Class 09: Mini Project

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1. Exploratory Data Analysis

```
# Place csv file into project directory, then assign it a variable name
fna.data <- "WisconsinCancer.csv"
# read.csv the csv file then assign it a name
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
```

The first column contains the pathologist's diagnosis of if the cells are malignant or benign, we want to remove it from our data set.

```
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
```

We still want to view the diagnosis column later to check, so we will save it as a vector.

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

Q1. How many observations are in this dataset?

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

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

There are 569 observations in the "WisconsinCancer.csv" data set.

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

Use grep to find how many "M" there are in our diagnosis vector OR use table of diagnosis.

```
length(grep(pattern="M", x=diagnosis))
```

```
## [1] 212
```

```
table(diagnosis)
```

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

There are 212 malignant diagnosis obersvations.

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

Use grep to find how many columns end in "_mean".

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

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

There are 10 variables / features in the data that are suffixed with "_mean".

2. Principal Component Analysis

```
# Check column means and their 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, we need to set the scale argument to true in order to scale the data.
wisc.pr <- prcomp(wisc.data, scale.=TRUE)
# Look at the summary of the PCA 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 PC1.

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

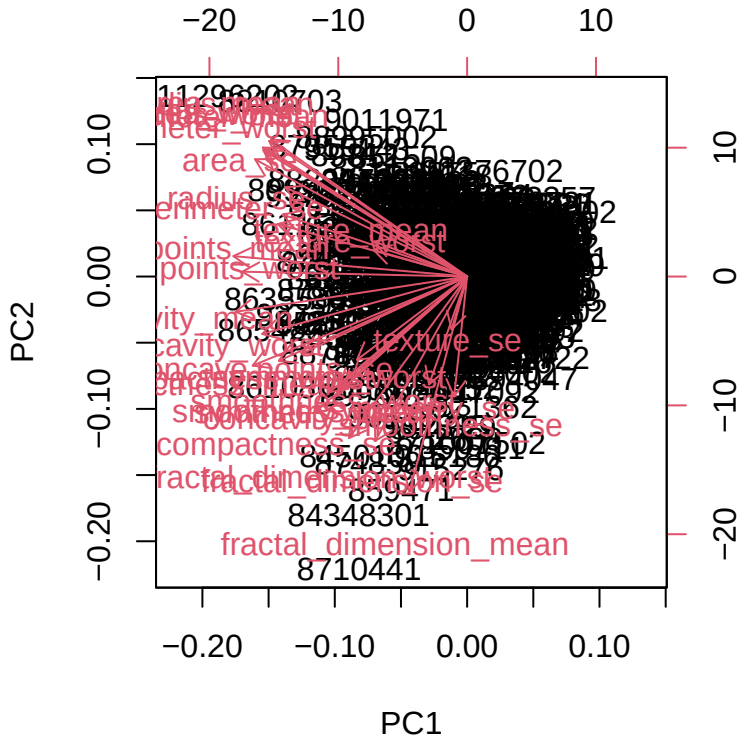
3 principal components are required to describe at least 70% of the original variance in the data.

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

7 principal components are required to descibe at least 90& of the original variance in the data.

Create a biplot of "wisc.pr"

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



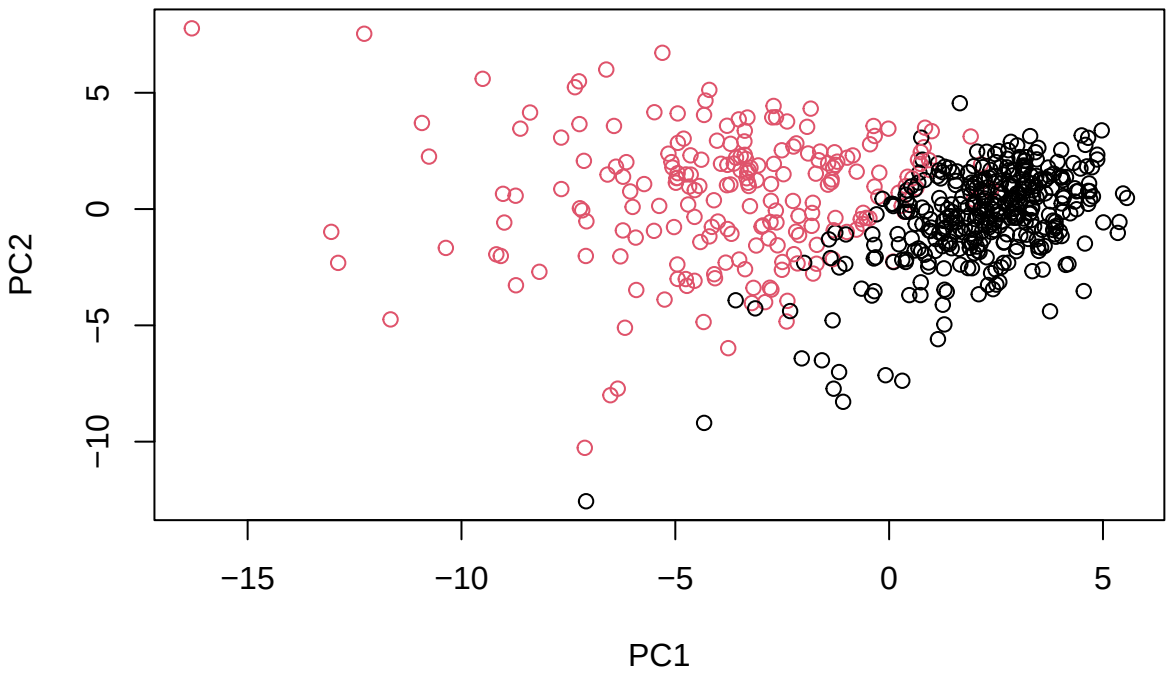
> **Q7.** What stands out to you about this plot? Is it easy or difficult to understand? Why?

This plot is very difficult to understand, it is just a giant blob of all the data set numbers and the column names.

We are after the score plot(aka "PCA plot", PC1 vs PC2)

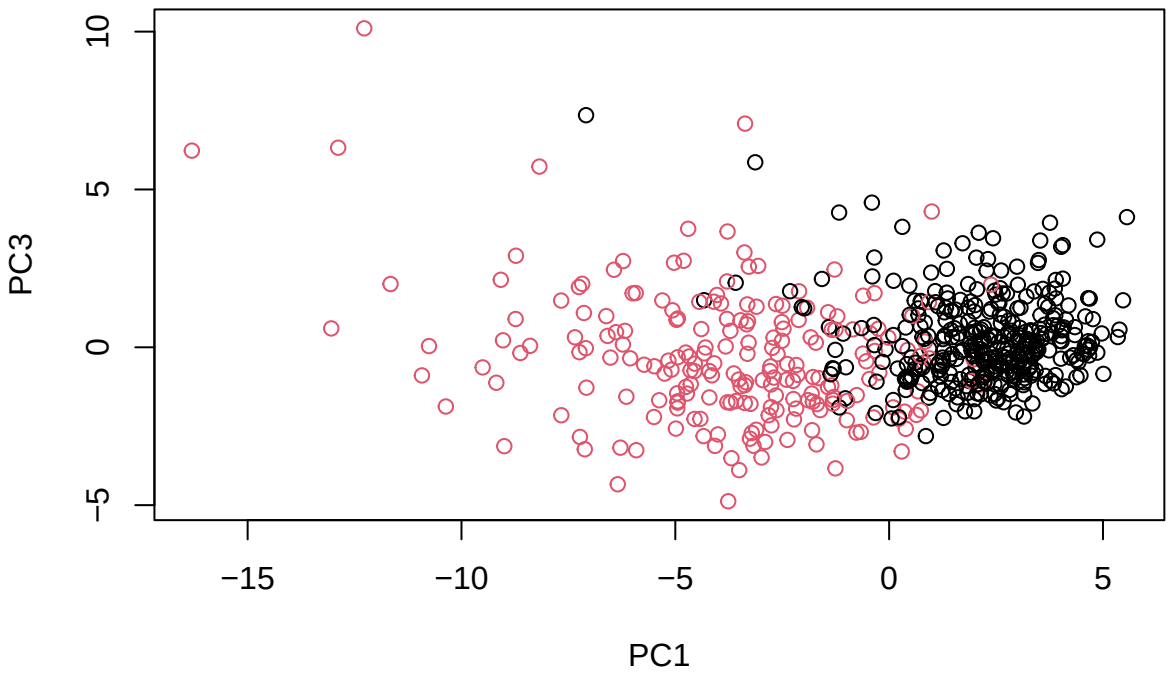
Let's generate a more standard scatter plot to make better sense of the observations along PC1 and PC2.

