Class09_Mini Project

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This project is examining patient data from fine needle aspiration of breast mass. The resulting data was collected from microscope analysis of cells to determine if they were normal or not.

Importing the data set make sure to save the WisconsinCancer.csv file to the mini project directory

```
# 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) #use read.csv to read the imported file
wisc.df.sub <- subset(wisc.df[,1:31]) #My import data added and x column to the end of the file to remo
```

View the file using 'head()' or by clicking the object and examining the table

```
head(wisc.df.sub)
```

```
##          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
```

Omit the first column which is the expert's diagnosis, since we will be determining that ourselves from the data

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

Store the diagnosis into a separate factor vector to use for plotting later

```
# Create diagnosis vector for later
diagnosis <- factor(wisc.df.sub[,1])
```

Q1. How many observations are in this dataset?

```
dim(wisc.data) # Displays the rows then columns
```

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

```
nrow(wisc.data) # Gives exactly the number of rows or obersvations
```

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

There are 569 patient samples or observations with 3 different categories describing the patient sample

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

```
?grep()
M <- grep(pattern="M", x= diagnosis)#returns all of the observations that were marked at M
length(M) # Use length to count the observations
```

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

It looks like there were 212 samples that were malignant

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

```
mean <- grep(pattern="_mean",x= colnames(wisc.data)) # use grep to find the pattern _mean, have it spec
length(mean) # use length to calculate the total number of matches
```

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

There were 10 variables with the suffix mean

```
# 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(x= wisc.data, scale = TRUE) #scale 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
```

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

PC1 captures 44.27% of the variance.

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

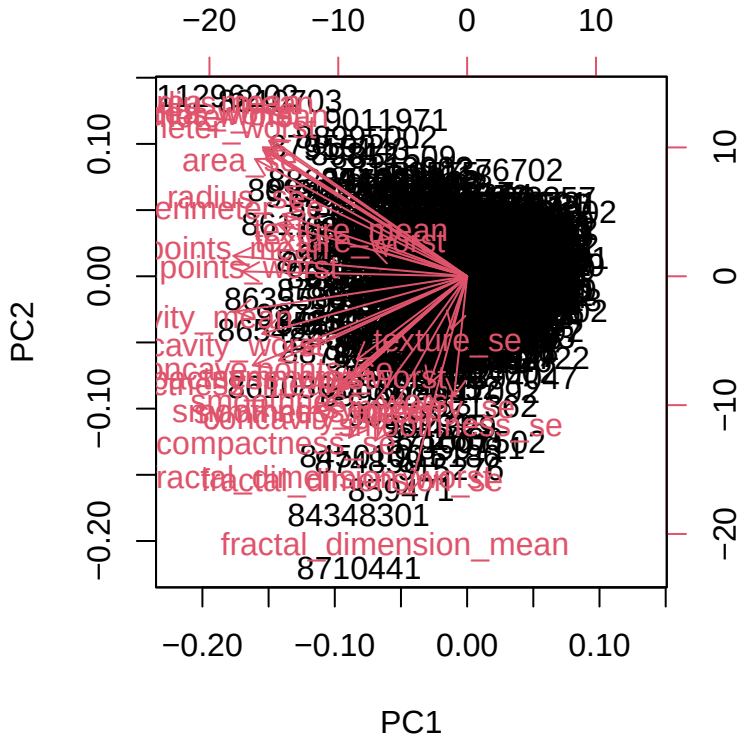
PC1, PC2, and PC3 capture 72.64% of the variance of the data.

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

The first 7 principal components explains 91% of the variation from this data set.

First plot of the data using 'biplot()'

