ML Mini Project

Haroon Riyaz (PID A15377799)

2/14/2022

1. Exploratory Data Anlysis

Downlaod and prepare data!

```
#Save Data into directory
fna.data <- "WisconsinCancer.csv"

#Store data as wisc.df
wisc.df <- read.csv(fna.data, row.names=1)
```

Remove data that already provides answers to lab questions (diagnosis)!

```
#Removes first column
wisc.data <- wisc.df[,-1]
```

Store diagnosis vector that can be used to check work later on!

```
#Create diagnosis vector to be used later on
diagnosis <- wisc.df[,1]
diagnosis
```

```
##   [1] "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M"
##  [19] "M" "B" "B" "B" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M"
##  [37] "M" "B" "M" "M" "M" "M" "M" "M" "M" "M" "B" "M" "B" "B" "B" "B" "B" "M"
##  [55] "M" "B" "M" "M" "B" "B" "B" "B" "M" "B" "M" "M" "B" "B" "B" "B" "M" "B"
##  [73] "M" "M" "B" "M" "B" "M" "M" "B" "B" "B" "M" "M" "B" "M" "M" "M" "B" "B"
##  [91] "B" "M" "B" "B" "M" "M" "B" "B" "B" "M" "M" "B" "B" "B" "B" "M" "B" "B"
## [109] "M" "B" "B" "B" "B" "B" "B" "B" "B" "M" "M" "M" "B" "M" "M" "B" "B" "B"
## [127] "M" "M" "B" "M" "B" "M" "M" "B" "M" "M" "B" "B" "M" "B" "B" "M" "B" "B"
## [145] "B" "B" "M" "B" "B" "B" "B" "B" "B" "B" "B" "B" "M" "B" "B" "B" "B" "M"
## [163] "M" "B" "M" "B" "B" "M" "M" "B" "B" "M" "M" "B" "B" "B" "B" "M" "B" "B"
## [181] "M" "M" "M" "B" "M" "B" "M" "B" "B" "B" "M" "B" "B" "M" "M" "B" "M" "M"
## [199] "M" "M" "B" "M" "M" "M" "B" "M" "B" "M" "B" "B" "M" "B" "M" "M" "M" "M"
## [217] "B" "B" "M" "M" "B" "B" "B" "M" "B" "B" "B" "B" "B" "M" "M" "B" "B" "M"
## [235] "B" "B" "M" "M" "B" "M" "B" "B" "B" "B" "M" "B" "B" "B" "B" "B" "M" "B"
## [253] "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "B" "B" "B" "B"
## [271] "B" "B" "M" "B" "M" "B" "B" "M" "B" "B" "M" "B" "M" "M" "B" "B" "B" "B"
## [289] "B" "B" "B" "B" "B" "B" "B" "B" "B" "M" "B" "B" "M" "B" "M" "B" "B" "B"
## [307] "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "M" "B" "B" "B" "M" "B" "M"
## [325] "B" "B" "B" "B" "M" "M" "M" "B" "B" "B" "B" "M" "B" "M" "B" "M" "B" "B"
## [343] "B" "M" "B" "B" "B" "B" "B" "B" "B" "M" "M" "M" "B" "B" "B" "B" "B" "B"
## [361] "B" "B" "B" "B" "B" "M" "M" "B" "M" "M" "M" "B" "M" "M" "B" "B" "B" "B"
## [379] "B" "M" "B" "B" "B" "B" "B" "M" "B" "B" "B" "M" "B" "B" "M" "M" "B" "B"
## [397] "B" "B" "B" "B" "M" "B" "B" "B" "B" "B" "B" "B" "M" "B" "B" "B" "B" "B"
## [415] "M" "B" "B" "M" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "M" "B"
## [433] "M" "M" "B" "M" "B" "B" "B" "B" "B" "M" "B" "B" "M" "B" "M" "B" "B" "M"
## [451] "B" "M" "B" "B" "B" "B" "B" "B" "B" "B" "M" "M" "B" "B" "B" "B" "B" "B"
## [469] "M" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "M" "B" "B" "B" "B" "B" "B"
## [487] "B" "M" "B" "M" "B" "B" "M" "B" "B" "B" "B" "B" "M" "M" "B" "M" "B" "M"
## [505] "B" "B" "B" "B" "B" "M" "B" "B" "M" "B" "M" "B" "M" "M" "B" "B" "B" "M"
## [523] "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "M" "B" "M" "M" "B" "B" "B"
## [541] "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B"
## [559] "B" "B" "B" "B" "M" "M" "M" "M" "M" "M" "B"
```

> Q1. How many observations are in this dataset?

Number of rows corresponds to observations so nrow will be used. Length of diagnosis can also be used.

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

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

```
length(diagnosis)
```

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

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

Use table to find number of malignant cells

```
num_malignant <- table(diagnosis)
num_malignant["M"]
```

```
##   M
## 212
```

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

Grep() can be used to identify features with "_mean" and length() can then count all features with "_mean"

```
#Assigns features to data_names vector
data_names <- colnames(wisc.data)

#Grep identifies features with "_mean" suffix and length counts all such features
length(grep("_mean",data_names))
```

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

2. Principal Component Analysis

Check mean and SD to see if data must be scaled!

```
# Check the means and SD of the data
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
```

```
# Perform PCA on wisc.data
wisc.pr <- prcomp((wisc.data), scale = TRUE)
```

Look at summary of results

```
#Summary
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)?

