# Class 8 Mini Project

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## Prepare the data

```
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
```

We would like to exclude the diagnosis column since we are doing an unsupervised learning.

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

Also we would like to store the diagnosis column into a separate factor vector:

```r
diagnosis <- factor(wisc.df[, 1])
```

# 1. Exploratory data analysis

### Q1. How many observations are in this dataset?

```r
nrow(wisc.data)
```

```
[1] 569
```

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

```r
sum(diagnosis == 'M')
```

```
[1] 212
```

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

```r
length(grep(pattern = "*_mean", x = colnames(wisc.data)))
```

```
[1] 10
```

# 2. Principle Component Analysis

### Performing PCA

```r
# Check column means and standard deviations
colMeans(wisc.data)
```

```
       radius_mean       texture_mean     perimeter_mean
      1.412729e+01       1.928965e+01       9.196903e+01
         area_mean    smoothness_mean   compactness_mean
      6.548891e+02       9.636028e-02       1.043410e-01
    concavity_mean concave.points_mean     symmetry_mean
```

```
          8.879932e-02           4.891915e-02           1.811619e-01
fractal_dimension_mean              radius_se             texture_se
          6.279761e-02           4.051721e-01           1.216853e+00
          perimeter_se                area_se          smoothness_se
          2.866059e+00           4.033708e+01           7.040979e-03
       compactness_se           concavity_se      concave.points_se
          2.547814e-02           3.189372e-02           1.179614e-02
           symmetry_se    fractal_dimension_se           radius_worst
          2.054230e-02           3.794904e-03           1.626919e+01
        texture_worst         perimeter_worst             area_worst
          2.567722e+01           1.072612e+02           8.805831e+02
     smoothness_worst       compactness_worst         concavity_worst
          1.323686e-01           2.542650e-01           2.721885e-01
  concave.points_worst          symmetry_worst fractal_dimension_worst
          1.146062e-01           2.900756e-01           8.394582e-02
```

```
apply(wisc.data,2,sd)
```

```
           radius_mean           texture_mean         perimeter_mean
          3.524049e+00           4.301036e+00           2.429898e+01
             area_mean        smoothness_mean       compactness_mean
          3.519141e+02           1.406413e-02           5.281276e-02
        concavity_mean     concave.points_mean          symmetry_mean
          7.971981e-02           3.880284e-02           2.741428e-02
fractal_dimension_mean              radius_se             texture_se
          7.060363e-03           2.773127e-01           5.516484e-01
          perimeter_se                area_se          smoothness_se
          2.021855e+00           4.549101e+01           3.002518e-03
       compactness_se           concavity_se      concave.points_se
          1.790818e-02           3.018606e-02           6.170285e-03
           symmetry_se    fractal_dimension_se           radius_worst
          8.266372e-03           2.646071e-03           4.833242e+00
        texture_worst         perimeter_worst             area_worst
          6.146258e+00           3.360254e+01           5.693570e+02
     smoothness_worst       compactness_worst         concavity_worst
          2.283243e-02           1.573365e-01           2.086243e-01
  concave.points_worst          symmetry_worst fractal_dimension_worst
          6.573234e-02           6.186747e-02           1.806127e-02
```

Then we perform PCA:

```
wisc.pr <- prcomp(wisc.data, scale=TRUE)
# Look at summary of results
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
```

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

```
wisc.pr$sdev[1] ** 2 / sum(wisc.pr$sdev ** 2)
```

```
[1] 0.4427203
```

0.4427

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

3.

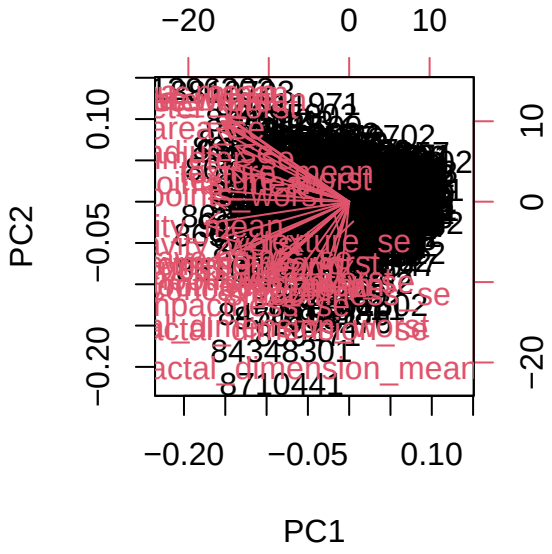
**Q6. How many principal components (PCs) are required to describe at least 90% of the original variance in the data?**

7.

