lab08_backup

Karina Cardenas

Table of contents

Background

The goal of this mini-project is for you to explore a complete analysis using the unsupervised learning techniques covered in class. You'll extend what you've learned by combining PCA as a preprocessing step to clustering using data that consist of measurements of cell nuclei of human breast masses. This expands on our RNA-Seq analysis from last day.

The mini project explores unsupervised learning techniques covered in class. interpreting principal component analysis (PCA) to reduce the dimensional of the data while retaining variance, and applying hierarchical clustering with different linkage methods. It also includes an optional section on K-means clustering for comparison. The ultimate goal is to combine PCA and clustering to better separate benign and malignant cell samples evaluating the results using metrics like sensitivity and specificity and finally demonstrating how to predict he classification of new samples using the developed PCA model.

Data Import

Our data comes from the University of Wisconsin Medical Center. Omit the ID column from the dataset.

```
# Save your input data file into your Project directory
fna.data <- "WisconsinCancer.csv"

# Complete the following code to input the data and store as wisc.df
wisc.df <- read.csv(fna.data, row.names=1)

head(wisc.df)
```

```
         diagnosis radius_mean texture_mean perimeter_mean area_mean
842302           M       17.99        10.38         122.80    1001.0
842517           M       20.57        17.77         132.90    1326.0
84300903         M       19.69        21.25         130.00    1203.0
84348301         M       11.42        20.38          77.58     386.1
84358402         M       20.29        14.34         135.10    1297.0
843786           M       12.45        15.70          82.57     477.1
         smoothness_mean compactness_mean concavity_mean concave.points_mean
842302           0.11840          0.27760         0.3001             0.14710
842517           0.08474          0.07864         0.0869             0.07017
84300903         0.10960          0.15990         0.1974             0.12790
84348301         0.14250          0.28390         0.2414             0.10520
84358402         0.10030          0.13280         0.1980             0.10430
843786           0.12780          0.17000         0.1578             0.08089
         symmetry_mean fractal_dimension_mean radius_se texture_se perimeter_se
842302          0.2419                0.07871    1.0950     0.9053        8.589
842517          0.1812                0.05667    0.5435     0.7339        3.398
84300903        0.2069                0.05999    0.7456     0.7869        4.585
84348301        0.2597                0.09744    0.4956     1.1560        3.445
84358402        0.1809                0.05883    0.7572     0.7813        5.438
843786          0.2087                0.07613    0.3345     0.8902        2.217
         area_se smoothness_se compactness_se concavity_se concave.points_se
842302    153.40      0.006399        0.04904      0.05373           0.01587
842517     74.08      0.005225        0.01308      0.01860           0.01340
84300903   94.03      0.006150        0.04006      0.03832           0.02058
84348301   27.23      0.009110        0.07458      0.05661           0.01867
84358402   94.44      0.011490        0.02461      0.05688           0.01885
843786     27.19      0.007510        0.03345      0.03672           0.01137
         symmetry_se fractal_dimension_se radius_worst texture_worst
```

```
842302       0.03003             0.006193       25.38         17.33
842517       0.01389             0.003532       24.99         23.41
84300903     0.02250             0.004571       23.57         25.53
84348301     0.05963             0.009208       14.91         26.50
84358402     0.01756             0.005115       22.54         16.67
843786       0.02165             0.005082       15.47         23.75
         perimeter_worst area_worst smoothness_worst compactness_worst
842302            184.60     2019.0           0.1622            0.6656
842517            158.80     1956.0           0.1238            0.1866
84300903          152.50     1709.0           0.1444            0.4245
84348301           98.87      567.7           0.2098            0.8663
84358402          152.20     1575.0           0.1374            0.2050
843786            103.40      741.6           0.1791            0.5249
         concavity_worst concave.points_worst symmetry_worst
842302            0.7119               0.2654         0.4601
842517            0.2416               0.1860         0.2750
84300903          0.4504               0.2430         0.3613
84348301          0.6869               0.2575         0.6638
84358402          0.4000               0.1625         0.2364
843786            0.5355               0.1741         0.3985
         fractal_dimension_worst
842302                   0.11890
842517                   0.08902
84300903                 0.08758
84348301                 0.17300
84358402                 0.07678
843786                   0.12440
```

Q. How many patient/samples are in this dataset? `nrow()`

```
nrow(wisc.df)
```

```
[1] 569
```

Q. How many of the observations have a malignant diagnosis? `table()`

```
#summarizes the quantity of diagnosis by malignant or benign
table(wisc.df$diagnosis)
```

```

  B   M 
357 212 
```

```r
#sums the number of malignant diagnosis
sum(wisc.df$diagnosis == "M")
```

```
[1] 212
```

> Q. How many variables/features in the data are suffixed with `_mean`?

```r
#column names
colnames(wisc.df)
```

```
 [1] "diagnosis"               "radius_mean"            
 [3] "texture_mean"            "perimeter_mean"         
 [5] "area_mean"               "smoothness_mean"        
 [7] "compactness_mean"        "concavity_mean"         
 [9] "concave.points_mean"     "symmetry_mean"          
[11] "fractal_dimension_mean"  "radius_se"              
[13] "texture_se"              "perimeter_se"           
[15] "area_se"                 "smoothness_se"          
[17] "compactness_se"          "concavity_se"           
[19] "concave.points_se"       "symmetry_se"            
[21] "fractal_dimension_se"    "radius_worst"           
[23] "texture_worst"           "perimeter_worst"        
[25] "area_worst"              "smoothness_worst"       
[27] "compactness_worst"       "concavity_worst"        
[29] "concave.points_worst"    "symmetry_worst"         
[31] "fractal_dimension_worst"
```

```r
#dimensions
dim(wisc.df)
```

```
[1] 569  31
```

```r
#grep gives index of which columns contain mean
length(grep("mean",colnames(wisc.df)))
```

```
[1] 10
```