```
#Scatter plot observations by PC1 and PC2
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")
```



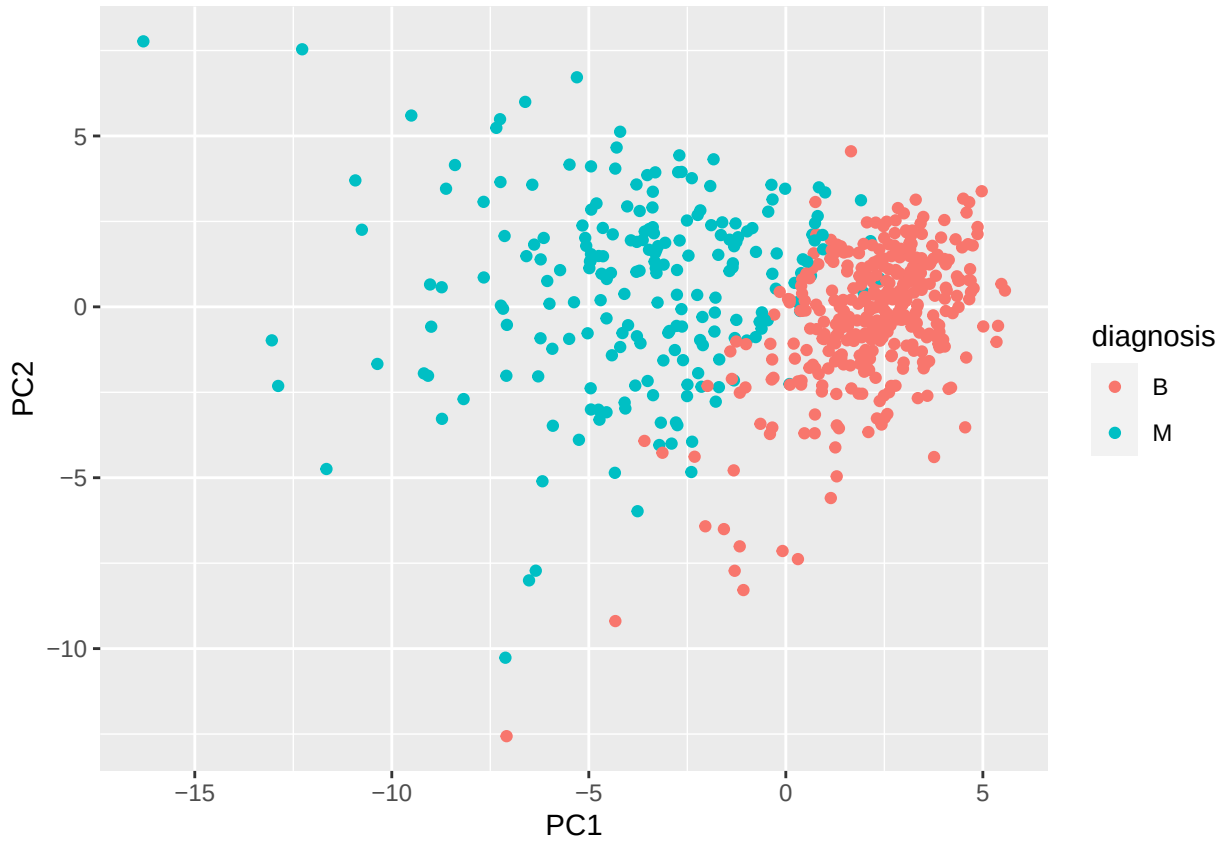
PC1 and PC2 are more clearly separated compared to PC1 and PC3. This is because PC2 describes more variance in the data than PC3.

Now, let's use ggplot to to make fancier figures.

