Class08 Mini-project

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Background

The goal of today's mini-project is to perform principal component analysis (PCA) and hierarchical clustering on a dataset containing features of breast cancer tumors.

Data import

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

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

Exploratory data analysis

```
dim(wisc.df)
```

```
[1] 569  31
```

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

```
[1] 212
```

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

```
[1] 357
```

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

```
[1] 10
```

Q1. 569 observations

Q2. 212 observations with a malignant diagnosis

Q3. 10 features

Principal Component Analysis

The main function in base R for PCA is called `prcomp()`. An optional argument `scale` should nearly always be set to `TRUE` for this function.

```r
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
wisc.pr <- prcomp(wisc.data, center = TRUE, scale. = TRUE)
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
```

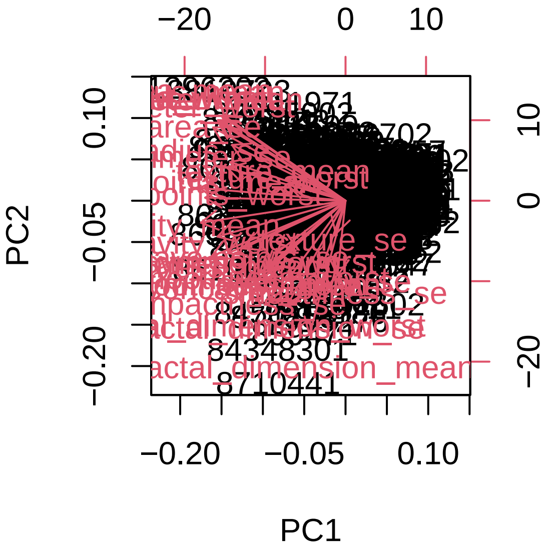
Q4. 44.27% of the variance is captured by PC1