Cleaning the Data

There is a diangosis column that is the clincian conensus that I want to exclude from any further analysis. We will come back later and comapre our results to this, so omit the Diagnosis column.

```
# We can use -1 here to remove the first column
wisc.data <- wisc.df[,-1]

head(wisc.data)
```

```
         radius_mean texture_mean perimeter_mean area_mean smoothness_mean
842302         17.99        10.38         122.80    1001.0         0.11840
842517         20.57        17.77         132.90    1326.0         0.08474
84300903       19.69        21.25         130.00    1203.0         0.10960
84348301       11.42        20.38          77.58     386.1         0.14250
84358402       20.29        14.34         135.10    1297.0         0.10030
843786         12.45        15.70          82.57     477.1         0.12780
         compactness_mean concavity_mean concave.points_mean symmetry_mean
842302            0.27760         0.3001             0.14710        0.2419
842517            0.07864         0.0869             0.07017        0.1812
84300903          0.15990         0.1974             0.12790        0.2069
84348301          0.28390         0.2414             0.10520        0.2597
84358402          0.13280         0.1980             0.10430        0.1809
843786            0.17000         0.1578             0.08089        0.2087
         fractal_dimension_mean radius_se texture_se perimeter_se area_se
842302                  0.07871    1.0950     0.9053        8.589  153.40
842517                  0.05667    0.5435     0.7339        3.398   74.08
84300903                0.05999    0.7456     0.7869        4.585   94.03
84348301                0.09744    0.4956     1.1560        3.445   27.23
84358402                0.05883    0.7572     0.7813        5.438   94.44
843786                  0.07613    0.3345     0.8902        2.217   27.19
         smoothness_se compactness_se concavity_se concave.points_se
842302        0.006399        0.04904      0.05373           0.01587
842517        0.005225        0.01308      0.01860           0.01340
84300903      0.006150        0.04006      0.03832           0.02058
84348301      0.009110        0.07458      0.05661           0.01867
84358402      0.011490        0.02461      0.05688           0.01885
843786        0.007510        0.03345      0.03672           0.01137
         symmetry_se fractal_dimension_se radius_worst texture_worst
842302       0.03003             0.006193        25.38         17.33
842517       0.01389             0.003532        24.99         23.41
```

```
84300903     0.02250              0.004571        23.57         25.53
84348301     0.05963              0.009208        14.91         26.50
84358402     0.01756              0.005115        22.54         16.67
843786       0.02165              0.005082        15.47         23.75
         perimeter_worst area_worst smoothness_worst compactness_worst
842302            184.60     2019.0           0.1622            0.6656
842517            158.80     1956.0           0.1238            0.1866
84300903          152.50     1709.0           0.1444            0.4245
84348301           98.87      567.7           0.2098            0.8663
84358402          152.20     1575.0           0.1374            0.2050
843786            103.40      741.6           0.1791            0.5249
         concavity_worst concave.points_worst symmetry_worst
842302            0.7119               0.2654         0.4601
842517            0.2416               0.1860         0.2750
84300903          0.4504               0.2430         0.3613
84348301          0.6869               0.2575         0.6638
84358402          0.4000               0.1625         0.2364
843786            0.5355               0.1741         0.3985
         fractal_dimension_worst
842302                   0.11890
842517                   0.08902
84300903                 0.08758
84348301                 0.17300
84358402                 0.07678
843786                   0.12440
```

```r
diagnosis <- as.factor(wisc.df$diagnosis)

head(diagnosis)
```