```
# 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 the variance of each principal component by squaring the sdev component of wisc.pr

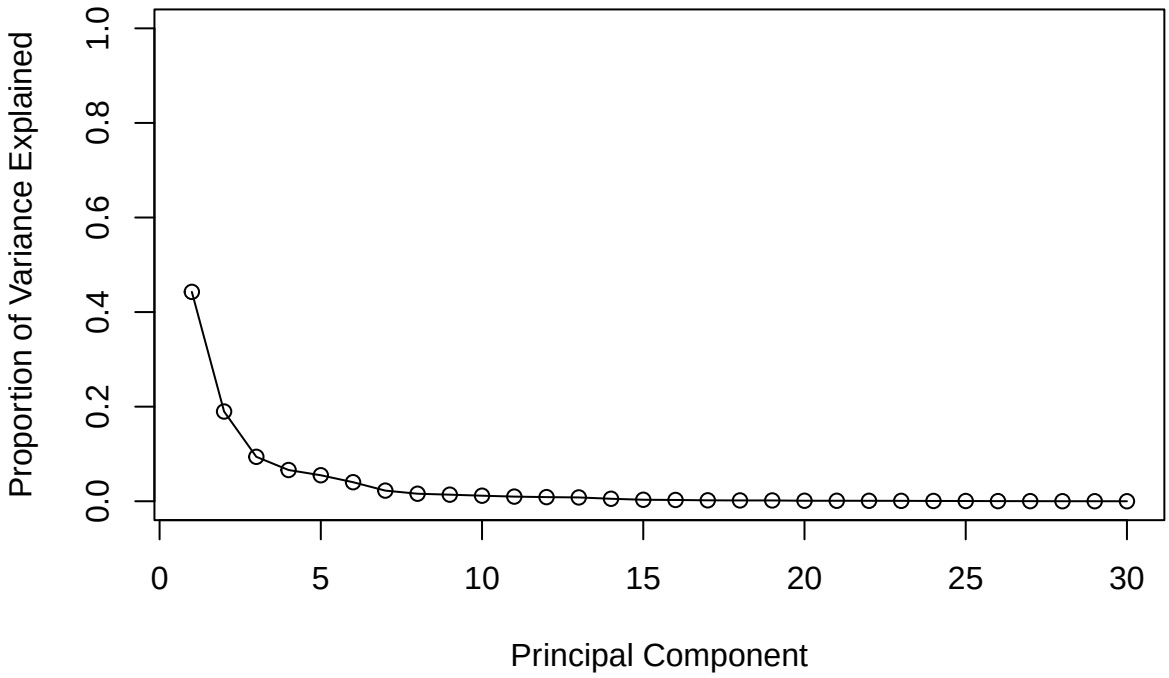
```
# Calculate variance of each component
pr.var <- wisc.pr$sdev^2
head(pr.var)
```