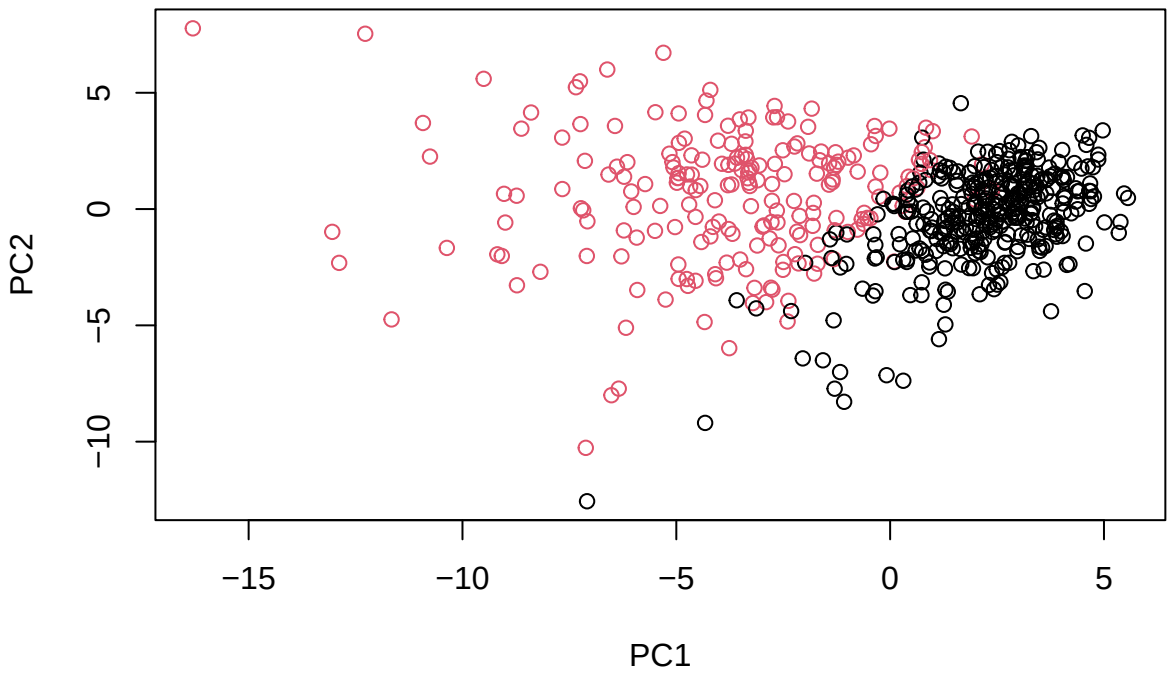
```
biplot(wisc.pr)
```



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

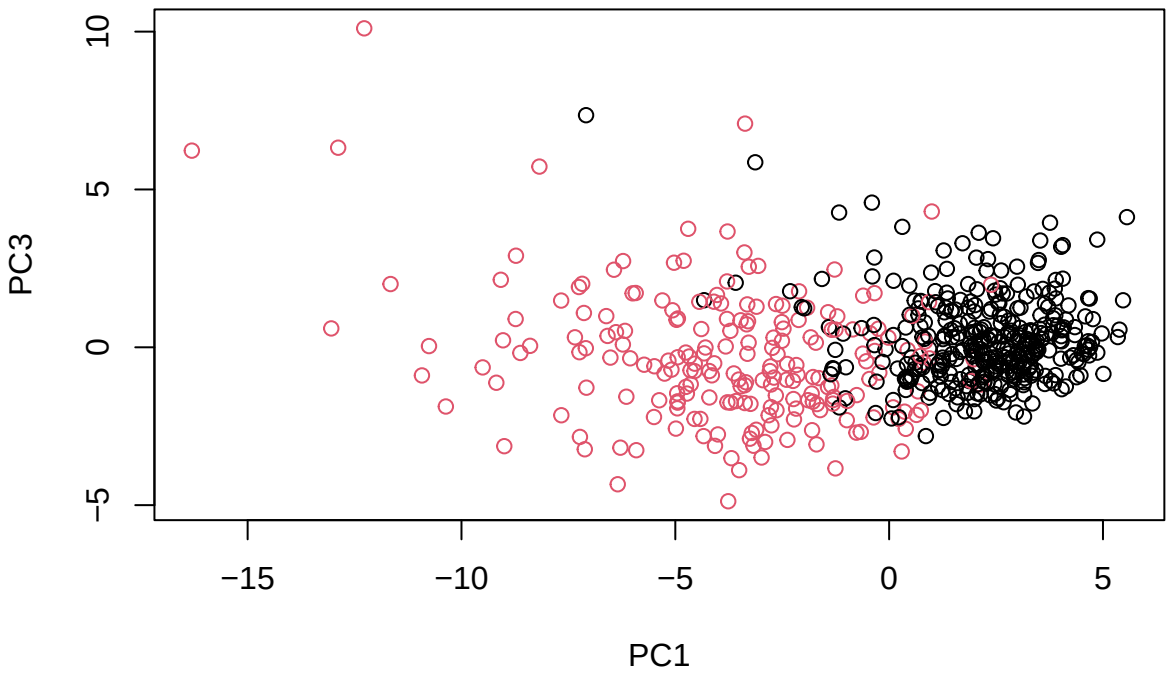
It looks like the black data points representing the patient samples are clustered in the middle and the variables are scattered farther away from the center denoted by the arrows.

```
# Scatter plot observations by components 1 and 2
plot(wisc.pr$x[,1], wisc.pr$x[,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")
```



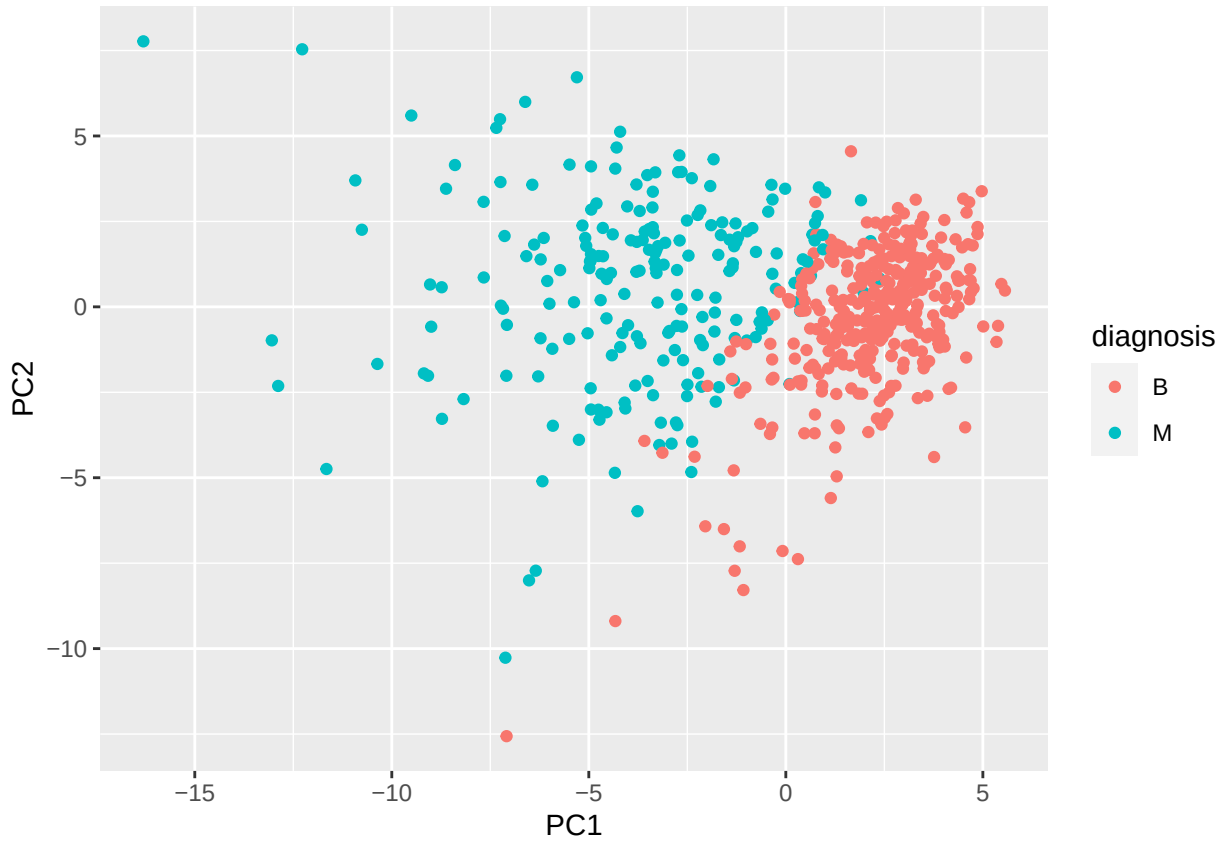
The plot overall has shifted downward towards PC1, additionally, the black points "normal" are more clustered together.

