class08

Import the data

```r
fna.data <- "WisconsinCancer.csv"
wisc.df <- read.csv(fna.data, row.names=1)

head(wisc.df, 3)
```

```
         diagnosis radius_mean texture_mean perimeter_mean area_mean
842302           M       17.99        10.38          122.8      1001
842517           M       20.57        17.77          132.9      1326
84300903         M       19.69        21.25          130.0      1203
         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
         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
         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
         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
         perimeter_worst area_worst smoothness_worst compactness_worst
842302             184.6       2019           0.1622            0.6656
842517             158.8       1956           0.1238            0.1866
```

```
84300903            152.5       1709           0.1444             0.4245
         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
         fractal_dimension_worst
842302                  0.11890
842517                  0.08902
84300903                0.08758
```

```
# remove first column
wisc.data <- wisc.df[,-1]
```

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

Q1. How many observations are in this dataset?

```
print(paste(nrow(wisc.df), "observation"))
```

```
[1] "569 observation"
```

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

```
print(paste(nrow(wisc.df[wisc.df$diagnosis=="M",]), 'malignant diagnosis'))
```

```
[1] "212 malignant diagnosis"
```

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

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

```
[1] 10
```

PCA

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

```
            radius_mean            texture_mean          perimeter_mean 
           1.412729e+01            1.928965e+01            9.196903e+01 
              area_mean         smoothness_mean        compactness_mean 
           6.548891e+02            9.636028e-02            1.043410e-01 
         concavity_mean     concave.points_mean           symmetry_mean 
           8.879932e-02            4.891915e-02            1.811619e-01 
 fractal_dimension_mean               radius_se              texture_se 
           6.279761e-02            4.051721e-01            1.216853e+00 
           perimeter_se                 area_se           smoothness_se 
           2.866059e+00            4.033708e+01            7.040979e-03 
         compactness_se            concavity_se       concave.points_se 
           2.547814e-02            3.189372e-02            1.179614e-02 
            symmetry_se    fractal_dimension_se            radius_worst 
           2.054230e-02            3.794904e-03            1.626919e+01 
          texture_worst         perimeter_worst              area_worst 
           2.567722e+01            1.072612e+02            8.805831e+02 
       smoothness_worst       compactness_worst         concavity_worst 
           1.323686e-01            2.542650e-01            2.721885e-01 
   concave.points_worst          symmetry_worst fractal_dimension_worst 
           1.146062e-01            2.900756e-01            8.394582e-02 
```

```
round(apply(wisc.data,2,sd), 2)
```

```
            radius_mean            texture_mean          perimeter_mean 
                   3.52                    4.30                   24.30 
              area_mean         smoothness_mean        compactness_mean 
                 351.91                    0.01                    0.05 
         concavity_mean     concave.points_mean           symmetry_mean 
                   0.08                    0.04                    0.03 
 fractal_dimension_mean               radius_se              texture_se 
                   0.01                    0.28                    0.55 
           perimeter_se                 area_se           smoothness_se 
                   2.02                   45.49                    0.00 
         compactness_se            concavity_se       concave.points_se 
                   0.02                    0.03                    0.01 
            symmetry_se    fractal_dimension_se            radius_worst 
                   0.01                    0.00                    4.83 
         texture_worst          perimeter_worst               area_worst
                  6.15                    33.60                   569.36
      smoothness_worst        compactness_worst          concavity_worst
                  0.02                     0.16                     0.21
  concave.points_worst           symmetry_worst fractal_dimension_worst
                  0.07                     0.06                     0.02
```

```
# so it's important to scale the data during pca
```

```
# Perform PCA on wisc.data by completing the following code
wisc.pr <- prcomp(wisc.data, scale=TRUE)
# Look at summary of results
summary(wisc.pr)
```

```
Importance of components:
                          PC1    PC2     PC3     PC4     PC5     PC6     PC7
Standard deviation     3.6444 2.3857 1.67867 1.40735 1.28403 1.09880 0.82172
Proportion of Variance 0.4427 0.1897 0.09393 0.06602 0.05496 0.04025 0.02251
Cumulative Proportion  0.4427 0.6324 0.72636 0.79239 0.84734 0.88759 0.91010
                           PC8    PC9    PC10   PC11    PC12    PC13    PC14
Standard deviation     0.69037 0.6457 0.59219 0.5421 0.51104 0.49128 0.39624
Proportion of Variance 0.01589 0.0139 0.01169 0.0098 0.00871 0.00805 0.00523
Cumulative Proportion  0.92598 0.9399 0.95157 0.9614 0.97007 0.97812 0.98335
                          PC15    PC16    PC17    PC18    PC19    PC20   PC21
Standard deviation     0.30681 0.28260 0.24372 0.22939 0.22244 0.17652 0.1731
Proportion of Variance 0.00314 0.00266 0.00198 0.00175 0.00165 0.00104 0.0010
Cumulative Proportion  0.98649 0.98915 0.99113 0.99288 0.99453 0.99557 0.9966
                          PC22    PC23   PC24    PC25    PC26    PC27    PC28
Standard deviation     0.16565 0.15602 0.1344 0.12442 0.09043 0.08307 0.03987
Proportion of Variance 0.00091 0.00081 0.0006 0.00052 0.00027 0.00023 0.00005
Cumulative Proportion  0.99749 0.99830 0.9989 0.99942 0.99969 0.99992 0.99997
                          PC29    PC30
Standard deviation     0.02736 0.01153
Proportion of Variance 0.00002 0.00000
Cumulative Proportion  1.00000 1.00000
```