Q5. 3 PC required

Q6. 7 PC required

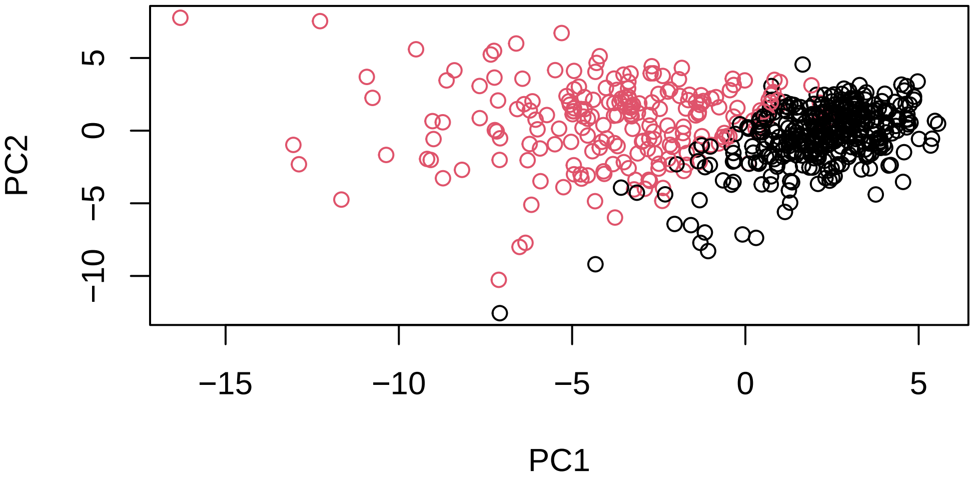
Interpreting PCA results

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

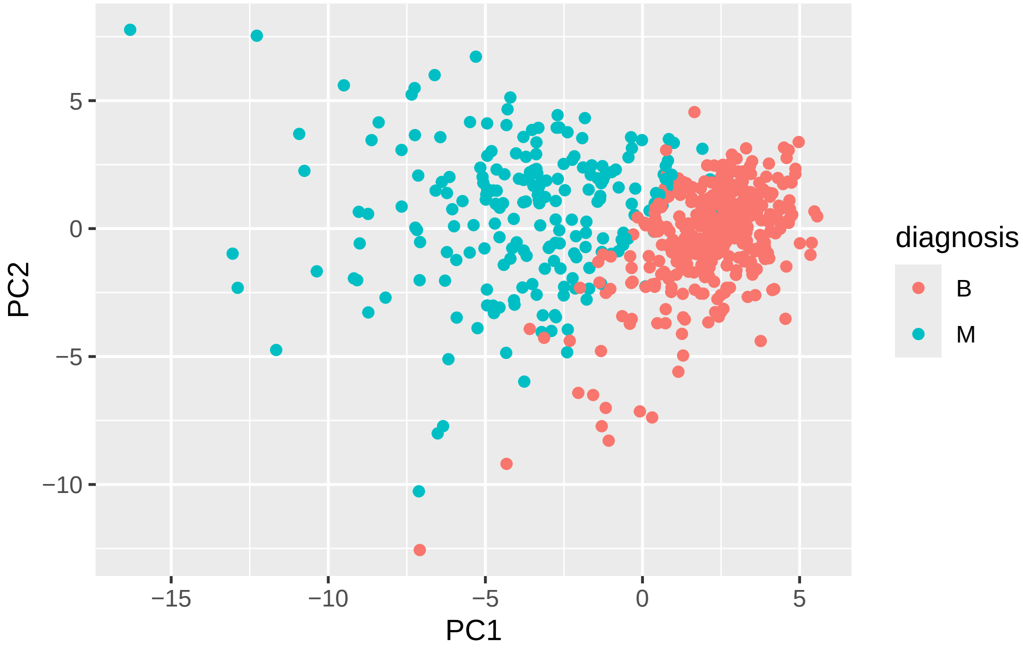


Q7. The variables are all over the place, making it extremly hard to understand visually.

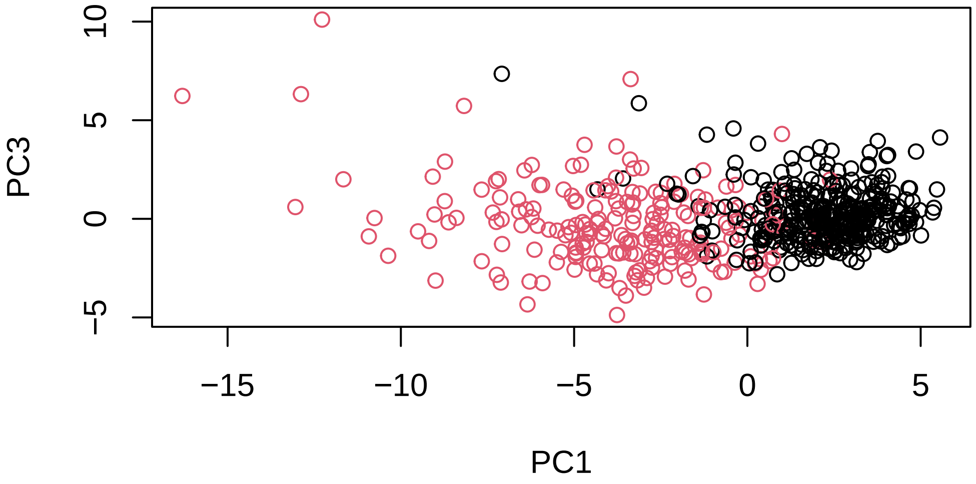
```r
plot(wisc.pr$x[, 1:2], col = diagnosis ,
     xlab = "PC1", ylab = "PC2")
```



```
library(ggplot2)
ggplot(wisc.pr$x[, 1:2], aes(x=PC1, y=PC2, color=diagnosis)) + geom_point()
```