```
pca.var <- wisc.pr$sdev^2

pca.var.per <- round(pca.var/sum(pca.var)*100,1)
pca.var.per[1]
```

```
## [1] 44.3
```

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

I manually added the PCs until reaching the specified variance.

```
pca.var.per[1] + pca.var.per[2] + pca.var.per[3]
```

```
## [1] 72.7
```

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?

```
pca.var.per[1] + pca.var.per[2] + pca.var.per[3] + pca.var.per[4] + pca.var.per[5] + pca.var.per[6] + p
```

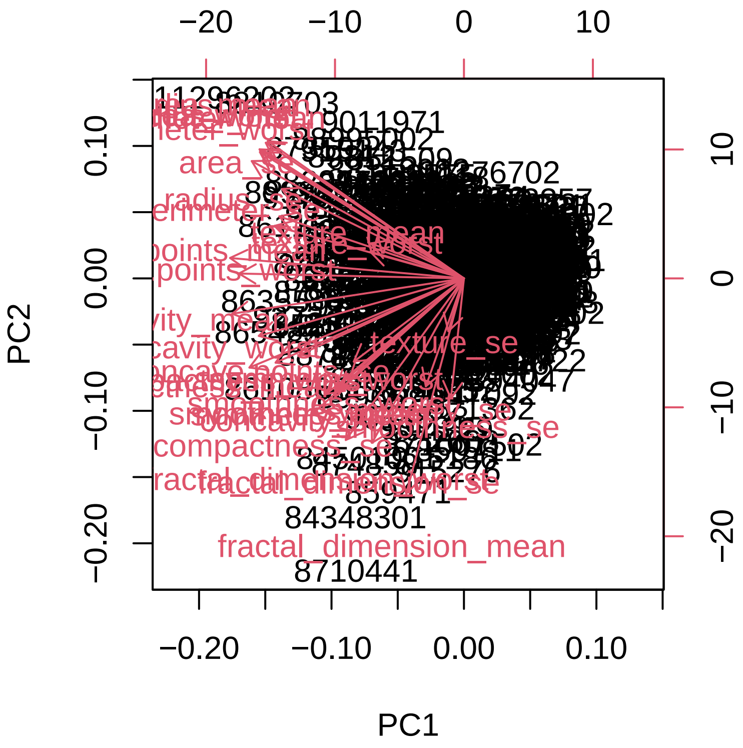
```
## [1] 91.1
```

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

Interpreting PCA Results

Biplot of wisc.pr

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

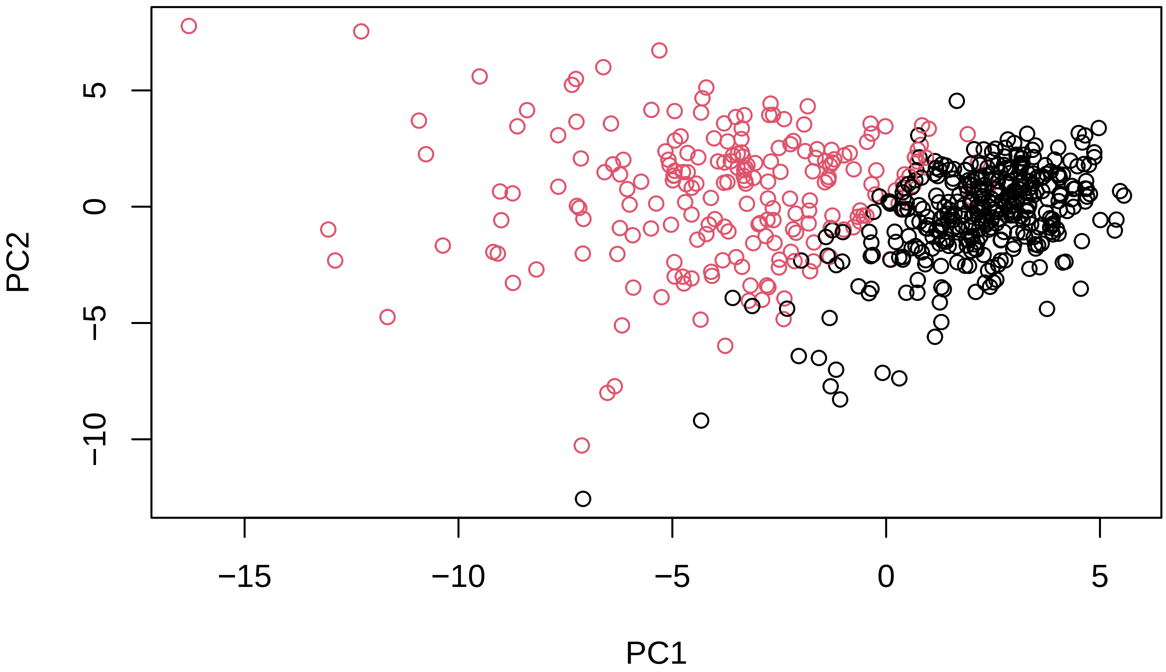


Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?

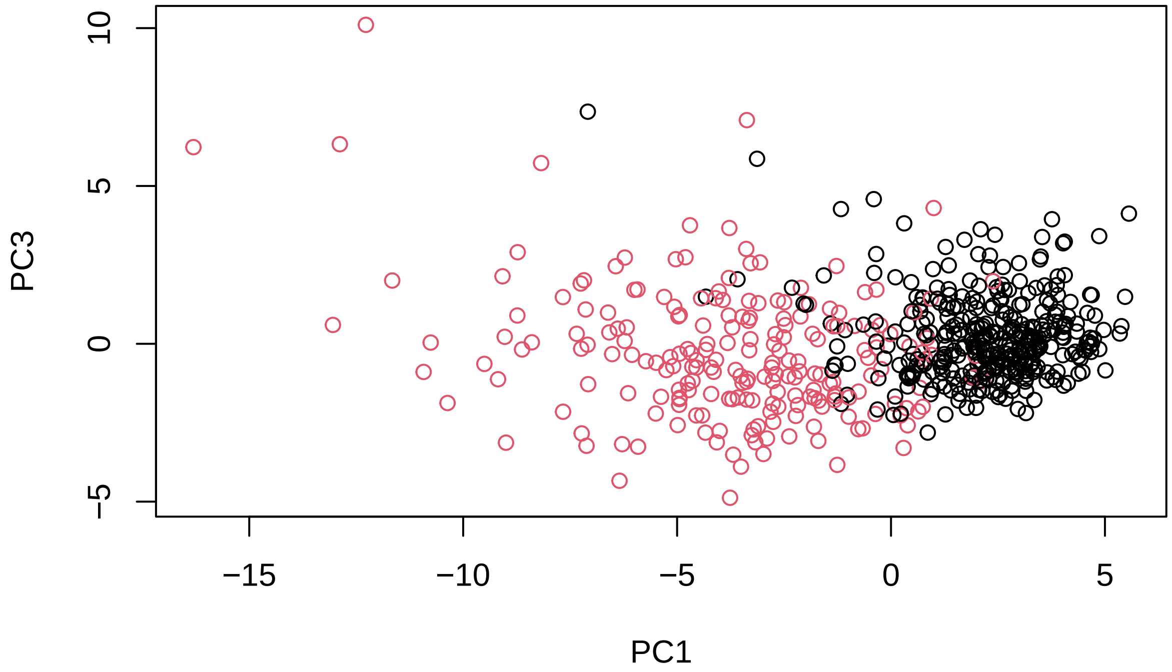
It is difficult to understand and is very messy due to the many labels and data points. Since row_names are used as plotting characters it is hard to see the data as the variable names block the graph. This plot also incorporates many hundreds of points which obscures individual data points.

Let's generate a more standard scatter plot!