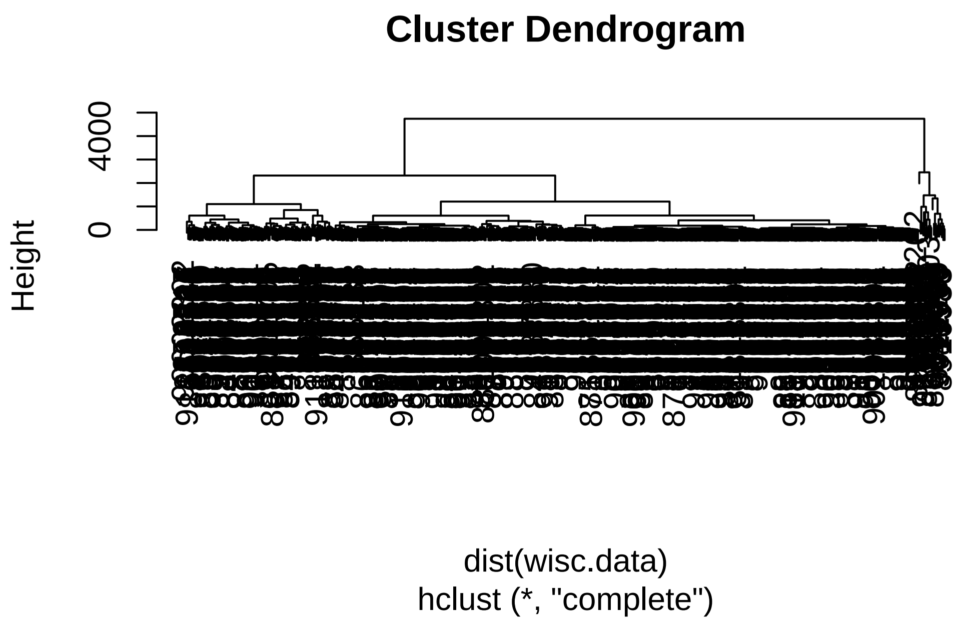
```
[1] M M M M M M
Levels: B M
```

Clustering

Let's try `hclust()`

```r
hc <- hclust(dist(wisc.data))

plot(hc)
```



We can extract clusters from this rather poor dendrogram/tree with the `cutree()`

```
grps <- cutree(hc, k = 2)
```

How many individuals in each cluster

```
table(grps)
```

```
grps
  1   2 
549  20 
```

We can generate a cross-table that compares our cluster `grps` vector

```
#tells
table(diagnosis, grps)
```

```
         grps
diagnosis   1   2
        B 357   0
        M 192  20
```

Principal Component Analysis (PCA)

The Importance of scaling

The main function for PCA in base R is `prcomp()` it has a default input parameter of `scale = FALSE`.

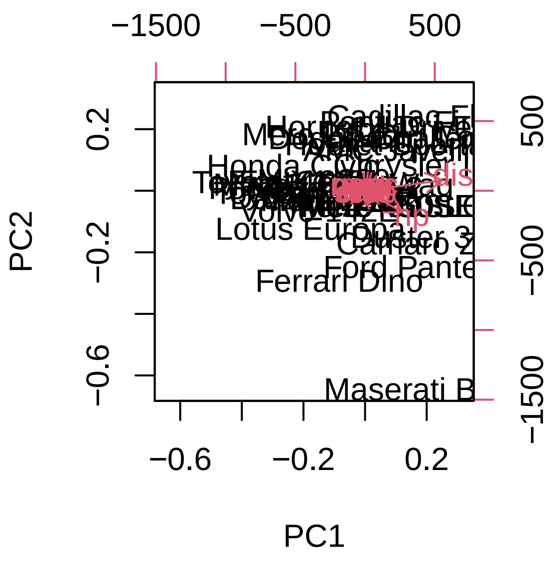
```
#prcomp()
head(mtcars)
```

```
                   mpg cyl disp  hp drat    wt  qsec vs am gear carb
Mazda RX4         21.0   6  160 110 3.90 2.620 16.46  0  1    4    4
Mazda RX4 Wag     21.0   6  160 110 3.90 2.875 17.02  0  1    4    4
Datsun 710        22.8   4  108  93 3.85 2.320 18.61  1  1    4    1
Hornet 4 Drive    21.4   6  258 110 3.08 3.215 19.44  1  0    3    1
Hornet Sportabout 18.7   8  360 175 3.15 3.440 17.02  0  0    3    2
Valiant           18.1   6  225 105 2.76 3.460 20.22  1  0    3    1
```

We could do a PCA of this data as is and it could be misleading...

```
pc <- prcomp(mtcars)

biplot(pc)
```



Lets look at the mean values of each column and their standard deviation

```r
colMeans(mtcars)
```

```
       mpg        cyl       disp         hp       drat         wt       qsec 
 20.090625   6.187500 230.721875 146.687500   3.596563   3.217250  17.848750 
        vs         am       gear       carb 
  0.437500   0.406250   3.687500   2.812500 
```

```r
apply(mtcars, 2, sd)
```

```
        mpg         cyl        disp          hp        drat          wt 
  6.0269481   1.7859216 123.9386938  68.5628685   0.5346787   0.9784574 
       qsec          vs          am        gear        carb 
  1.7869432   0.5040161   0.4989909   0.7378041   1.6152000 
```

We can "scale" this data data before PCA to get a much better representation and analysis of all the columns.

```r
mtscale <- scale(mtcars)
```

```r
round(colMeans(mtscale))
```

```
 mpg  cyl disp   hp drat   wt qsec   vs   am gear carb 
   0    0    0    0    0    0    0    0    0    0    0 
```

```r
apply(mtscale, 2, sd)
```