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

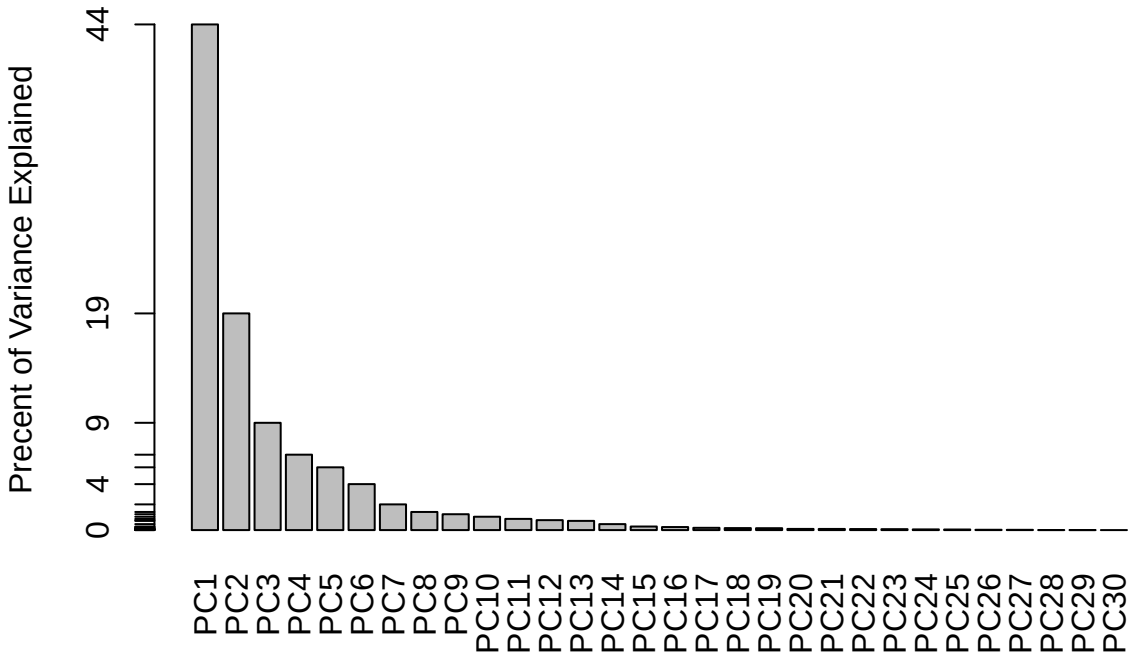
Calculate the variance explained by each principal component by dividing by the total variance explained of all principal components

```
# 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 = "o")
```



