class09_mini_project

Hyeonseok Jang (PID# A59011126)

10/27/2021

1. Exploratory data analysis

```
# 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)
```

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

```
# Create diagnosis vector for later
diagnosis <- as.factor(wisc.df$diagnosis)
```

> Q1. How many observations are in this dataset?

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

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

There are 569 observations in the dataset.

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

```
table(diagnosis)
```

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

212 observations have a malignant diagnosis.

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

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

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

There are 10 variables in the data with the '_mean' suffix.

2. Principal Component Analysis Performing PCA

```
# 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
```

```
# Perform PCA on wisc.data by completing the following code
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)?

44.27% of the original variance is captured by the PC1.

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

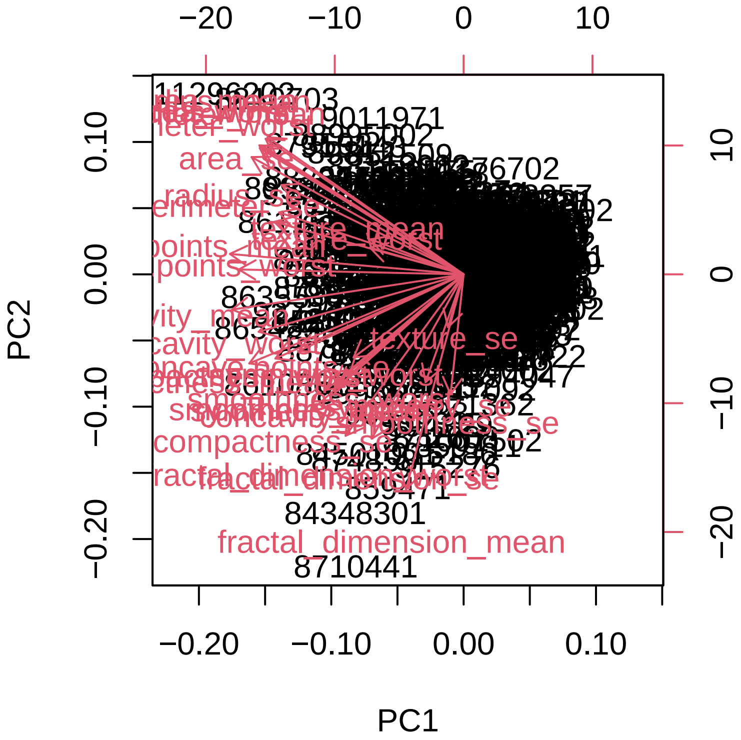
Three PCs

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

seven PCs

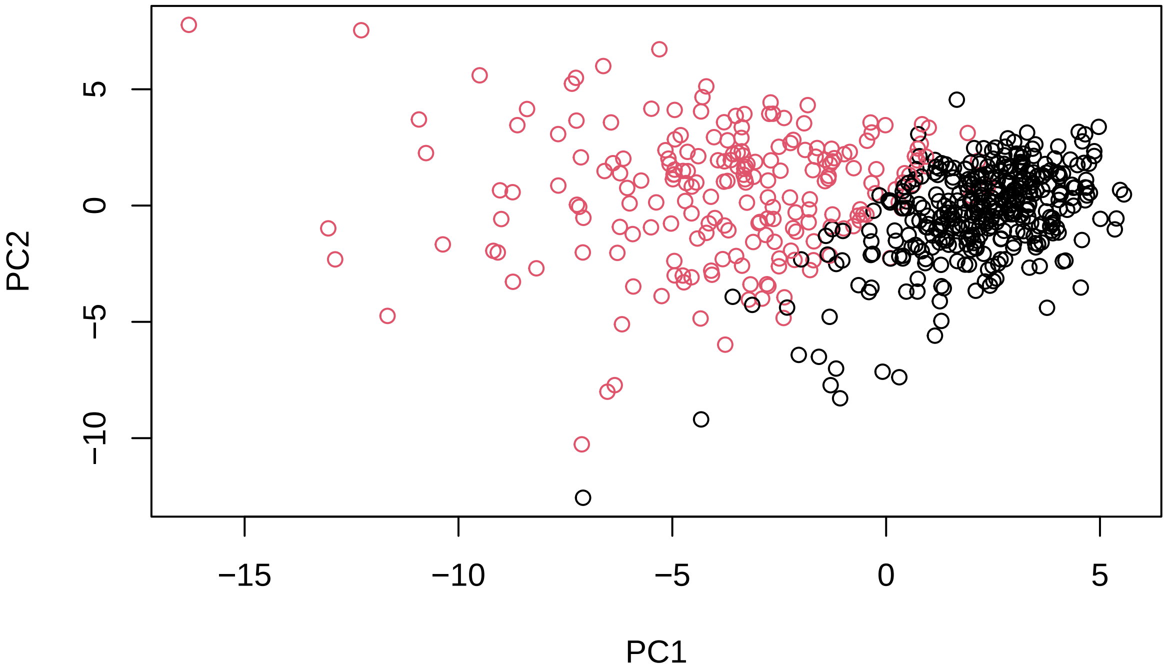
> Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?

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



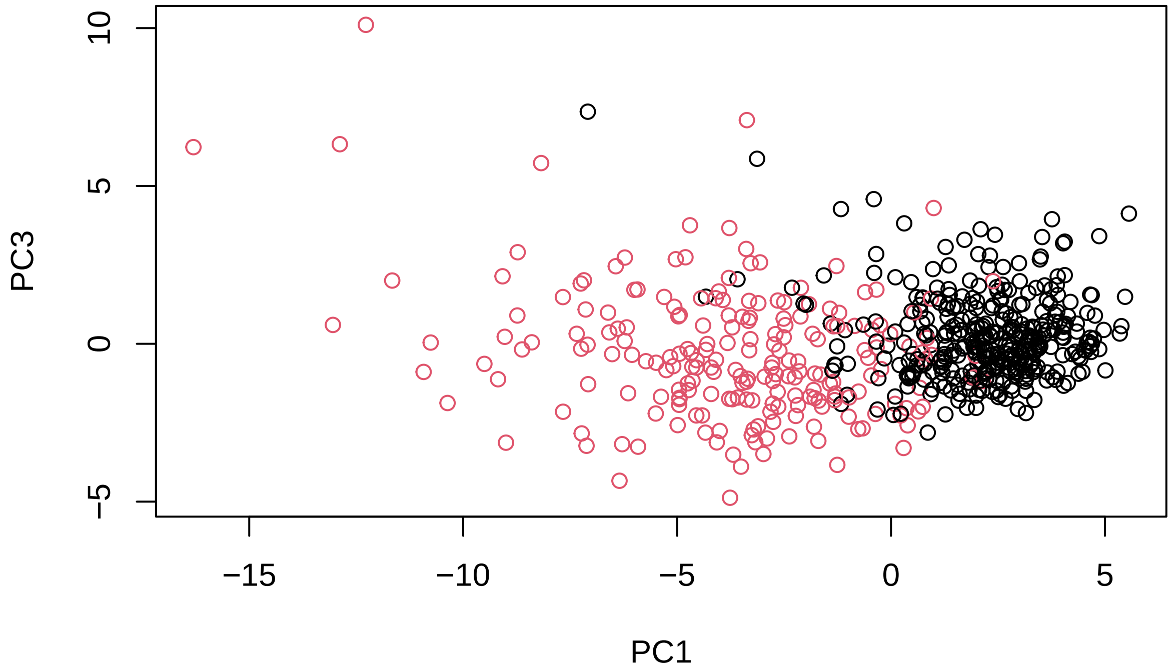
Rownames are used as the plotting character for biplots like this one which can make trends rather hard to see.