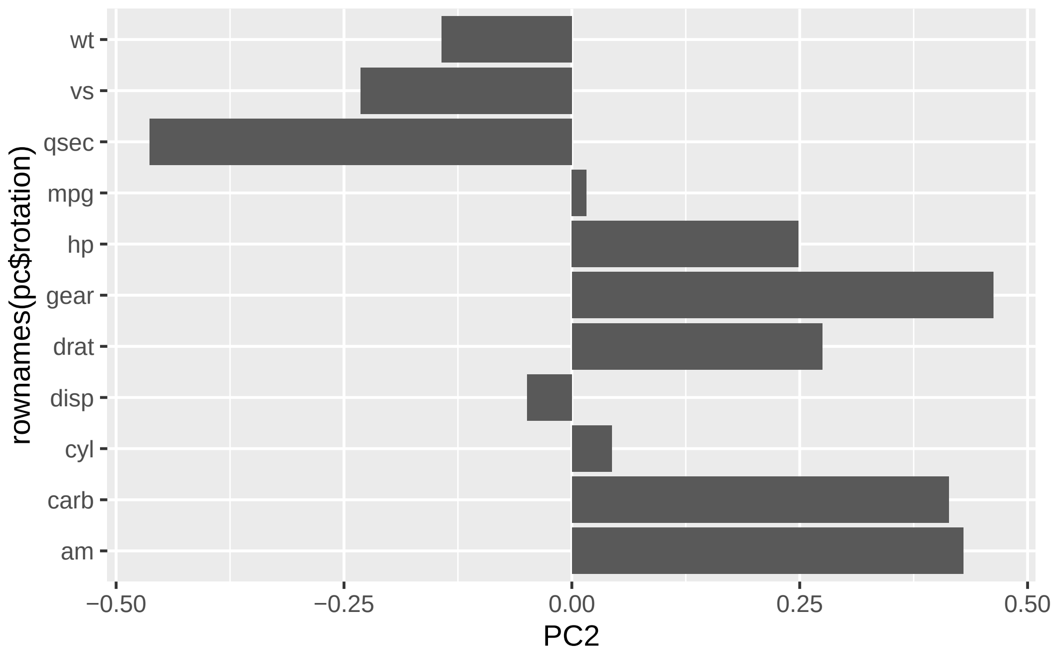
```
 mpg  cyl disp   hp drat   wt qsec   vs   am gear carb 
   1    1    1    1    1    1    1    1    1    1    1 
```

```r
pc.scale <- prcomp(mtscale)
```

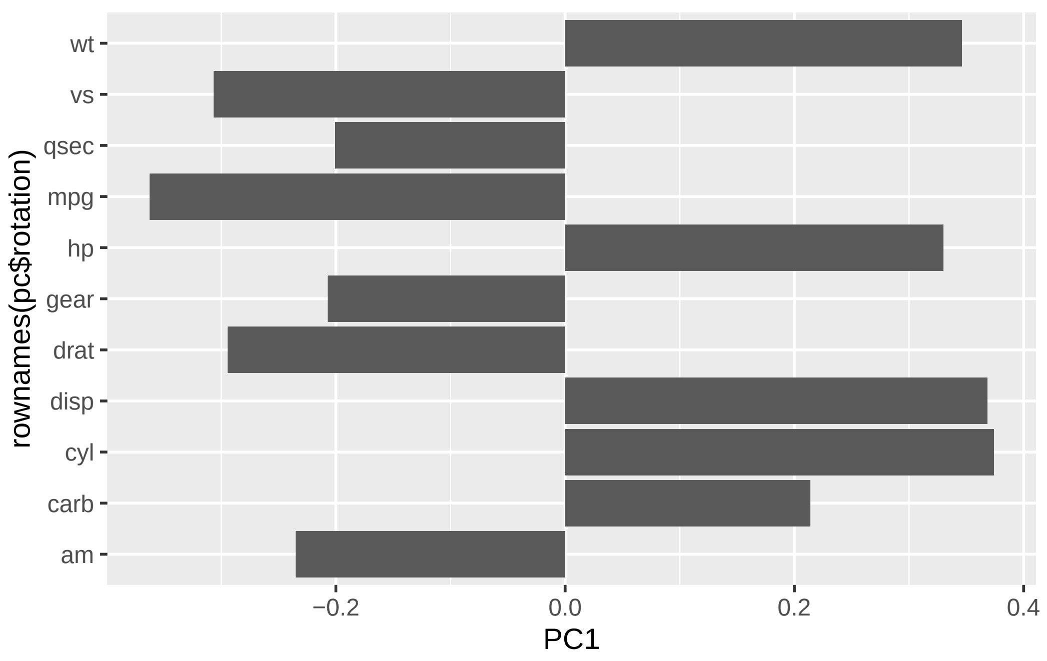
We can look at the two main results figures from PCA - the "PC plot" aka (score plot, ordienation plot, or PC1 vs PC2 plot). The "loadings plot" how the original variables contribute to the new PCs

```r
library(ggplot2)

ggplot(pc.scale$rotation) +
       aes(PC2, rownames(pc$rotation)) +
      geom_col()
```