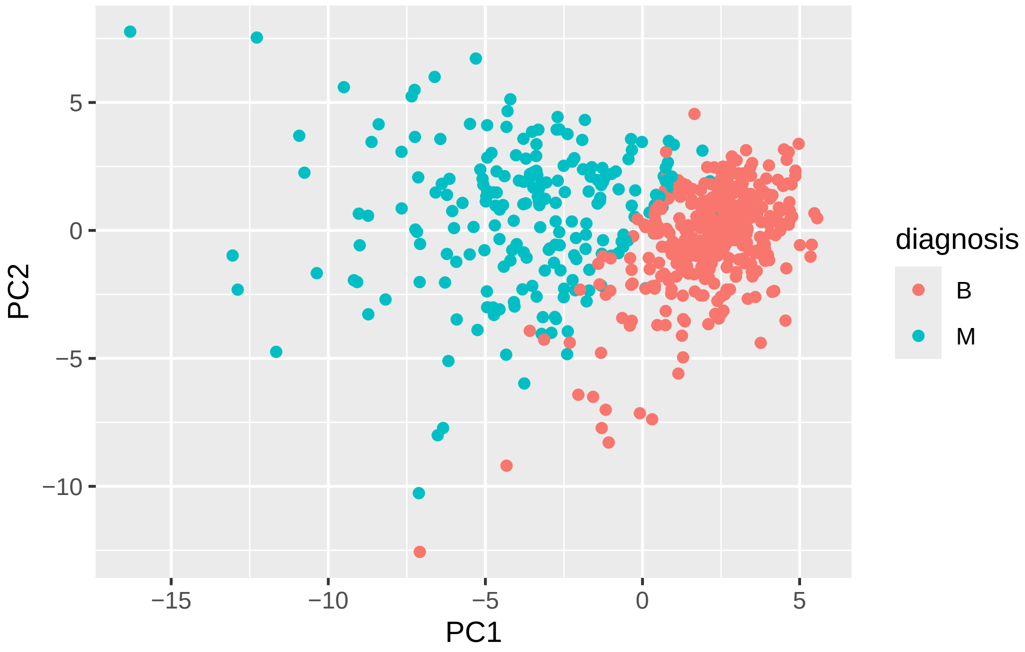


```
plot(wisc.pr$x[, c(1,3)], col = diagnosis ,
     xlab = "PC1", ylab = "PC3")
```



Q8. Black dots are clustered together while red dots are more spread out, indicating that benign tumors have more similarity within the group.

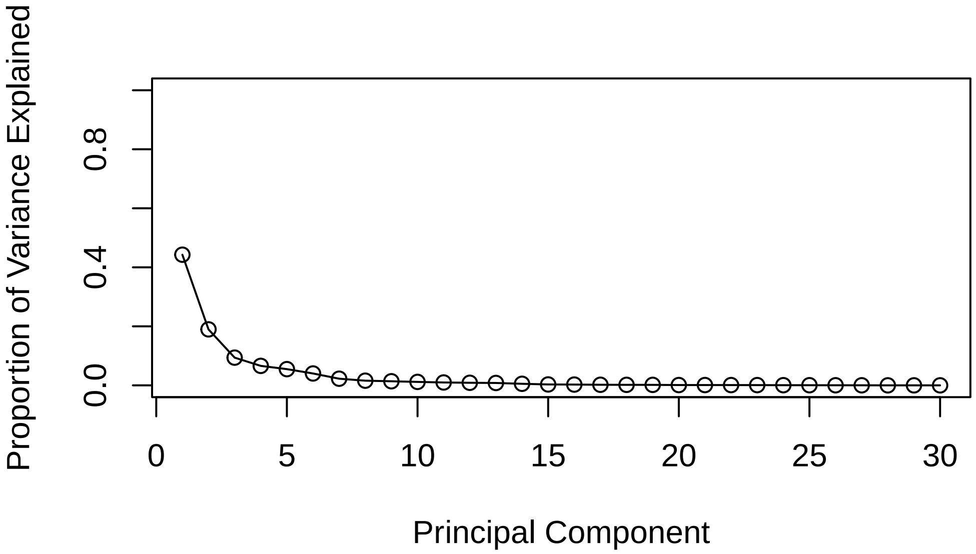
```
# Create a data.frame for ggplot
df <- as.data.frame(wisc.pr$x)
df$diagnosis <- diagnosis

# Load the ggplot2 package
library(ggplot2)

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



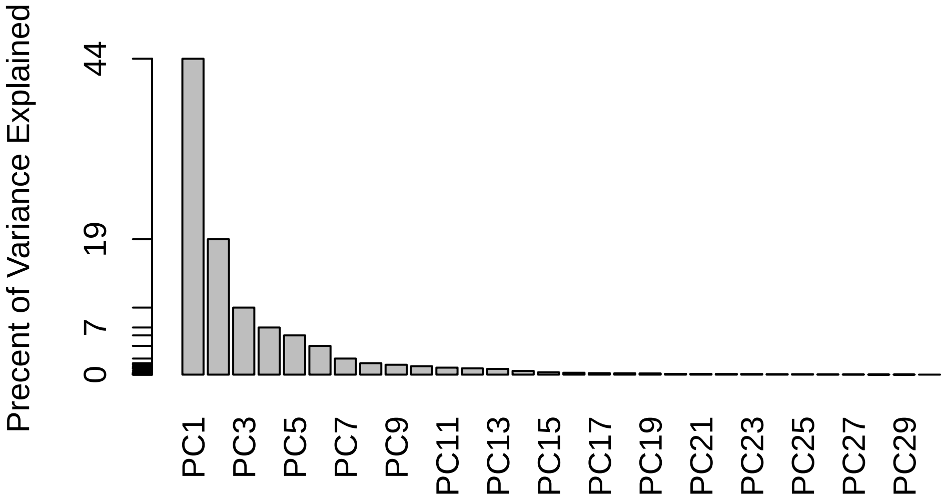
```
pr.var <- wisc.pr$sdev^2
head(pr.var)
```

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