```
# 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?

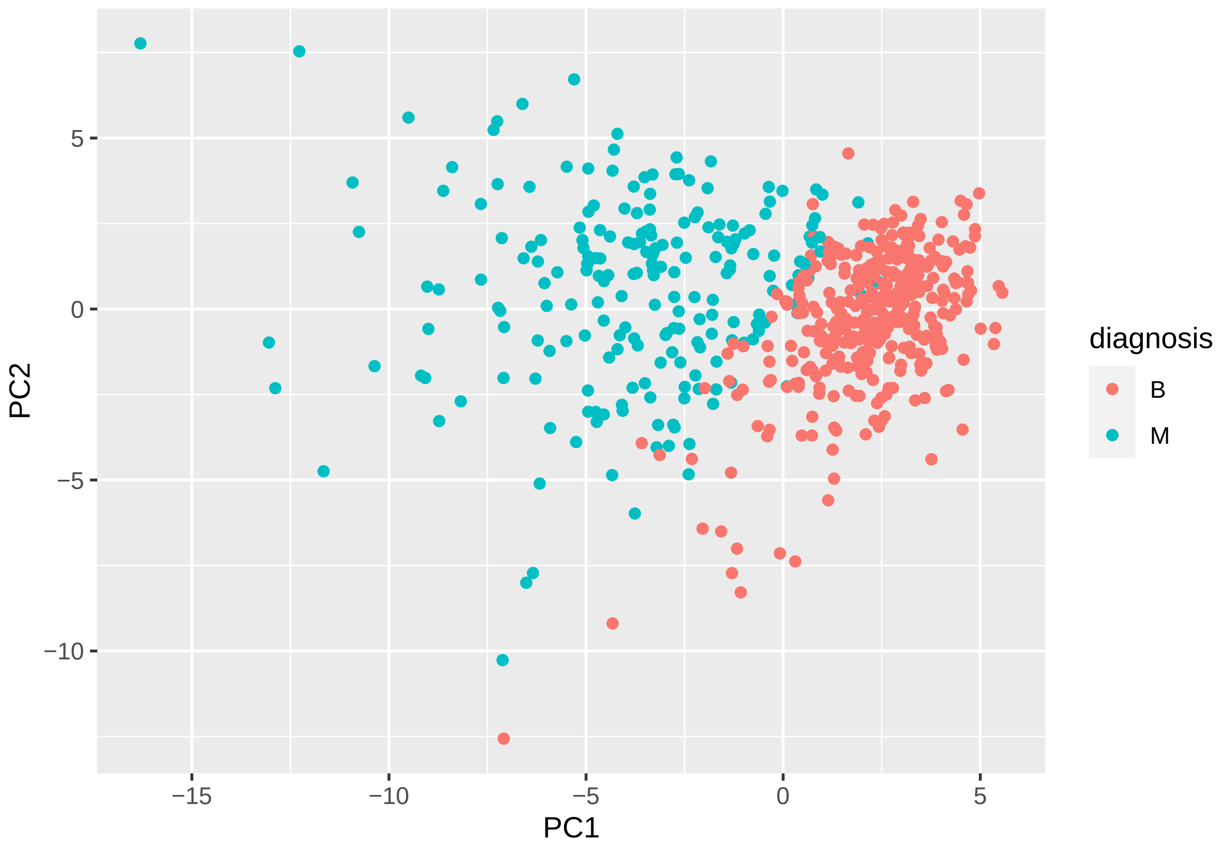
```
plot(wisc.pr$x[,c(1, 3)], col = diagnosis, xlab = "PC1", ylab = "PC3")
```



```
# 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()
```