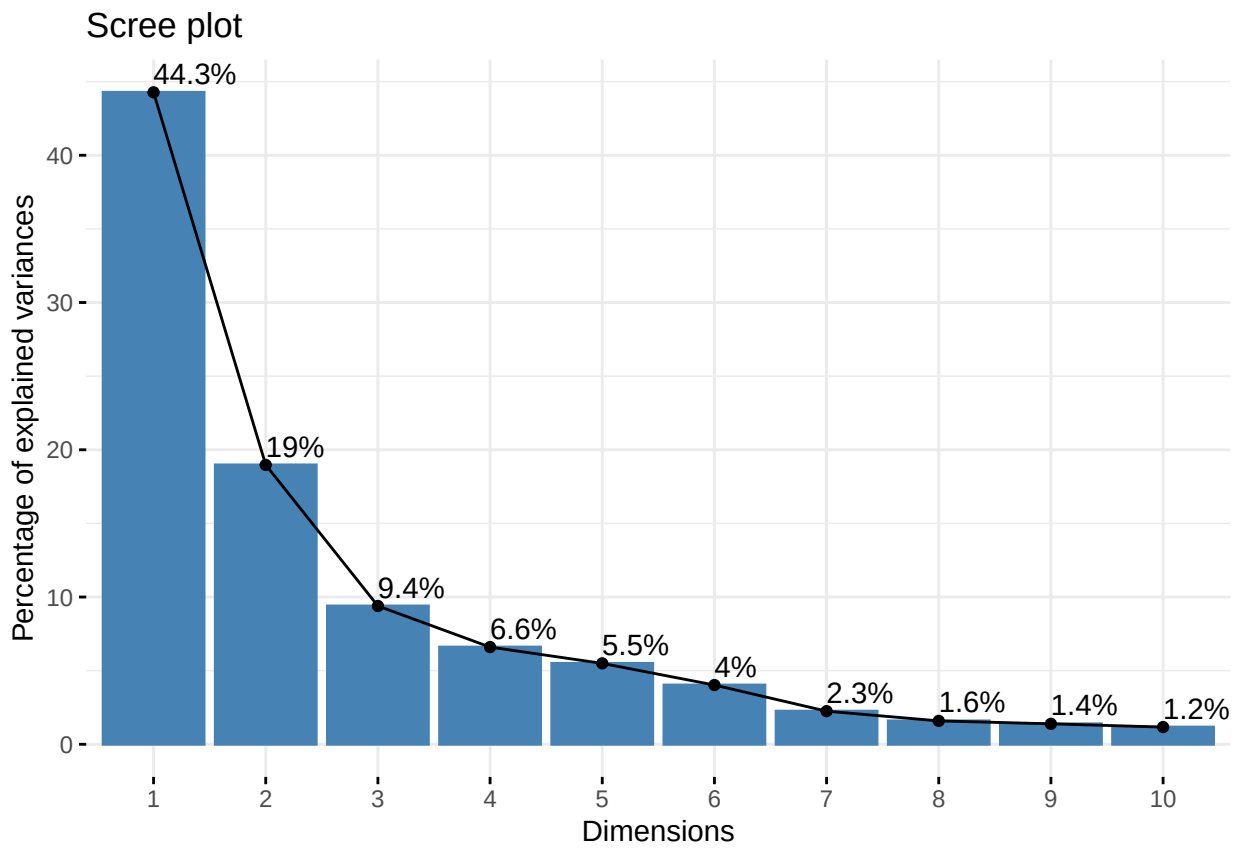

```
# Make an alternative scree plot of the same data
barplot(pve, ylab = "Precent of Variance Explained",
     names.arg=paste0("PC",1:length(pve)), las=2, axes = FALSE)
axis(2, at=pve, labels=round(pve,2)*100 )
```




```
## ggplot based 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)
```



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
```

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

```
## [1] -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
```

5 PC's are required 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)
```

Calculate the (Euclidean) distances between all pairs of observations in the new scaled dataset and assign the result to data.dist.

