Class 9 Mini Project

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#Unsupervised Learning Analysis of Human Breast Cancer Cells

Here we read data from the University of Wisconsin Medical Center on breast cancer patients

```
wisc.df <- read.csv("WisconsinCancer.csv", 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
```

Use -1 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
```

Diagnosis of vector

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

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

Exploring data analysis

> Q1. How many observations are in this dataset?

```
dim(wisc.data)
```

```
## [1] 569  30
```

How many rows

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

```
## [1] 569
```

How many columns (i.e. variables)

```
ncol(wisc.data)
```

```
## [1] 30
```

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

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

```
##
##   B   M
## 357 212
```

A useful function we will use lots and lots -> table()

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

```
length(grep("_mean", colnames(wisc.df)))
```

```
## [1] 10
```

Principle Component Analysis

Performing PCA

Here we need to scale the data before PCA as the various variable (i.e. columns) have very different scales.

Checking 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
```

```r
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
```

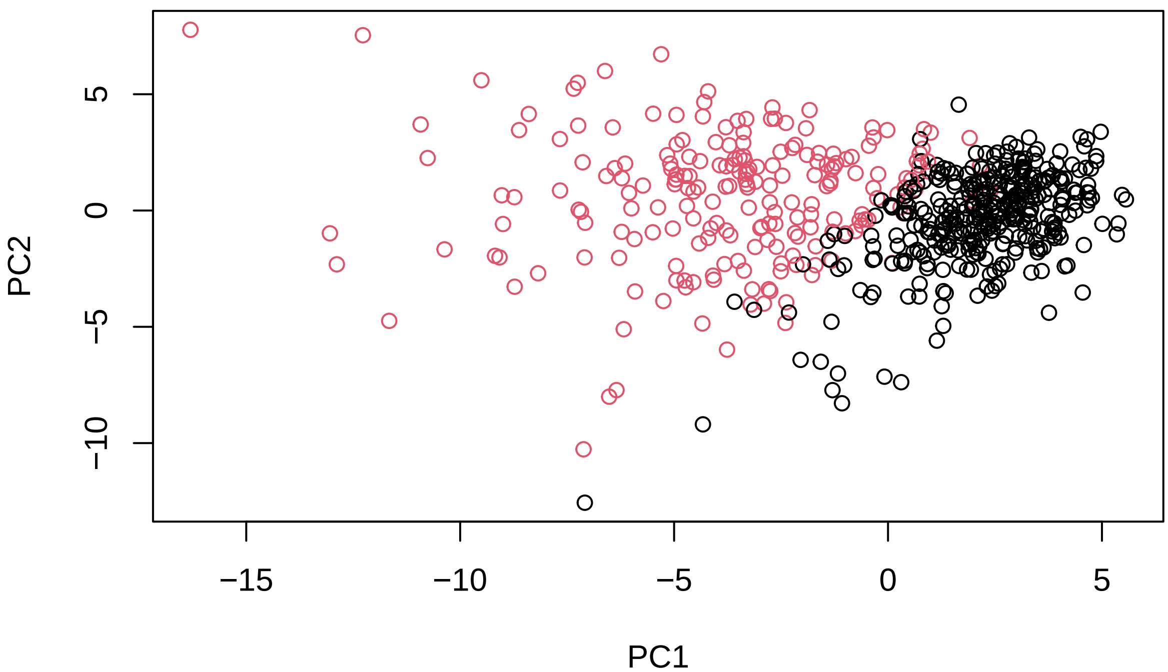
Performing PCA on wisc.data

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

Now we will make my main result: the “PCA plot” (a.k.a. “score plot”, PC1 vs. PC2 plot)

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



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

44.27%

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

3 principle components (PC3)