## Interpreting PCA results

Create a biplot for the pca result.

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

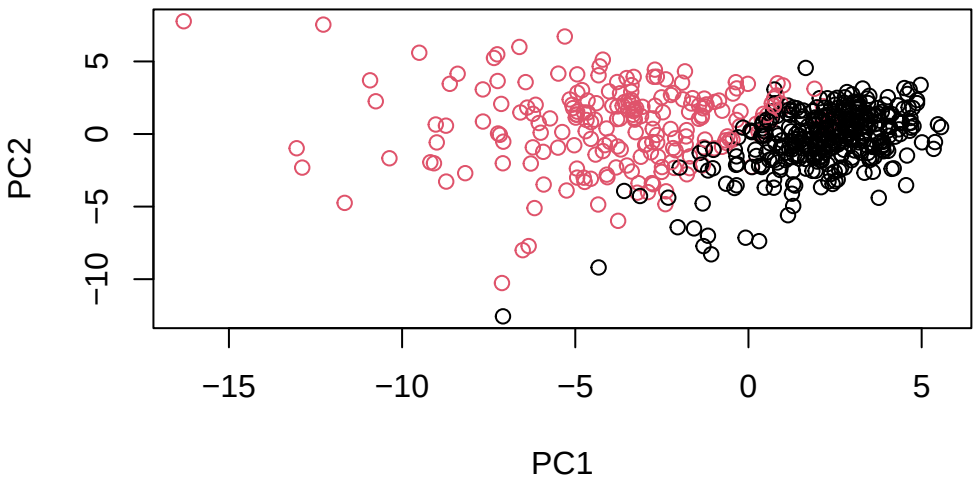



**Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?**

It is a mess and difficult to understand, because the label is very messy and occupies a lot of space.

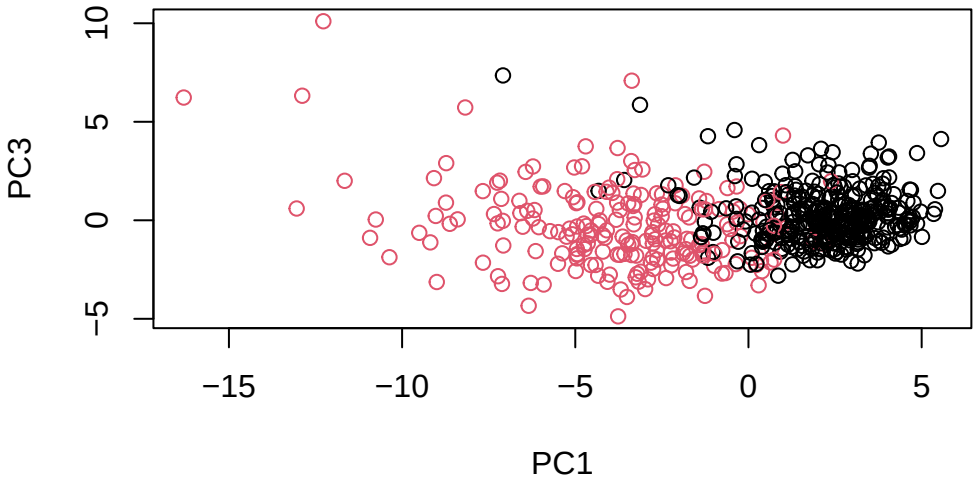
We would rather use `plot` to get a scatter plot.