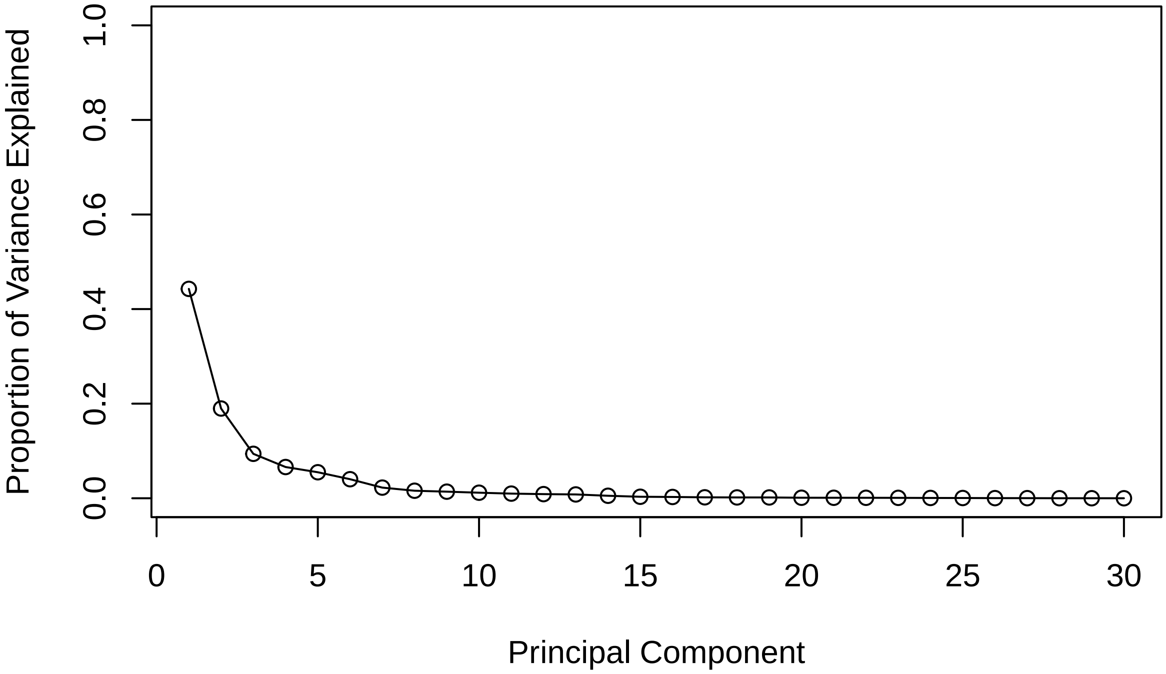


```
# Calculate variance of each component
pr.var <- wisc.pr$sdev^2
head(pr.var)
```

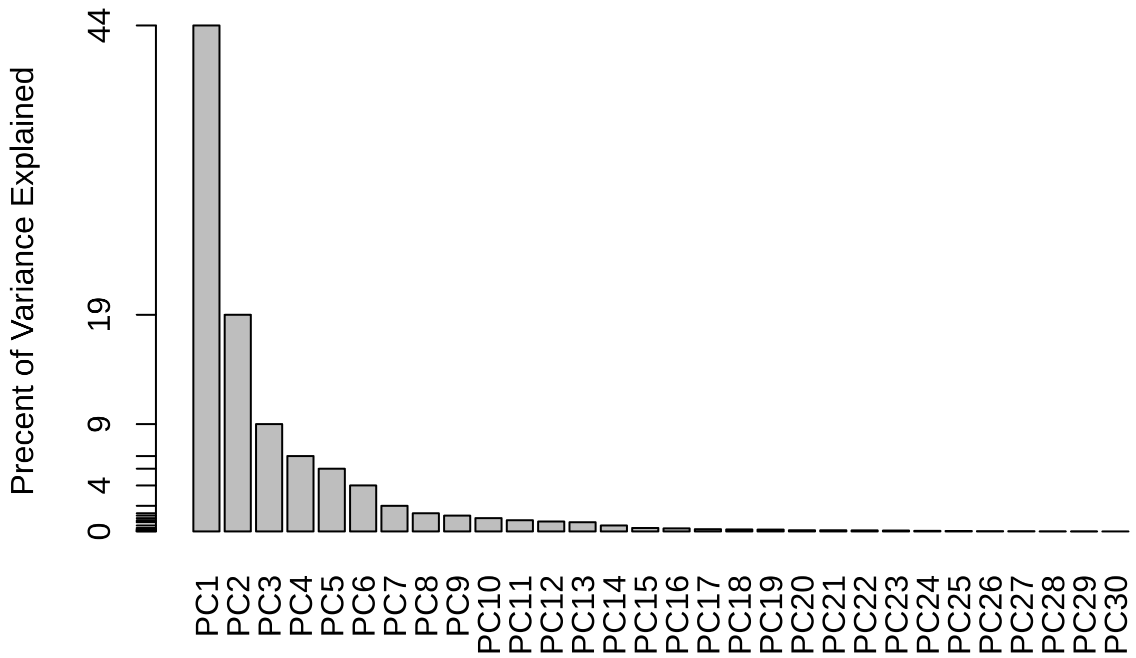
```
## [1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

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

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



```
# 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 =
axis(2, at=pve, labels=round(pve,2)*100 )
```



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]["concave.points_mean"]
```

```
## concave.points_mean 
##          -0.2608538
```