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

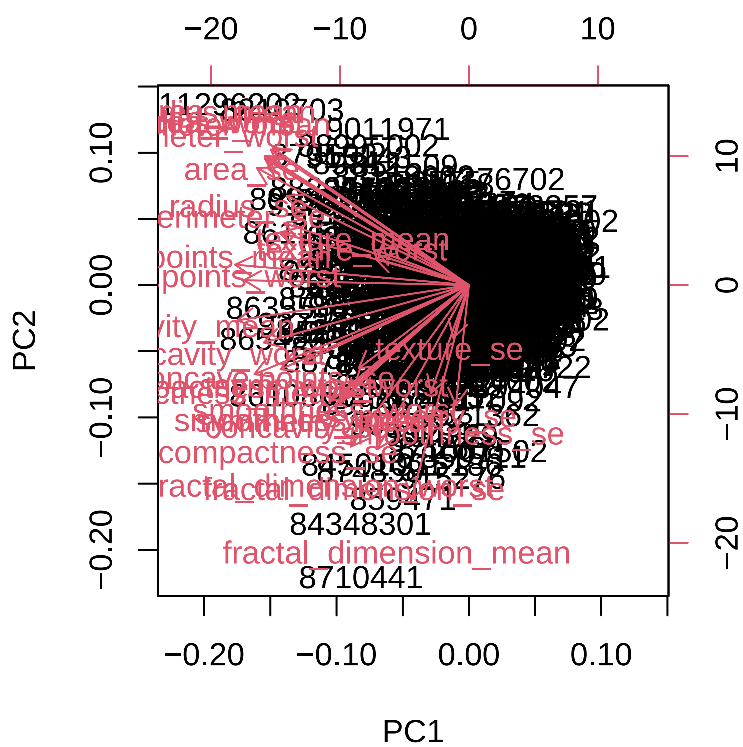
7 principle components (PC7)

Interpreting PCR results

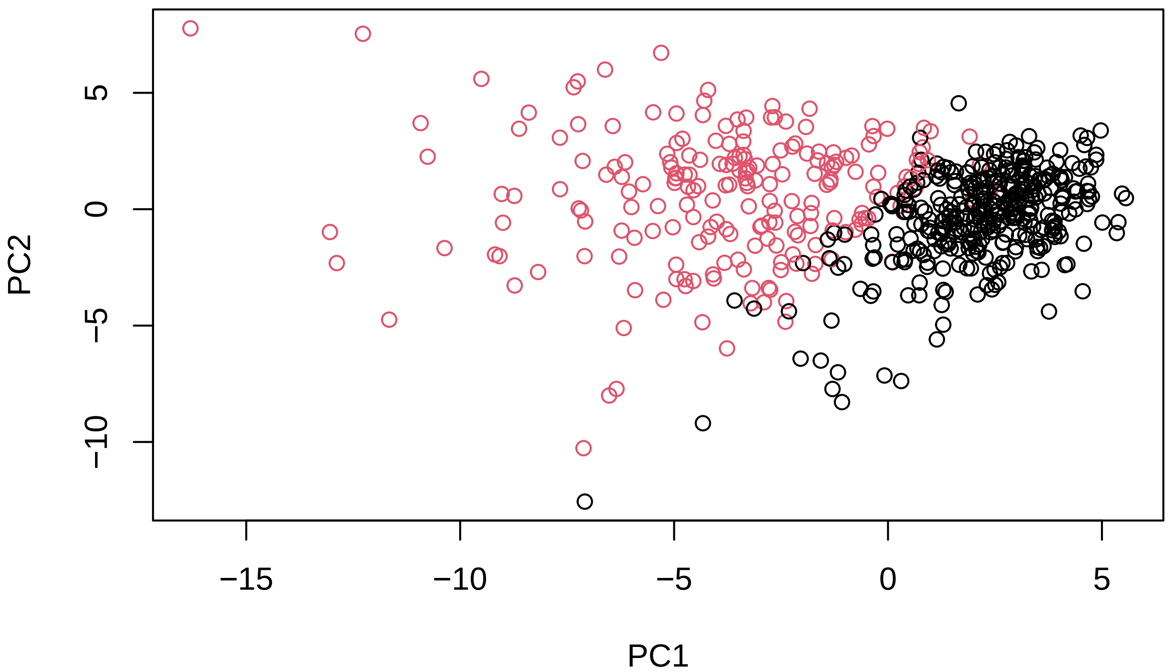
> Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?

The plot is very messy and difficult to understand because all components are being observed on the plot.