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




**Q8. Generate a similar plot for principal components 1 and 3. What do you notice about these plots?**

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



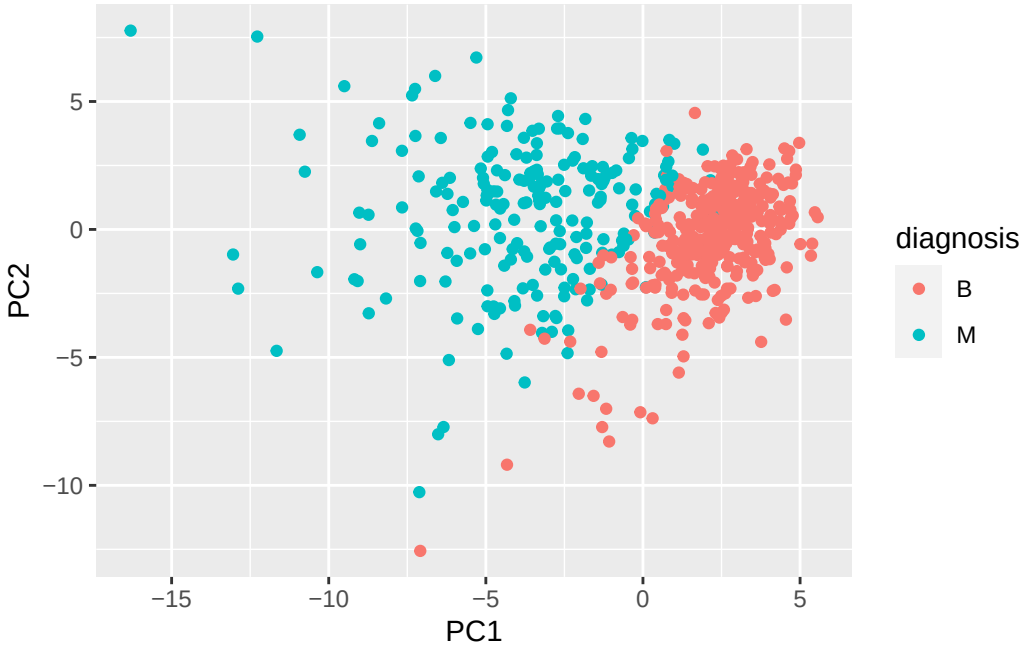

It is similarly separable to the PC1-PC2 scatter plot.

Let's use ggplot to make a fancier plot.

```
# Create a data.frame for ggplot
df <- as.data.frame(wisc.pr$x)
df$diagnosis <- diagnosis

# Load the ggplot2 package
library(ggplot2)

# Make a scatter plot colored by diagnosis
ggplot(df) +
  aes(PC1, PC2, col=diagnosis) +
  geom_point()
```