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

```
print(paste(round((summary(wisc.pr)[[1]][1]^2 / sum(summary(wisc.pr)[[1]]^2)) * 100, 2), "
[1] "44.27%"
```

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

```r
sde <- summary(wisc.pr)[[1]]


n_PC <- function(percentage_variance) {
  for (i in 1:length(sde) ) {
    if ( (sum(sde[1:i]^2) / sum(sde^2)) * 100 >= percentage_variance) {
      break
    }
  }
i
}

print(paste(n_PC(70), "PCs are required"))
```

```
[1] "3 PCs are required"
```

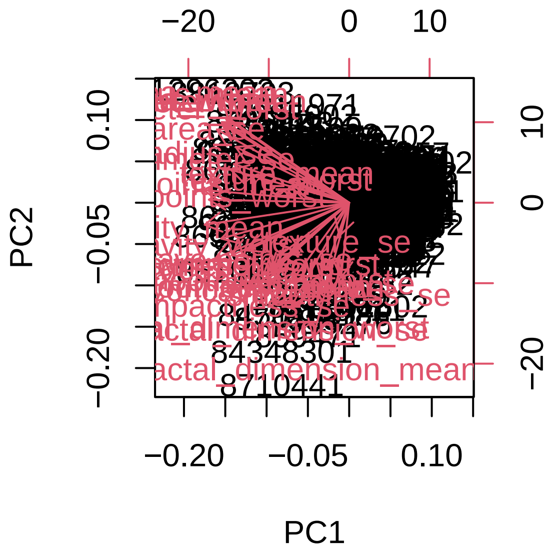
> Q6. How many principal components (PCs) are required to describe at least 90% of the original variance in the data?

```r
print(paste(n_PC(90), "PCs are required"))
```

```
[1] "7 PCs are required"
```