```r
# Scatter plot of components 1 and 2

#diagnosis[grep("M", diagnosis)] <- "red"
#diagnosis[grep("B", diagnosis)] <- "black"

plot(wisc.pr$x[,1], wisc.pr$x[,2], col = as.factor(diagnosis) ,xlab="PC1", ylab="PC2")
```



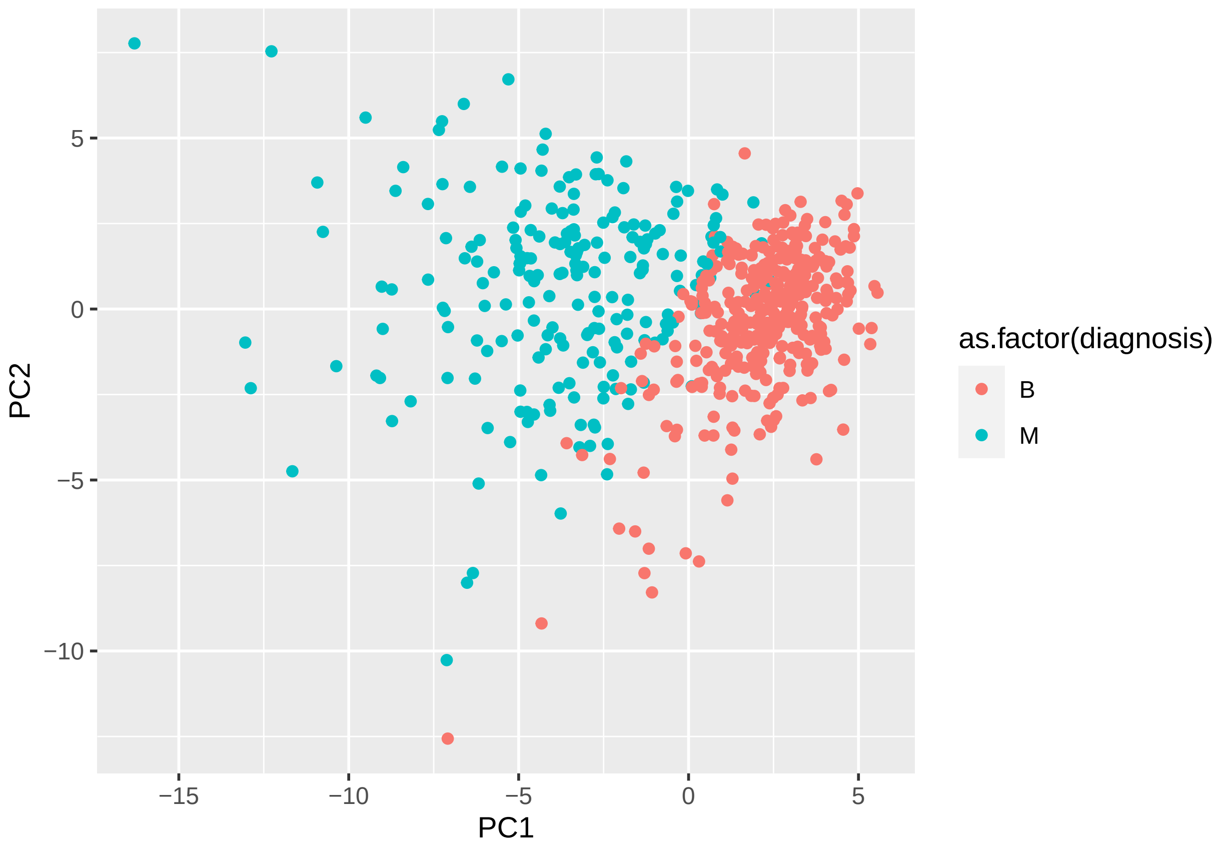
```r
# Scatter plot of components 1 and 2

