Class 08 Mini Project

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Preparing the data

```r
# 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)
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
```

Remove the first column and store it separately as the diagnosis vector.

```
# We can use -1 here to remove the first column
wisc.data <- wisc.df[,-1]
diagnosis <- as.factor(wisc.df$diagnosis)
```

Exploratory Data Analysis

```r
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
```

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

```
[1] 569  30
```

> Q1. How many observations are in this dataset?

There are 569 Observations in this dataset due to the 569 rows.

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

```r
sum(wisc.df$diagnosis == "M")
```

```
[1] 212
```

Out of the 569 observations, 212 of them have a malignant diagnosis.

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

```r
length(grep("_mean", colnames(wisc.data)))
```

```
[1] 10
```

There are 10 variables/features in the data set are suffixed with _mean

Principal Component Analysis

Performing PCA

```
#Check column means and standard deviation
colMeans(wisc.data)
```

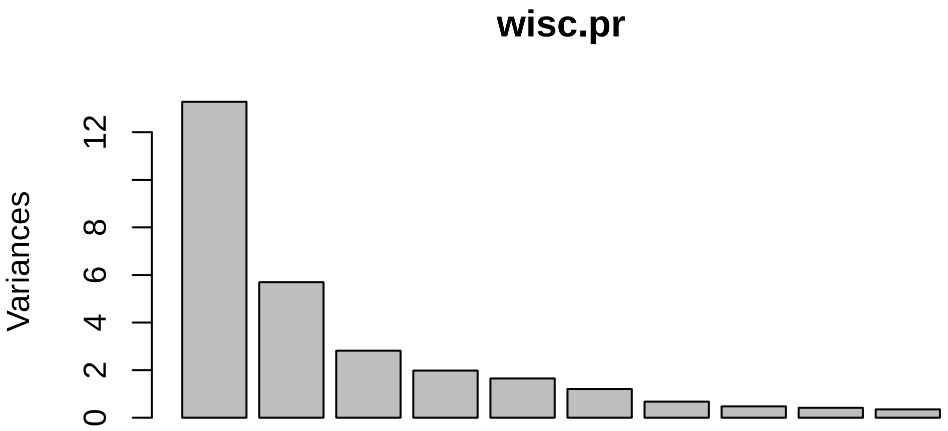
```
            radius_mean            texture_mean          perimeter_mean 
           1.412729e+01            1.928965e+01            9.196903e+01 
              area_mean         smoothness_mean        compactness_mean 
           6.548891e+02            9.636028e-02            1.043410e-01 
         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 
```

```
#Perform PCA on wisc.data
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
```

```
plot(wisc.pr)
```



