
f. Use cutree() to obtain the cluster assignments using your decision in (d). Recode this as a factor object. Plot the mpg versus wt and use the different colors according to your cluster assignment.

```
library(ggplot2)
#Using cutree() to obtain the cluster assignments for every linkage and converting to dataframe
comp.cluster.mtcars <- cbind(mtcars.scaled, "cluster" = as.factor(cutree(complete.mtcars,h=4)))
comp.cluster.mtcars_df<-data.frame(comp.cluster.mtcars)</pre>
```

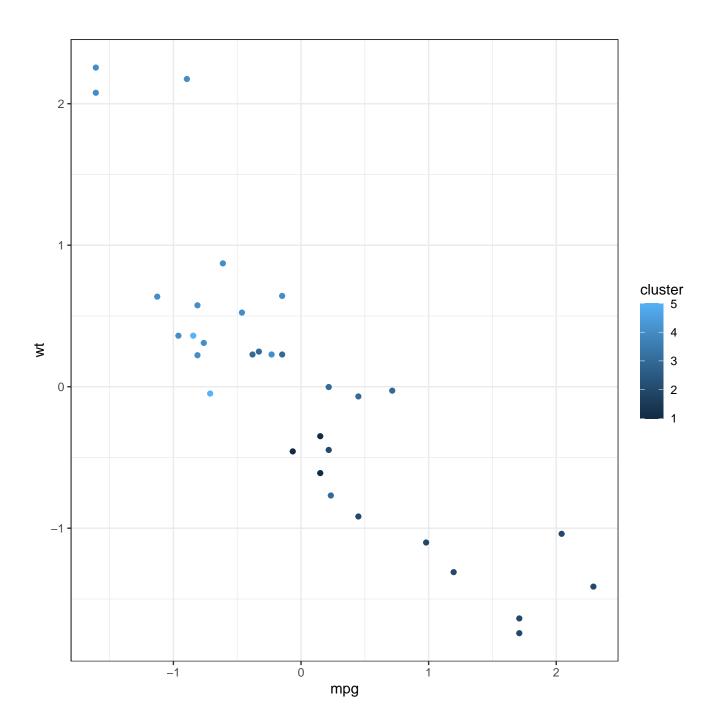
```
av.cluster.mtcars <- cbind(mtcars.scaled, "cluster" = as.factor(cutree(average.mtcars,h=4)))
av.cluster.mtcars_df<-data.frame(comp.cluster.mtcars)

sing.cluster.mtcars <- cbind(mtcars.scaled, "cluster" = as.factor(cutree(single.mtcars,h=4)))
sing.cluster.mtcars_df<-data.frame(comp.cluster.mtcars)

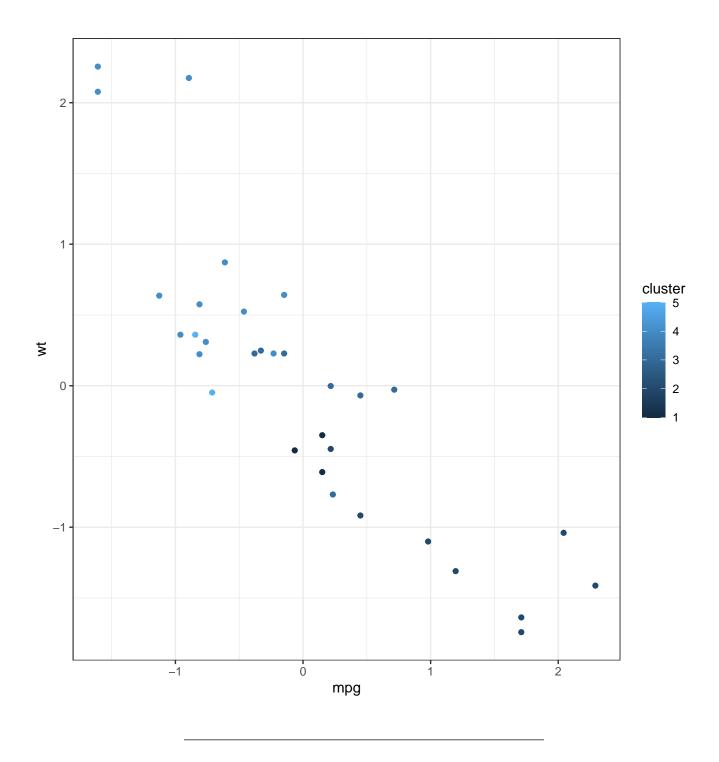
#Plotting mpg vs wt using different colors for complete linkage
ggplot(comp.cluster.mtcars_df,aes(x=mpg,y=wt,color=cluster))+theme_bw()+geom_point()</pre>
```