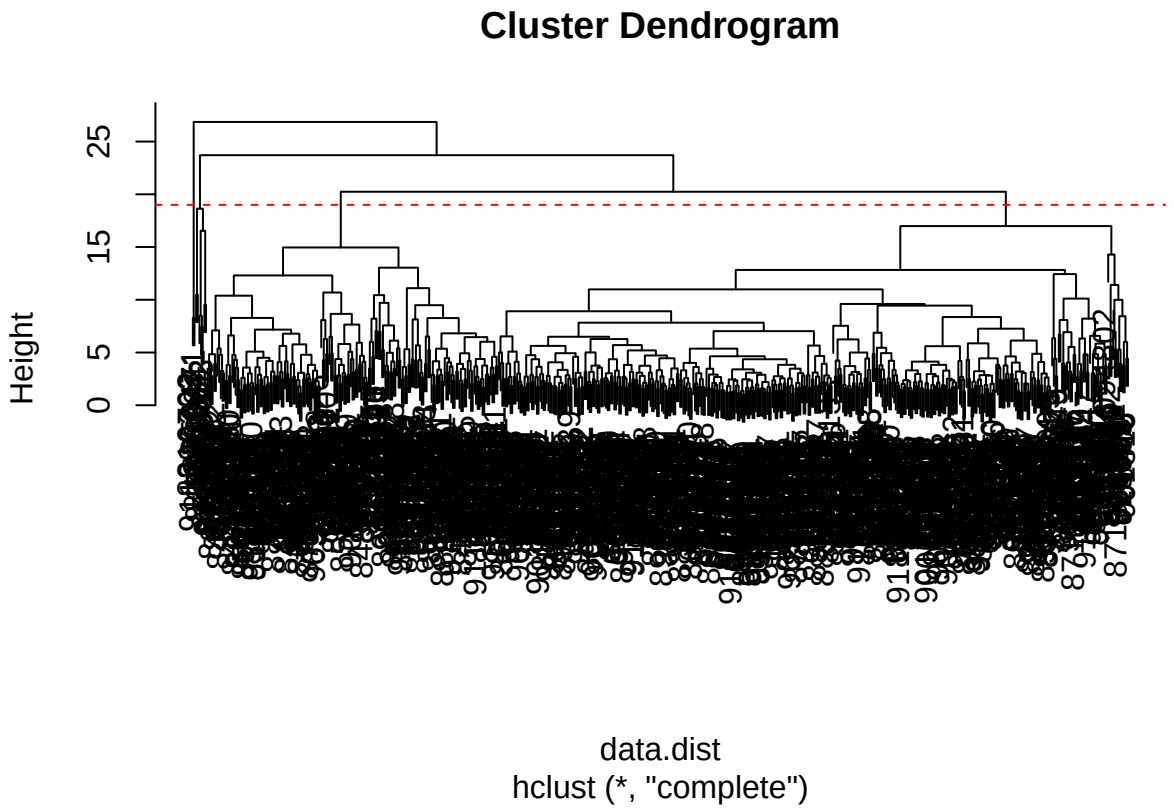
```
data.dist <- dist(data.scaled)
```

Create a hierarchical clustering model using complete linkage. Manually specify the method argument to hclust() and assign the results to wisc.hclust.

```
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=19, col="red", lty=2)
```



Height 19 is when the clustering model has 4 clusters.

Use "cutree()" function to assign 4 clusters to wisc.hclust, then use "table()" to compare our cutree() cluster with the diagnosis.

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

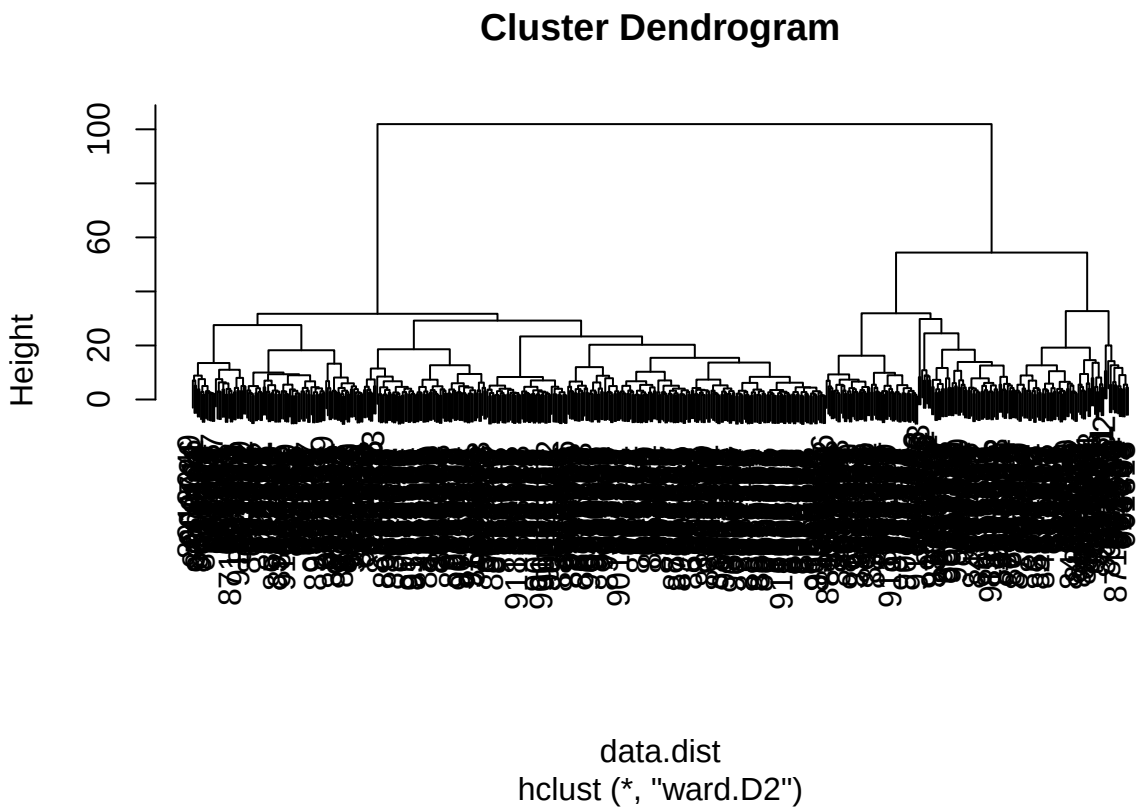
```
##                     diagnosis
## wisc.hclust.clusters   B   M
##                    1  12 165
##                    2   2   5
##                    3 343  40
##                    4   0   2
```

