# Lab 8

**Anagha Pashilkar**

```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
```

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

```
# Create diagnosis vector for later
diagnosis <- wisc.df$diagnosis
```

Q1. How many observations are in this dataset?

```r
nrow(wisc.df)
```

```
[1] 569
```

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

```r
sum(diagnosis == "M")
```

```
[1] 212
```

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

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

```
[1] 10
```

### Principle Component Analysis

```r
# 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 
```

```r
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 
```

```r
# Perform PCA on wisc.data by completing the following code
wisc.pr <- prcomp( wisc.data, scale=T)
```

```r
# 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)?

```r
# Proportion of variance explained by PC1
prop_var_PC1 <- wisc.pr$sdev[1]^2 / sum(wisc.pr$sdev^2)
prop_var_PC1
```

```
[1] 0.4427203
```

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

```r
# Cumulative proportion of variance
cum_var <- cumsum(wisc.pr$sdev^2) / sum(wisc.pr$sdev^2)

# Number of PCs needed to capture at least 70% of the variance
n_PC_70 <- min(which(cum_var >= 0.7))
n_PC_70
```

```
[1] 3
```

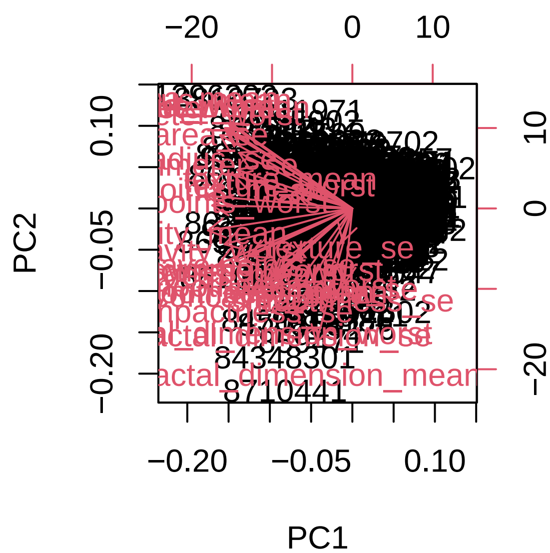
Q6. How many principal components (PCs) are required to describe at least 90% of the original variance in the data?

```
# Number of PCs needed to capture at least 90% of the variance
n_PC_90 <- min(which(cum_var >= 0.9))
n_PC_90
```