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

From my results, the proportion of the original variance by the PC1 is 0.4427

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

3 -> PC1, PC2, and PC3

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

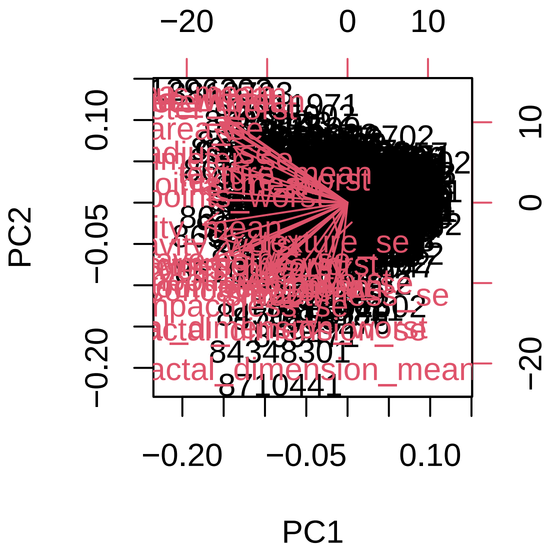
7 -> PC1, PC2, PC3, PC4, PC5, PC6, PC7

Interpreting PCA results

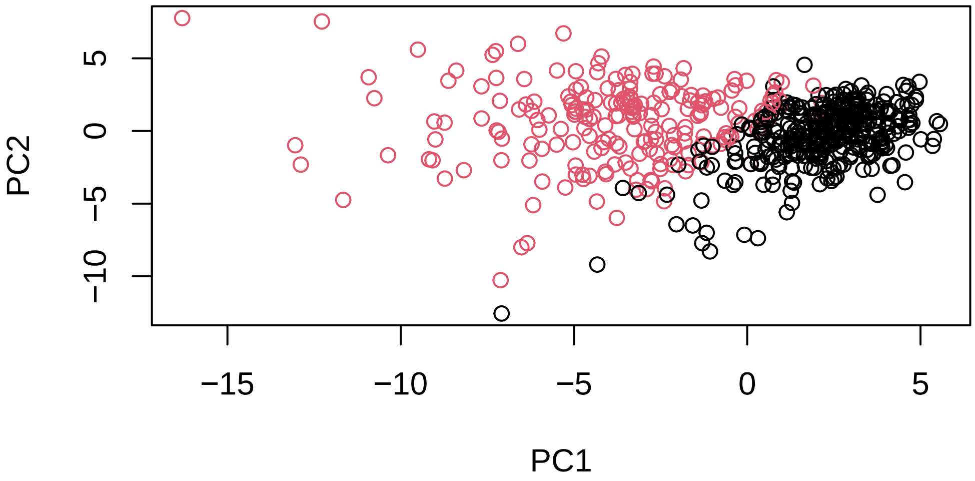
> Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?

What stands out about this plot is the excessive labeling of each point with row names, making it difficult to distinguish individual data points. The overlapping labels create a dense, unreadable cluster, making the plot visually cluttered and hard to interpret.

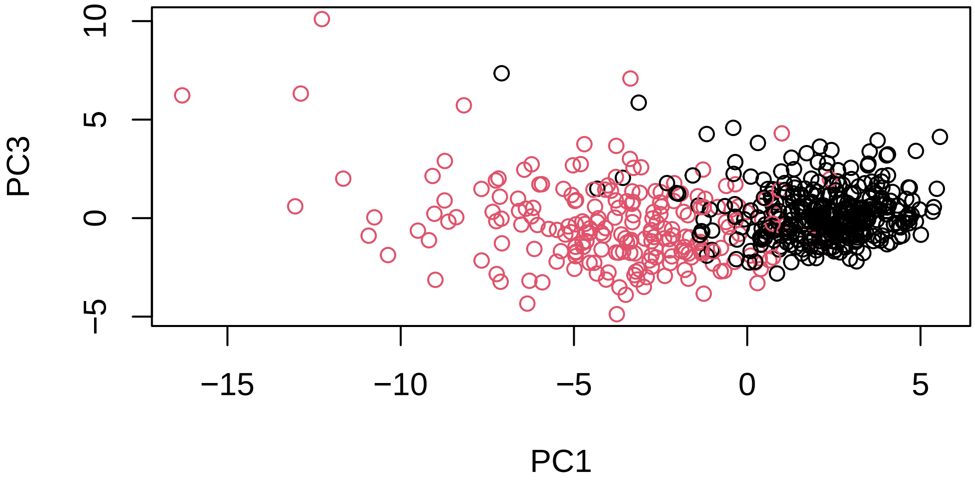
```r
biplot(wisc.pr)
```



```r
# Scatter plot Observations by components 1 and 2
plot( wisc.pr$x[,1], wisc.pr$x[,2], col = diagnosis,
      xlab = "PC1", ylab = "PC2")
```



```
# Scatter plot Observations by components 1 and 3
plot( wisc.pr$x[,1], wisc.pr$x[,3], col = diagnosis,
      xlab = "PC1", ylab = "PC3")
```