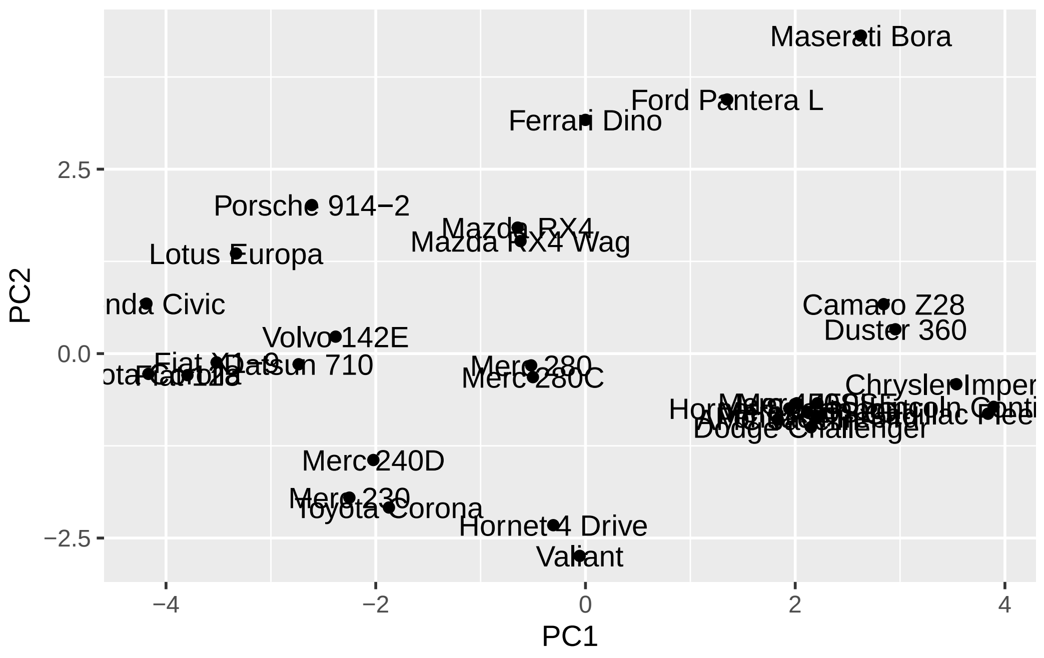
```r
ggplot(pc.scale$rotation) +
  aes(PC1, rownames(pc$rotation)) +
  geom_col()
```



PC plot of scaled PCA results

```r
library(ggrepel)

ggplot(pc.scale$x) +
  aes(PC1, PC2, label = rownames(pc.scale$x)) +
  geom_point() +
  geom_text()
```



Key point: In general we will set `scale = TRUE` when we do PCA. This is not the default but porably should be…

Scaling the Wisconsin data

We can check the SD and mean of the different columns in `wisc.data` to see if we need to scale - hint: we do !

```r
wisc.pr <- prcomp(wisc.data, scale = TRUE)
```

To see how well PCA is doing here in terms of capturing the variance(spread) in the data we can use the `sumarry()` function

```r
summary(wisc.pr)
```

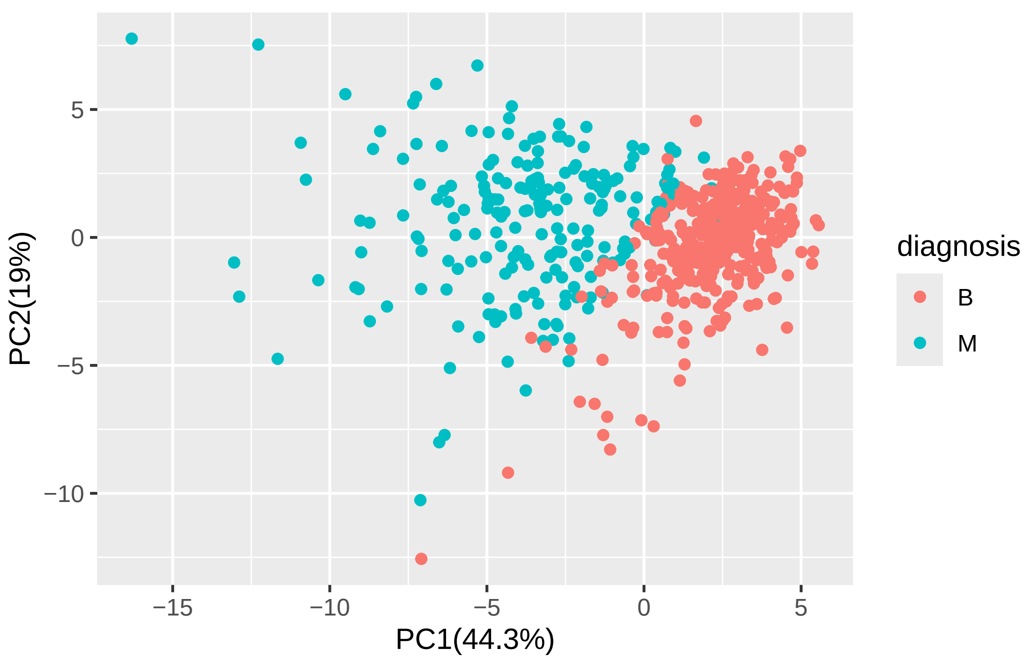
```
Importance of components:
                          PC1    PC2     PC3     PC4     PC5     PC6     PC7
Standard deviation     3.6444 2.3857 1.67867 1.40735 1.28403 1.09880 0.82172
Proportion of Variance 0.4427 0.1897 0.09393 0.06602 0.05496 0.04025 0.02251
Cumulative Proportion  0.4427 0.6324 0.72636 0.79239 0.84734 0.88759 0.91010
                           PC8    PC9    PC10   PC11    PC12    PC13    PC14
```

```
Standard deviation     0.69037 0.6457 0.59219 0.5421 0.51104 0.49128 0.39624
Proportion of Variance 0.01589 0.0139 0.01169 0.0098 0.00871 0.00805 0.00523
Cumulative Proportion  0.92598 0.9399 0.95157 0.9614 0.97007 0.97812 0.98335
                          PC15    PC16    PC17    PC18    PC19    PC20   PC21
Standard deviation     0.30681 0.28260 0.24372 0.22939 0.22244 0.17652 0.1731
Proportion of Variance 0.00314 0.00266 0.00198 0.00175 0.00165 0.00104 0.0010
Cumulative Proportion  0.98649 0.98915 0.99113 0.99288 0.99453 0.99557 0.9966
                          PC22    PC23   PC24    PC25    PC26    PC27    PC28
Standard deviation     0.16565 0.15602 0.1344 0.12442 0.09043 0.08307 0.03987
Proportion of Variance 0.00091 0.00081 0.0006 0.00052 0.00027 0.00023 0.00005
Cumulative Proportion  0.99749 0.99830 0.9989 0.99942 0.99969 0.99992 0.99997
                          PC29    PC30
Standard deviation     0.02736 0.01153
Proportion of Variance 0.00002 0.00000
Cumulative Proportion  1.00000 1.00000
```

