Class 8: Breast cancer mini project

Linh Dang (PID: A16897764)

Table of contents

Background 1
Data import 1
Clustering 3
Principal Component Analysis 5
The importance data scaling 5
PCA of wisc.data 9
5. Combining methods 14
Clustering on PCA results 14
7. Prediction 15

Background

This mini-project explores unsupervised learning techniques applied to a dataset of human breast cancer cell measurements. The goal is to use Principal Component Analysis (PCA) as a pre-processing step before applying clustering algorithms to identify patterns in the data without prior knowledge of diagnosis. The data, originating from the Wisconsin Breast Cancer Diagnostic Data Set, contains measurements of cell nuclei features from fine needle aspiration (FNA) biopsies. The analysis involves exploratory data analysis, performing and interpreting PCA, and then applying and evaluating both hierarchical clustering and k-means clustering methods, including a comparison of clustering results with known diagnoses and a discussion of sensitivity and specificity. Finally, the project demonstrates how to predict the principal components for new data points.

Data import

Our data come from the U. of Wisconsin Medical Center

```r
wisc.df <- read.csv("WisconsinCancer.csv", row.names = 1)
```

> Q1. How many patients/samples are in this dataset?

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

```
[1] 569
```

> Q2. How many of the observations have a malignant diagnosis?

```r
table(wisc.df$diagnosis)
```

```

  B   M 
357 212 
```

```r
sum(wisc.df$diagnosis == "M")
```

```
[1] 212
```

> Q3. How many variables/features in the data are suffixed with _mean?

```r
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"
```

```
length( grep("mean", colnames(wisc.df), value=T) )
```

```
[1] 10
```

There is a diagnosis column that is the clinician consensus that I want to exclude from any further analysis. We will come back later and compare our results to this diagnosis.

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

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

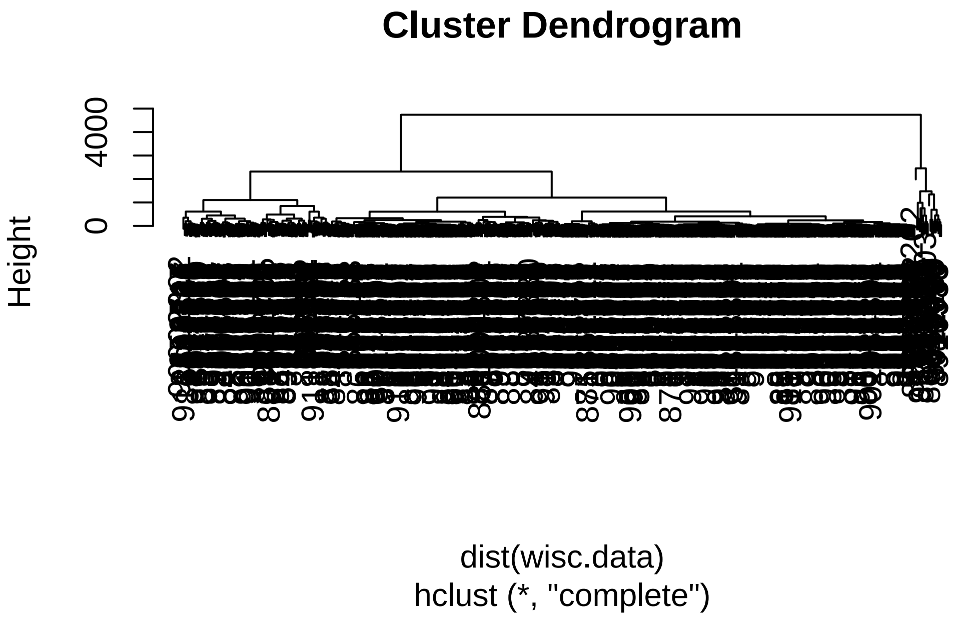
Now we can remove it from the `wisc.df`

```
wisc.data <- wisc.df[,-1]
```

Clustering

Let's try a `hclust()`

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



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

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

How many individuals in each cluster?

```
table(grps)
```

```
grps
  1   2 
549  20 
```

```
table(diagnosis)
```

```
diagnosis
  B   M 
357 212 
```