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

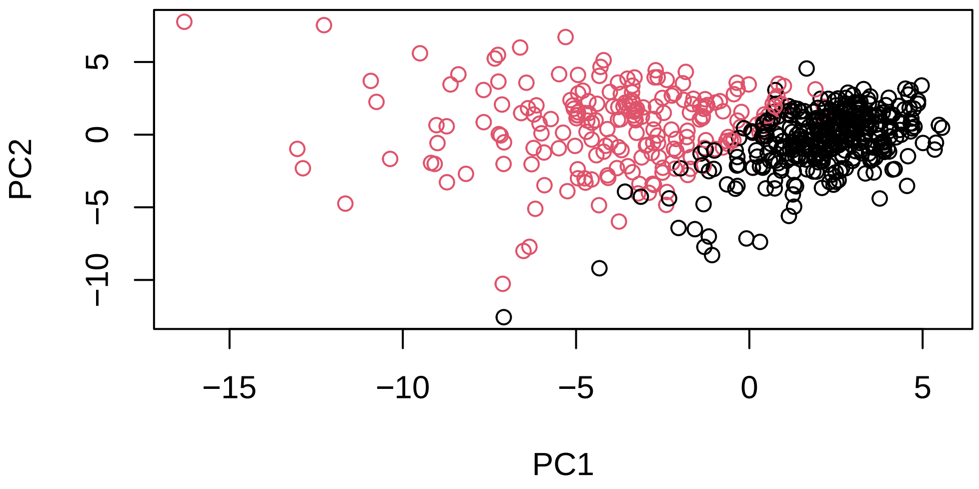
```r
biplot(wisc.pr)
```



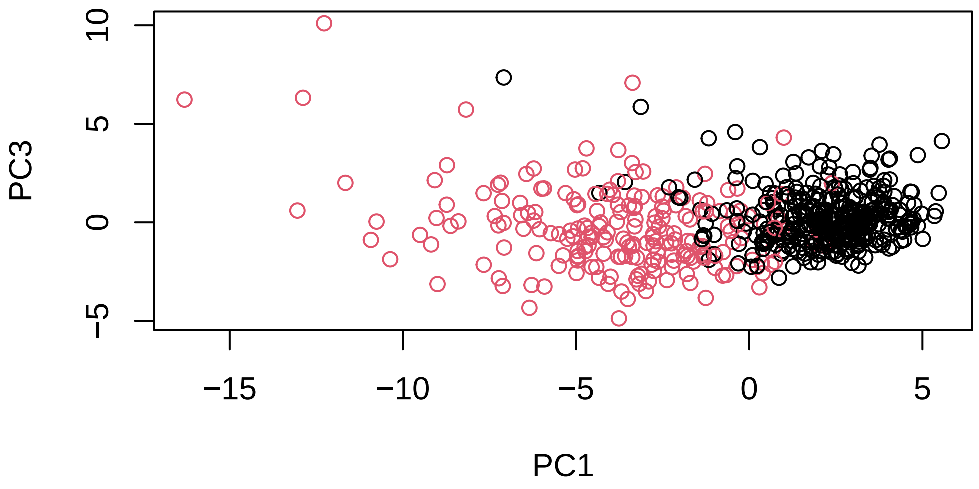
The plot is very crowded and difficult to read. The text overlap with the points and make the data points unreadable. The length of the red arrow of each point should represent the weight of each sample contributing to each features in dimension of first two components.

Q8

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

plot(wisc.pr$x[, 1:2], col = diagnosis,
     xlab = "PC1", ylab = "PC2")
```

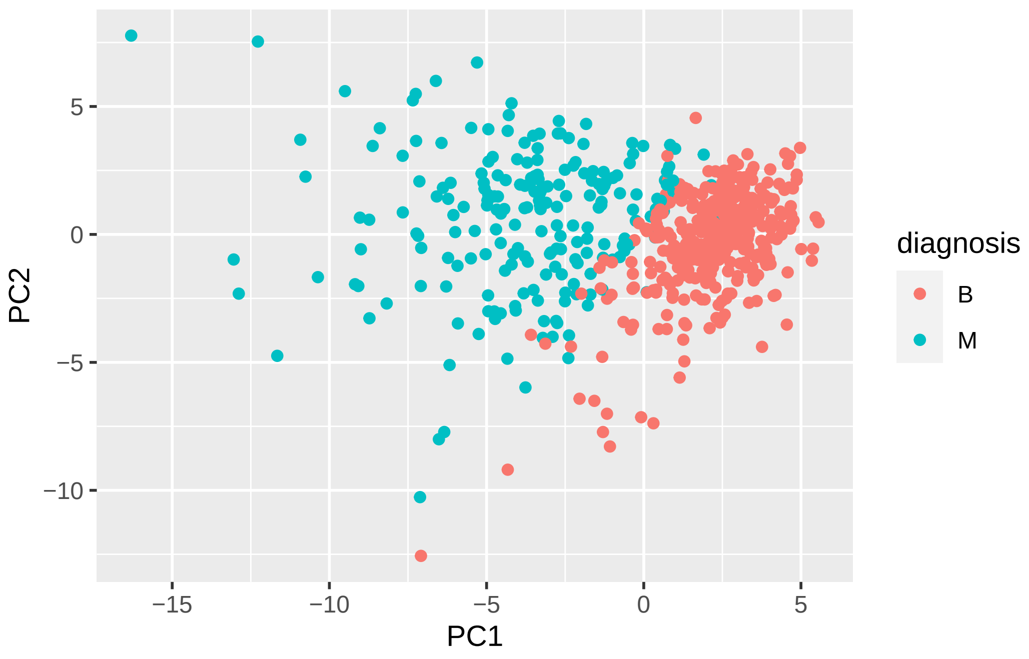