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

# Load the ggplot2 package
library(ggplot2)
```

```
## Warning in register(): Can't find generic 'scale_type' in package ggplot2 to
## register S3 method.
```

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



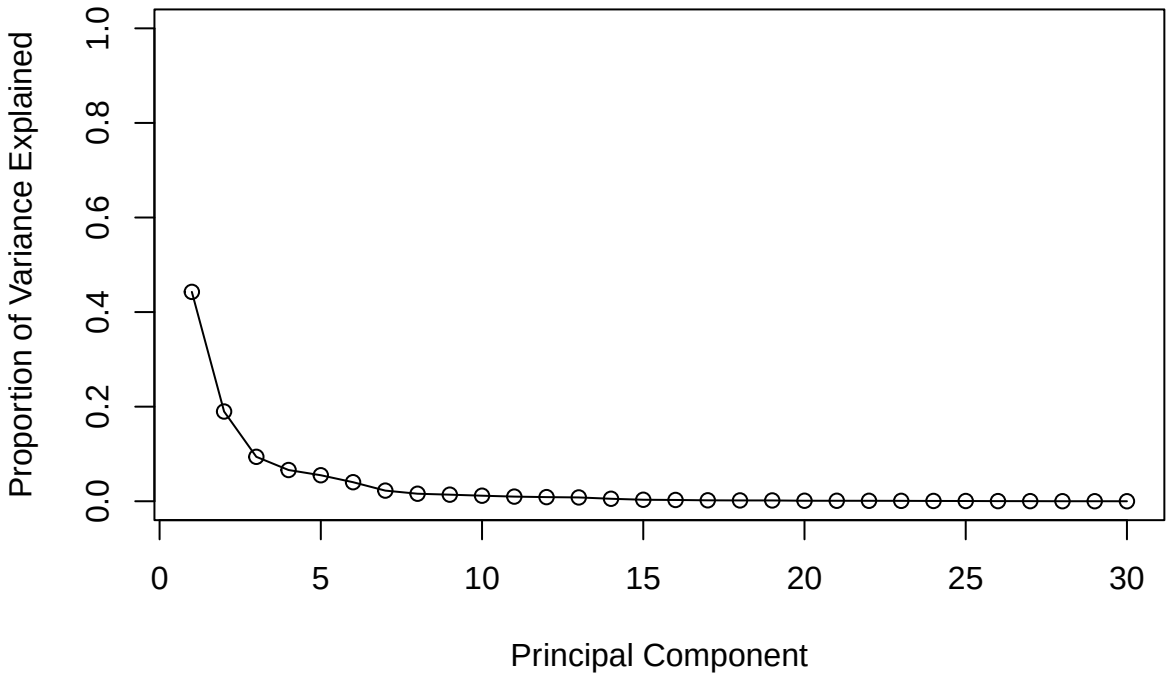
Variance is calculated by the square of the standard deviation

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

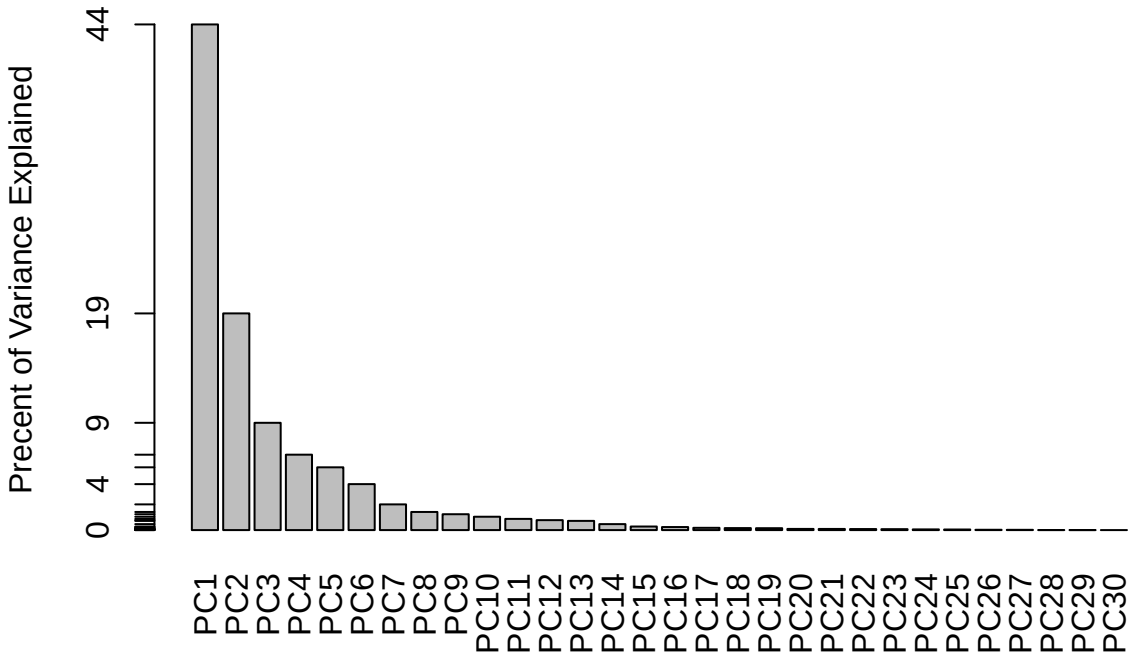
```
## [1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