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
```

We need at least 5 of principal components to explain 80% of the variance of the data.

3. Hierarchical clustering

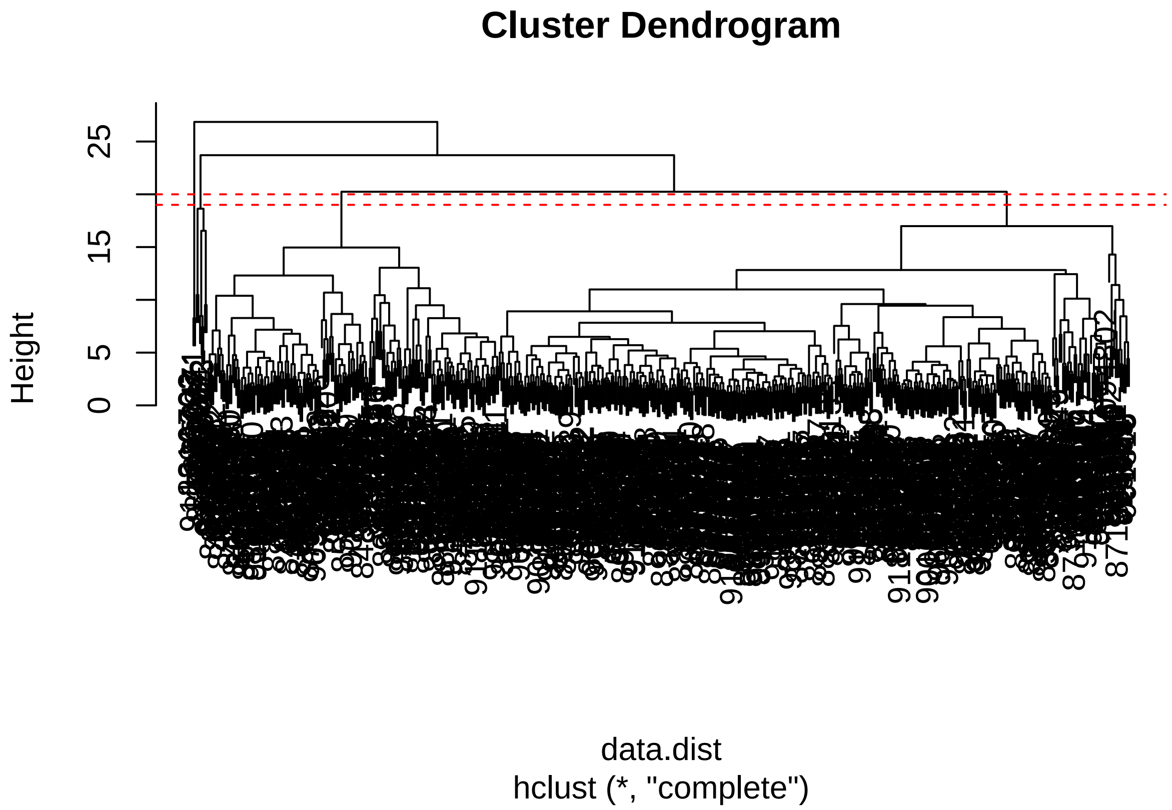
```
# Scale the wisc.data data using the "scale()" function
data.scaled <- scale(wisc.data)
```

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

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

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

```
plot(wisc.hclust)
abline(h=c(19, 20), col="red", lty=2)
```



The clustering model has 4 clusters at the heights of 19 and 20.

```
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?

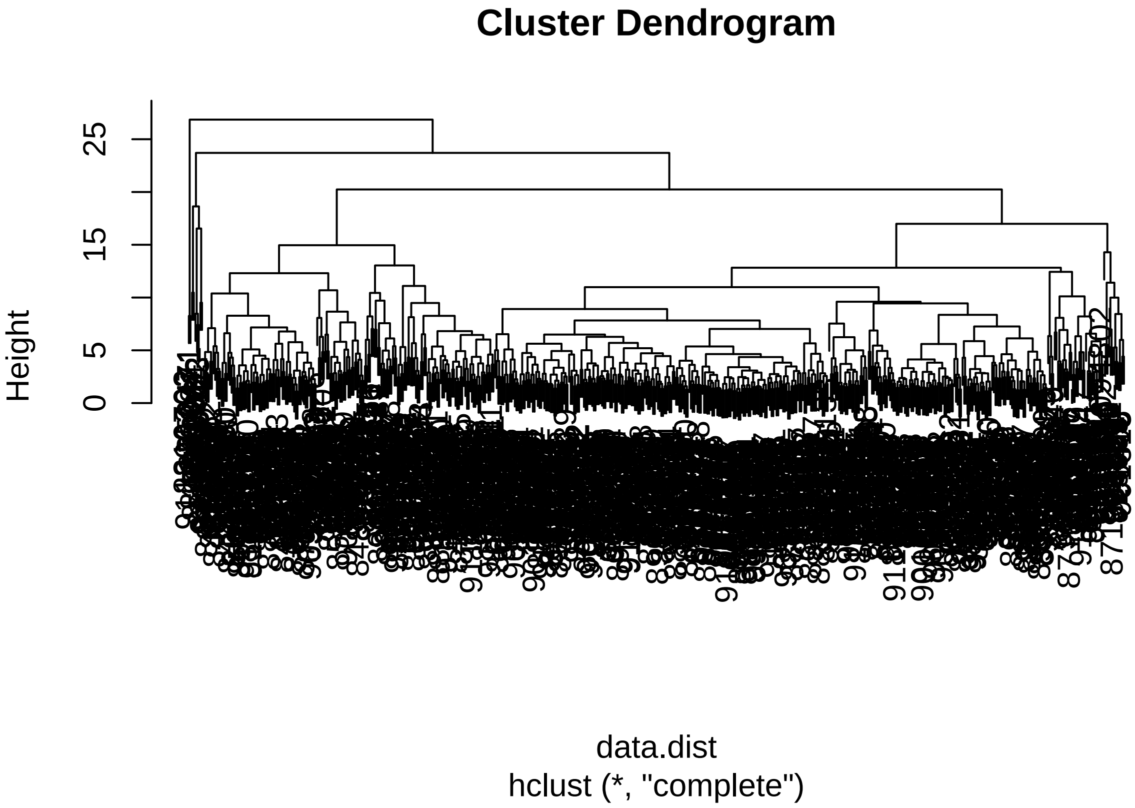
```
for (i in 2:10) {
  clusters <- cutree(wisc.hclust, k=i)
  print(table(clusters, diagnosis))
}
```

```
##         diagnosis
## clusters   B   M
##        1 357 210
##        2   0   2
##          diagnosis
## clusters   B   M
##        1 355 205
##        2   2   5
##        3   0   2
##          diagnosis
## clusters   B   M
##        1  12 165
##        2   2   5
##        3 343  40
##        4   0   2
##          diagnosis
## clusters   B   M
##        1  12 165
##        2   0   5
##        3 343  40
##        4   2   0
##        5   0   2
##          diagnosis
## clusters   B   M
##        1  12 165
##        2   0   5
##        3 331  39
##        4   2   0
##        5  12   1
##        6   0   2
##          diagnosis
## clusters   B   M
##        1  12 165
##        2   0   3
##        3 331  39
##        4   2   0
##        5  12   1
##        6   0   2
##        7   0   2
##          diagnosis
## 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
##          diagnosis
## clusters   B   M
##        1  12  86
##        2   0  79
##        3   0   3
##        4 331  39
##        5   2   0
##        6  12   0
##        7   0   2
##         8   0   2
##         9   0   1
##          diagnosis
## 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
```