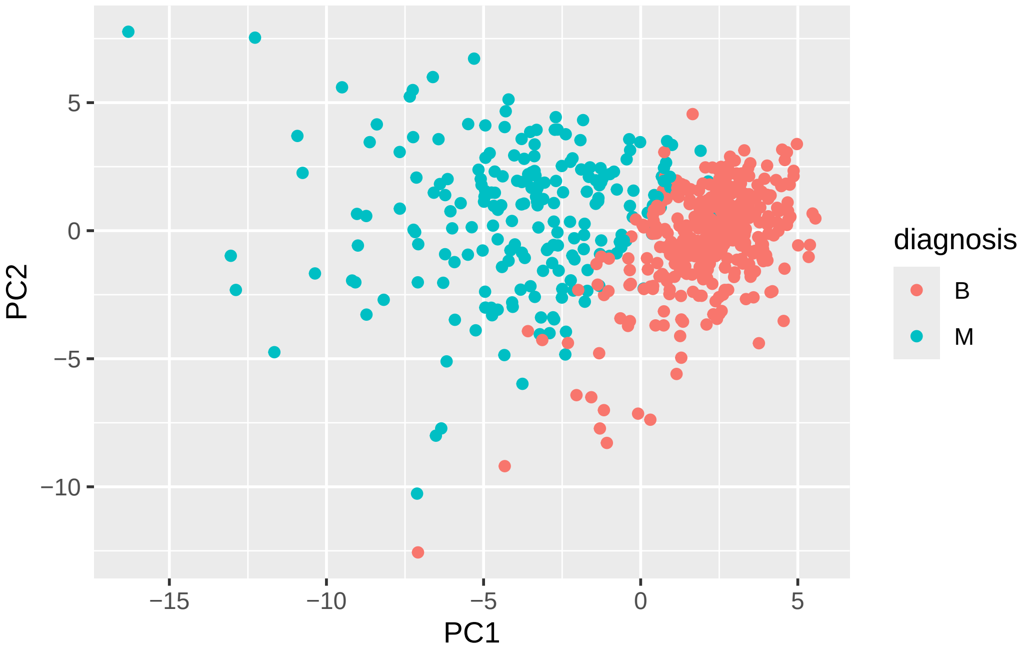
Q8. Generate a similar plot for principal components 1 and 3. What do you notice about these plots?

The first plot between PC1 & PC2 has a more observant separation while the second plot between PC1 & PC3 has more data points overlapping

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

```
# Load the ggplot 2 package
library(ggplot2)

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



Variance Explained

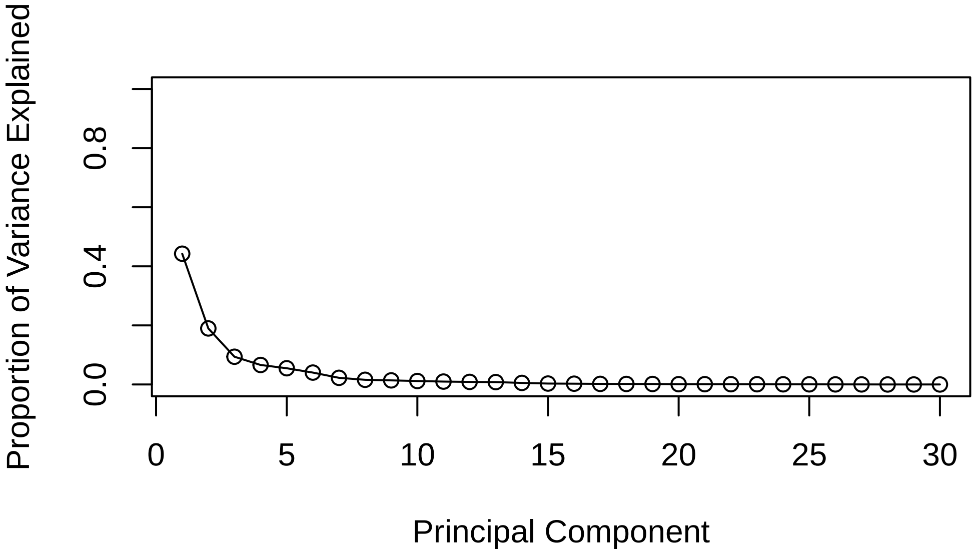
```
#Calculate variance of each component
pr.var <- wisc.pr$sdev^2
head(pr.var)
```

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

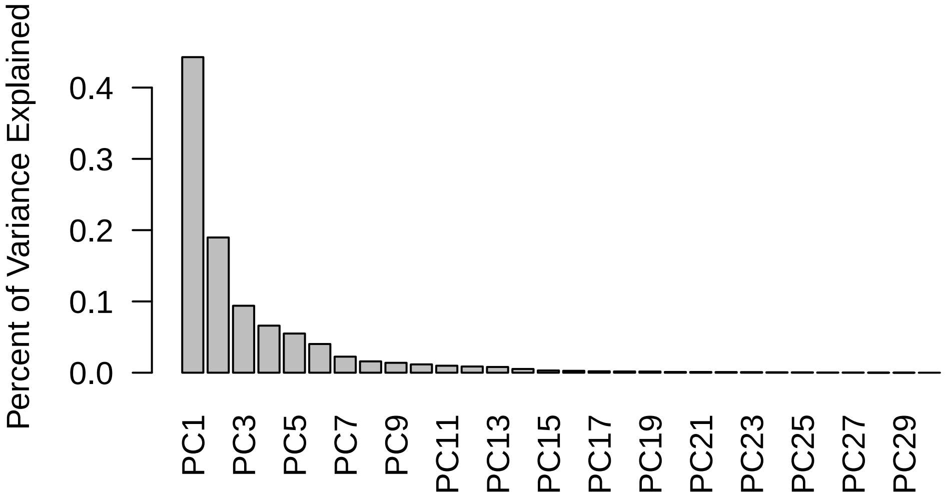
```
#Variance explained by each principal component: pve
pve <- pr.var/sum(pr.var)