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



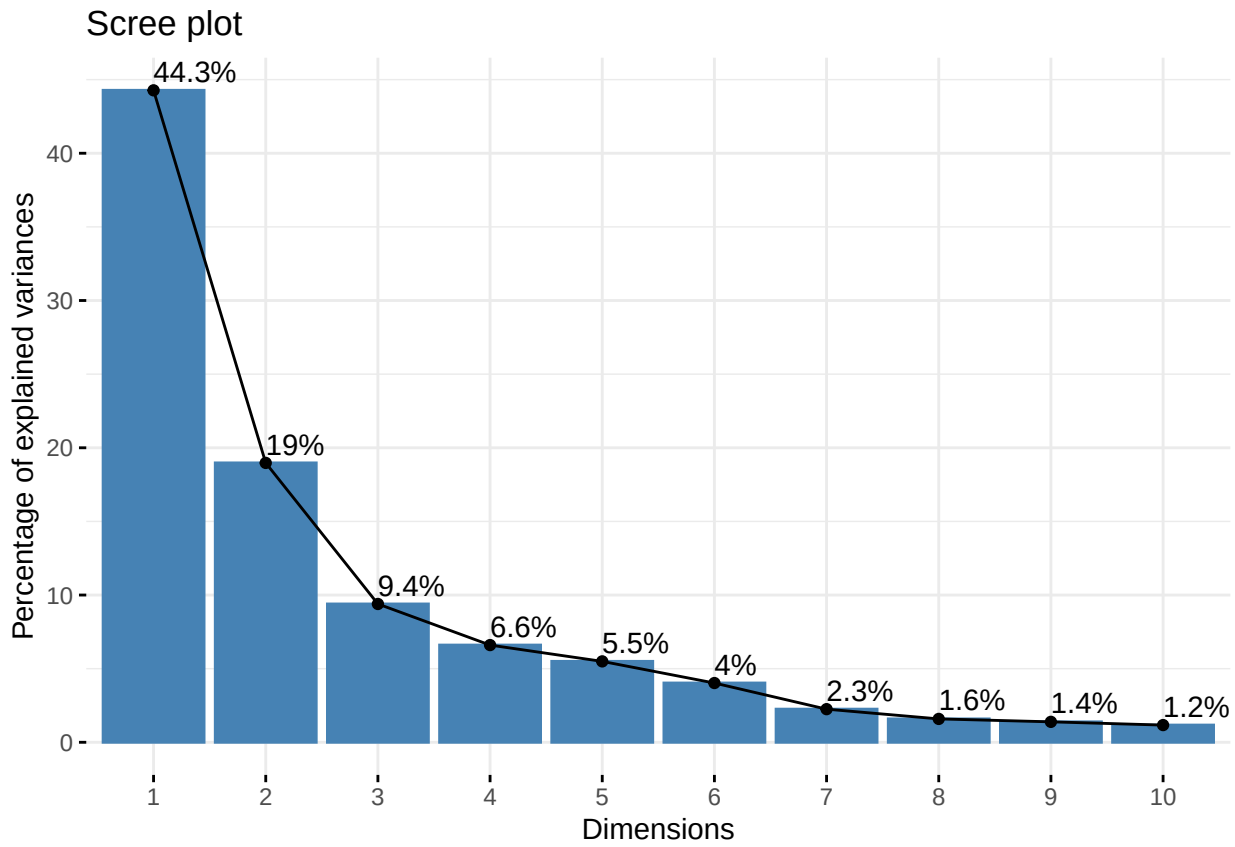

```
# Alternative scree plot of the same data, note data driven y-axis
barplot(pve, ylab = "Precent of Variance Explained",
     names.arg=paste0("PC",1:length(pve)), las=2, axes = FALSE)
axis(2, at=pve, labels=round(pve,2)*100 )
```




```
## ggplot based 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)
```



This graph is much easier to see which principal component explains the data

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?

-0.26085376

```
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
```

```
#concave.points_mean
#-0.26085376
```

The components are ordered from most variance explained to least variance explained

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

Referring to the graph made with factoextra, it takes 5 principal components to explain 80% of the variance in the data.

Hierarchical Clustering

Use function 'scale()'

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

Use function 'dist()'