We can generate a cross-table that compares our cluster `grps` vectors with our `diagnosis` vector values

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

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

Principal Component Analysis

The importance data scaling

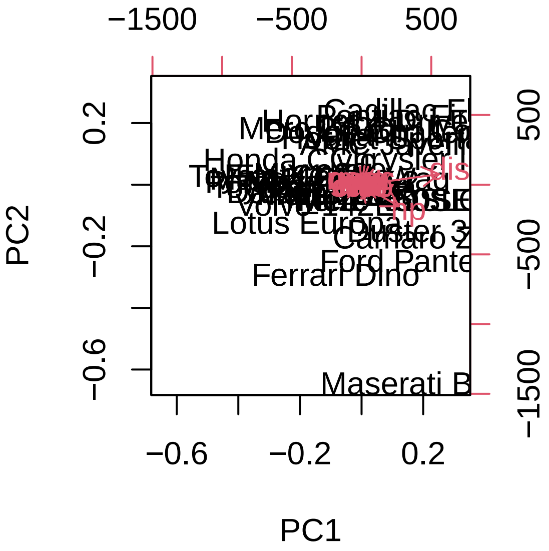
The main function for PCA in base R is `prcomp()` it has a default input parameter of `scale=FALSE`.

```
#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 mis-leading…

```
pc <- prcomp(mtcars)
biplot(pc)
```



Let’s 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 before PCA to get a much bettter 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 
```