### Variance explained

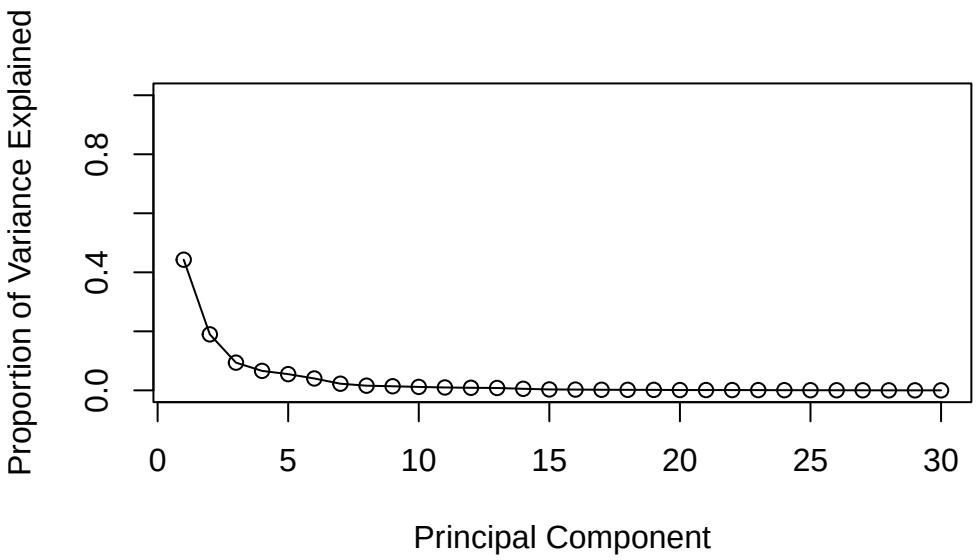
```
# Calculate variance of each component
wisc.pr.var <- wisc.pr$sdev ^ 2
head(wisc.pr.var)
```

```
[1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

Then we can plot the variance explained.

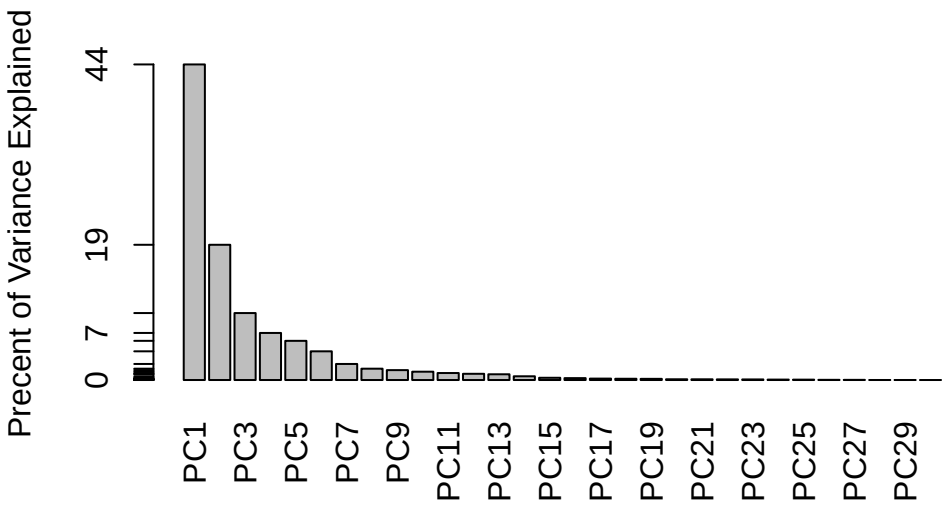
```
# Variance explained by each principal component: pve
pve <- wisc.pr.var / sum(wisc.pr.var)

# Plot variance explained for each principal component
plot(pve, xlab = "Principal Component",
     ylab = "Proportion of Variance Explained",
     ylim = c(0, 1), type = "o")
```




Or using barplot:

```
# Alternative scree plot of the same data, note data driven y-axis
barplot(pve, ylab = "Precent of Variance Explained",
     names.arg=paste0("PC",1:length(pve)), las=2, axes = FALSE)
axis(2, at=pve, labels=round(pve,2)*100 )
```




### Communicating PCA results

**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? This tells us how much this original feature contributes to the first PC.**

```
wisc.pr$rotation[, 1]["concave.points_mean"]
```

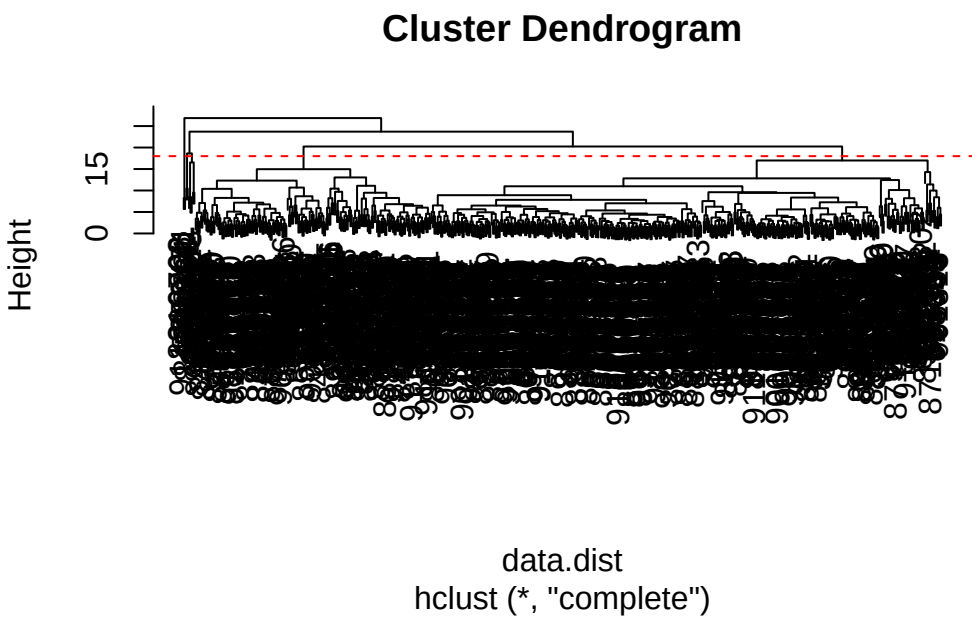
```
concave.points_mean
         -0.2608538
```

It is negatively contributing to the first PC.

## 3. Hierarchical clustering