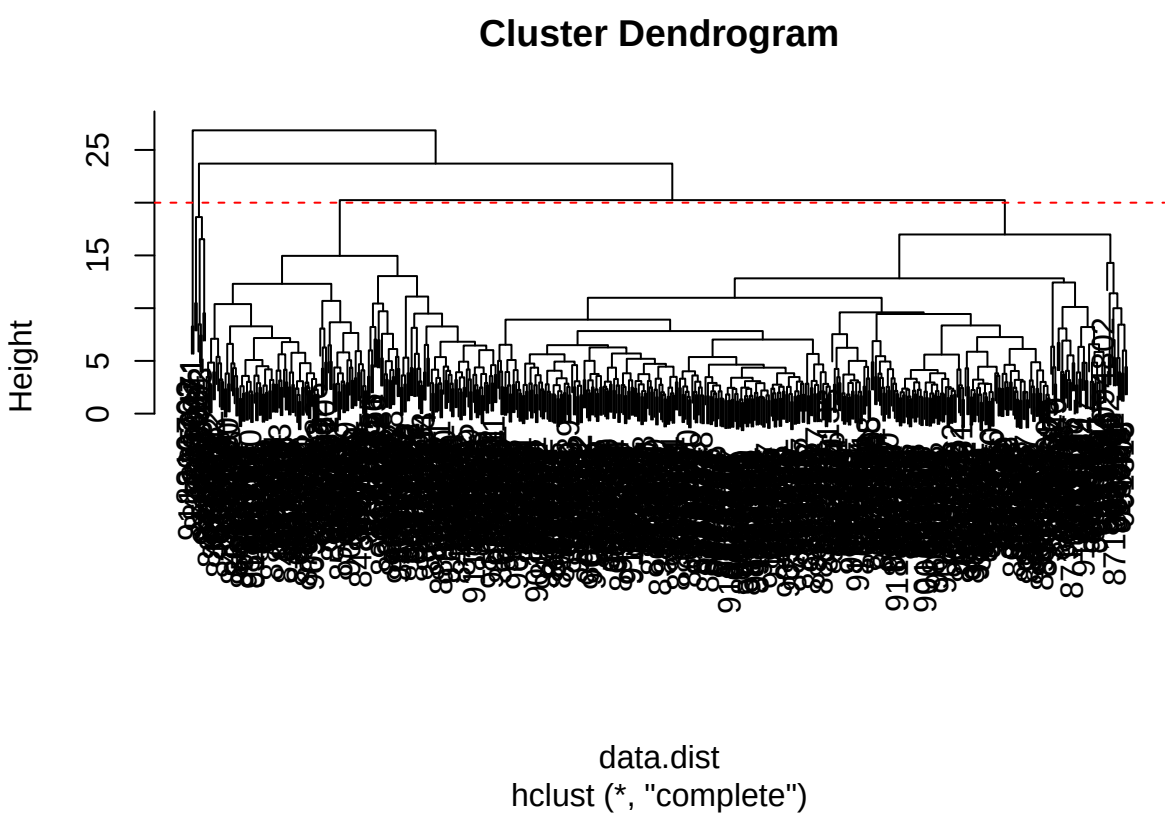
```
data.dist <- dist(data.scaled)
```

Use function 'hclust()' and tell it what type of linkage you want to use

```
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=20, col="red", lty=2) # It looks like at 20 it differentiates into 4 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?

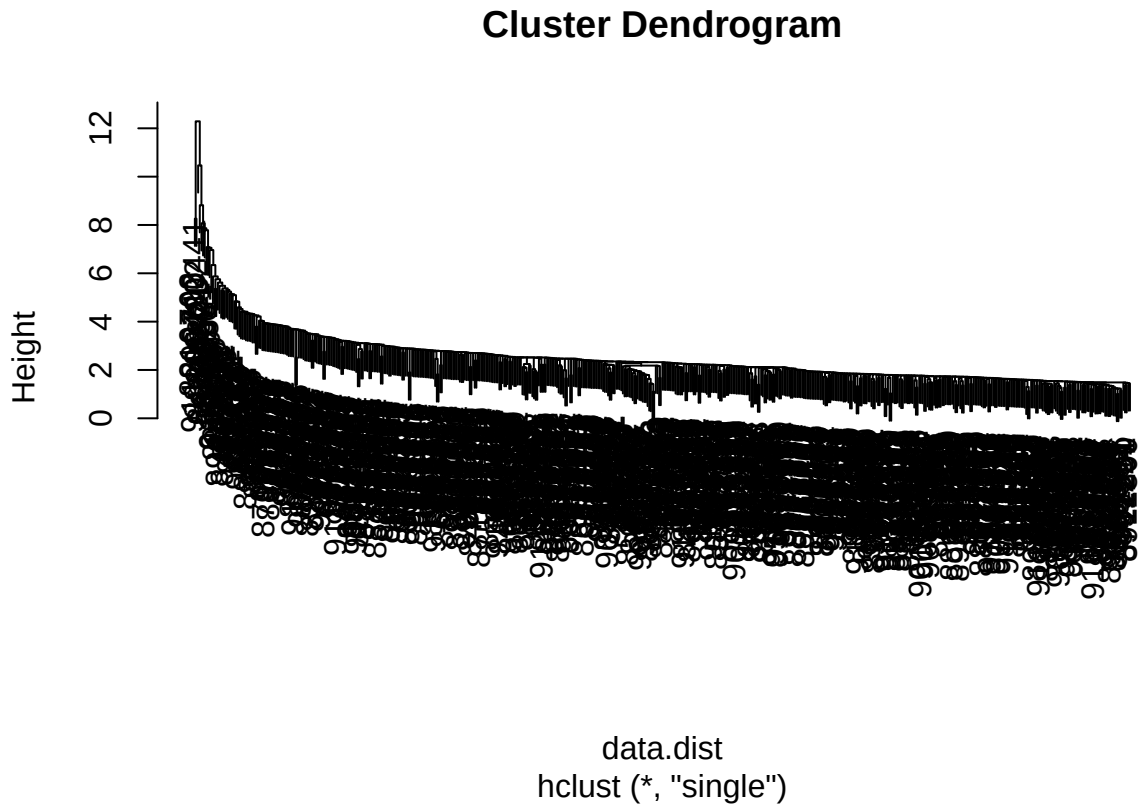
If we choose 2 then it separates all of our diagnoses to either 0 or 2 matching benign or malignant, with not false positives or false negatives.

```
wisc.hclust.clusters.test <- cutree(wisc.hclust, k = 2)
table(wisc.hclust.clusters.test, diagnosis)
```

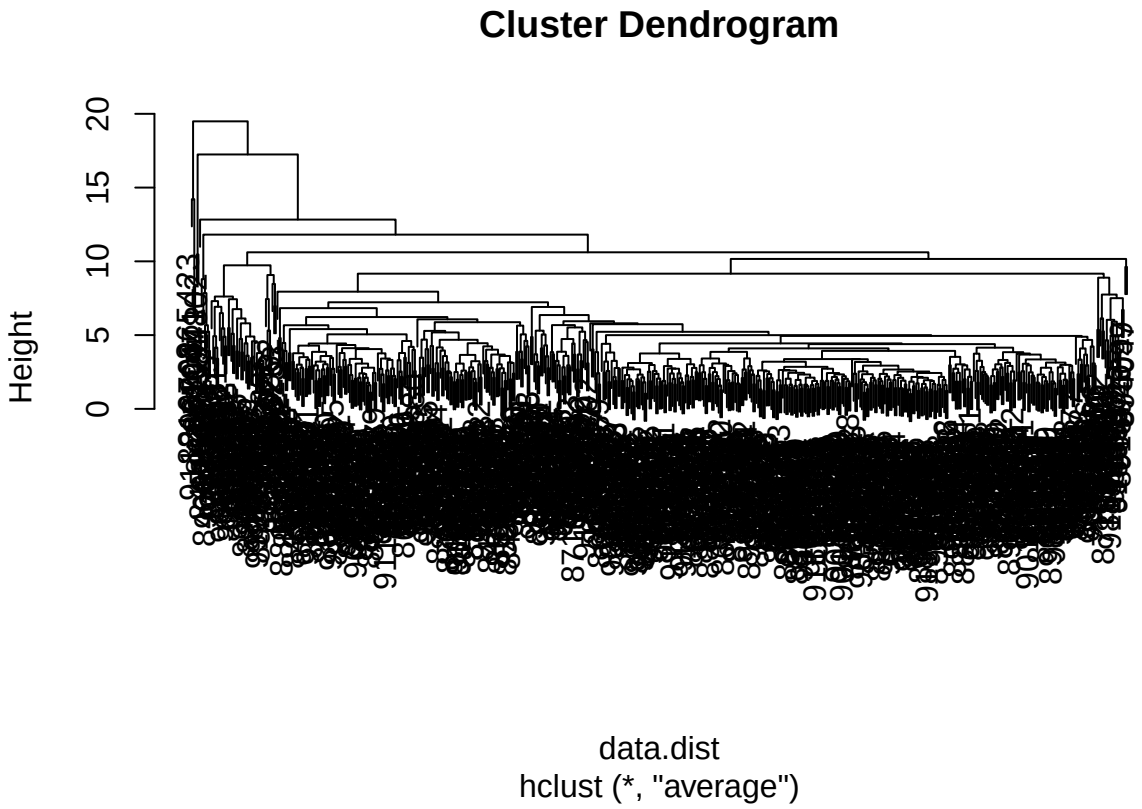
```
##                          diagnosis
## wisc.hclust.clusters.test   B   M
##                         1 357 210
##                         2   0   2
```

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

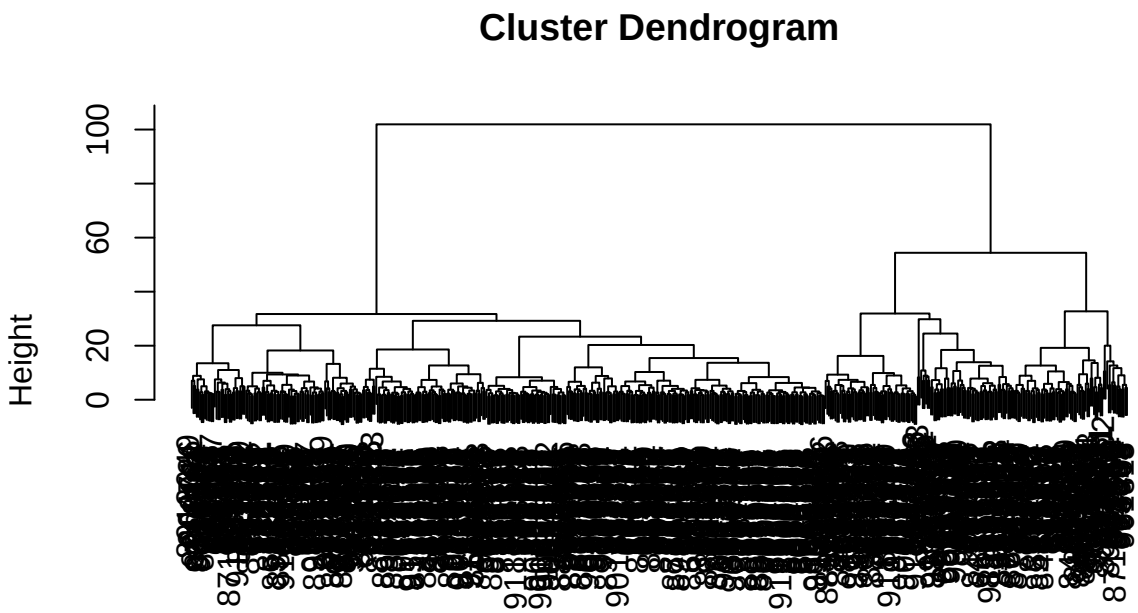
```
wisc.hclust.single <- hclust(data.dist, method = "single")
plot(wisc.hclust.single)
```