#Plotting mpg vs wt using different colors for average linkage
ggplot(av.cluster.mtcars_df,aes(x=mpg,y=wt,color=cluster))+theme_bw()+geom_point()



#Plotting mpg vs wt using different colors for single linkage
ggplot(sing.cluster.mtcars_df,aes(x=mpg,y=wt,color=cluster))+theme_bw()+geom_point()



Discussion: While you can see some clustering that makes sense, some of the clusters seem to intermixed with each other. Remember, the clustering was determined not using only the mpg and wt variables alone, but using all of the information from all of the variables in the dataset. So the clusters are formed in multidimensional space. This can be difficult to visualize when the number of dimensions is bigger than 3.

One solution is to rotate the multidimensional variable coordinate system into the principal component coordinate system as we will show in the next problem. This means that if most of the variation is in the first 2 principal components, it might be possible to more easily see the clusters in higher dimensional space using the lower dimensional representation.

Problem 3: [15 pts Extra Credit] PCA + Hierarchical Clustering.

Consider the mtcars dataset once again.

a. Use PCA to rotate the observations from the mtcars dataset into a new coordinate system using the principal components. Remember that you have to do either scale. = TRUE if using prcomp() or cor = TRUE if using princomp(). We want the component scores which will either be pca.result\$x if you used prcomp() or pca.result\$scores if you use princomp().

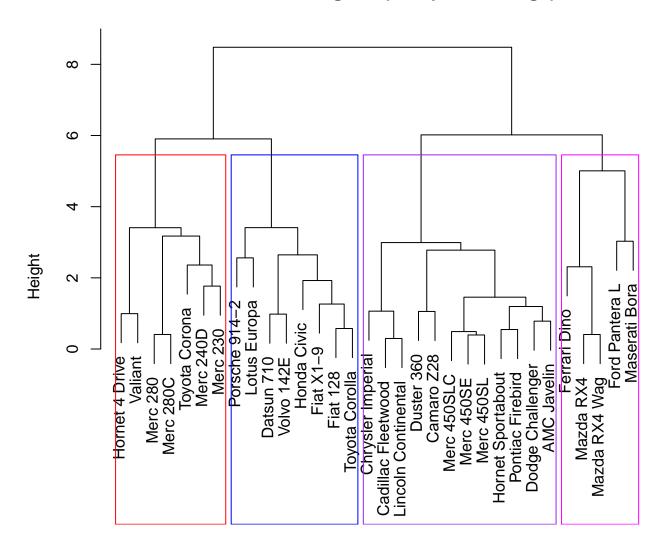
```
#PCA+Hierarchical Clustering using prcomp
pca.result<-prcomp(mtcars,scale. = T)
pca.result$x</pre>
```