```
pve <- pr.var/sum(pr.var)
plot(pve, xlab = "Principal Component",
     ylab = "Proportion of Variance Explained",
     ylim = c(0, 1), type = "o")
```



```
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 )
```

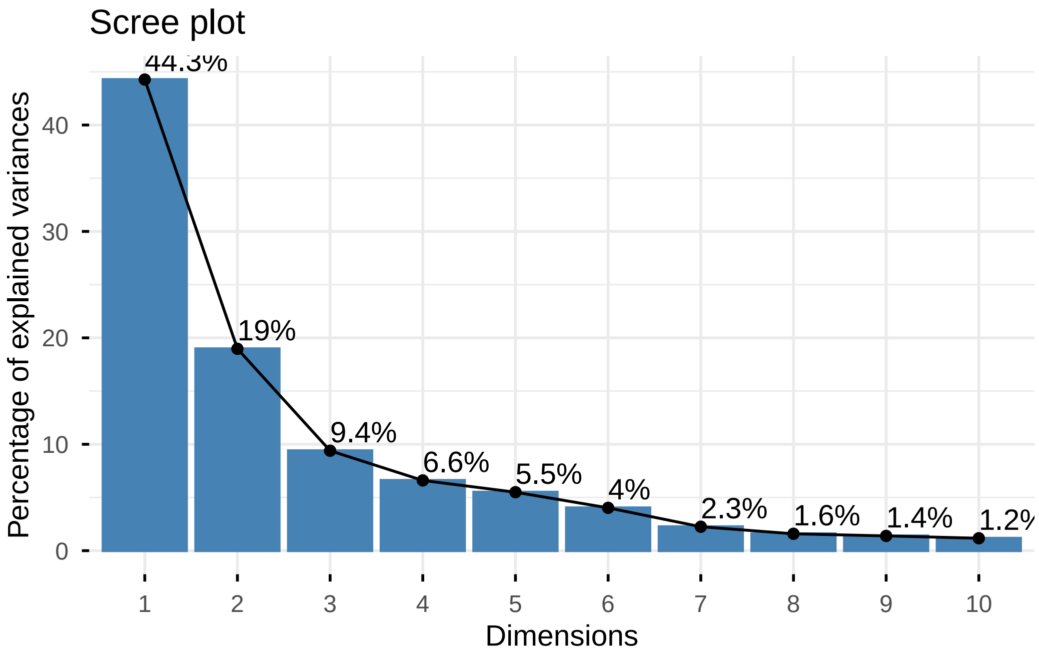