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

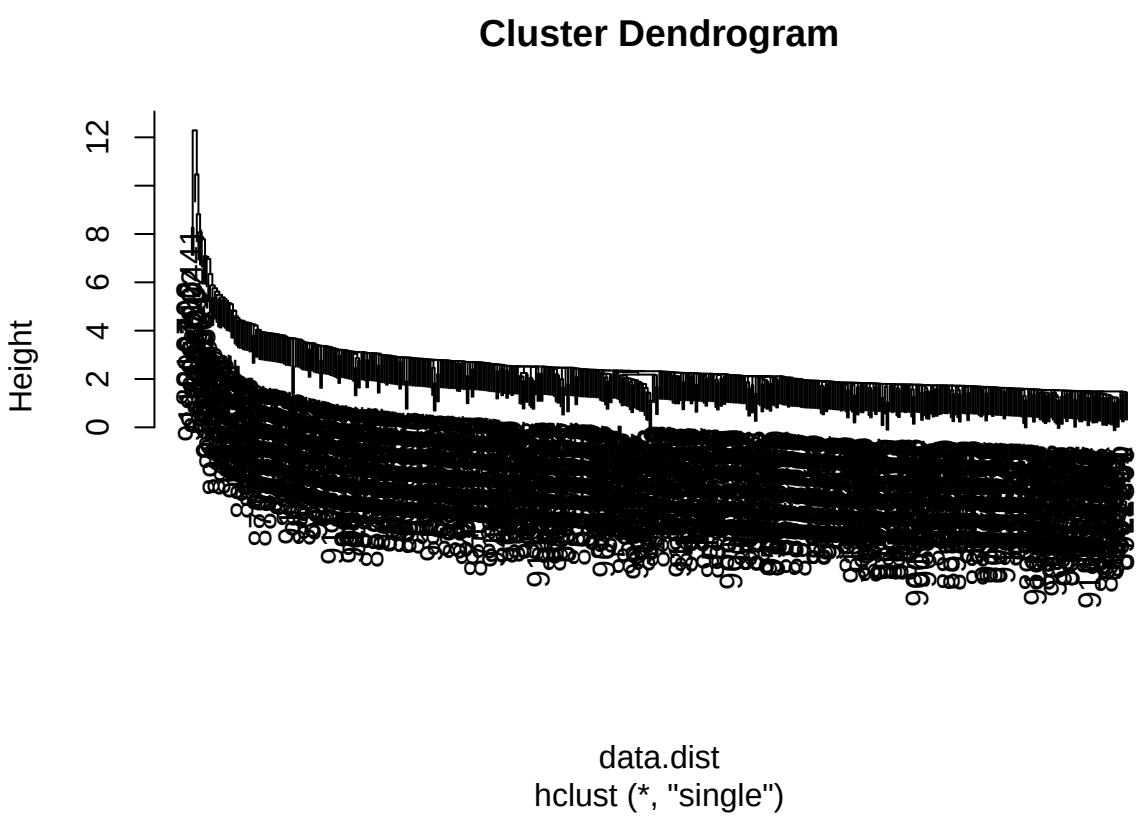
'No, it looks like 4 clusters seem to be the best amount to separate the different diagnoses.