```r
plot(wisc.pr$x[, c(1,3)], col = diagnosis,
     xlab = "PC1", ylab = "PC3")
```



The two different diagnosis looks seperated in these plot, suggesting that PC1 and PC2 or PC1 and PC3 (mostly PC1) captures enough differences to the extend that the same diagnosis clustered together in the dimension of only two PCs. It's also much easier to read than the previous one.

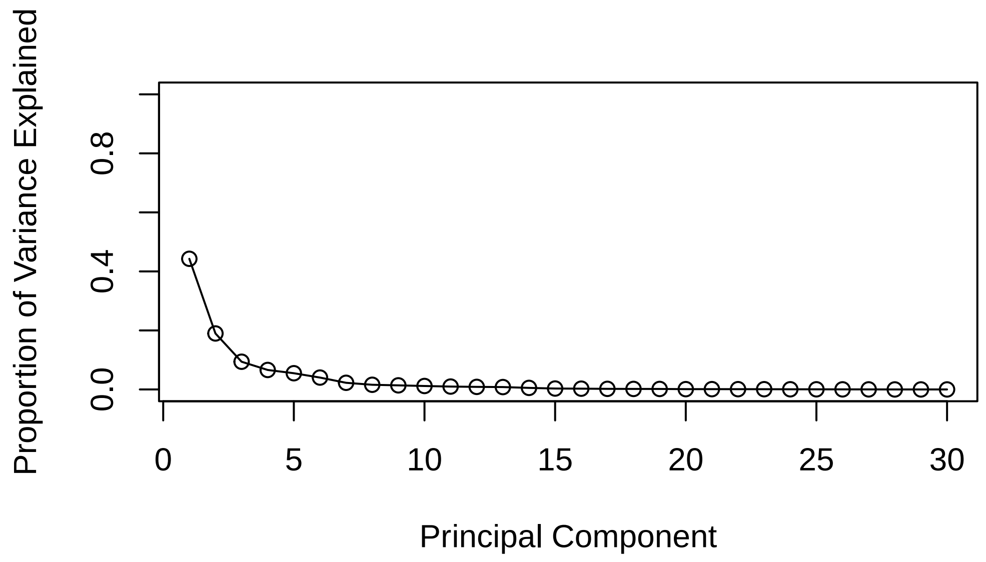
```r
# Create a data.frame for ggplot
df <- as.data.frame(wisc.pr$x)
df$diagnosis <- diagnosis

# Load the ggplot2 package
library(ggplot2)

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



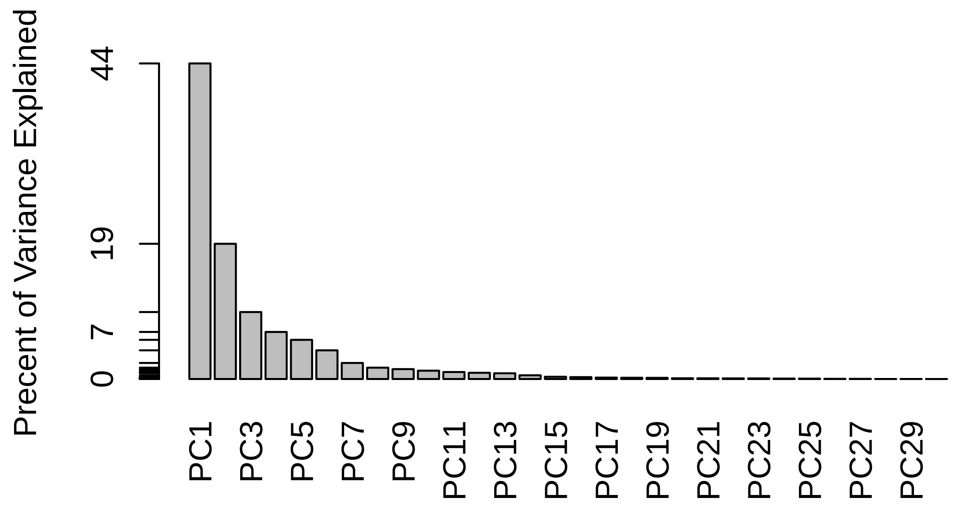
```r
pr.var <- wisc.pr$sdev^2
head(pr.var)
```

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

```r
# 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")
```



```r
# 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 )
```



Q9.