```
#Optional CRAN package:

library(factoextra)
```

```
Welcome! Want to learn more? See two factoextra-related books at https://goo.gl/ve3WBa
```

```
fviz_eig(wisc.pr, addlabels = TRUE)
```

```
Warning in geom_bar(stat = "identity", fill = barfill, color = barcolor, :
Ignoring empty aesthetic: `width`.
```



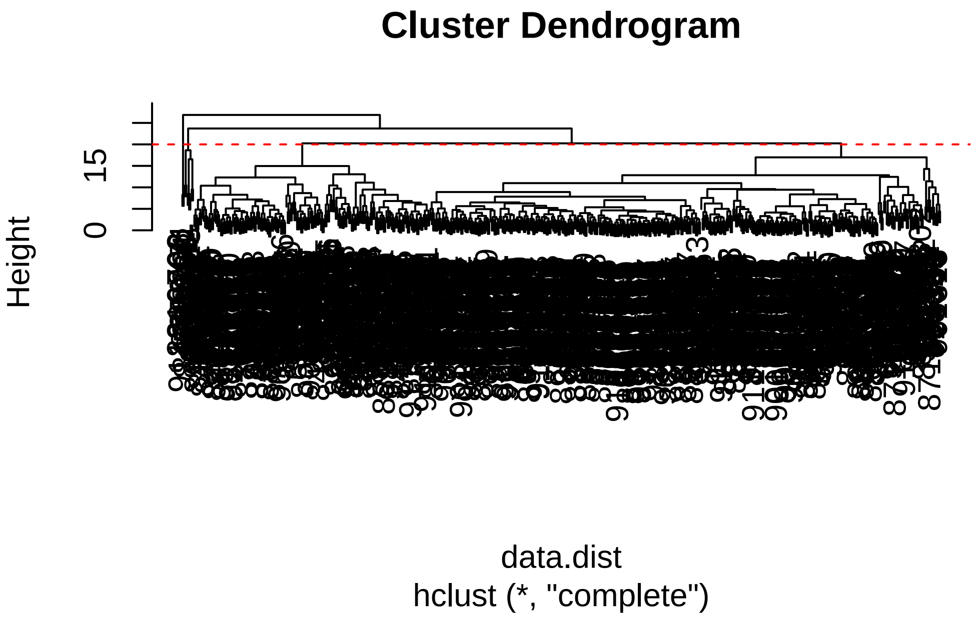
Q9. -0.2608538. High concave point usually points to low PC1 value.

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

```
[1] -0.2608538
```

Hierarchical Clustering

```
data.scaled <- scale(wisc.data)
data.dist <- dist(data.scaled)
wisc.hclust <- hclust(data.dist)
plot(wisc.hclust)
abline(h = 20, col = "red", lty = 2)
```



Q10. h=20