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



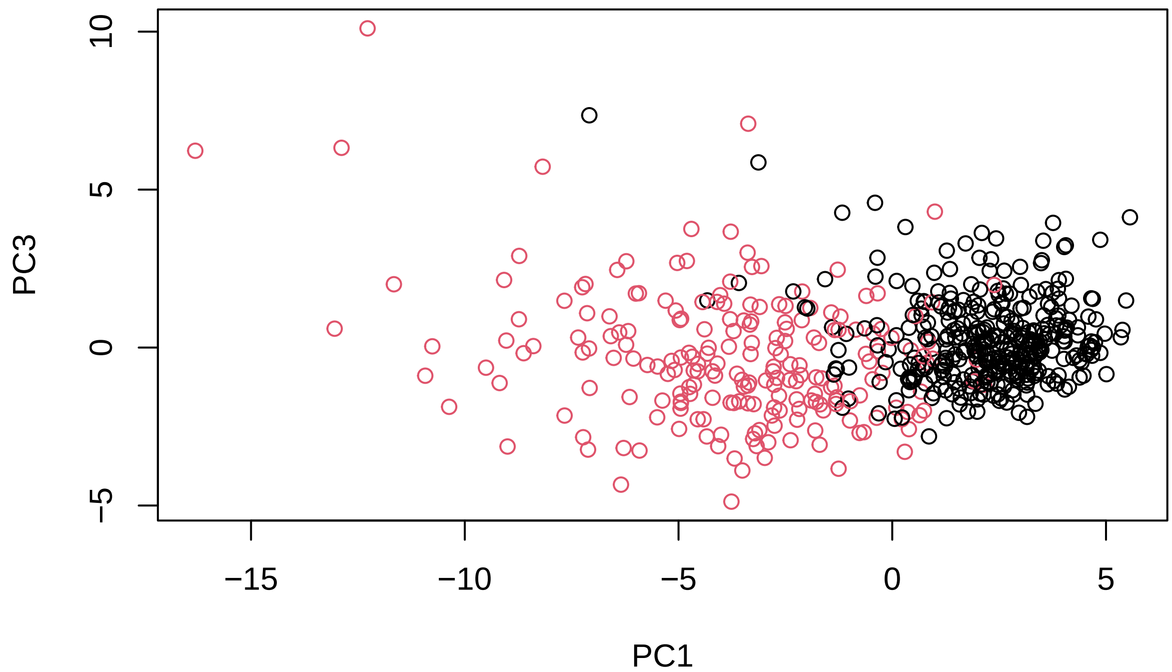

```r
plot(wisc.pr$x , col = diagnosis ,
     xlab = "PC1", ylab = "PC2")
```



8. Generate a silimar plot for principal components 1 and 3. What do you notice about these plots?

These plots contain less variance than principle component 2 and the principle component 1 is capturing a separation of malignant from benign.