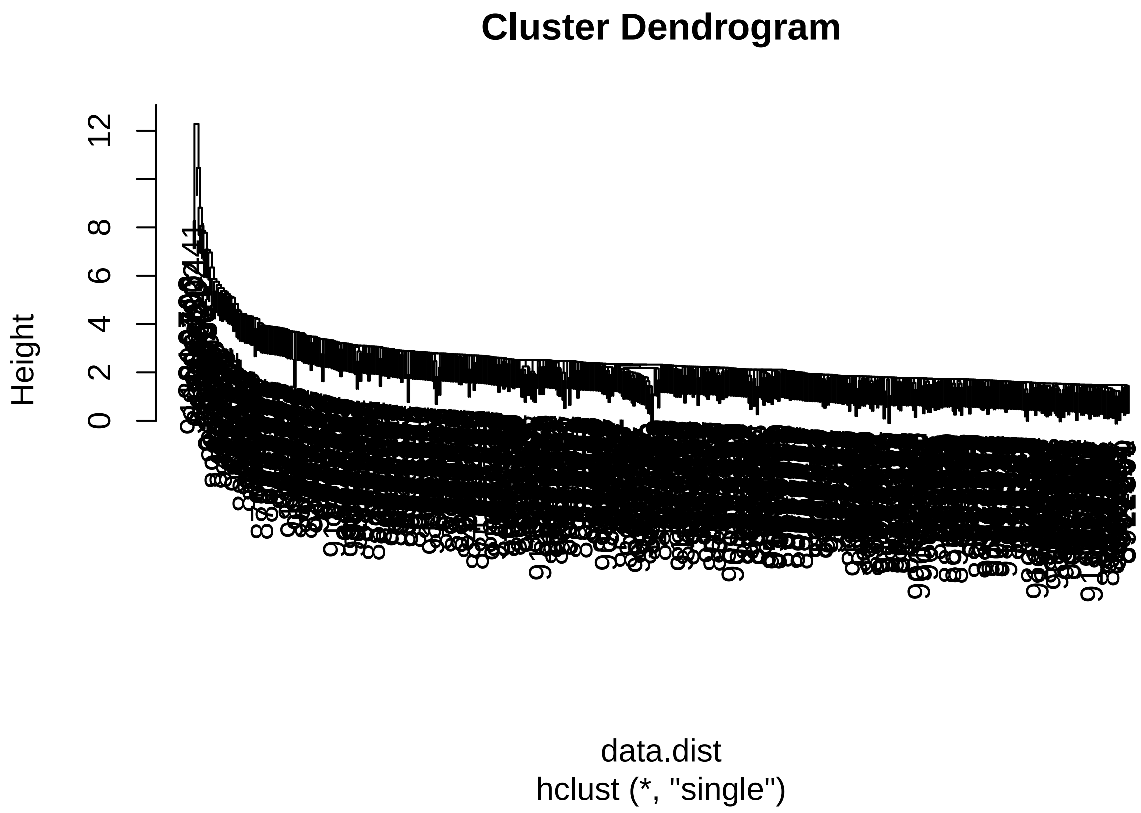
I think that cutting into 4 clusters is the best in regard to diagnosis.

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

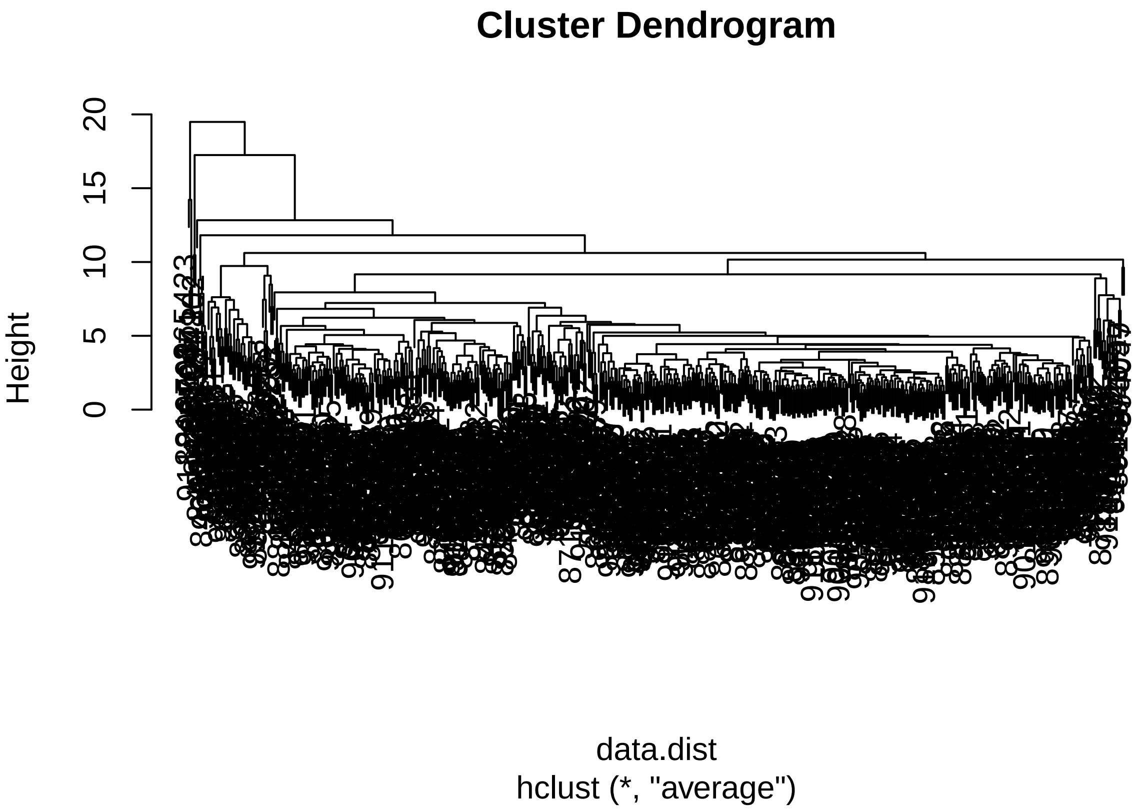
```
wisc.hclust.complete <- hclust(data.dist, method="complete")
plot(wisc.hclust.complete)
```