```
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
```

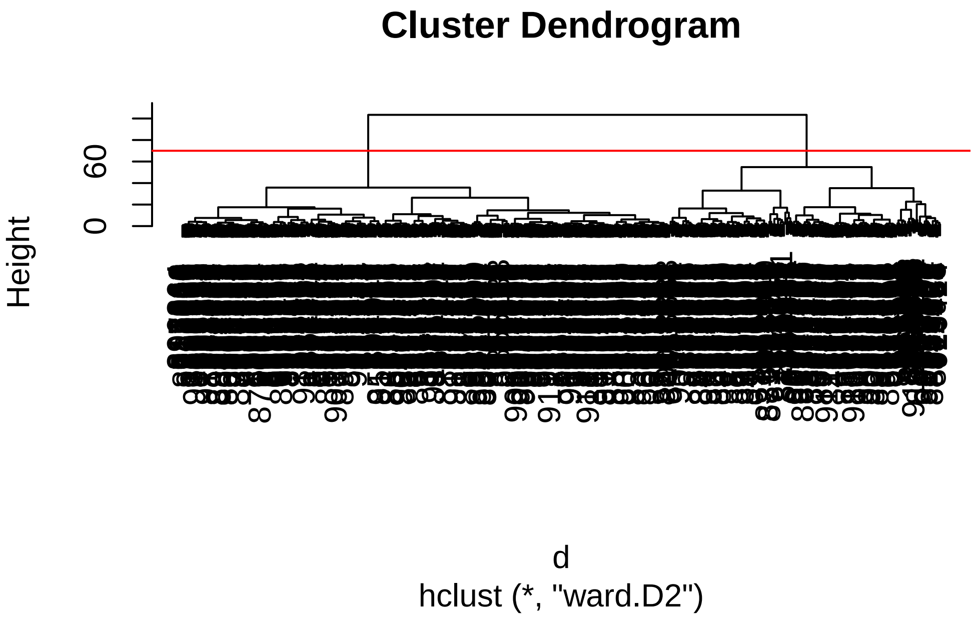
```
for(i in 2:10){
  wisc.hclust.clusters.i <- cutree(wisc.hclust, k = (i))
  print(table(wisc.hclust.clusters.i, diagnosis))
}
```

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

Q11. Either 4 or 5 clusters seem to provide the best separation.

Q12. No method stands out as my favorite as the plot all appears messy with large data set. Results wise, ward.D2 seems to perform slightly better than other methods. TP=179 FP=24

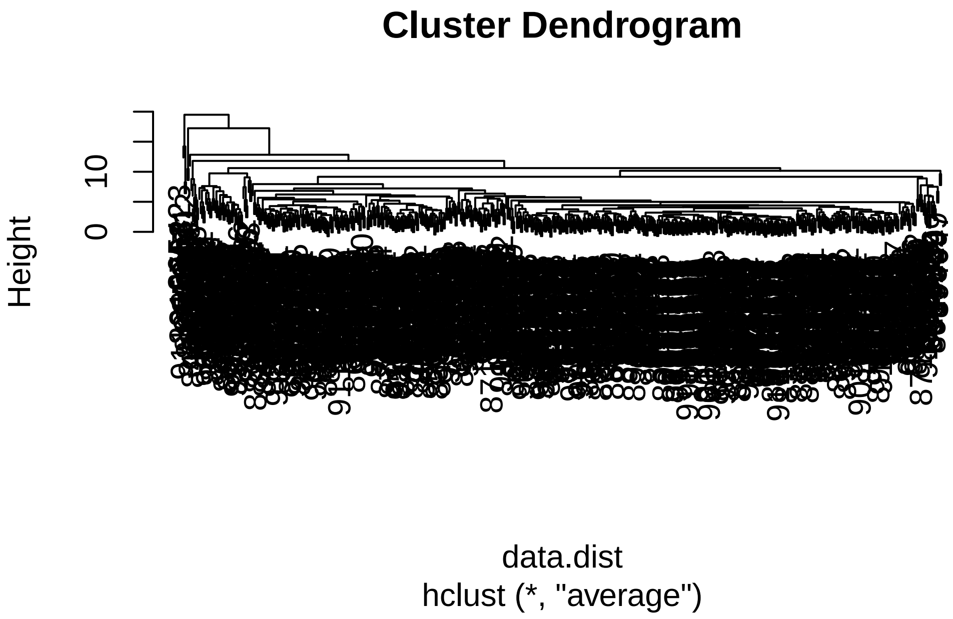
```
d <- dist(wisc.pr$x[,1:3]) #Finding distance between the first 3 columns of the PCA result.