Wisconsin PCA plots

Let's make the main PC1 vs PC2

```r
ggplot(wisc.pr$x) +
  aes(PC1, PC2, col = diagnosis) +
  geom_point() +
  xlab("PC1(44.3%)") +
  ylab("PC2(19%)")
```



> Q. From your results, what proportion of the original variance is captured by the first principal components (PC1)?

0.4427

> Q. How many principal components (PCs) are required to describe at least 70% of the original variance in the data?

at least 3 PCs

> Q. How many principal components (PCs) are required to describe at least 90% of the original variance in the data?

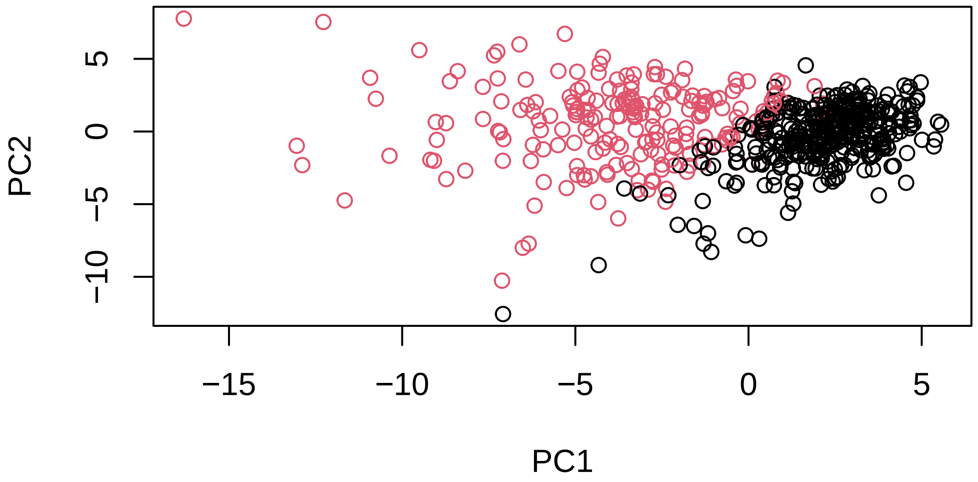
at least 4 PCs

> Q. What stands out to you about this plot? Is it easy or difficult to understand? Why?

The biplot of mtcars is not easy to understand, it is very messy compact and diffucult to understand the relationship of anything.

> Q. Generate a similar plot for principal components 1 and 3. What do you notice about these plots?

```r
# Scatter plot observations by components 1 and 2
plot( wisc.pr$x , col = diagnosis ,
     xlab = "PC1", ylab = "PC2")
```



The plots appear to be the same spread but flipped, 1 and 2 are slightly higher on the axis vs 1 and 3 are lower on the axis. The spread/variance however remains the same, the main difference being if you flipped PC1 and PC2 downwards you would have the same result as PC1 and PC3.

> Q. For the first principal component, what is the component of the loading vector (i.e. `wisc.pr$rotation[,1]`) for the feature `concave.points_mean`?

```r
wisc.pr$rotation[,1]
```

```
           radius_mean           texture_mean         perimeter_mean 
           -0.21890244            -0.10372458            -0.22753729 
             area_mean        smoothness_mean       compactness_mean 
           -0.22099499            -0.14258969            -0.23928535 
        concavity_mean    concave.points_mean          symmetry_mean 
           -0.25840048            -0.26085376            -0.13816696 
fractal_dimension_mean              radius_se             texture_se 
           -0.06436335            -0.20597878            -0.01742803 
          perimeter_se                 area_se           smoothness_se 
           -0.21132592             -0.20286964             -0.01453145 
        compactness_se            concavity_se       concave.points_se 
           -0.17039345             -0.15358979             -0.18341740 
           symmetry_se    fractal_dimension_se            radius_worst 
           -0.04249842             -0.10256832             -0.22799663 
         texture_worst         perimeter_worst              area_worst 
           -0.10446933             -0.23663968             -0.22487053 
      smoothness_worst       compactness_worst         concavity_worst 
           -0.12795256             -0.21009588             -0.22876753 
  concave.points_worst          symmetry_worst fractal_dimension_worst 
           -0.25088597             -0.12290456             -0.13178394 
```

concave.points_mean it is -0.26085376

> Q. What is the minimum number of principal components required to explain 80% of the variance of the data?