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



Creating data.frame for ggplot

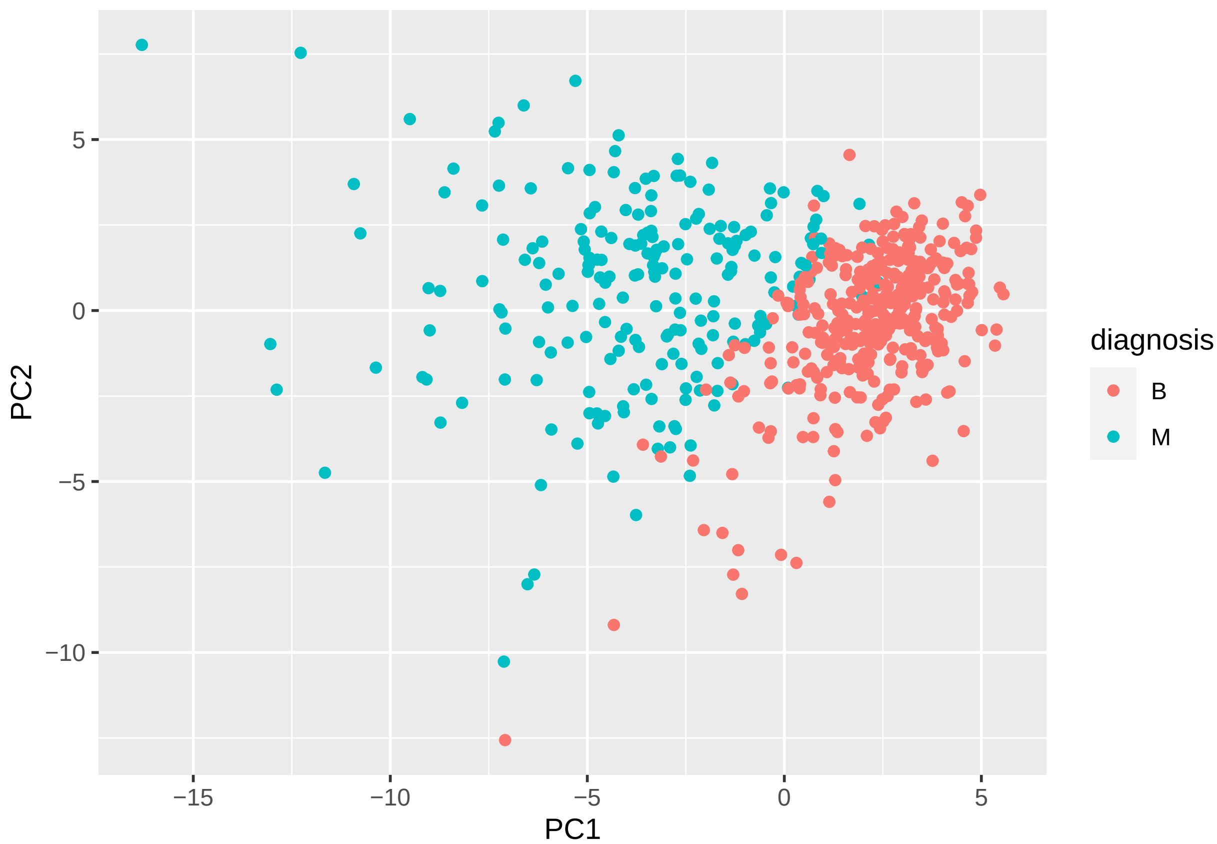
```
df <- as.data.frame(wisc.pr$x)
df$diagnosis <- diagnosis
```

Loading ggplot2 package

```
library(ggplot2)
```

Making a scatter plot colored by diagnosis

```
ggplot(df) +
  aes(PC1, PC2, col= diagnosis) +
  geom_point()
```



Variance explained

Calculating variance of each component

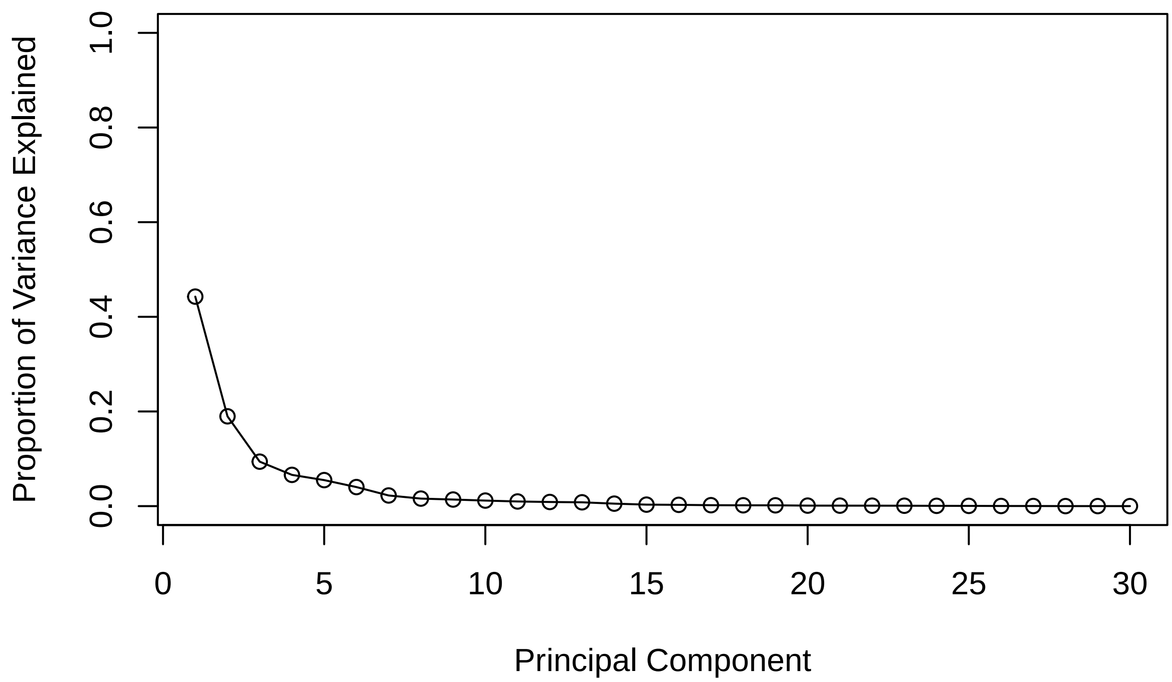
```
pr.var <- wisc.pr$sdev^2
head(pr.var)
```