#diagnosis[grep("M", diagnosis)] <- "red"
#diagnosis[grep("B", diagnosis)] <- "black"

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



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

There is less distinction between malignant and benign cells (more mixture) for components 1 and 3 compared to components 1 and 2 since components 1 and 2 highlight patterns the most while component 3 does less so and shows less variation, hence why both the malignant and benign data are more mixed.

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

# Load ggplot2
library(ggplot2)

# Scatter plot colored by diagnosis
ggplot(df) +
  aes(PC1, PC2, col= as.factor(diagnosis)) +
  geom_point()
```



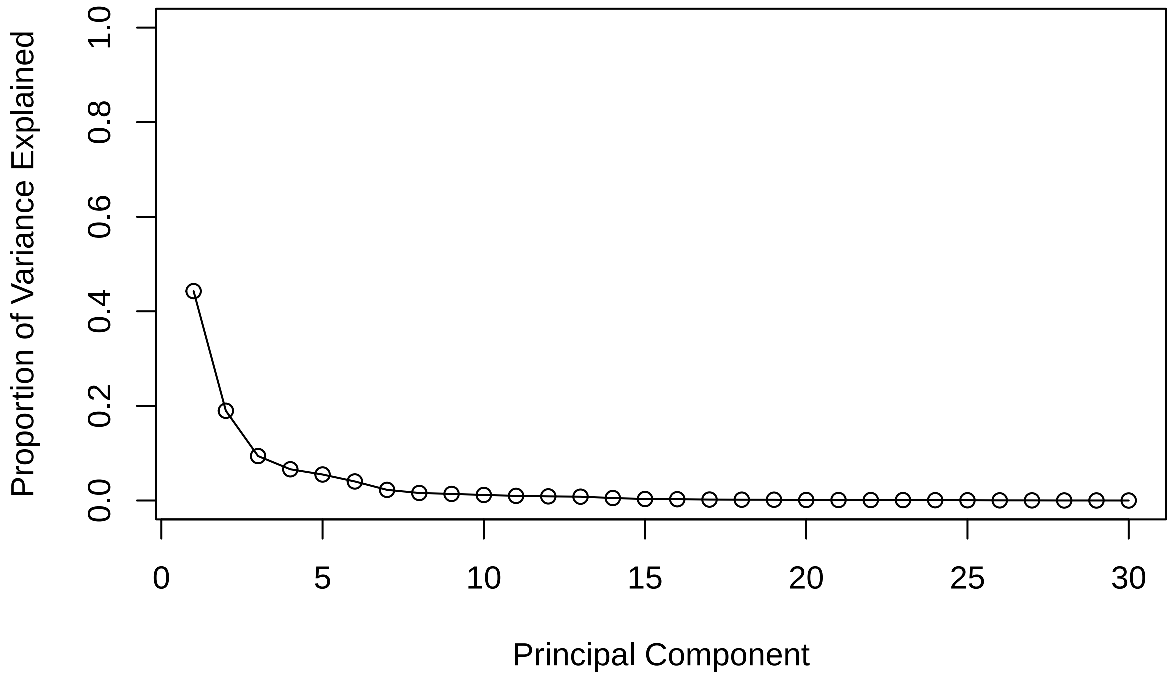
### Variance Explained

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

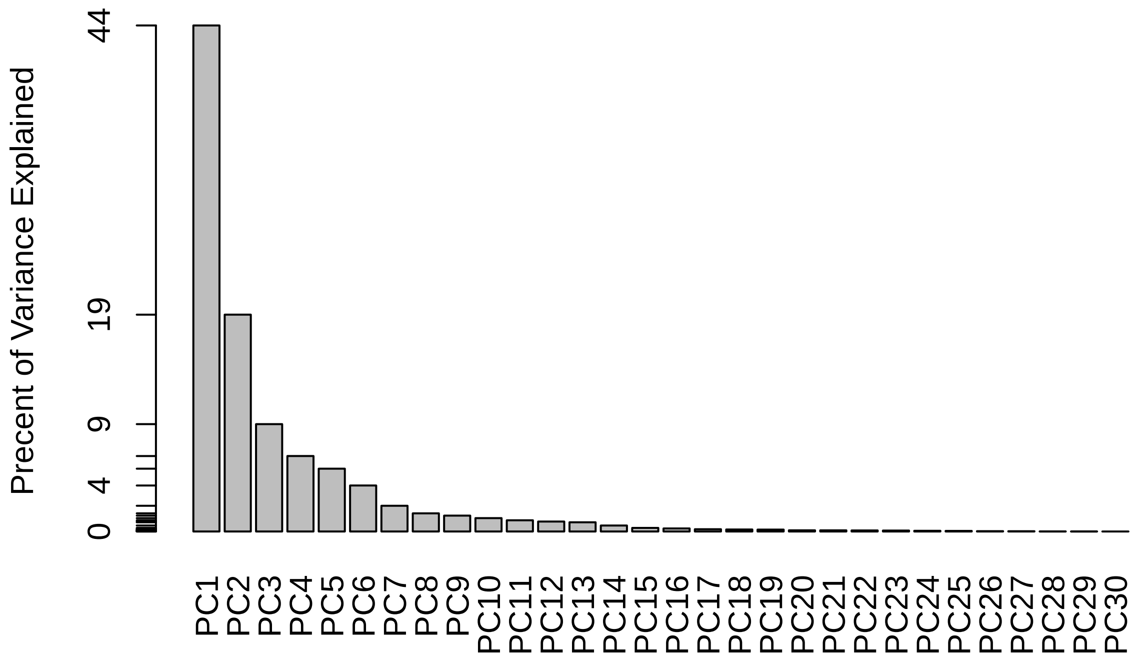
```
## [1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