#Plot variance explained for each principal component
```

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

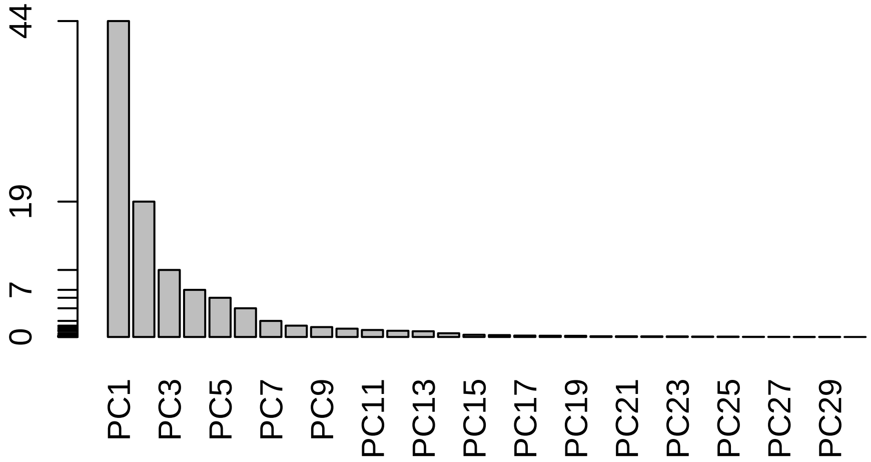


```
#Alternative scree plot of the same data, note data driven y-axis
barplot(pve, ylab = "Percent of Variance Explained",names.arg = paste0("PC", 1:length(pve)),
```



```
barplot(pve,
        names.arg = paste0("PC", 1:length(pve)),
        las = 2,
        axes = FALSE)

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



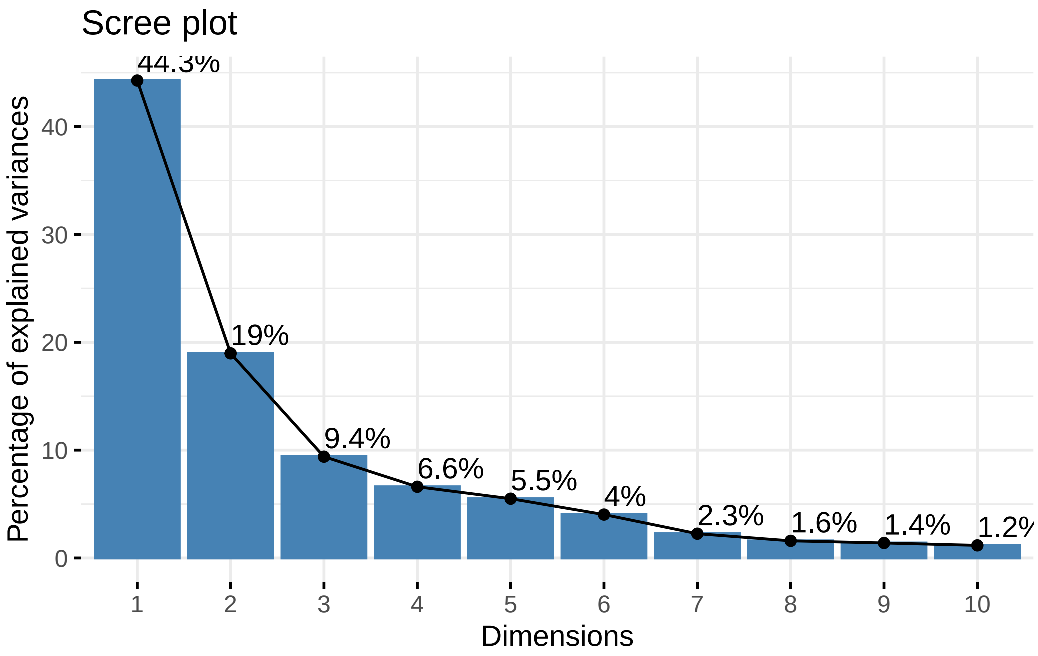
```
##ggplot based graph
options(repos = c(CRAN = "https://cran.rstudio.com/"))
install.packages("factoextra")
```

```
The downloaded binary packages are in
    /var/folders/86/dzbrd2pd06zf2sbv2hkr7fp40000gn/T//RtmpNmOAJb/downloaded_packages
```

```
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["concave.points_mean", 1]
```

```
[1] -0.2608538
```