	PC1	PC2	PC3	PC4
Mazda RX4	-0.6468627420			
Mazda RX4 Wag	-0.6194831460			
Datsun 710	-2.7356242748	-0.1441501	-0.2374391	
Hornet 4 Drive	-0.3068606268			
Hornet Sportabout	1.9433926844			0.074461963
Valiant	-0.0552534228			-0.975167425
Duster 360	2.9553851233			
Merc 240D	-2.0229593244			-0.142129082
Merc 230	-2.2513839535	-1.9522879	1.7689364	0.287210957
Merc 280	-0.5180912217	-0.1594610	1.4692603	0.066263362
Merc 280C	-0.5011860079	-0.3187934	1.6570701	0.094357222
Merc 450SE	2.2124096339			-0.129797905
Merc 450SL	2.0155715693	-0.6724606	-0.4768341	-0.210991001
Merc 450SLC	2.1147047372	-0.7891129	-0.2904620	-0.175332868
Cadillac Fleetwood	3.8383725118	-0.8149087	0.6370972	0.290505877
Lincoln Continental	3.8918495626	-0.7218314	0.7092612	0.405336898
Chrysler Imperial	3.5363862158	-0.4145024	0.5402468	0.665665306
Fiat 128	-3.7955510831	-0.2920783	-0.4161681	0.055191058
Honda Civic	-4.1870356784	0.6775721	-0.2035831	1.167526096
Toyota Corolla	-4.1675359344	-0.2748890	-0.4589124	0.183313028
Toyota Corona	-1.8741790870	-2.0864529	0.1543265	0.050514126
Dodge Challenger	2.1504414942	-0.9982442	-1.1503639	-0.584982249
AMC Javelin	1.8340369797	-0.8921886	-0.9472872	0.005694071
Camaro Z28	2.8434957523	0.6701037	-0.1605593	0.814340105
Pontiac Firebird	2.2105479148	-0.8600504	-1.0279577	0.146420497
Fiat X1-9	-3.5176818134	-0.1192950	-0.4464716	-0.013427353
Porsche 914-2	-2.6095003965	2.0141425	-0.8172519	0.568564789
Lotus Europa	-3.3323844512	1.3568877	-0.4467167	-1.153197531
Ford Pantera L	1.3513346957	3.4448780	-0.1343943	0.590098358
Ferrari Dino	-0.0009743305	3.1683750	0.3957610	-0.938933017
Maserati Bora	2.6270897605	4.3107016	1.3315940	-0.877332804
Volvo 142E	-2.3824711412	0.2299603	0.4052798	0.223549117
	PC5	PO	C6 P	PC7 PC8
Mazda RX4	-0.945523363	-0.016987373	33 -0.426486	552 -0.009631217
Mazda RX4 Wag	-1.016680740	-0.241724643	34 -0.416200	046 -0.084520213
Datsun 710	0.398762288	-0.348767813	38 -0.608841	.46 0.585255765
Hornet 4 Drive	0.549208936	0.019296998	34 -0.040360	75 -0.049583029
Hornet Sportabout	0.207515698	0.149192760	06 0.383508	316 -0.160297757
Valiant	0.211665375	-0.243835854	46 -0.294641	.60 0.256612420
Duster 360	0.343847875	0.712692086	68 -0.136077	92 -0.171103449
Merc 240D	-0.316651386	-0.000988939	91 0.639462	214 0.163156195
Merc 230	-0.333682355	-0.333870338	34 0.622010	34 -0.105779936
Merc 280	-0.069624161	0.816530836	65 0.161170	0.099983313
Merc 280C	-0.148803650	0.730838379	57 0.092544	30 0.197306566
Merc 450SE	-0.378611141	0.131701476	62 -0.016454	98 -0.194092435

```
Merc 450SL
                  Merc 450SLC
                  Cadillac Fleetwood -0.048245223 -0.8844735483 -0.16615296 0.138398783
Lincoln Continental
                   0.003899176 -0.8625868981 -0.19250873 0.129305868
                   0.208027112 -0.6536447300 0.03449804 -0.391104141
Chrysler Imperial
                   0.219981109 -0.4675796343 -0.03749941 -0.625278746
Fiat 128
Honda Civic
                   0.097674091 \quad 0.5180554279 \quad -0.25316291 \quad -0.395045565
Toyota Corolla
                   Toyota Corona
                   0.039299002 0.7236992559 -0.28027808
                                                       0.207237627
Dodge Challenger
                  -0.226237802 0.1062181942 0.09489585
                                                       0.316055390
AMC Javelin
                  -0.252565496
                               0.2888101997
                                            0.08161916
                                                       0.321900593
Camaro Z28
                   0.389118986  0.9468795171  -0.21157976
                                                       0.038657331
Pontiac Firebird
                   0.299261925 - 0.1983310387 \quad 0.47269865 - 0.234144182
Fiat X1-9
                   0.206753365 -0.1449905641 -0.35850305
                                                       0.089109764
Porsche 914-2
                  -0.597313744 -0.3394265065 0.82032965