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

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




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

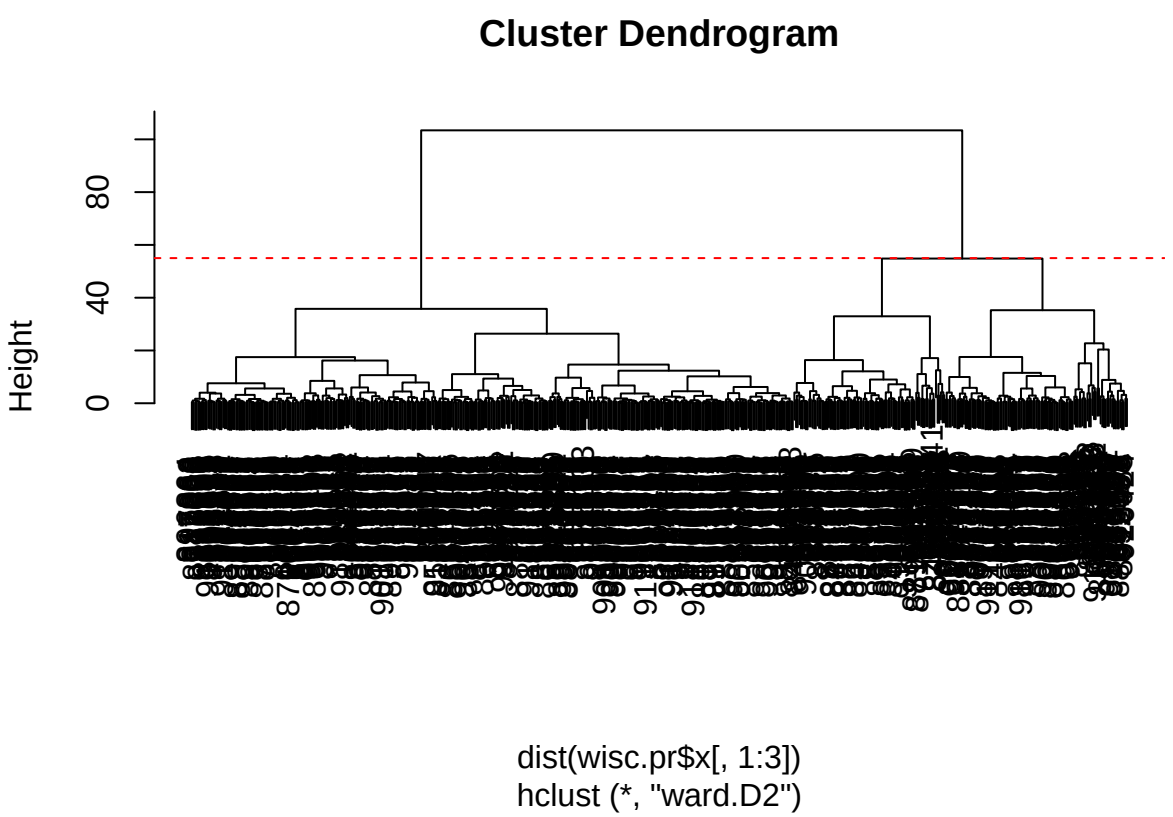


I prefer the "ward.D2" method as it gives the cleanest clustering model.

5. Combining Methods

We take the results of our PCA analysis and cluster in this space 'wisc.pr$x'

```
wisc.pr.hclust <- hclust(dist (wisc.pr$x[,1:3]), method = "ward.D2")
plot(wisc.pr.hclust)
abline(h=55, col="red", lty=2)
```



Cut the tree into k=2 groups

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

```
## grps
##   1   2
## 203 366
```

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

Check to see if the 2 groups correspond to Benign and Malignant by doing a cross table.

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

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

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
```

```
# We skipped the kmeans section so we only have 1 option
```

6. Sensitivity and Specificity

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

Accuracy What proportion did we get correct if we call cluster 1 M and cluster 2 B?

```
(333+179)/nrow(wisc.data)
```

```
## [1] 0.8998243
```

Now Calculate the Sensitivity and Specificity

```
#Sensitivity <- TP/(TP + FP)
179/(179+33)
```

```
## [1] 0.8443396
```

```
#Specificity <- TN/(TN + FN)
333/(333+24)
```

```
## [1] 0.9327731
```

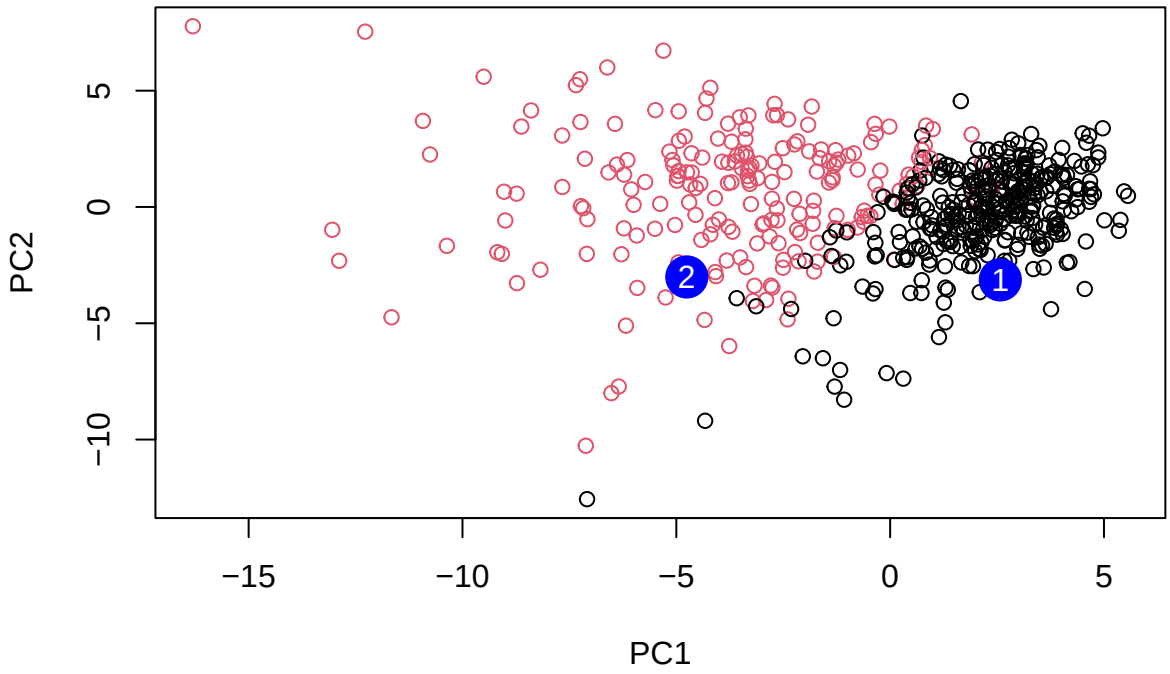
7. Prediction

```
#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=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?

We should prioritize patient 2 for follow up because the red signifies patient 2 has malignant cancer cells, where as patient 1 is diagnosed with benign cells.