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

```
[1] -0.2608538
```

10.

```
print(paste(n_PC(80), "PCs are required"))
```

```
[1] "5 PCs are required"
```

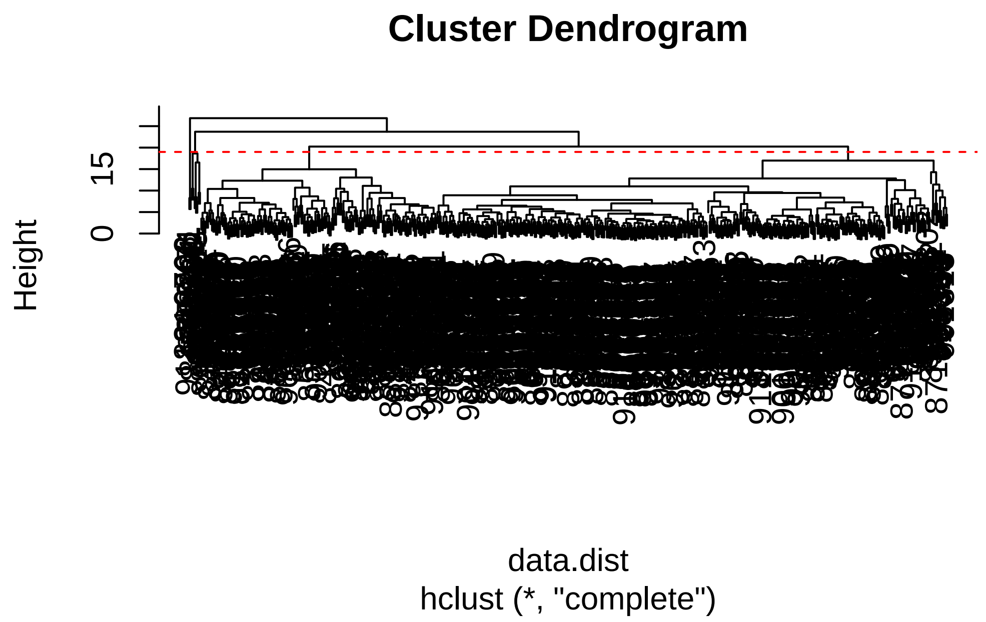
Hierarchical clustering

```
# Scale the wisc.data data using the "scale()" function
data.scaled <- scale(wisc.data)
# calculate euclidian distance
data.dist <- dist(data.scaled, method = "euclidean")
#clustering
```

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

11.

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



The height is 19.

```r
wisc.hclust.clusters <- cutree(wisc.hclust, 4)

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

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

12.

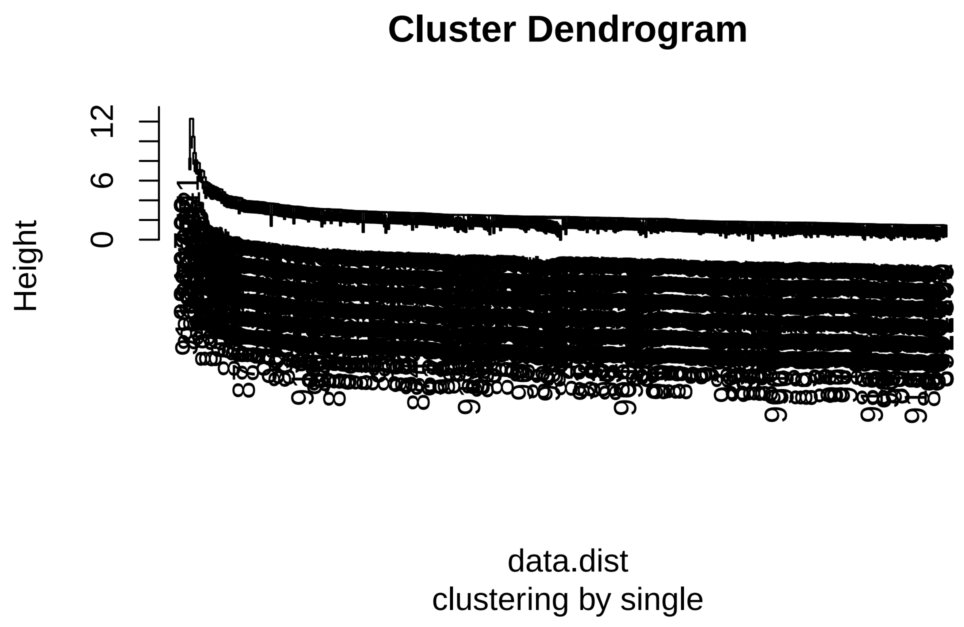
```r
wisc.hclust.clusters <- cutree(wisc.hclust, 6)

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

```
                    diagnosis
wisc.hclust.clusters   B   M
                   1  12 165
                   2   0   5
                   3 331  39
                   4   2   0
                   5  12   1
                   6   0   2
```