In this instance it is a minimum of 5 PCs

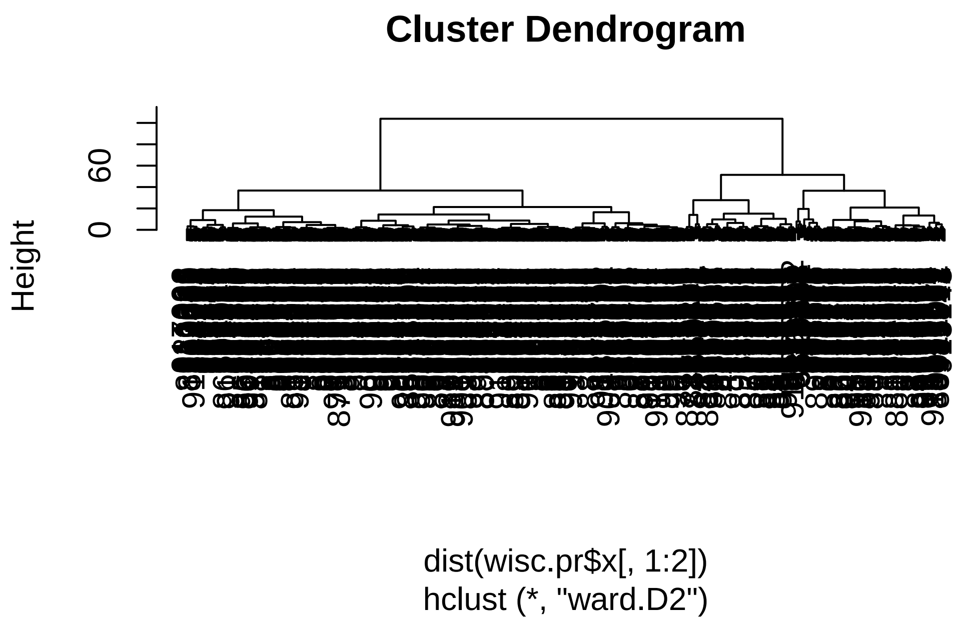
Combining methods

Clustering on PCA results

We can take our PCA results and use them as a basis set for other analysis such as clustering

```r
wisc.pr.hclust <- hclust(dist(wisc.pr$x[,1:2]), method = "ward.D2")

plot(wisc.pr.hclust)
```



We can "cut" this tree to yield our clusters(groups):

```r
pc.grps <- cutree(wisc.pr.hclust, k = 2)

table(pc.grps)
```

```
pc.grps
  1   2 
195 374 
```

> Q. Can you find a better cluster vs diagnoses match by cutting into a different number of clusters between 2 and 10?

no, creating more clusters creates a mess of a diagram and table.

How do my cluster grps compare to the expert diagnosis

```r
table(diagnosis, pc.grps)
```

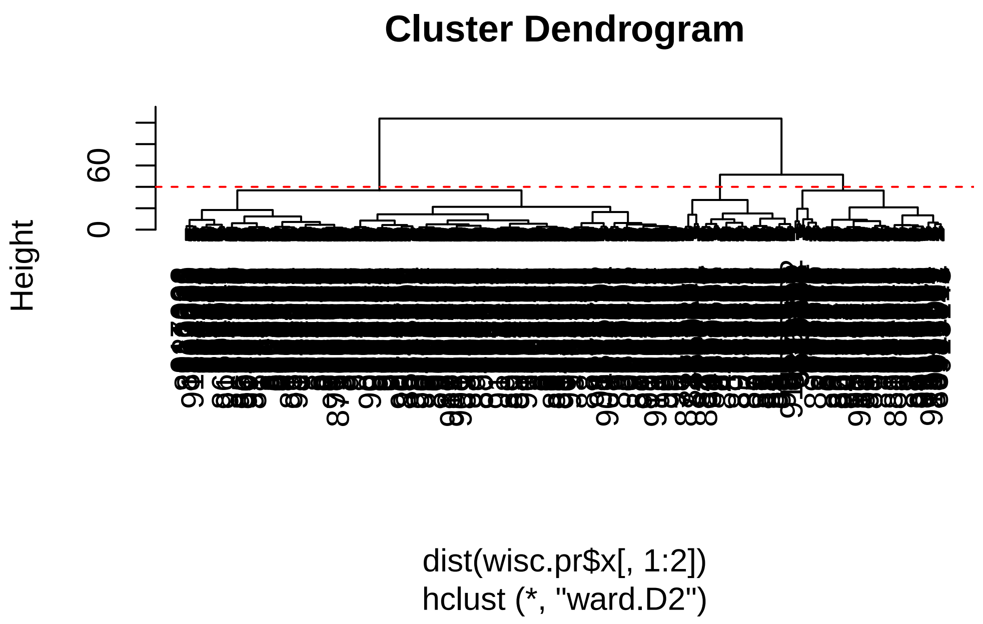
```
         pc.grps
diagnosis   1   2
        B  18 339
        M 177  35
```

```r
table(diagnosis, grps)
```

```
         grps
diagnosis   1   2
        B 357   0
        M 192  20
```

Q. Using the plot() and abline() functions, what is the height at which the clustering model has 4 clusters?

```r
plot(wisc.pr.hclust)
abline( h = 40, col="red", lty=2)
```