                                                       0.634987241
                   0.694667640 0.0165037718 0.51018011
                                                       0.004140777
Lotus Europa
Ford Pantera L
                   1.101648091 -0.1746156635 0.41358868
                                                       0.609167214
                  -0.848833976 -0.0097569921 0.02967883
Ferrari Dino
                                                       0.014187801
Maserati Bora
                   0.455265189 -0.0156094416 -0.18813730 -0.558646792
Volvo 142E
                   0.321777017 -0.3263029217 -0.77995741 0.476634473
                          PC9
                                    PC10
                                                PC11
                   0.14642303 -0.06670350 0.179693570
Mazda RX4
Mazda RX4 Wag
                   0.07452829 -0.12692766 0.088644265
Datsun 710
                  -0.13122859 0.04573787 -0.094632914
Hornet 4 Drive
                   0.22021812 -0.06039981 0.147611269
Hornet Sportabout
                  -0.02117623 -0.05983003 0.146406899
Valiant
                  -0.03222907 -0.20165466
                                         0.019545064
Duster 360
                  -0.17844547 0.36086641 0.171863162
Merc 240D
                   Merc 230
                  -0.86455356 -0.11597058
                                        0.159688512
Merc 280
                   0.54092449 -0.22093750 -0.124486227
Merc 280C
                   0.30876072 -0.34417564 -0.034578568
Merc 450SE
                  -0.05614966 -0.06531727 -0.396445135
Merc 450SL
                  -0.20501055 -0.10761308 -0.197616838
Merc 450SLC
                  -0.38704169 -0.21191036 -0.142498830
Cadillac Fleetwood
                   0.19333387  0.06184979  0.262886205
Lincoln Continental 0.19523562 0.12094849
                                         0.039191100
Chrysler Imperial
                   0.27447514 0.27588169 -0.224420191
Fiat 128
                   0.10550311 -0.02717077 -0.208865888
Honda Civic
                   0.23711675 -0.15433928 0.246835364
Toyota Corolla
                  -0.11313627 -0.12606845 -0.031747839
Toyota Corona
                  Dodge Challenger
                   0.10435633 -0.13641143 0.049594456
AMC Javelin
                  -0.12237636 -0.29628634 0.045293027
Camaro Z28
                  -0.05282991 0.32624525 -0.099386307
Pontiac Firebird
                   0.20849043 0.01547674 0.122593248
Fiat X1-9
                  -0.02228967 -0.08414018 -0.005746448
Porsche 914-2
                  -0.12999660 0.34968156 -0.111596656
Lotus Europa
                   0.29680350 0.23980308 0.030015592
Ford Pantera L
                  -0.23280792 -0.50262890 -0.042242570
Ferrari Dino
                   0.09813571 0.14491815 0.043006835
Maserati Bora
                  -0.34081133 0.04706368 0.062135486
Volvo 142E
                  -0.04473670 0.11767108 -0.145329008
```

b. For the principal component "variables" for the cars (which are the component scores), use the hierarchical clustering techniques that you learned in Problem 2. Use this to determine the optimal number of clusters, show the dendrogram and put a box around these clusters. **Use Complete Linkage only.** How does this compare with your answer result from the previous problem when you used complete linkage on the original variables?

Cluster Dendrogram (Complete Linkage)



dist_pca
hclust (*, "complete")

#It gives me the same answer as the previous problem when used complete linkage

c. Using k=4 for the number of clusters, plot PC2 versus PC1 and use different colors to show the clusters. You will need to use cutree() to get the cluster assignments. Can you see the clusters a bit better than you did compared to plotting mpg versus wt in the previous problem?

#Getting cluster assignments using cutree()
as_cluster<-as.factor(cutree(pca.cluster.comp,h=4))</pre>