```
[1] 7
```

**Interpreting PCA Results**

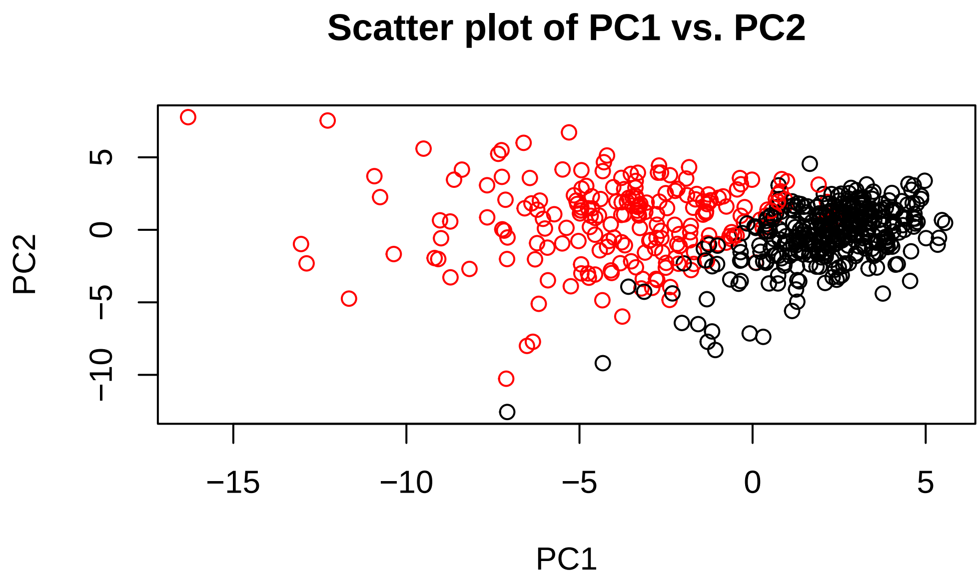
```
biplot(wisc.pr)
```




Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why? very difficult to understand. too much going on.

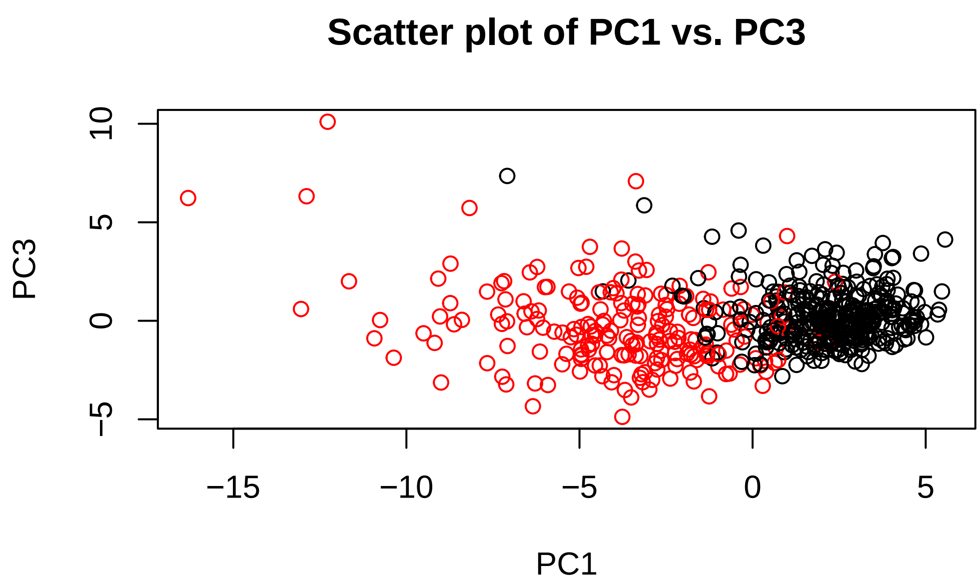
```
# Scatter plot observations by components 1 and 2

plot(wisc.pr$x[, c(1, 2)], col = ifelse(diagnosis == "M", "red", "black"),
     xlab = "PC1", ylab = "PC2", main = "Scatter plot of PC1 vs. 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 = ifelse(diagnosis == "M", "red", "black"),
     xlab = "PC1", ylab = "PC3", main = "Scatter plot of PC1 vs. PC3")
```

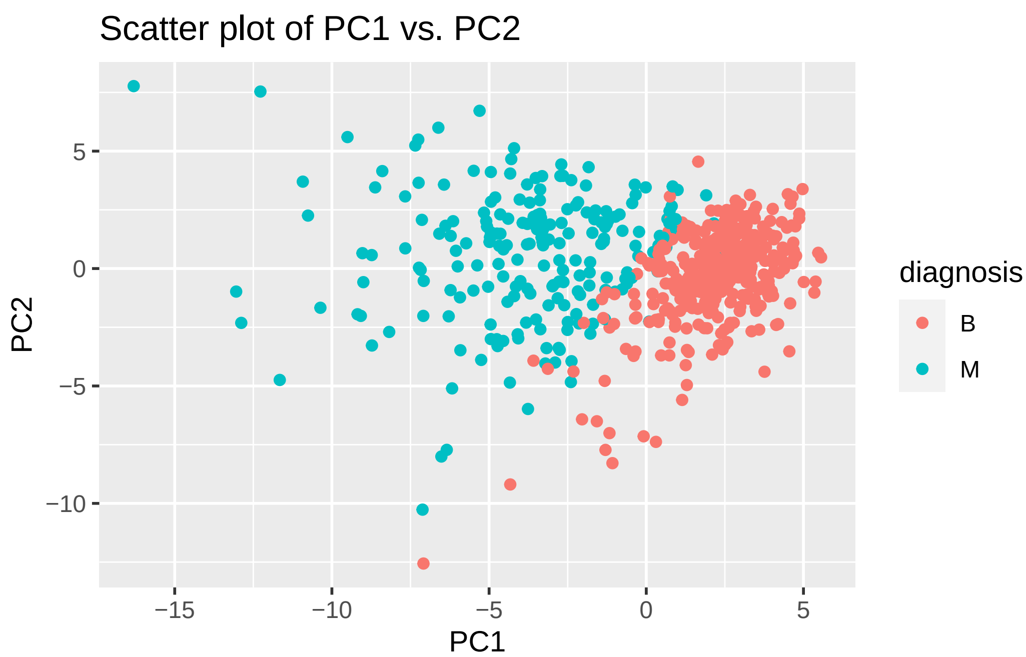



**create ggplot**