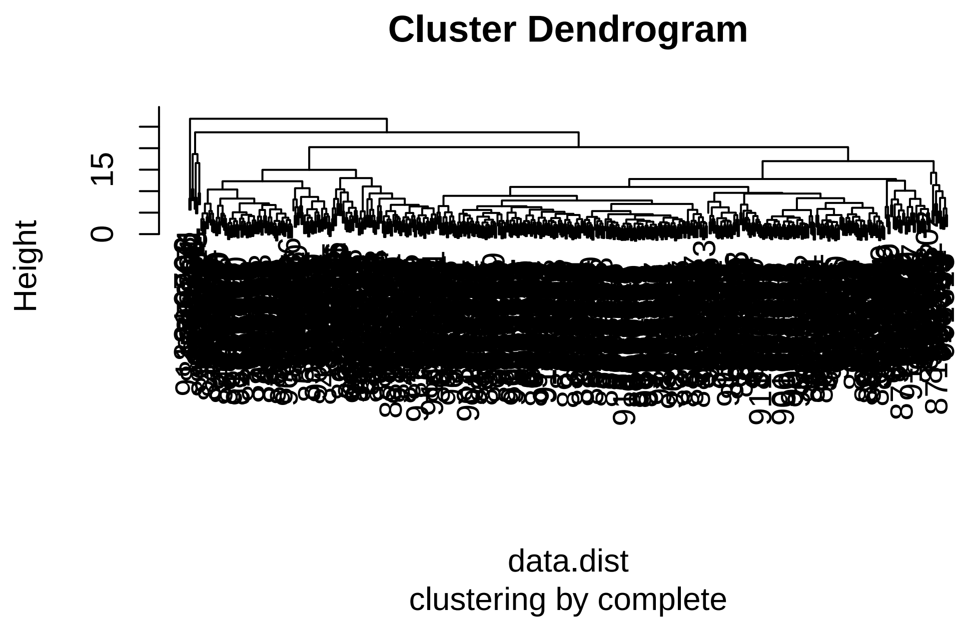
I cannot find a better cut. Anything below 4 will cause majority of B and M to be clustered together. Anything above 4 will cause smaller clusters to form that are not obvious representative B or M.

Q13

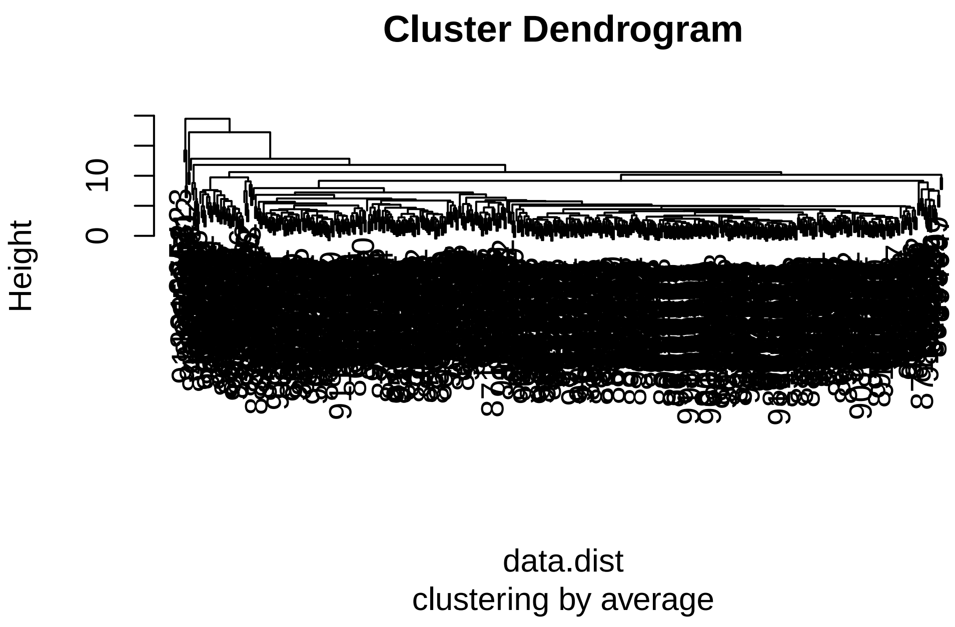
```r
for (med in c("single", "complete", "average", "ward.D2")) {
  wisc.hclust <- hclust(data.dist, method=med)
  plot(wisc.hclust, sub = paste("clustering by", med))
  wisc.hclust.clusters <- cutree(wisc.hclust, 2)
  print(med)
  print(table(wisc.hclust.clusters, diagnosis))
}
```