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

Calculating variance explained by each principle component : pve

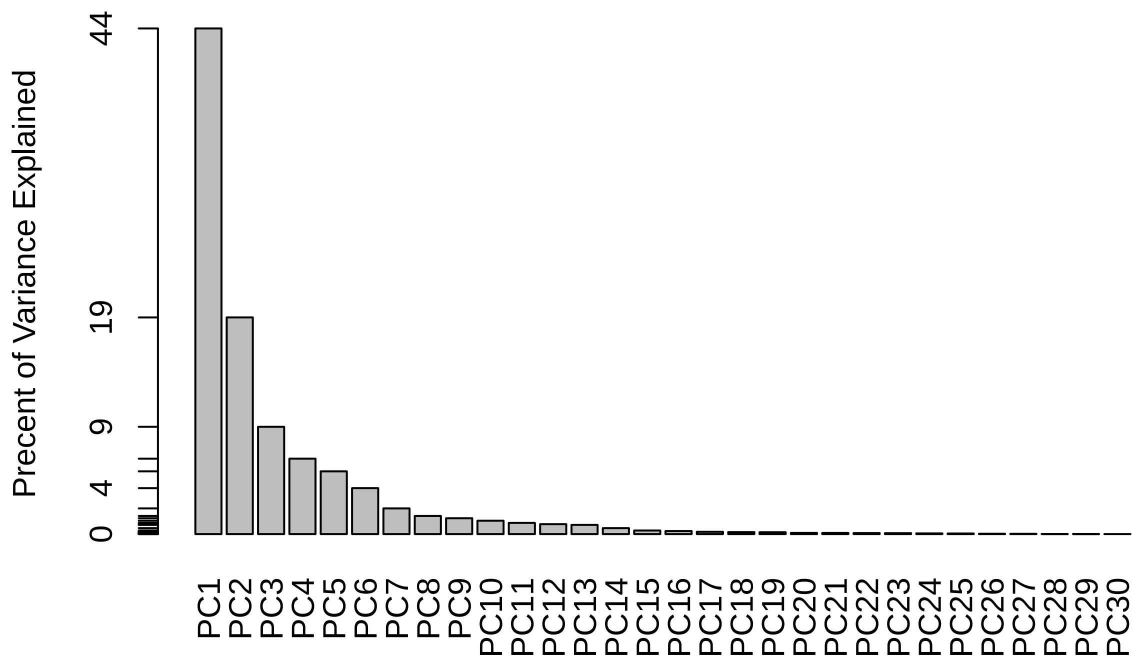
```
pve <-  pr.var/ sum(pr.var)

plot(pve, xlab = "Principal Component",
     ylab = "Proportion of Variance Explained",
     ylim = c(0, 1), type = "o")
```