```
# 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() +
  xlab("PC1") +
  ylab("PC2") +
  ggtitle("Scatter plot of PC1 vs. PC2")
```



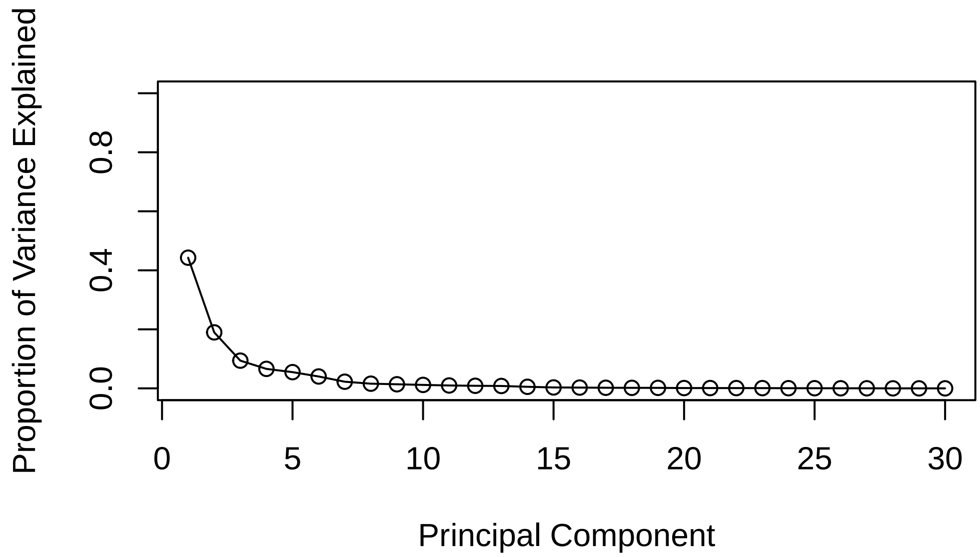

### Variance

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

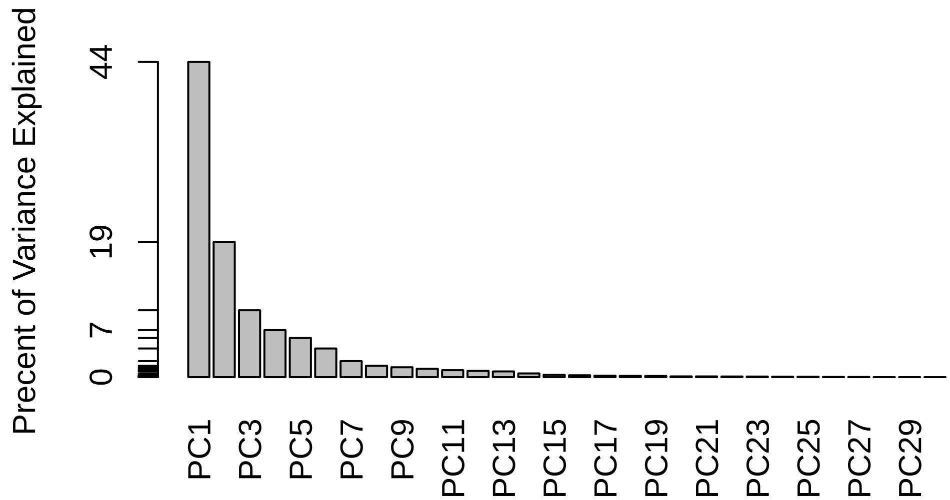
```
[1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

```
# 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")
```