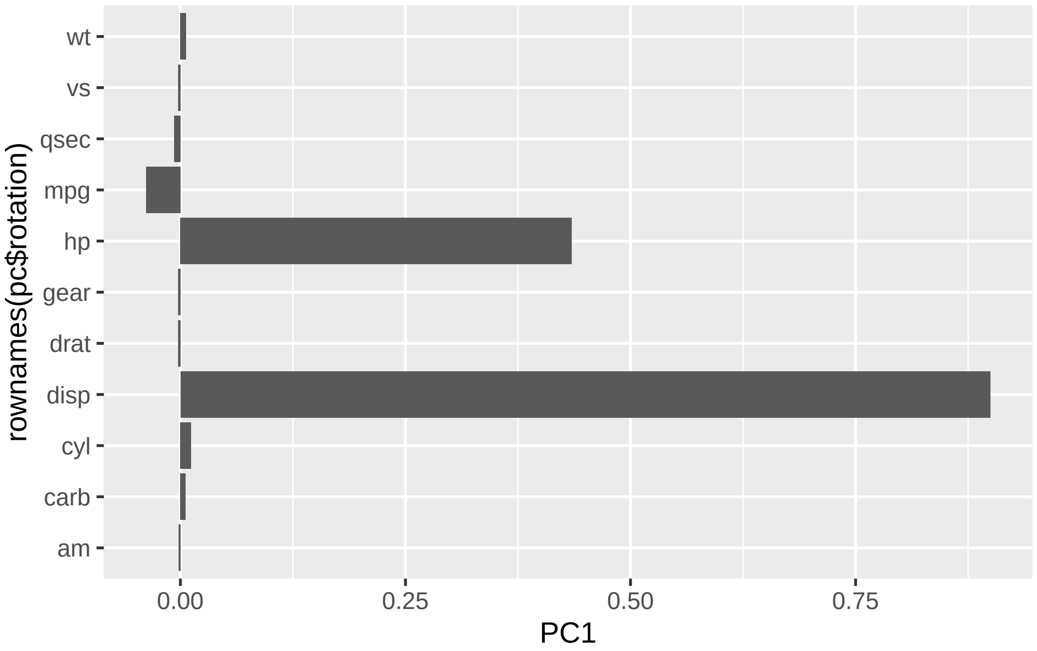
```r
pc.scale <- prcomp(mtscale)
```

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

A loadings plot of the unscaled PCA results

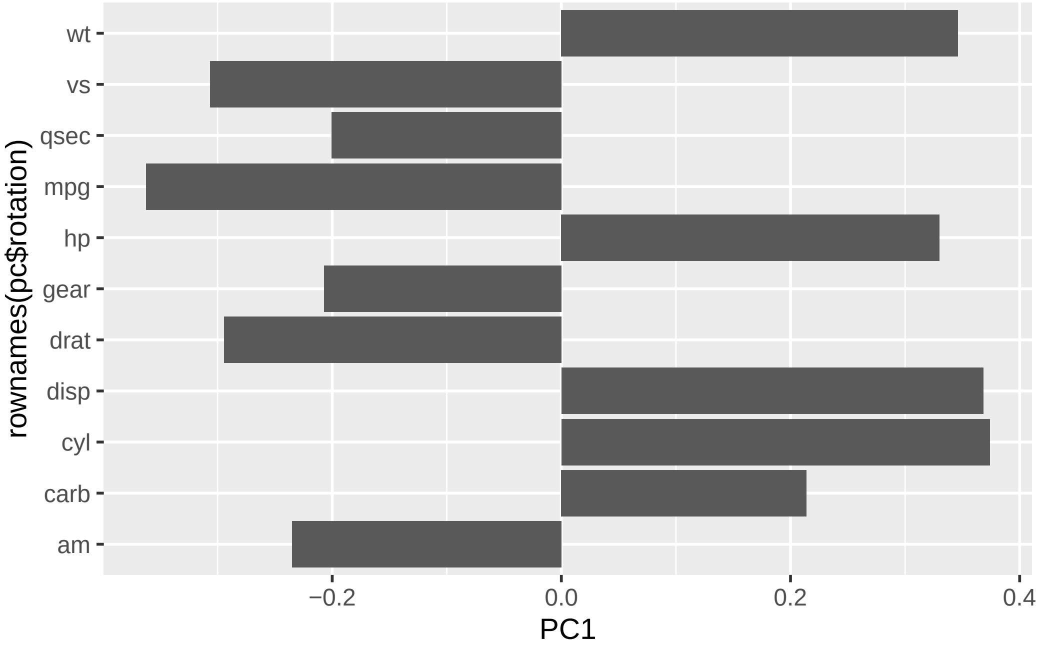
```r
library(ggplot2)

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



Loadings plot of the scaled data.

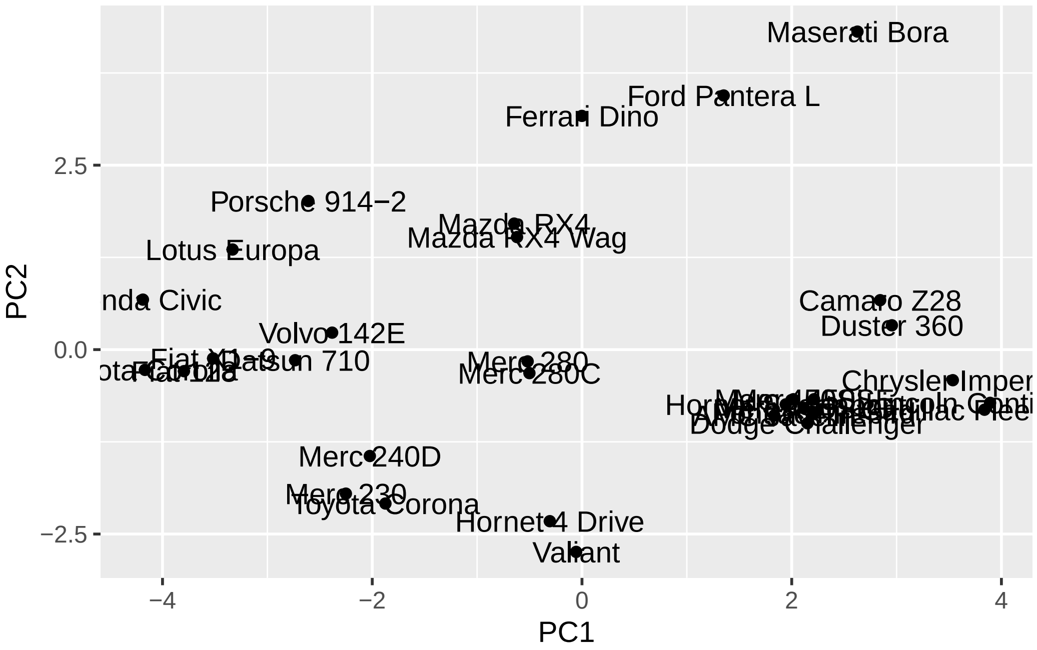
```
ggplot(pc.scale$rotation) +
  aes(PC1, rownames(pc$rotation) ) +
  geom_col()
```



PC plot of scaled PCA results

```
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 probably should be...