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 )
```

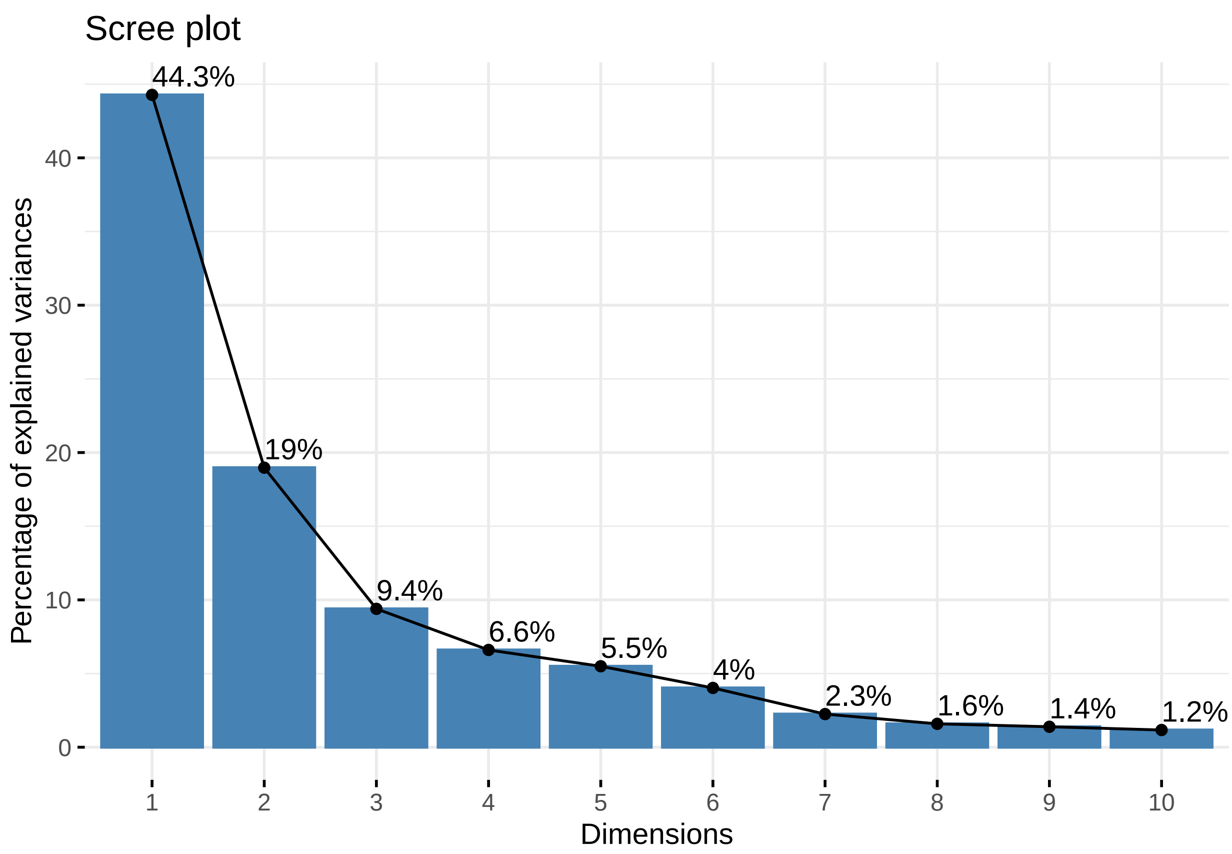


ggplot based on graph

```
#install.packages("factoextra")
library(factoextra)
```

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

```
fviz_eig(wisc.pr, addlabels = TRUE)
```



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?

```
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
```

The loading vector for the concave.points_mean is -0.26085376.

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

```
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
```

5 principle component (PC5)

Hierarchial CLustering

Scaling the wisc.data using "scale()" function

```
data.scaled <- scale(wisc.data)
```

Calculating the distances between all pairs of observations and assigning to data.dist