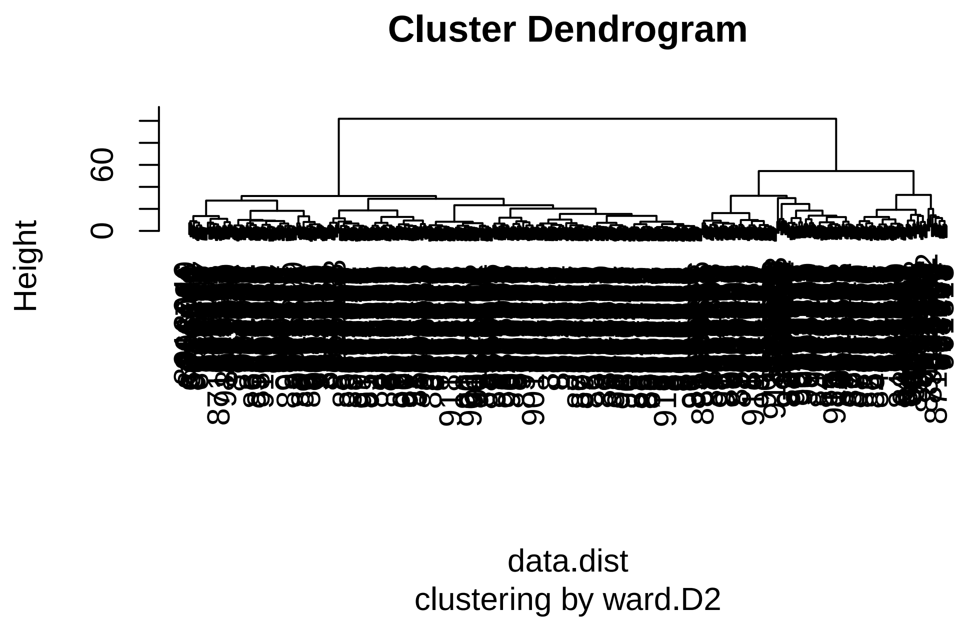
```
[1] "single"
                    diagnosis
wisc.hclust.clusters   B   M
                   1 357 210
                   2   0   2
```



```
[1] "complete"
                   diagnosis
wisc.hclust.clusters   B   M
                   1 357 210
                   2   0   2
```



```
[1] "average"
                  diagnosis
wisc.hclust.clusters   B   M
                   1 357 209
                   2   0   3
```



```
[1] "ward.D2"
                    diagnosis
wisc.hclust.clusters   B   M
                   1  20 164
                   2 337  48
```

Looks like ward.D2 gives the best result. At only two clusters, it shows a good cluster vs diagnoses match. The second best is the complete, which shows apparent match at cluster=4. The other two doesn't show apparent matches, as the clusters are too stringy and not compact. This could be because the "single" and "average" methods are affected too much by the noise to give good matches.

Combining methods

```
# select principle components

wisc.pr.90 <- wisc.pr$x[, 1:n_PC(90)]

# calculate euclidian distance
wisc.pr.90.dist <- dist(wisc.pr.90, method = "euclidean")
```

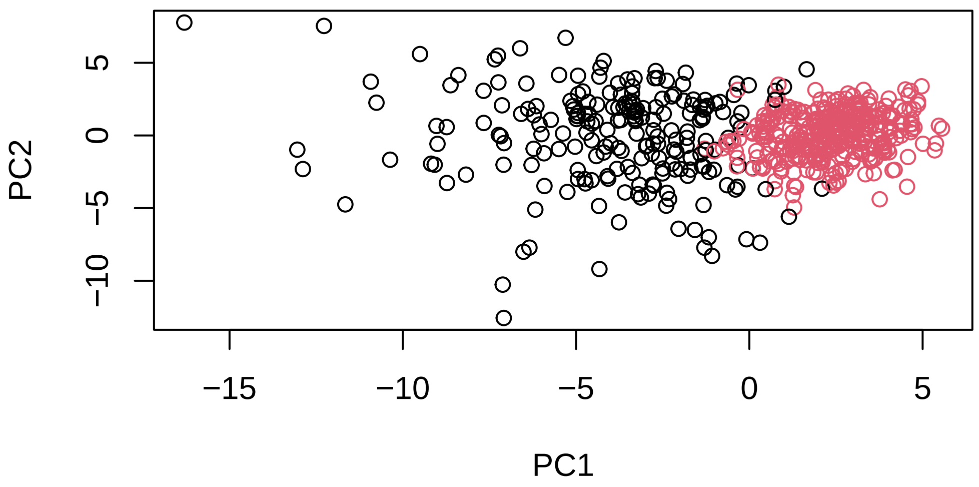
```
# build clusters
wisc.pr.hclust <- hclust(wisc.pr.90.dist, method="ward.D2")
grps <- cutree(wisc.pr.hclust, k=2)
table(grps)
```

```
grps
  1   2 
216 353 
```