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

PCA of wisc.data

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

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

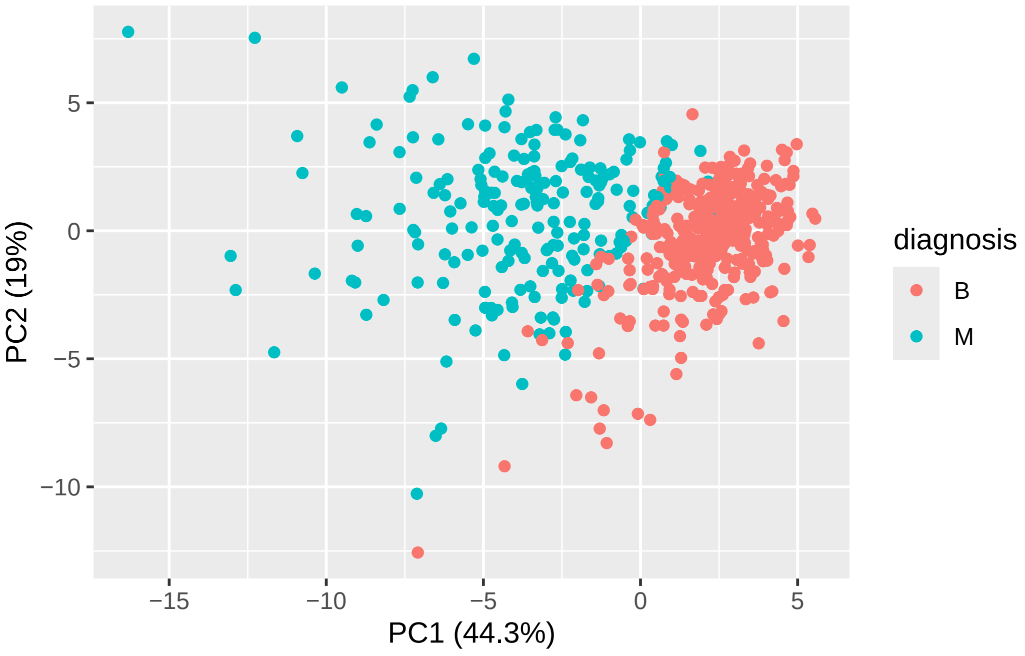
```
summary(wisc.pr)
```

```
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
```

Let's make the main PC1 vs PC2

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



> Q4. From your results, what proportion of the original variance is captured by the first principal components (PC1)?

44.3% is captured by the first principal components (PC1).

> Q5. How many principal components (PCs) are required to describe at least 70% of the original variance in the data?

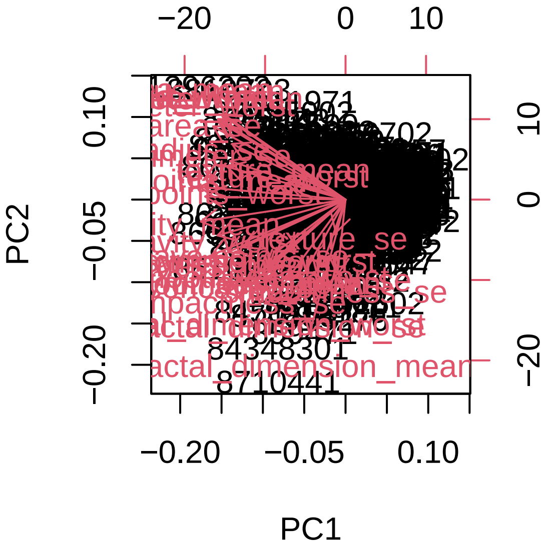
3 PCs are required to describe at least 70% of the original variance in the data.

> Q6. How many principal components (PCs) are required to describe at least 90% of the original variance in the data?