```
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 would say that either Ward.D2 or Complete are my favorite methods, because they were able to differentiate the two groups the easiest. They are also much clearer in how they separate the groups so visually they are easier to read.

Optional K-means clustering

```
wisc.km <- kmeans(wisc.data, centers= 2, nstart= 20)
table(wisc.km$cluster, diagnosis)
```

```
##    diagnosis
##       B   M
##   1   1 130
##   2 356  82
```

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

k-means is able to separate the Benign diagnosis better since there is only one sample that doesn't group with B. For the Malignant diagnosis there were most of the samples grouped into the 1st cluster, but there was still a lot of samples grouped into the second cluster. So it wasn't perfect in sorting the diagnoses.

```
# Compare k-means to hierarchical clustering
table(wisc.hclust.clusters, wisc.km$cluster)
```

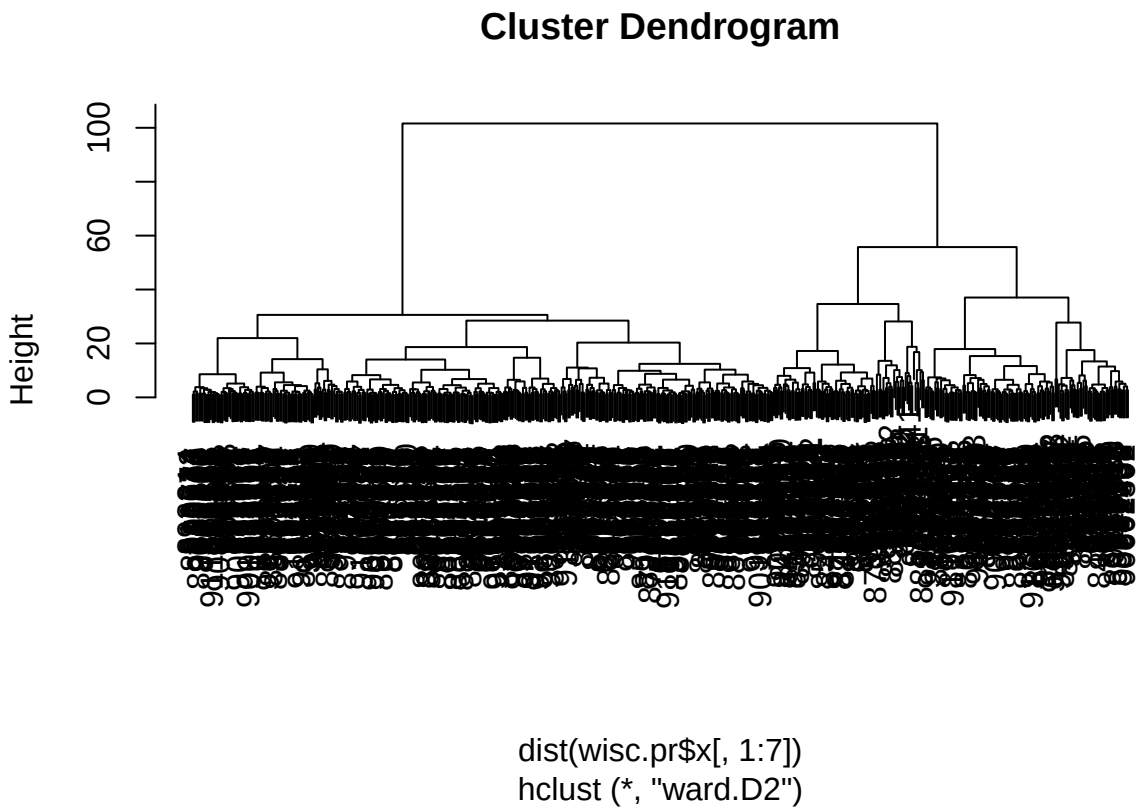
```
##
## wisc.hclust.clusters   1   2
##                    1 109  68
##                    2   2   5
##                    3  18 365
##                    4   2   0
```

From this clustering it looks like from hierarchical clustering groups 1 and 4 belong to group 1 and then 3 belongs to group 2. Group 2 has some patient samples for each so it could be more in group 2 than 1.