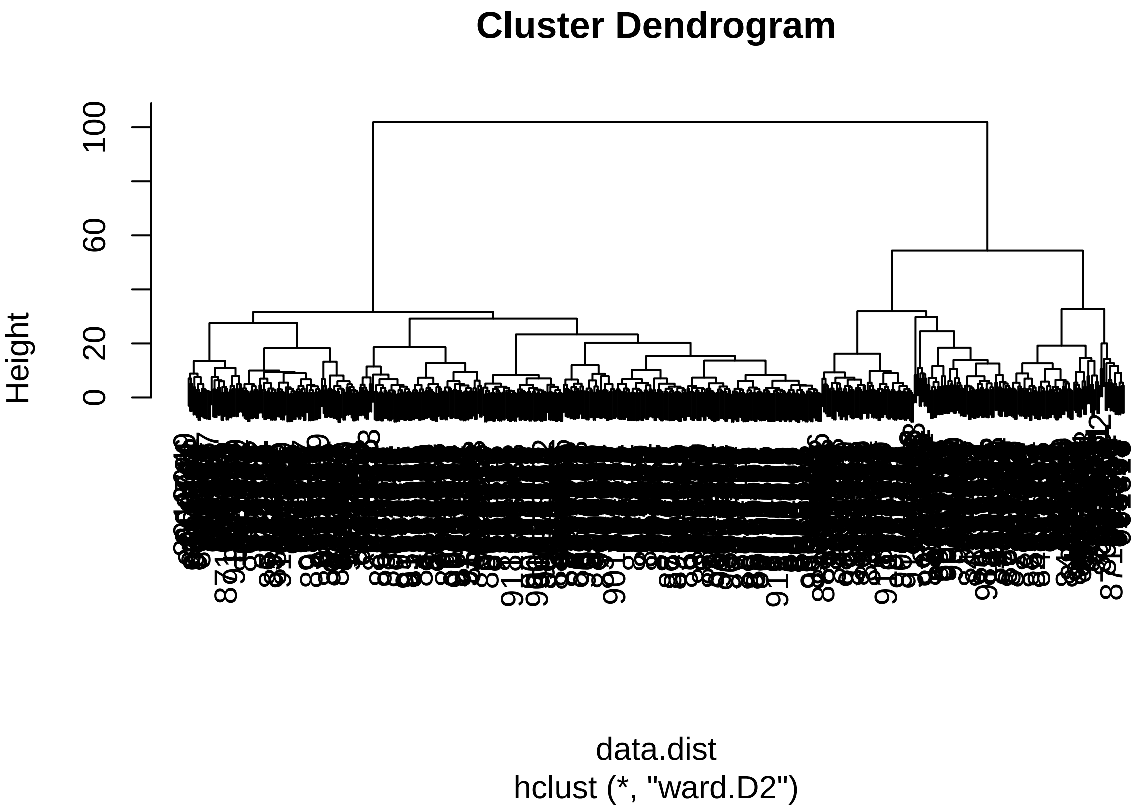
```
wisc.hclust.single <- hclust(data.dist, method="single")
plot(wisc.hclust.single)
```



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



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



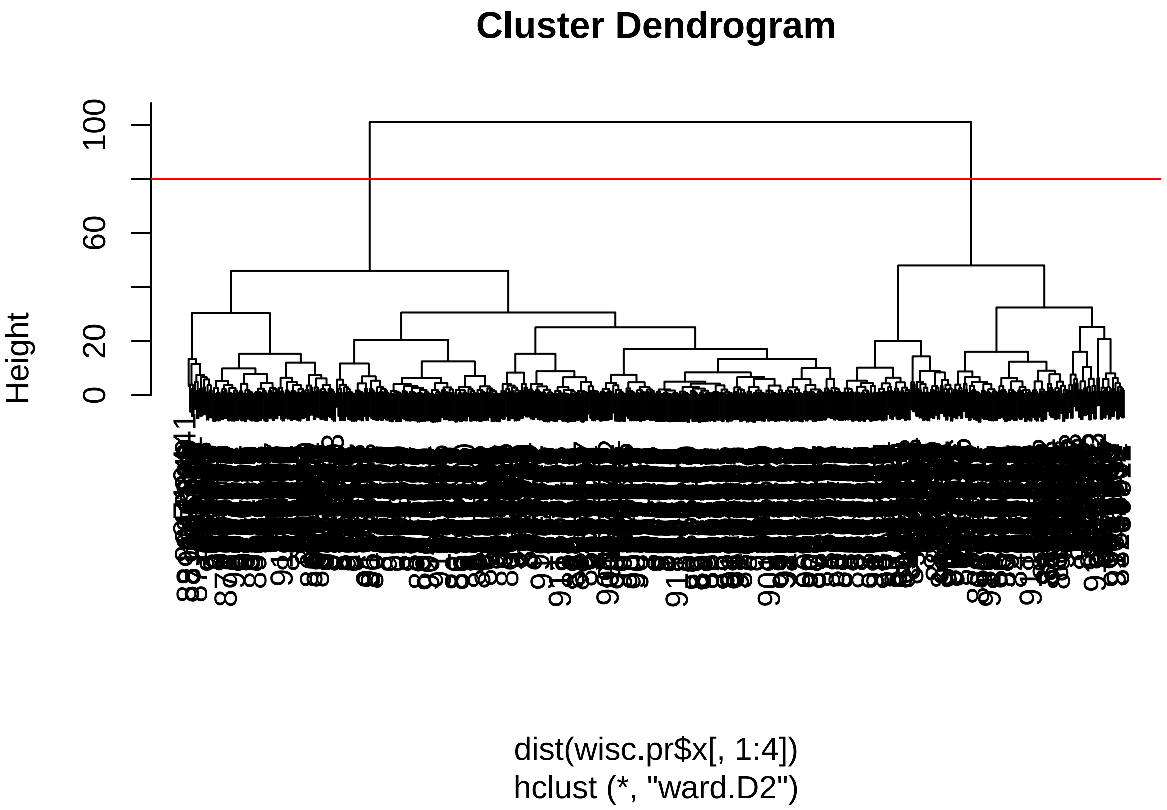
I think that "ward.D2" method gives me favorite results compared with others. I can get a good cluster vs diagnoses match only with the 2 clusters using this method.