wisc.pr.hclust <- hclust(d, method="ward.D2")
plot(wisc.pr.hclust)
abline(h=70, col="red")
```



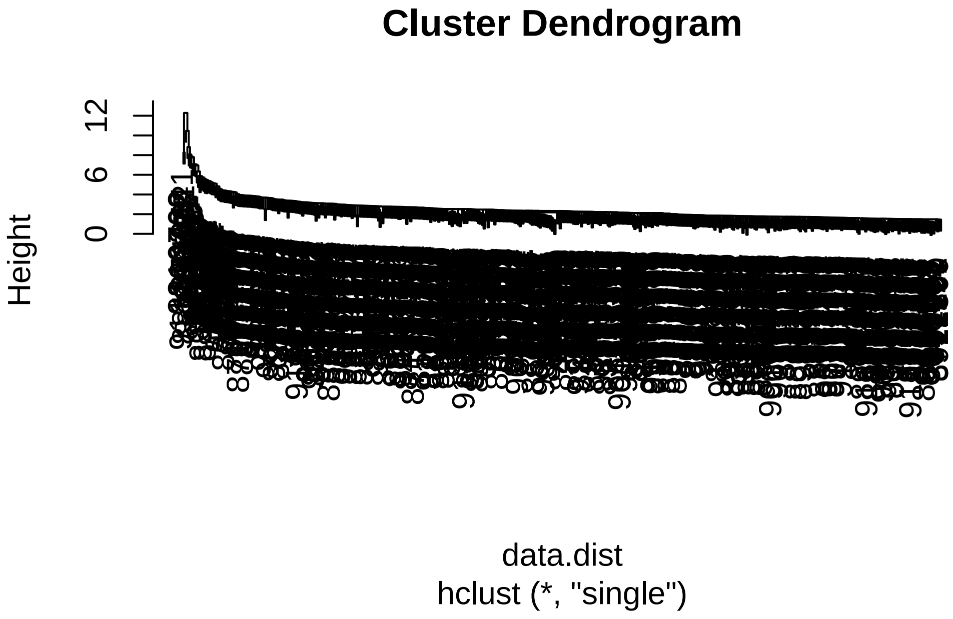
```r
grps <- cutree(wisc.pr.hclust, k=2)
table(grps, diagnosis)
```

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

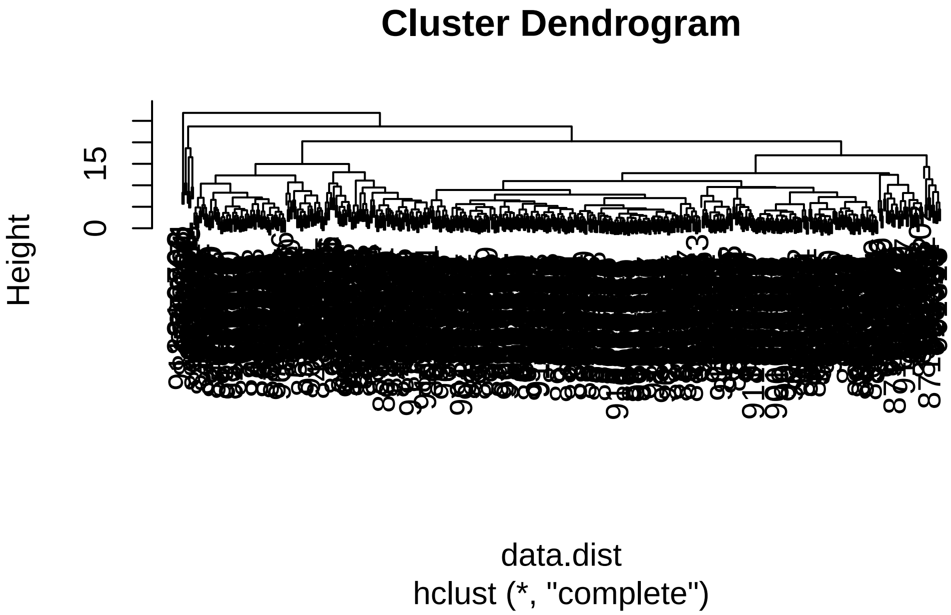
```r
wisc.hclust.average <- hclust(data.dist,method="average")
plot(wisc.hclust.average)
```



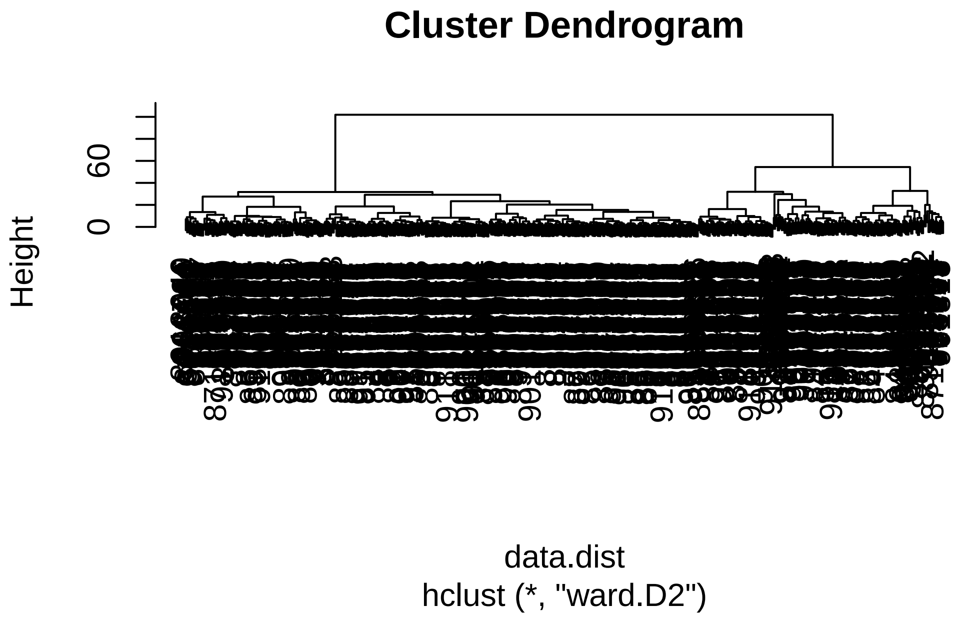
```
wisc.hclust.single <- hclust(data.dist,method="single")
plot(wisc.hclust.single)
```



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