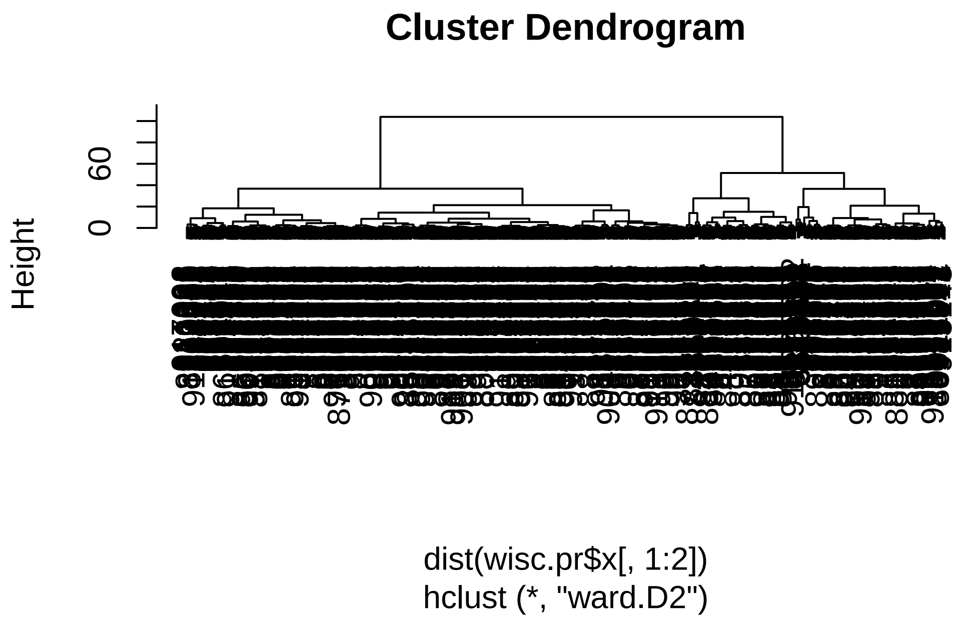


Q. Which method gives your favorite results for the same data.dist dataset? Explain your reasoning.

ward.D2 method gives me my favorite results, this is because the overall diagram is much easier to look at and therefor undersand. The clusters are simplified to be minimal and allow for easier visualization of clustering. The other methods produced very complicated chain/branching diagrams making it more difficult to understand the clusters and the relationships.

```r
hc2 <- hclust(dist(wisc.pr$x[,1:2]), method = "ward.D2")

plot(hc2)
```



> How well does k-means separate the two diagnoses? How does it compare to your hclust results?

kmeans is less effective than hclust results. comparing the kmeans clusters to diagnosis had 356 benign and 82 malignant in 1 and 1 benign, 130 malignant in 2. However the hclust options identified 18 people as B in group 1 and 338 in group 2 whereas malignant diagnosis were 177 in group 1 and 35 in group 2.

```r
wisc.km <- kmeans(wisc.data, centers = 2)

table(wisc.km$cluster, diagnosis)
```

```
   diagnosis
      B   M
  1 356  82
  2   1 130
```

> Q. How well does the newly created model with four clusters separate out the two diagnoses?

```r
clust4 <- cutree(wisc.pr.hclust, k = 4)
table(clust4)
```

```
clust4
  1   2   3   4 
112  83 250 124 
```

creating four clusters to separate the diagnosis is not recommended. It splits only two diagnosis intwo four different groups of which we are not aware are malignant or benign. It also makes understanding the table results more confusing.

> Q. How well do the k-means and hierarchical clustering models you created in previous sections (i.e. before PCA) do in terms of separating the diagnoses? Again, use the table() function to compare the output of each model (wisc.km$cluster and wisc.hclust.clusters) with the vector containing the actual diagnoses.

They did really badly, we do much better after PCA - the new PCA variables (what we call a basis set) give us much better separation of M and B

Prediction

We can use our PCA model for the analysis of the new "unseen" data. In this case from U. Michigan.

```r
#url <- "new_samples.csv"
url <- "https://tinyurl.com/new-samples-CSV"
new <- read.csv(url)
npc <- predict(wisc.pr, newdata=new)
npc
```

```
           PC1       PC2        PC3        PC4       PC5        PC6        PC7
[1,]  2.576616 -3.135913  1.3990492 -0.7631950  2.781648 -0.8150185 -0.3959098
[2,] -4.754928 -3.009033 -0.1660946 -0.6052952 -1.140698 -1.2189945  0.8193031
            PC8       PC9       PC10      PC11      PC12      PC13     PC14
[1,] -0.2307350 0.1029569 -0.9272861 0.3411457  0.375921 0.1610764 1.187882
[2,] -0.3307423 0.5281896 -0.4855301 0.7173233 -1.185917 0.5893856 0.303029
          PC15       PC16        PC17        PC18        PC19       PC20
[1,] 0.3216974 -0.1743616 -0.07875393 -0.11207028 -0.08802955 -0.2495216
[2,] 0.1299153  0.1448061 -0.40509706  0.06565549  0.25591230 -0.4289500
           PC21       PC22       PC23       PC24        PC25         PC26
[1,]  0.1228233 0.09358453 0.08347651  0.1223396  0.02124121  0.078884581
```

```
[2,] -0.1224776 0.01732146 0.06316631 -0.2338618 -0.20755948 -0.009833238
            PC27        PC28         PC29         PC30
[1,]  0.220199544 -0.02946023 -0.015620933  0.005269029
[2,] -0.001134152  0.09638361  0.002795349 -0.019015820
```

> Q18. Which of these new patients should we prioritize for follow up based on your results?

We should prioritize all the patients that are under the malignant category of groups 1 and 2.