```
# Scale the wisc.data data using the "scale()" function
data.scaled <- scale(wisc.data)
data.dist = dist(data.scaled)
wisc.hclust <- hclust(data.dist, method="complete")
```

```
plot(wisc.hclust)
abline(h=18, col="red", lty=2)
```




### Selecting number of clusters

```
wisc.hclust.clusters <- cutree(wisc.hclust, 4)
table(wisc.hclust.clusters, diagnosis)
```

```
                    diagnosis
wisc.hclust.clusters   B   M
                   1  12 165
                   2   2   5
                   3 343  40
                   4   0   2
```

**Q11. OPTIONAL: Can you find a better cluster vs diagnoses match by cutting into a different number of clusters between 2 and 10? How do you judge the quality of your result in each case?**

```
wisc.hclust.clusters <- cutree(wisc.hclust, 10)
table(wisc.hclust.clusters, diagnosis)
```

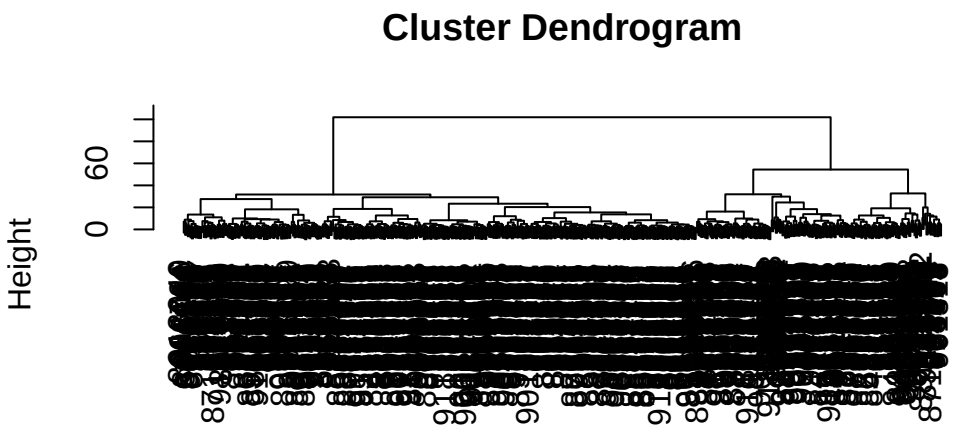
```
                    diagnosis
wisc.hclust.clusters   B   M
                   1   12  86
                   2    0  59
                   3    0   3
                   4  331  39
                   5    0  20
                   6    2   0
                   7   12   0
                   8    0   2
                   9    0   2
                   10   0   1
```

I think it is better to get a more separable distribution of number of samples in each cluster. I will prefer using 10 clusters.

### Using different methods

**Q12. Which method gives your favorite results for the same data.dist dataset? Explain your reasoning.**

```
wisc.pr.hclust <- hclust(data.dist, method="ward.D2")
plot(wisc.pr.hclust)
```