4. OPTIONAL: K-means clustering

5. Combining methods

```
wisc.pr.hclust <- hclust(dist(wisc.pr$x[,1:4]), method="ward.D2")
```

```
plot(wisc.pr.hclust)
abline(h=80, col="red")
```



Let’s find out cluster membership vector by cutting this tree into k=2 group.

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

```
## grps
##   1   2
## 171 398
```

Now let’s compare to the expert M and B vector.

```
table(diagnosis)
```

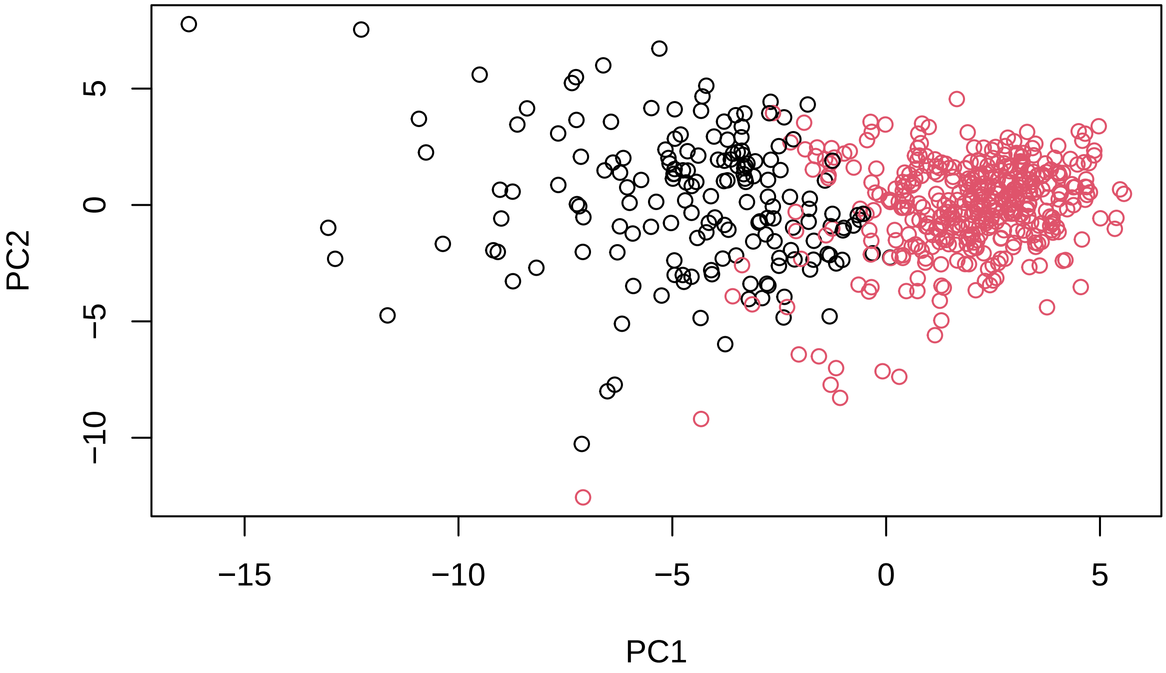
```
## diagnosis
##   B   M
## 357 212
```

We can do a cross-table by giving the ‘table()’ function two inputs.

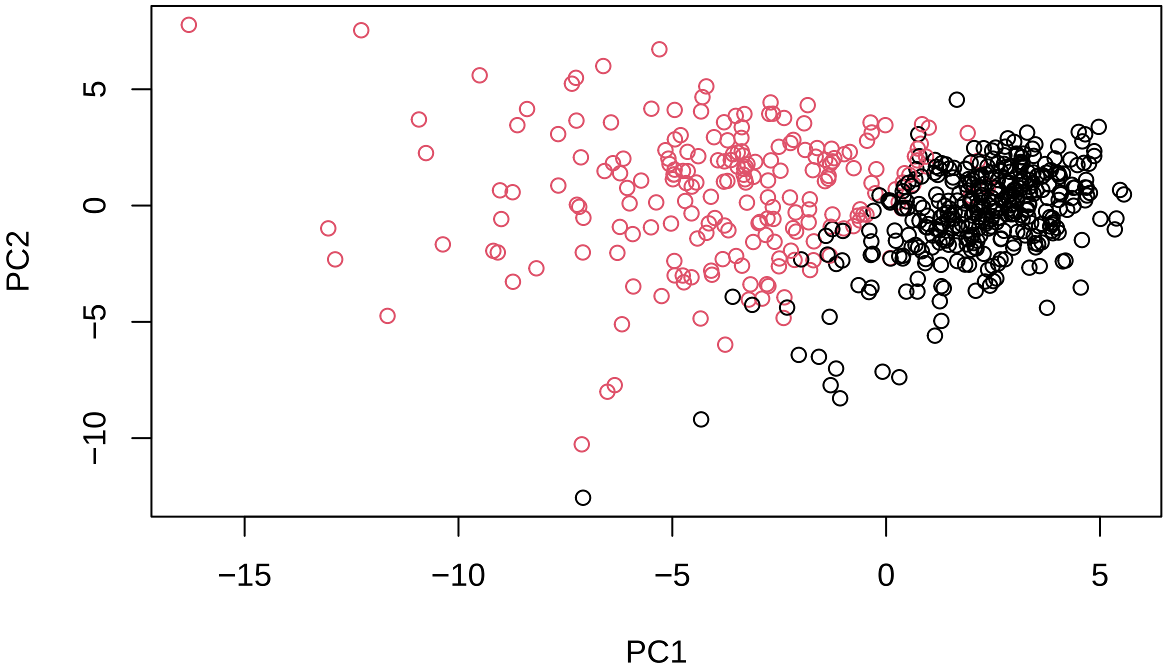
```
table(grps, diagnosis)
```

```
##     diagnosis
## grps   B   M
##    1   6 165
##    2 351  47
```