Principal Variance Proportion

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

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



```r
# Alternative screen plot of the same data
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?

```
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
```

-0.26085376

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

```
pca.var.per[1] + pca.var.per[2] + pca.var.per[3] + pca.var.per[4] + pca.var.per[5]
```

```
## [1] 84.8
```

5 PCs are required to describe at least 80% of the original variance in the data.

3. Hierarchical Clustering

```
# Scale wisc.data data with scale()
data.scaled <- scale(wisc.data)
```

Calculate euclidean distance between observations

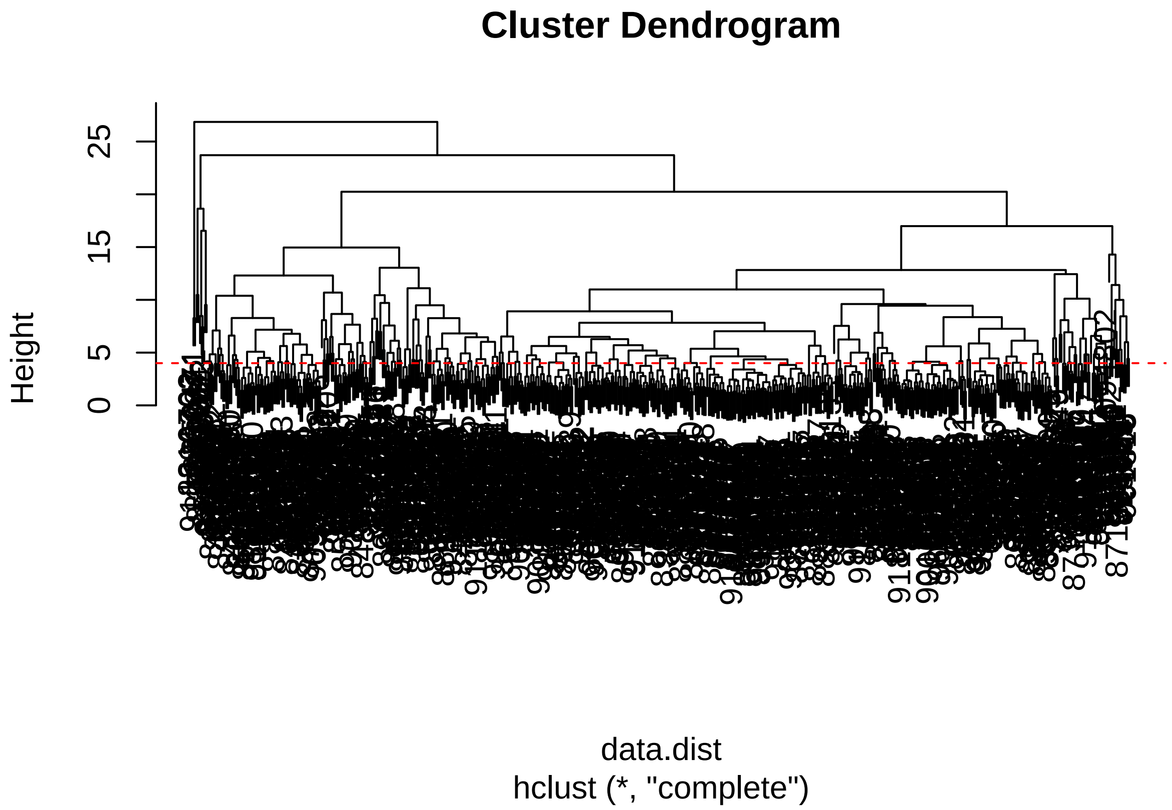
```
data.dist <- dist(data.scaled)
```

Create a hierarchical clustering model

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

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