```
data.dist <- dist(data.scaled)
```

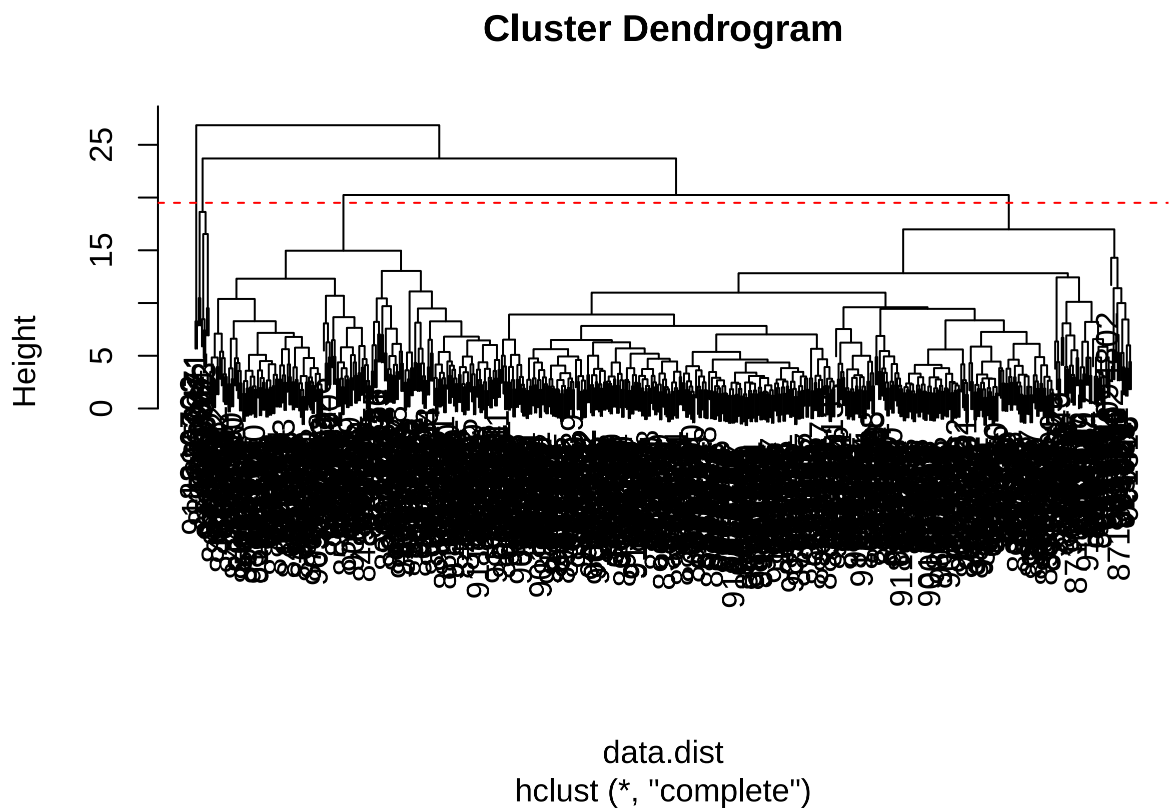
Creating hierarchical clustering model

```
wisc.hclust <- hclust(data.dist, method= "complete" )
```

Results of hierarchical clustering

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

```
plot(wisc.hclust)
abline(h= 19.5, col="red", lty=2)
```



Height= 19.5 at which the clustering model has 4 clusters. ### Selecting number of clusters