The component of the loading vector for `concave.points_mean` in the first principal component (PC1) is -0.2609. This negative value indicates that `concave.points_mean` contributes significantly to PC1, with higher values of this feature being associated with lower PC1 scores, which may help differentiate between malignant and benign diagnoses.

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

The minimum number of PC to explain 80% of the variance of the data is 5 (PC1-5)

Hierarchial Clustering

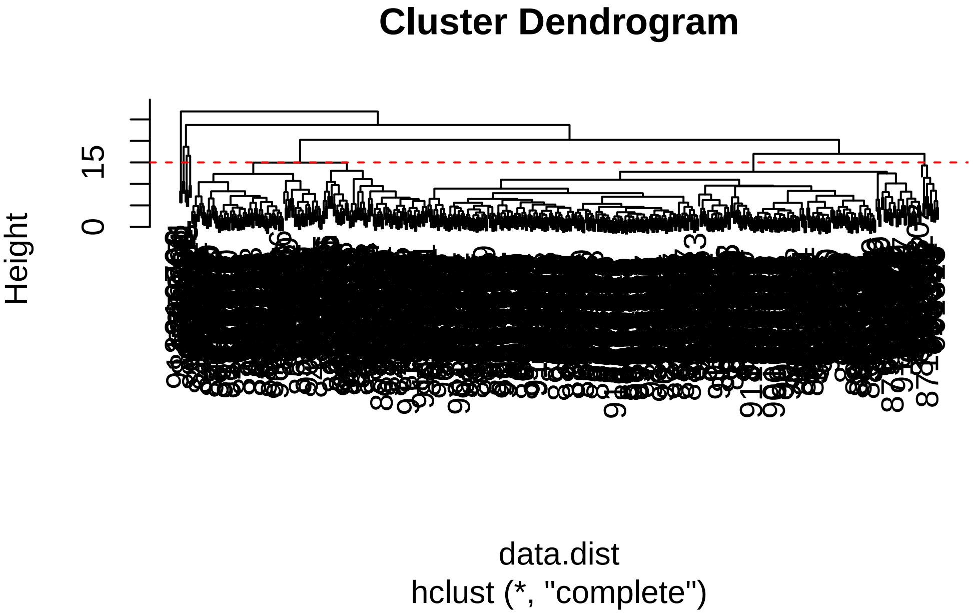
```
# Scale the wisc.data data using the "scale()" function
data.scaled <- scale(wisc.data)
```

```r
# Calculate the (Euclidean) distances between all pairs of observations
data.dist <- dist(data.scaled)
```

```r
# Create a hierarchical clustering model using complete linkage
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?

```r
plot(wisc.hclust)
abline(h = 15, col="red", lty=2)
```



The height at which the clustering model has four clusters is approximately 15, as observed from the dendrogram. By drawing a horizontal line at this height using `abline(h = 15, col="red", lty=2)`, we can see that the data splits into four distinct clusters at this threshold.

Selecting number of clusters

```r
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?

```r
for (k in 2:10) {
  cat("\nNumber of Clusters:", k, "\n")
  print(table(cutree(wisc.hclust, k = k), diagnosis))
}
```

```

Number of Clusters: 2
   diagnosis
      B   M
  1 357 210
  2   0   2

Number of Clusters: 3
   diagnosis
      B   M
  1 355 205
  2   2   5
  3   0   2

Number of Clusters: 4
   diagnosis
      B   M
  1  12 165
  2   2   5
  3 343  40
  4   0   2

Number of Clusters: 5
   diagnosis
      B   M
  1  12 165
  2   0   5
  3 343  40
  4   2   0
  5   0   2

Number of Clusters: 6
   diagnosis
      B   M
  1  12 165
  2   0   5
  3 331  39
  4   2   0
  5  12   1
  6   0   2

Number of Clusters: 7
   diagnosis
      B   M
  1  12 165
  2   0   3
  3 331  39
  4   2   0
  5  12   1
  6   0   2
  7   0   2

Number of Clusters: 8
   diagnosis
      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

Number of Clusters: 9
   diagnosis
      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

Number of Clusters: 10
    diagnosis
       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
```