7 PCs are required to describe at least 90% of the original variance in the data.

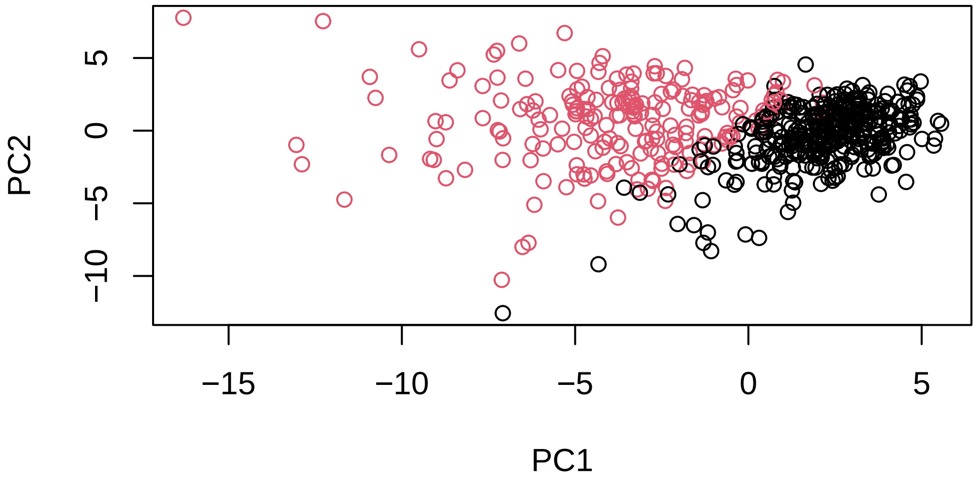
> Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?

```r
biplot(wisc.pr)
```



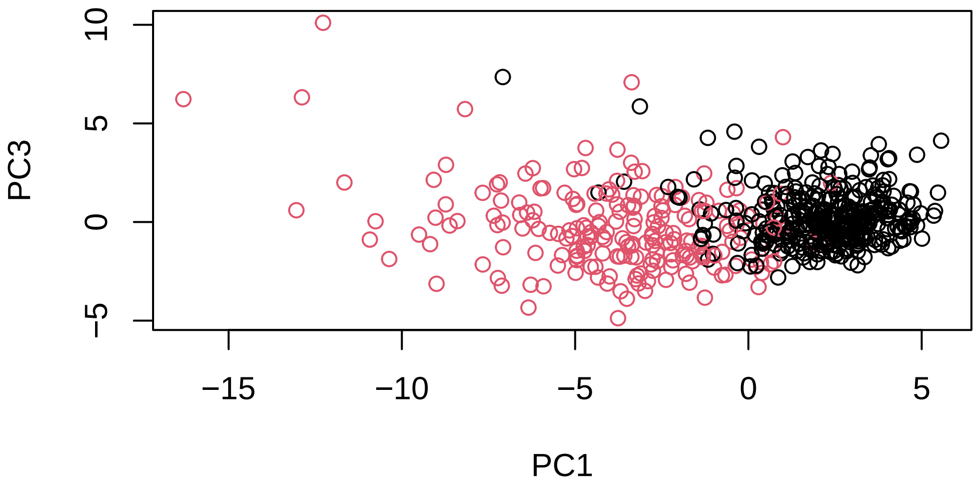
This plot is very difficult to understand because there are too many points on the same graph.

```r
plot(wisc.pr$x, col =diagnosis,
     xlab = "PC1", ylab = "PC2")
```



Q8. Repeat the same for principal components 1 and 3. What do you notice about these plots?

```
plot(wisc.pr$x[, c(1, 3)], col = (diagnosis),
     xlab = "PC1", ylab = "PC3")
```



These plots show very similar separation of the two groups, red cluster group (malignant) to the left or negative direction while black cluster group (benign) to the right or positive direction.

> Q9. 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?

-0.26085376, 5

```
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
```

> Q10. What is the minimum number of principal components required to explain 80% of the variance of the data?