```
wisc.hclust.clusters <- cutree(wisc.hclust, h=19.5)
```

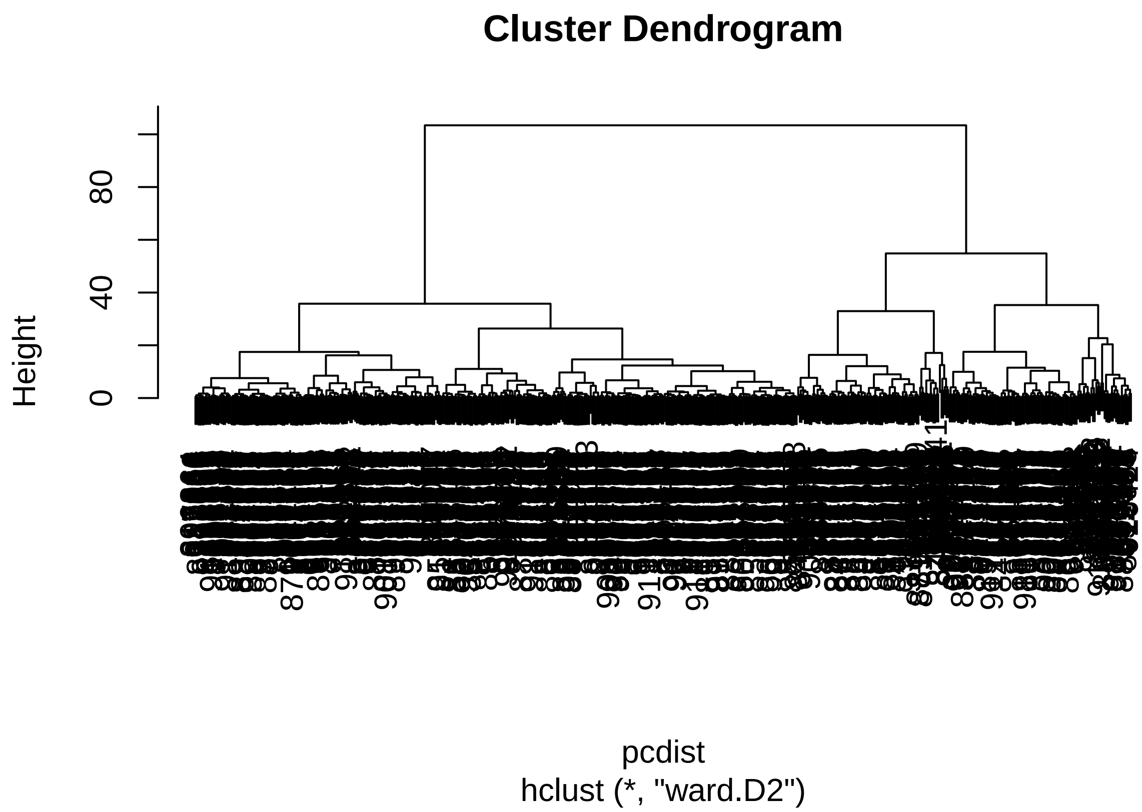
Using "table()" function to compare the cluster membership to actual diagnosis.

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

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

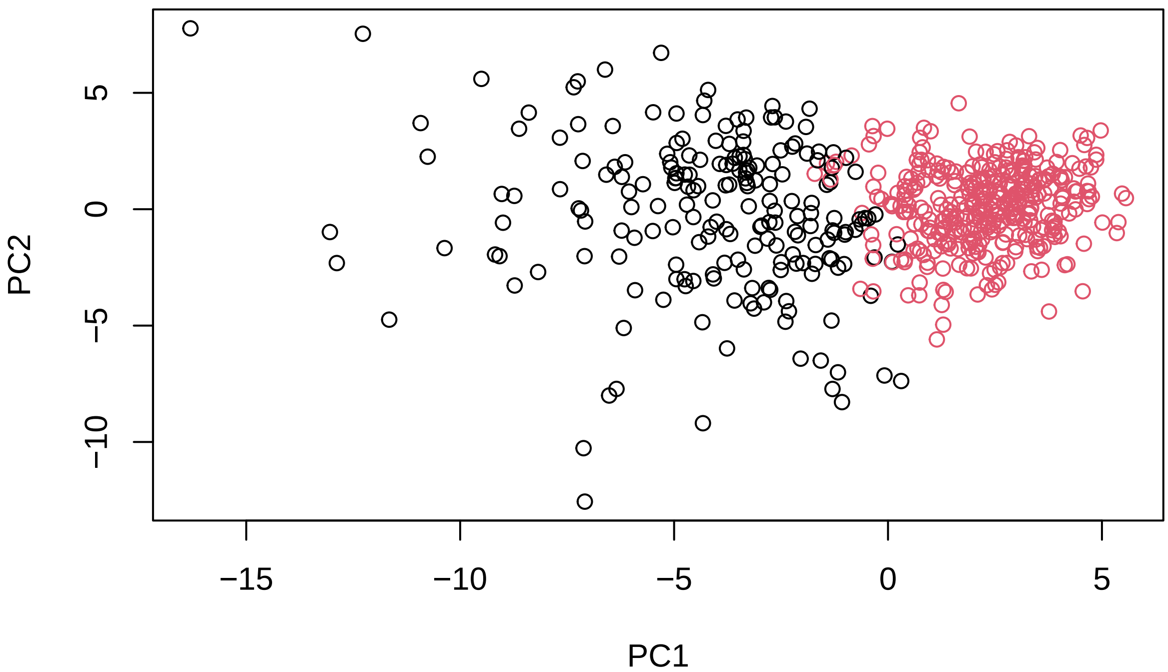
First 3 PCs for clustering

```
pcdist <- dist(wisc.pr$x[,1:3])
wisc.pr.hclust <- hclust(pcdist, method="ward.D2")
plot(wisc.pr.hclust)
```




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

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



How well do my clusters agree with the expert M/B values

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

```
##          grps
## diagnosis   1   2
##         B  24 333
##         M 179  33
```