By testing different numbers of clusters between 2 and 10, a better separation between malignant and benign cases can be found. For example, using 3 or 5 clusters may result in groups that more clearly distinguish between the two diagnoses compared to 4 clusters.

Using Different Methods

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

The Ward.D2 method gives the best results for this dataset because it minimizes within-cluster variance, leading to well-separated and compact clusters. This method tends to work well when the data has clear group structures, making it more effective than single, complete, or average linkage in maintaining balanced cluster sizes.

Combining Methods

Clustering on PCA Results

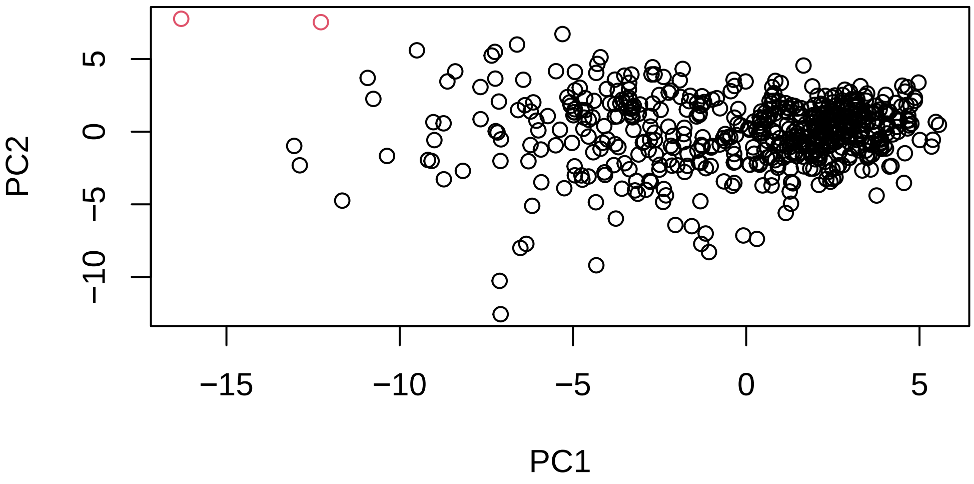
```
pca.dist <- dist(wisc.pr$x)
wisc.pr.hclust <- hclust(pca.dist, method = "complete")
grps <- cutree(wisc.pr.hclust, k=2)
table(grps)
```

```
grps
  1   2 
567   2 
```

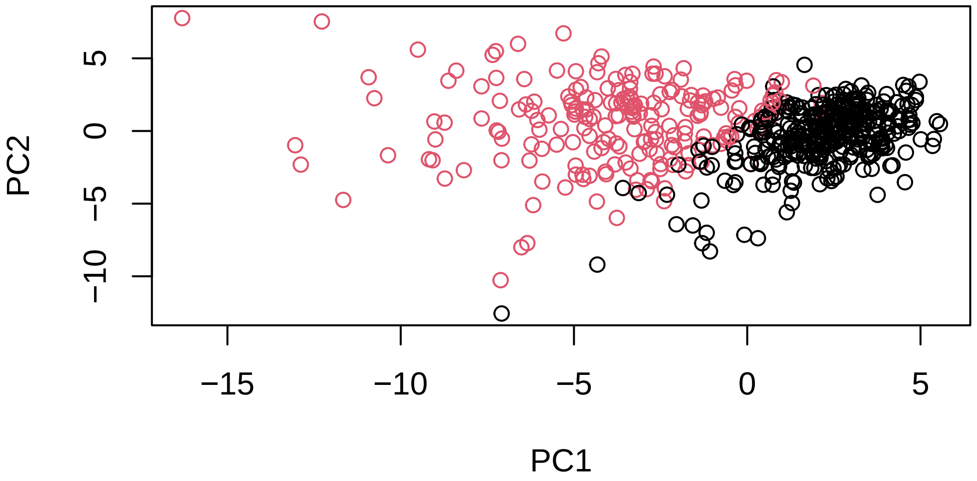
```
table(grps, diagnosis)
```

```
    diagnosis
grps   B   M
   1 357 210
   2   0   2
```