Combining Methods

Create a hierarchical clustering model using ward.D2 which is similar to PCA since they are both created on multidimensional analysis

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



We see two clear groups in this graph

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

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

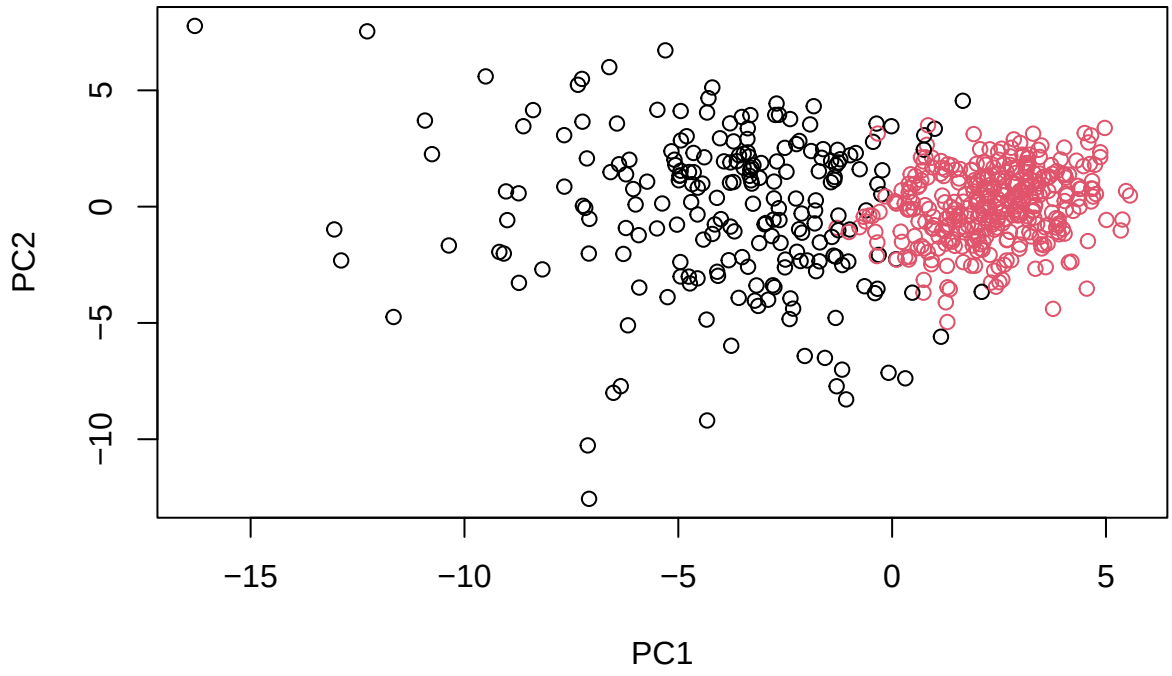
Gives us two clear groups

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

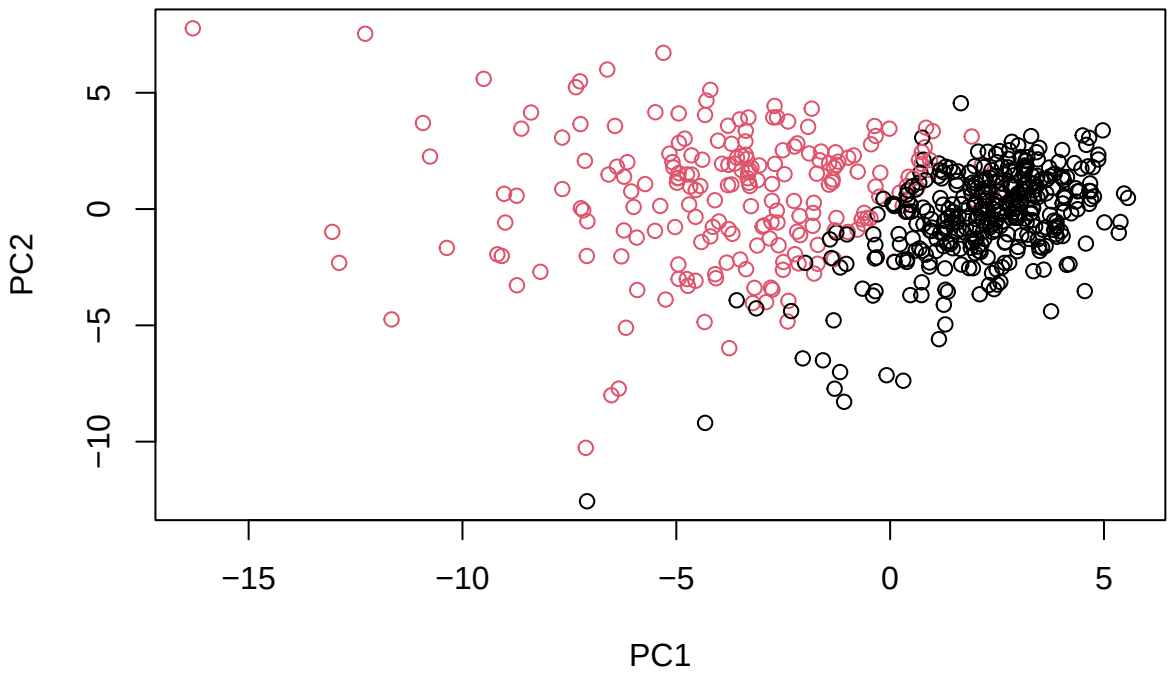
```
##     diagnosis
## grps   B   M
##    1  28 188
##    2 329  24
```