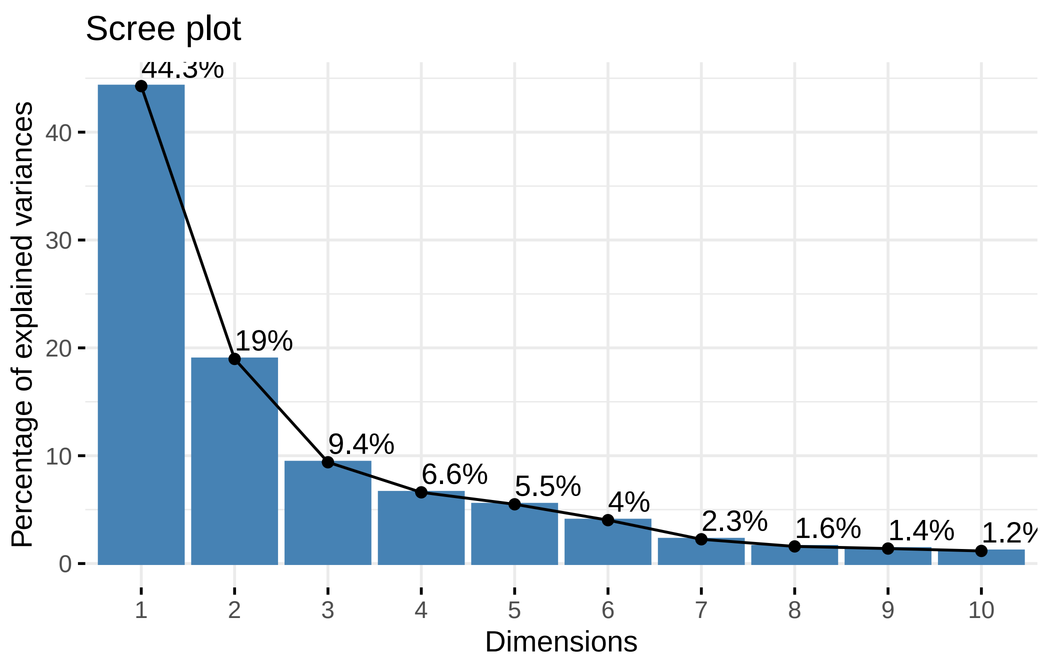

```
# Alternative scree plot of the same data, note data driven y-axis
barplot(pve, ylab = "Precent of Variance Explained",
     names.arg=paste0("PC",1:length(pve)), las=2, axes = FALSE)
axis(2, at=pve, labels=round(pve,2)*100 )
```




```
## 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)
```




### Communicating PCA Results

Q9. For the first principal component, what is the component of the loading vector (i.e. wisc.pr$rotation[,1]) for the feature concave.points_mean?

```
# Find the component of the loading vector for concave.points_mean for PC1
loading_concave_points_mean <- wisc.pr$rotation["concave.points_mean", 1]
loading_concave_points_mean
```

```
[1] -0.2608538
```

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

```
# Calculate cumulative proportion of variance explained by each PC
cumulative_var <- cumsum(pve)

# Find the minimum number of PCs required to explain 80% of variance
min_num_pcs <- min(which(cumulative_var >= 0.8))

min_num_pcs
```

```
[1] 5
```

## 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)
```

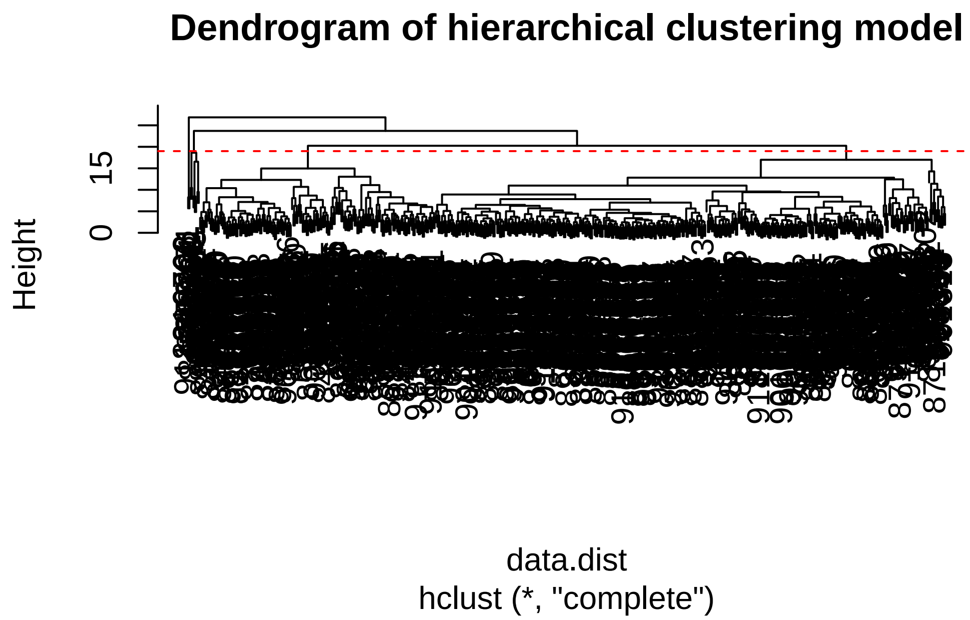
Create a hierarchical clustering model using complete linkage. Manually specify the method argument to `hclust()` and assign the results to `wisc.hclust`.