```
plot(wisc.hclust)
abline(h=4, col="red", lty=2)
```



The clustering model has 4 clusters at a height of 20

Selecting Number of Clusters

```
wisc.hclust.clusters <- cutree(wisc.hclust, k = 4)
```

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

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

> Q12. Can you find a better cluster vs diagnoses match by cutting into a different number of clusters between 2 and 10?

```
wisc.hclust_test.clusters <- cutree(wisc.hclust, k = 3)
table(wisc.hclust_test.clusters, diagnosis)
```

```
##                            diagnosis
## wisc.hclust_test.clusters    B   M
##                          1 355 205
##                          2   2   5
##                          3   0   2
```

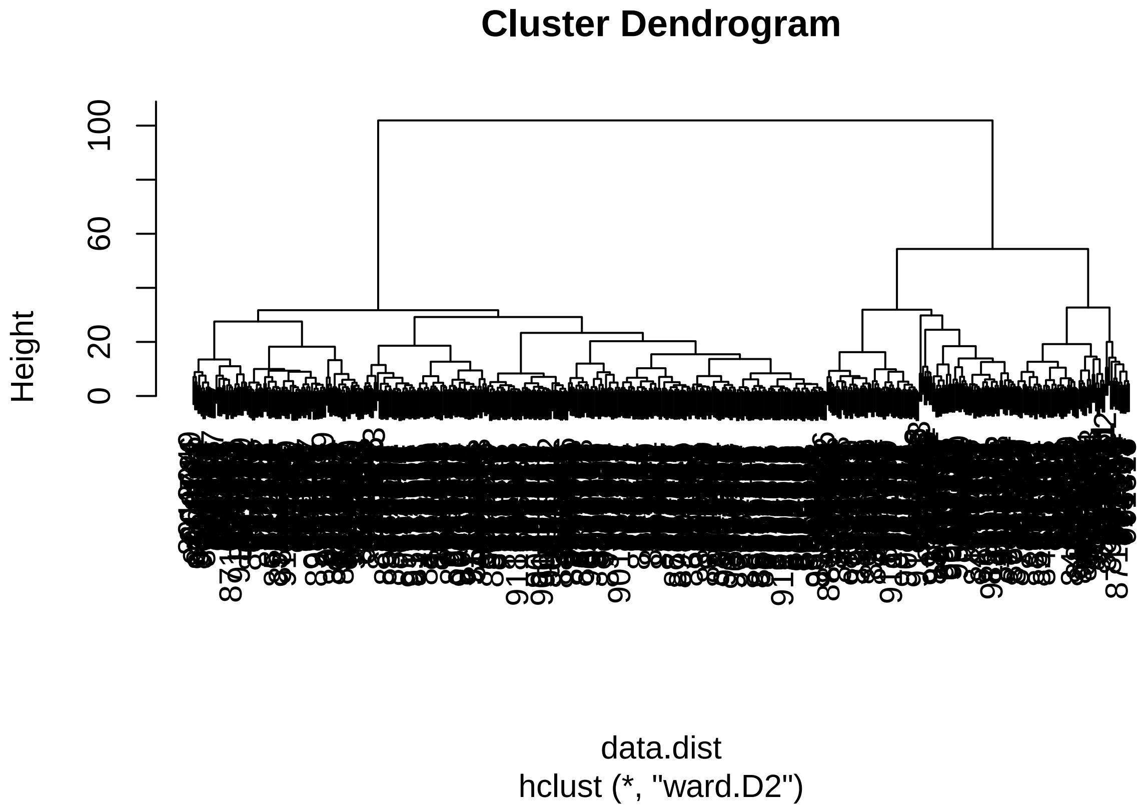
```
wisc.hclust_test.clusters <- cutree(wisc.hclust, k = 8)
table(wisc.hclust_test.clusters, diagnosis)
```

```
##                            diagnosis
## wisc.hclust_test.clusters   B   M
##                          1  12  86
##                          2   0  79
##                          3   0   3
##                          4 331  39
##                          5   2   0
##                          6  12   1
##                          7   0   2
##                          8   0   2
```

No, having a cluster number lower than 4 results in a majority of the benign and malignant cells being in the same cluster. Have more then 4 clusters does differentiate malignant and beignin cells more than the one with 4 clusters.

> Q13. Which method gives your favorite results for the same data.dist dataset? Explain your reasoning.