Let's plot the results to see the difference in grp

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




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



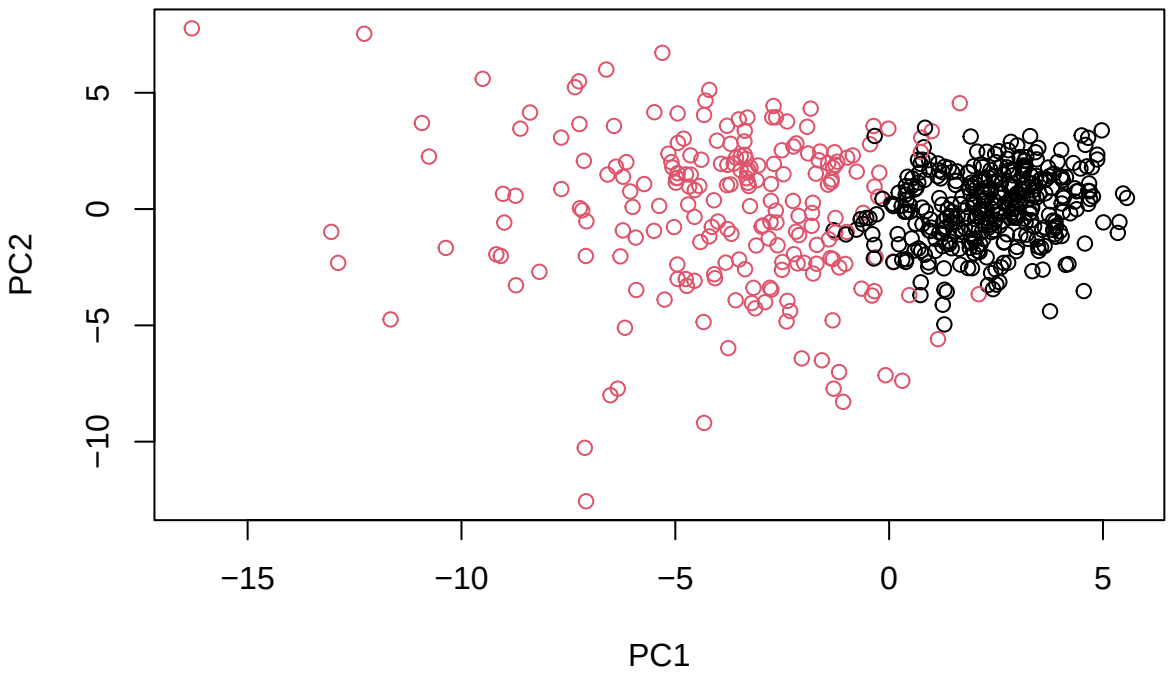

```
g <- as.factor(grps)
levels(g)
```

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

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

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

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




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

```
## Use the distance along the first 7 PCs for clustering i.e. wisc.pr$x[, 1:7]
wisc.pr.hclust <- hclust(dist(wisc.pr$x[, 1:7]), method="ward.D2")
```

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

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

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

The newly created model does a fairly good job clustering the two diagnosis, but there are ~24-28 patients that are clustering outside of what their diagnoses were. These samples probably were between the two centers of the clusters and therefore could be grouped either way by the program. Opposed to an expert that was using two distinct categories to separate samples.

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.km$cluster, diagnosis)
```

```
##    diagnosis
##       B   M
##   1   1 130
##   2 356  82
```

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

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

The k-means model did a better job seperating the two groups, however we told it to give two centers.

On the other hand the hierarchical clustering model separated our samples into 4 groups, but the majority of the sample are falling into either the Benign or Malignant. There were about ~50 samples not grouped compared to k-means had 83 samples not grouped under the two diagnoses.

Sensitivity

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

k-means was the most specific because it was able to group the benign patients the most closely, only 1 patient miss categorized.

The hierarchical ward.D2 model was the most sensitive since it was able to sort 188 patient samples into malignant when there was a total of 212 malignant samples, giving the most correctly detectec ill patients.

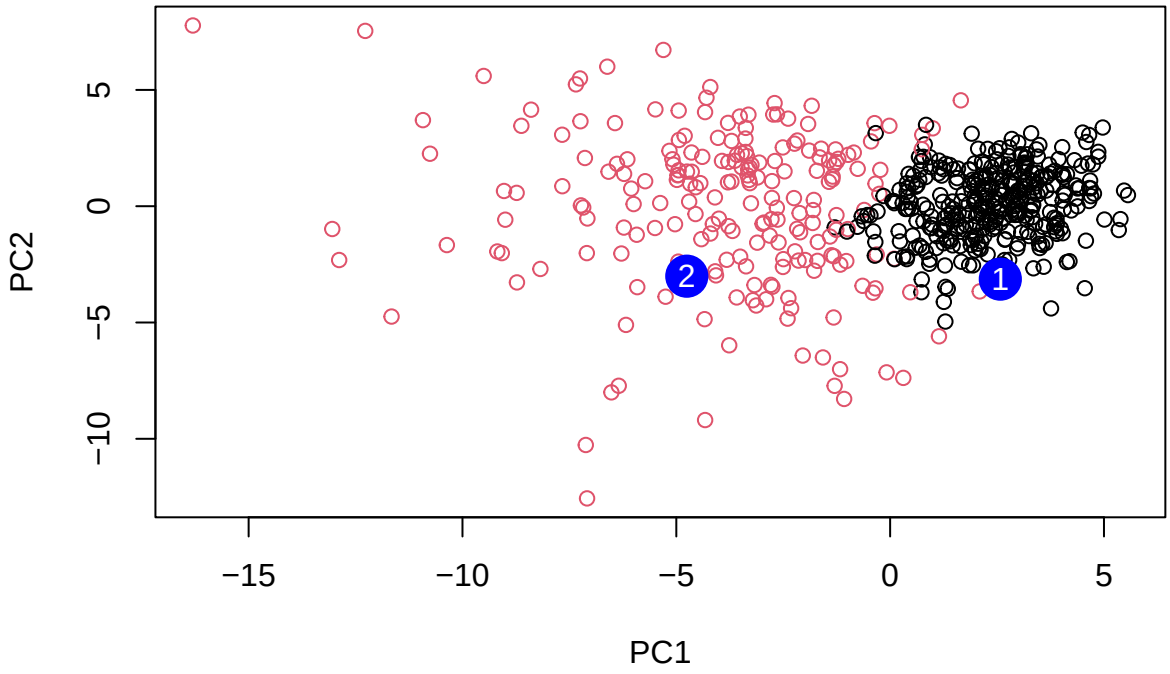
Prediction

```
#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?

We should focus on patients in cluster 2, since they are clustered with more variation. The separation between the two groups is seen with PCA1 which explains the majority of the variation in the data set. It is likely that these samples are malignant since they would have more variation opposed to normal samples which would likely cluster closely toghther.