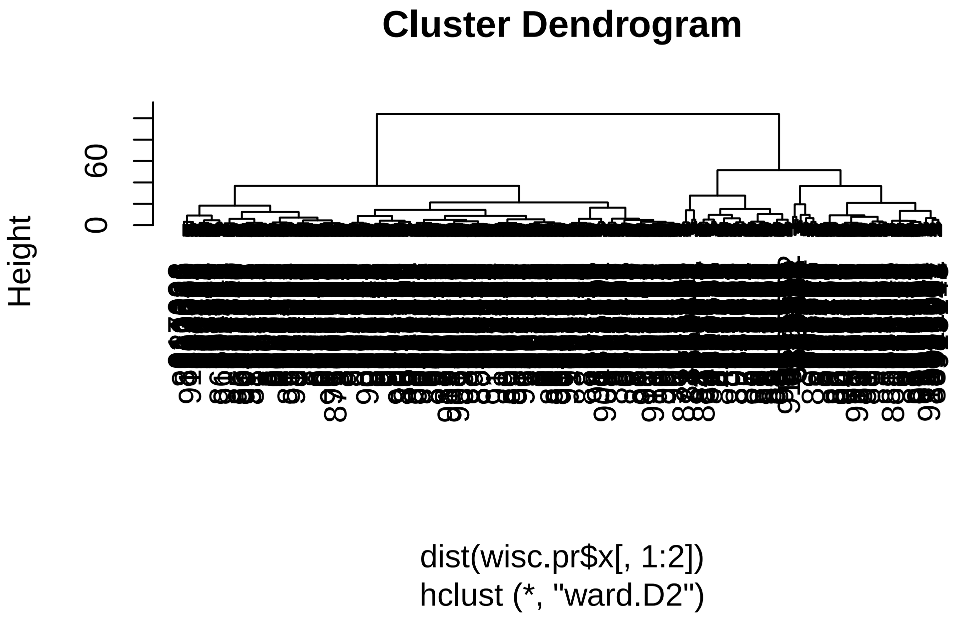
5 principal components are required to explain 80% of the variance.

5. Combining methods

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

Clustering on PCA results

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



> Q11. Using the plot() and abline() functions, what is the height at which the clustering model has 4 clusters?

At height 20, clustering model has 4 clusters.

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

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

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

How do my cluster grps compare to the expert diagnosis

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

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

> Q15. How well does the newly created model with four clusters separate out the two diagnoses?

The newly created model with four clusters separate out the two diagnoses are not good.

> Q16. 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.

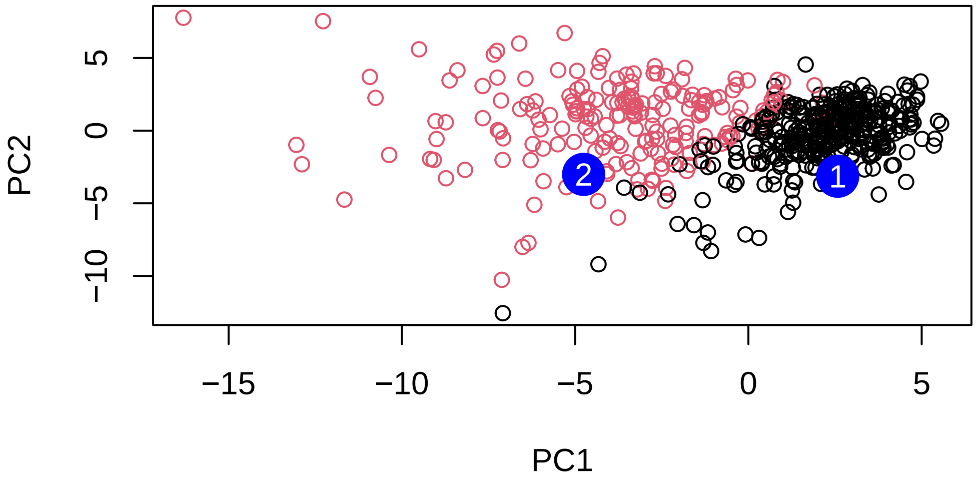
7. Prediction

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

```
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
```

```
plot(wisc.pr$x[,1:2], col=diagnosis)
points(npc[,1], npc[,2], col="blue", pch=16, cex=3)
text(npc[,1], npc[,2], c(1,2), col="white")
```



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

PCA shows a nice separation in either positive and negative scores for the 2 groups. Red cluster is malignant while black cluster is benign. New patients (red spots) that deviate away most from the clusters should we prioritize for follow up because they are in malignant group and have the most variation from the rest of other patients.