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



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



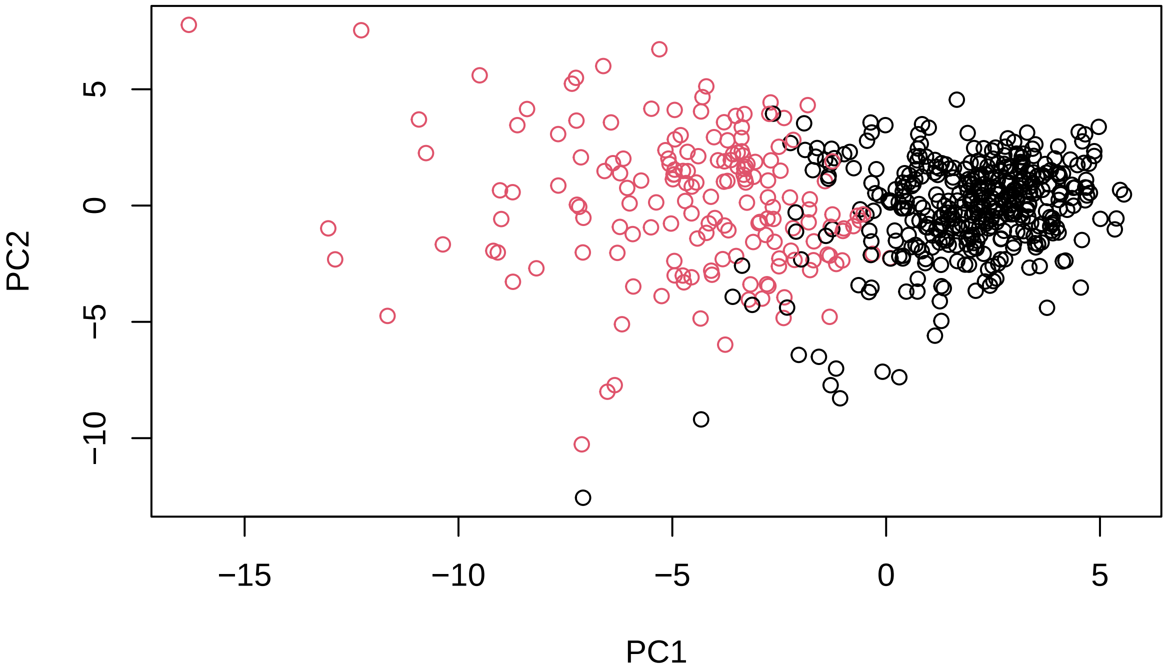
```r
g <- as.factor(grps)
levels(g)
```

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

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

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

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



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

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

```
##     diagnosis
## grps   B   M
##    1   6 165
##    2 351  47
```

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.

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

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

(As section 4 is optional, I do not have the output of the k-means model)

6. Sensitivity/Specificity

Accuracy, essentially how many did we get correct?

```
(165+351)/nrow(wisc.data)
```

```
## [1] 0.9068541
```

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

Sensitivity

```
(165)/(165+47)
```

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

Specificity

```
(351)/(351+47)
```

```
## [1] 0.8819095
```

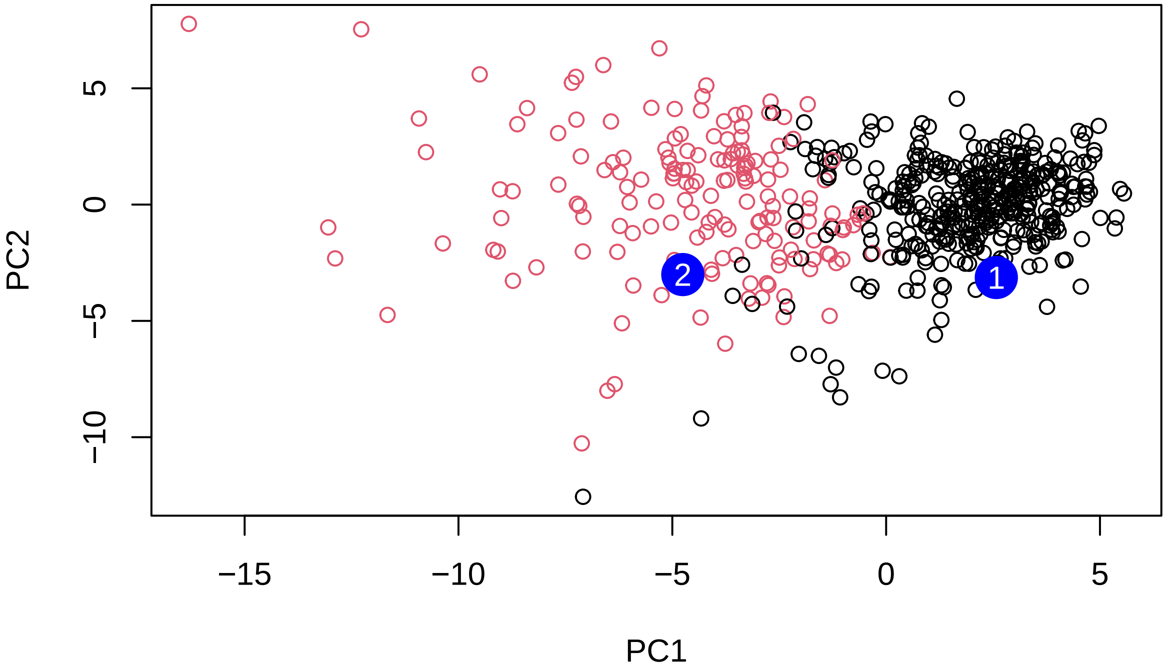
I just calculated the specificity and the sensitivity of the model with the "ward.D2" method.

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
```

```
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")
```



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

Based on the results, the patients in the group 2 should be priortized for follow up.