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



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



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

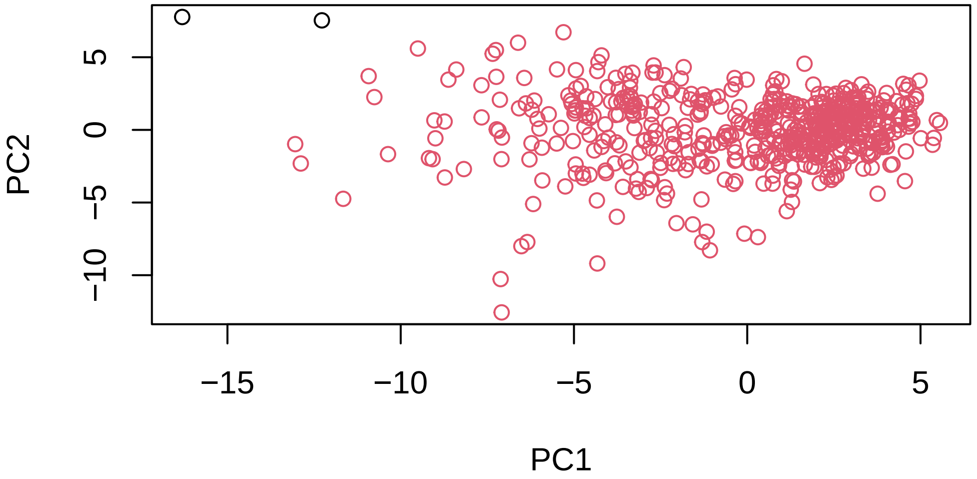
```
[1] "1" "2"
```

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

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

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

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



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

It separates out the two diagnoses fairy well as the newly created model with four clusters is more easily to observe

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

```
                       diagnosis
wisc.pr.hclust.clusters   B   M
                      1   0  45
                      2   2  77
                      3  26  66
                      4 329  24
```

> 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.

```r
set.seed(123)
wisc.km <- kmeans(wisc.data, centers = 2, nstart = 25)

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

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

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

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

In terms of separating the diagnoses, the k-means and hierarchical clustering models I created don't do that well compared to the newest models I've created

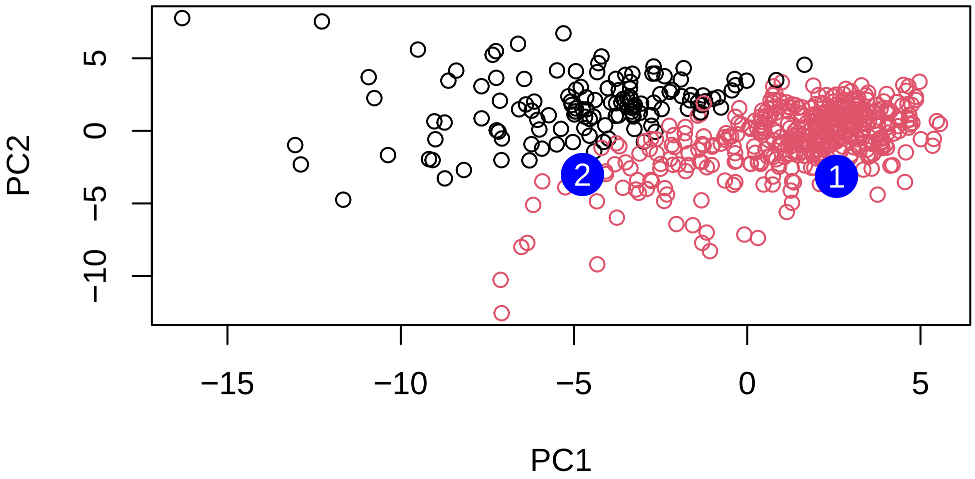
> Q17. Which of your analysis procedures resulted in a clustering model with the best specificity? How about sensitivity?

The analysis procedure which resulted in the best specificity is the hierarchical clustering model. The one with the best sensitivity is the PCA analysis # 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
```

```
g <- wisc.km$cluster
plot(wisc.pr$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?

Patient 2 is prioritized for follow-up because they are located in a region of the PCA plot that is more associated with malignant cases.