```
plot(hclust(data.dist, method = "ward.D2"))
```



Ward.D2 gives my favorite results since the branches are more organized and not as messy as the other methods since variance within clusters is lessened.

4. K-means Clustering

```
wisc.km <- kmeans(scale(wisc.data), centers= 2, nstart= 20)
```

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

```
##    diagnosis
##       B   M
##   1 343  37
##   2  14 175
```

```
# Black = Benign, Red = Malignant
```

> Q14. How well does k-means separate the two diagnoses? How does it compare to your hclust results?

The two diagnoses are as well-separated as in the hclust results. Both hclust and k-means show the majority of malignant and benign cells being separated into different clusters and each cluster only has a small proportion of cells which are the opposite (few malignant cells in benging cluster, vice versa). The diagnoses are separated well with both methods.

```
table(wisc.hclust.clusters, wisc.km$cluster)
```

```
##                     
## wisc.hclust.clusters   1   2
##                    1  17 160
##                    2   0   7
##                    3 363  20
##                    4   0   2
```

5. Combining Methods

```
wisc.pr.hclust <- hclust(dist(wisc.pr$x[,1:7]),"ward.D2")
```

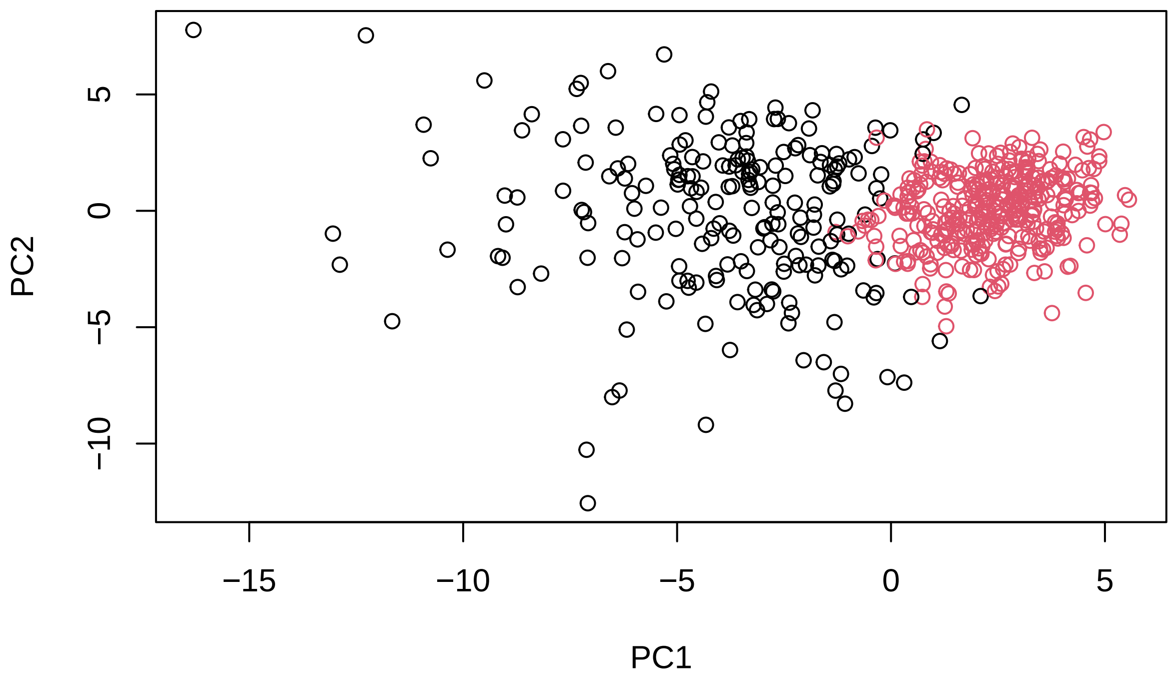
```
grps <- cutree(wisc.pr.hclust, k=2)
table(grps)
```

```
## grps
##   1   2 
## 216 353
```

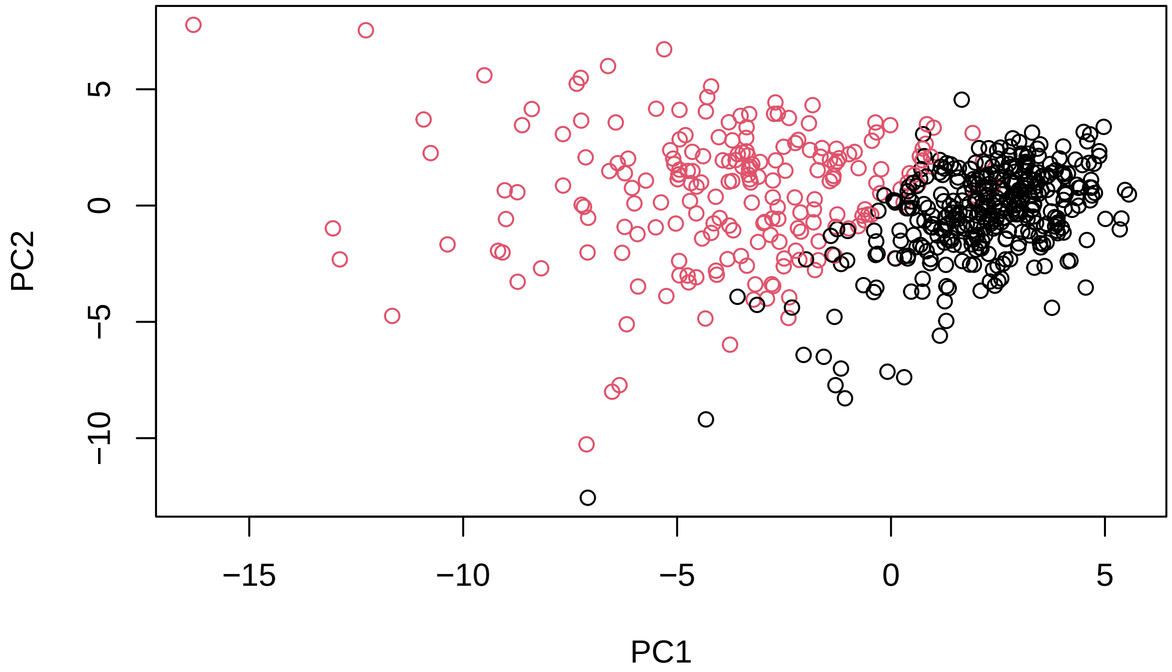
```
table(grps, diagnosis)
```

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

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