```
# abline(h=18, col="red", lty=2)
```

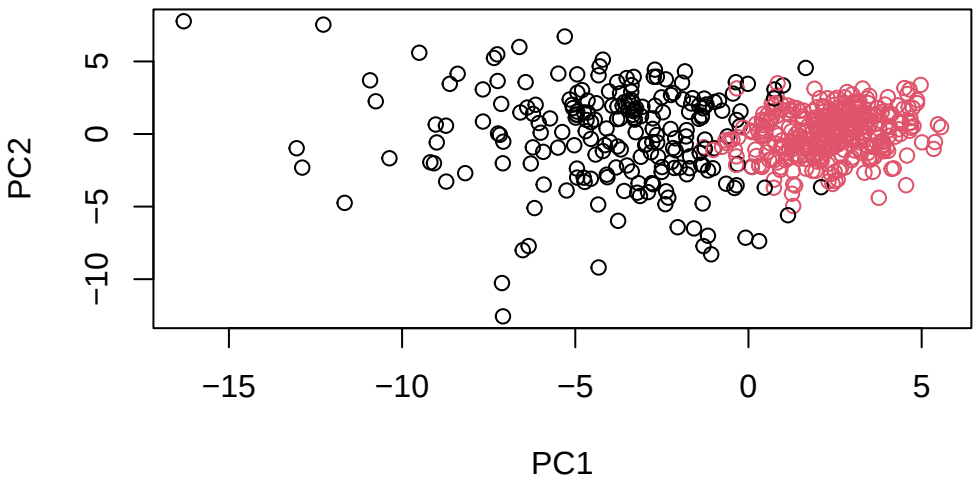
I like the D2 method, because it gives a more balance hierarchical clustering results.

## 4. Combining methods

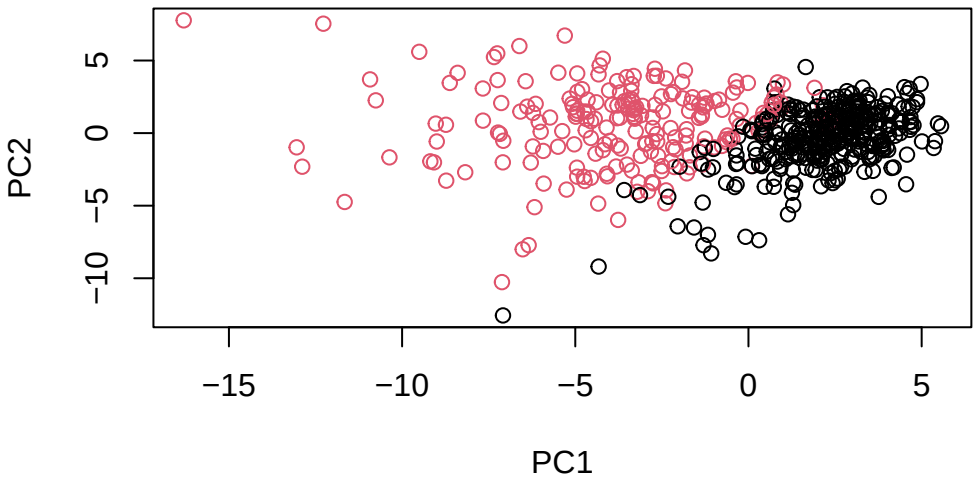
```
wisc.pr.hclust <- hclust(dist(wisc.pr$x[, 1:7]), method="ward.D2")
grps <- cutree(wisc.pr.hclust, k=2)
table(grps, diagnosis)
```