```
# Create a hierarchical clustering model using complete linkage
wisc.hclust <- hclust(data.dist, method = "complete")
```

### Results of hierarchical clustering

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

```
plot(wisc.hclust, main = "Dendrogram of hierarchical clustering model")
abline(h = 19, col = "red", lty = 2)
```




### Selecting number of clusters

```
# Use cutree() to cut the tree so that it has 4 clusters
wisc.hclust.clusters <- cutree(wisc.hclust, k = 4)
```

We can use the `table()` function to compare the cluster membership to 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
```

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

```
# Cut the tree into 2-10 clusters and display the resulting cluster vs diagnosis tables
for (k in 2:10) {
```

```r
  wisc.hclust.clusters <- cutree(wisc.hclust, k)
  tab <- table(wisc.hclust.clusters, diagnosis)
  print(tab)
}
```

```
                    diagnosis
wisc.hclust.clusters   B   M
                   1 357 210
                   2   0   2
                    diagnosis
wisc.hclust.clusters   B   M
                   1 355 205
                   2   2   5
                   3   0   2
                    diagnosis
wisc.hclust.clusters   B   M
                   1  12 165
                   2   2   5
                   3 343  40
                   4   0   2
                    diagnosis
wisc.hclust.clusters   B   M
                   1  12 165
                   2   0   5
                   3 343  40
                   4   2   0
                   5   0   2
                    diagnosis
wisc.hclust.clusters   B   M
                   1  12 165
                   2   0   5
                   3 331  39
                   4   2   0
                   5  12   1
                   6   0   2
                    diagnosis
wisc.hclust.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
wisc.hclust.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
wisc.hclust.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
wisc.hclust.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
```

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

ward.D2 since it minimizes variance within clusters. Since there is a lot of data, this method is most useful and will give cleanest results.

### K-means

```
# Create k-means model
wisc.km <- kmeans(scale(wisc.data), centers=2, nstart=20)

# Compare to actual diagnoses
table(wisc.km$cluster, diagnosis)
```

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

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

```
   wisc.hclust.clusters
      1   2   3   4   5   6   7   8   9  10
  1  17   0   0 358   0   0   5   0   0   0
  2  81  59   3  12  20   2   7   2   2   1
```

## Combining methods

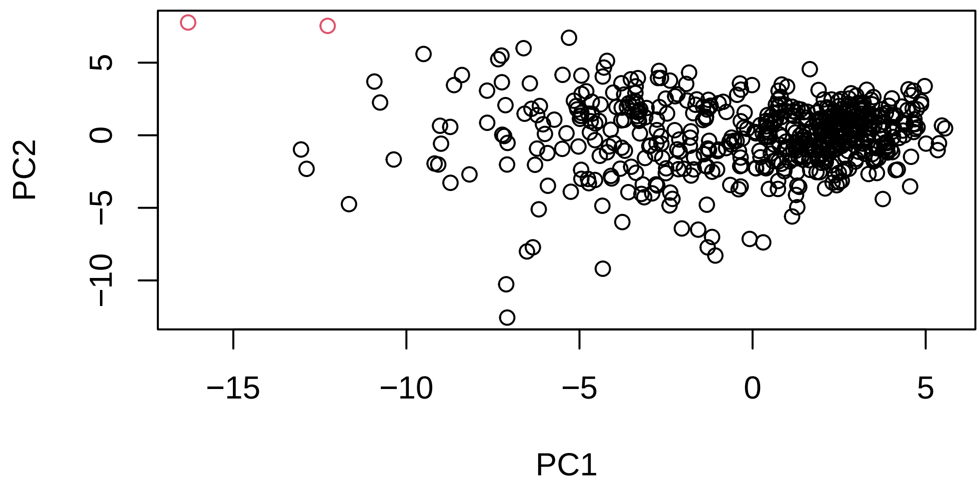
```
grps <- cutree(wisc.hclust, k=2)
table(grps)
```

```
grps
  1   2
567   2
```