```
#diagnosis[grep("M", diagnosis)] <- "red"
#diagnosis[grep("B", diagnosis)] <- "black"

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



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

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

```
# Compare to actual diagnoses
# Black = Benign, Red = Malignant
table(wisc.pr.hclust.clusters, diagnosis)
```

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

The model separates both well as each cluster possesses more than a majority of one type of cell. Each cluster is realtively homogenous and contains few of the other cell type.

> 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.

Both models do a good job at separating the diagnoses as the benign and malignant cells are mostly in separate clusters.

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

```
##    diagnosis
##       B   M
##   1 343  37
##   2  14 175
```

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

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

```
# Compare to actual diagnoses
# Black = Benign, Red = Malignant
```

6. Sensitivity/Specifciity

> Q17. Which of your analysis procedures resulted in a clustering model with the best specificity? How about sensitivity?

```
#KM
SensKM <- 175/(175+37)
SensKM
```

```
## [1] 0.8254717
```

```
SensHclust <- 165/(165+5+40+2)
SensHclust
```

```
## [1] 0.7783019
```

```
SpecKM <- 343/(343+13)
SpecKM
```

```
## [1] 0.9634831
```

```
SpecHclust <- 343/(343+12+2)
SpecHclust
```

```
## [1] 0.9607843
```

K-means had the best specificity but this was only by a very small margin (.963 vs .961).

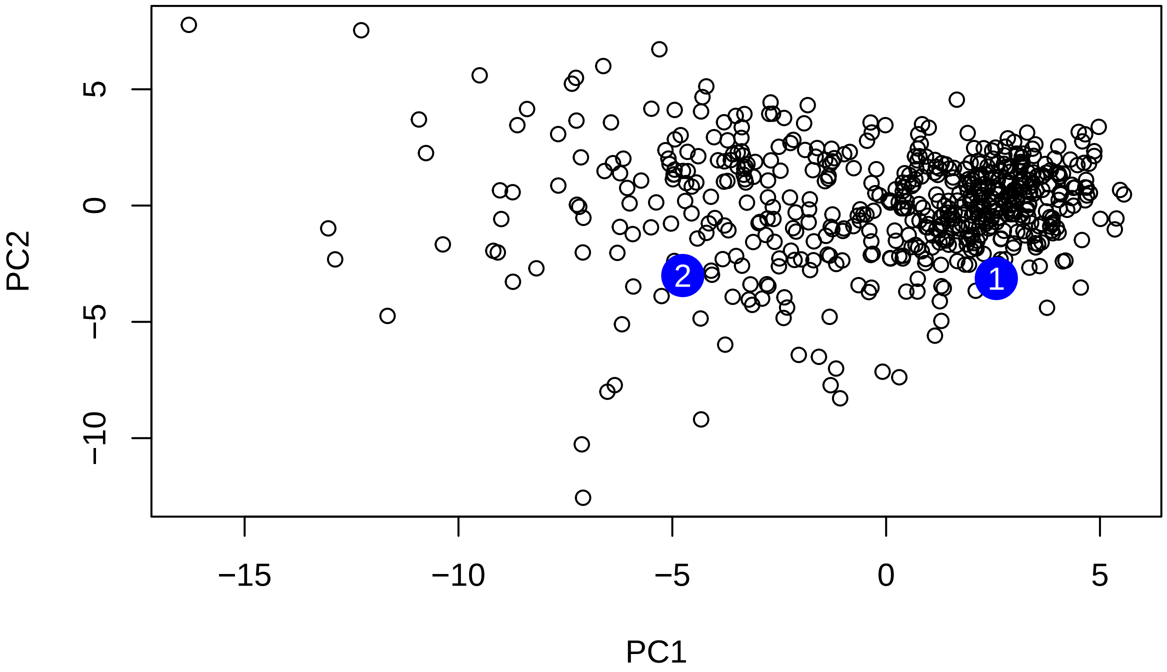
K-means had the best sensitivity (0.83).

7.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
```

```
# col = g WAS NOT WORKING!
plot(wisc.pr$x[,1:2])
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?

Patient 2 should be followed up since his data was in the same region as malignant cell data indicating he has cancer.