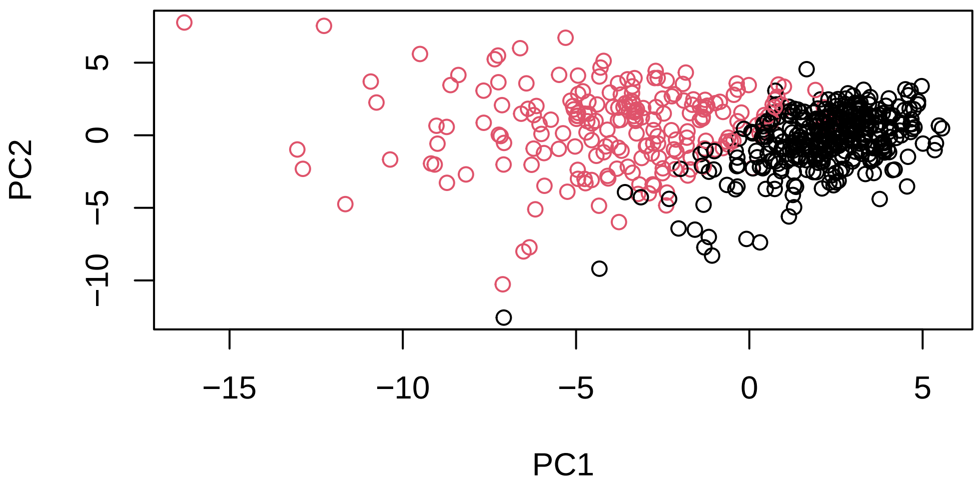
```
table(grps, diagnosis)
```

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

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



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



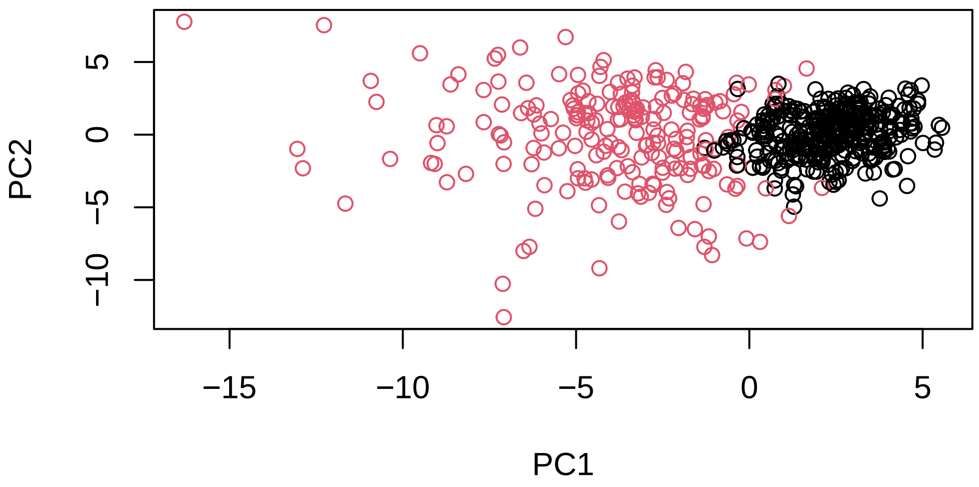
```r
g <- as.factor(grps)
levels(g)
```

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

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

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

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



```r
# 3d ploting
library(rgl)
# plot3d(wisc.pr$x[,1:3], xlab="PC 1", ylab="PC 2", zlab="PC 3", cex=1.5, size=1, type="s"
# rglwidget(width = 400, height = 400)
```

```r
## Use the distance along the first 7 PCs for clustering i.e. wisc.pr$x[, 1:7]

# calculate euclidian distance
wisc.pr.dist <- dist(wisc.pr$x[, 1:7], method = "euclidean")

# build clusters
wisc.pr.hclust <- hclust(wisc.pr.dist, method="ward.D2")

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


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

```
                       diagnosis
wisc.pr.hclust.clusters   B   M
```

```
  1   28 188
  2 329   24
```

Q15

The model separated the two diagnoses pretty well. If we assign the first cluster as “diagnosis M” and the second as “diagnosis B”, the fpr is 0.11 and the fnr is 0.08. The accuracy is 90.9%. It performs better than ward.D2 without PCA, proving that PCA indeed helps with dimension reduction and gives us a better model.