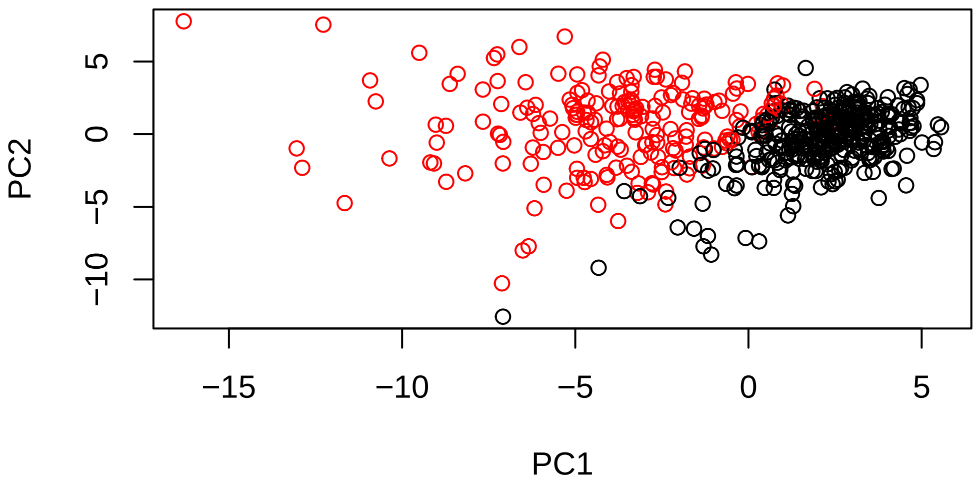
```
table(grps, diagnosis)
```

```
    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=  ifelse(diagnosis == "M", "red", "black"))
```



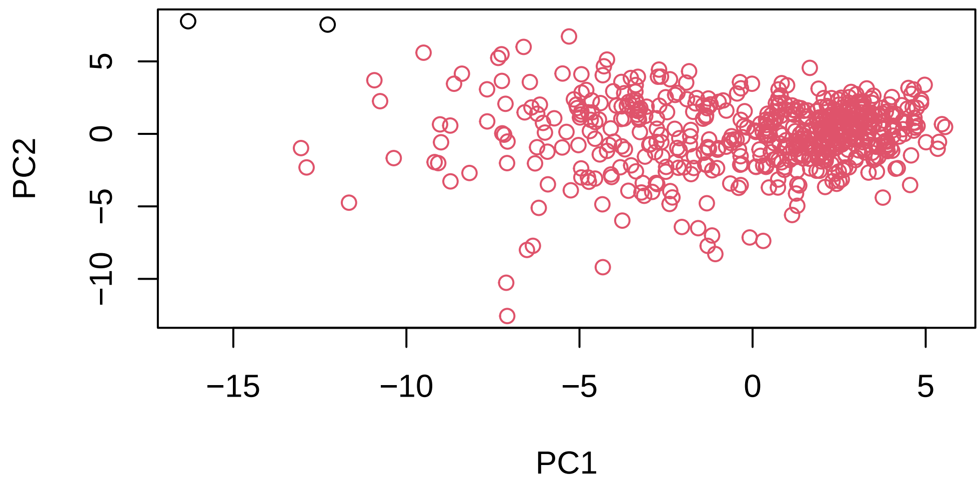

```
g <- as.factor(grps)
levels(g)
```

```
[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)
```




```
## 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)
```

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

```
# Compare to actual diagnoses
table(wisc.pr.hclust.clusters, diagnosis)
```

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

It clearly separates the clusters into two diagnoses (M and B)

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

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

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

```
                    diagnosis
wisc.hclust.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
```

K-means is much more efficient at separating the diagnosis. However, hclust helps us see a relationship between different datapoints at different levels.

## Sensitivity/ Specificity

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