```
    diagnosis
grps   B   M
   1  28 188
   2 329  24
```

```
plot(wisc.pr$x[,1:2], col=grps)
```




```
plot(wisc.pr$x[,1:2], col=diagnosis)
```



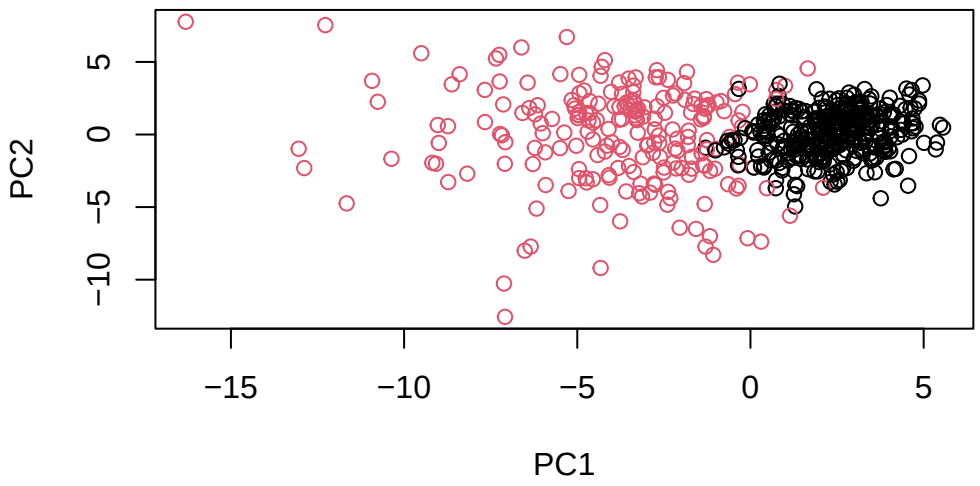
```
g <- as.factor(grps)
levels(g)
```

```
[1] "1" "2"
```

```
g <- relevel(g,2)
levels(g)
```

```
[1] "2" "1"
```

```
# Plot using our re-ordered factor
plot(wisc.pr$x[,1:2], col=g)
```




```
library(rgl)
```

```
Warning: package 'rgl' was built under R version 4.3.2
```

```
plot3d(wisc.pr$x[,1:3], xlab="PC 1", ylab="PC 2", zlab="PC 3", cex=1.5, size=1, type="s",
```

**Q13. How well does the newly created model with four clusters separate out the two diagnoses?**

```
wisc.pr.hclust <- hclust(dist(wisc.pr$x[, 1:7]), method="ward.D2")
wisc.pr.hclust.clusters <- cutree(wisc.pr.hclust, k=2)
table(wisc.pr.hclust.clusters, diagnosis)
```

```
                     diagnosis
wisc.pr.hclust.clusters   B   M
                      1  28 188
                      2 329  24
```

```
table(wisc.hclust.clusters, diagnosis)
```

```
                    diagnosis
wisc.hclust.clusters   B   M
                   1  12  86
                   2   0  59
                   3   0   3
                   4 331  39
                   5   0  20
                   6   2   0
                   7  12   0
                   8   0   2
                   9   0   2
                   10  0   1
```

It is definitely better.

**Q14. How well do the 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.**

Slightly worse, since it is not seperating different diagonosis well.

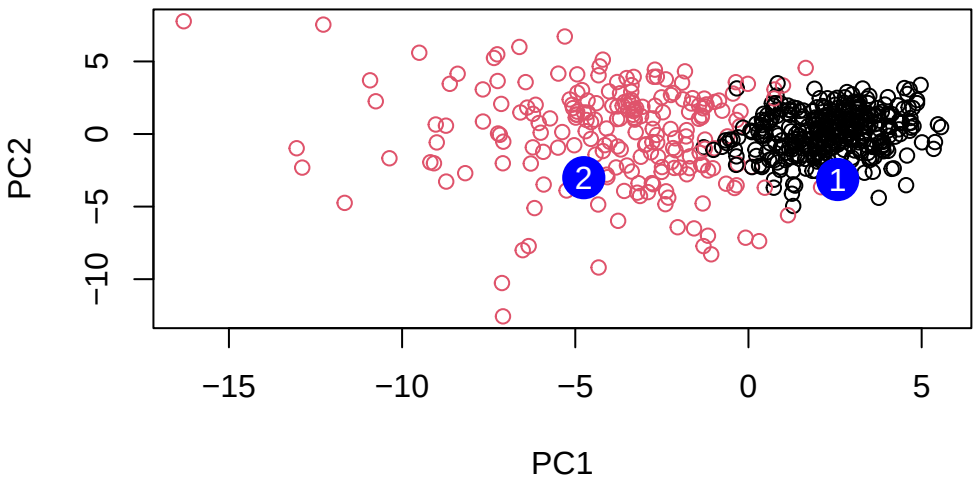
## 5. Sensitivity/Specificity

## 6. Prediction

```
#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
```

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




**Q16. Which of these new patients should we prioritize for follow up based on your results?**

The second patient should be prioritized. It is within the high-risk cluster.