```
wisc.pr.hclust <- hclust(data.dist,method="ward.D2")
plot(wisc.pr.hclust)
```



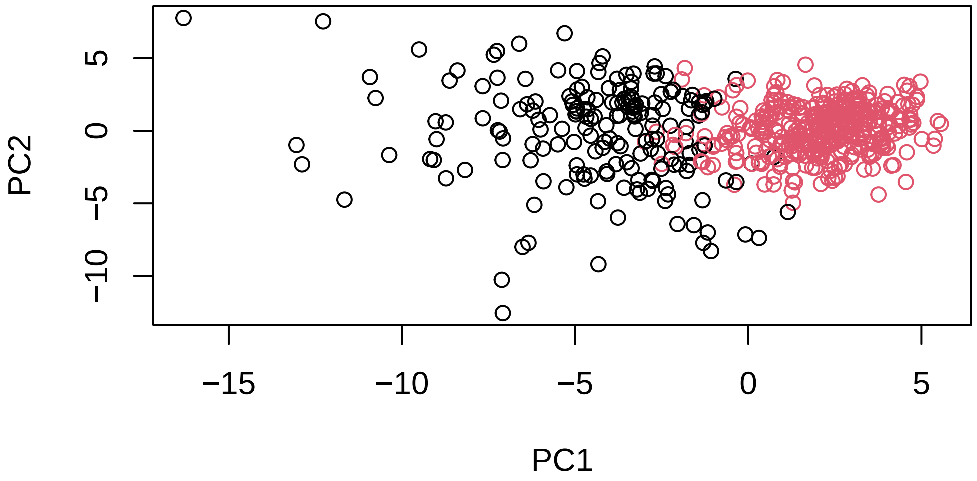
```
grps <- cutree(wisc.pr.hclust, k=2)
table(grps)
```

```
grps
  1   2 
184 385 
```

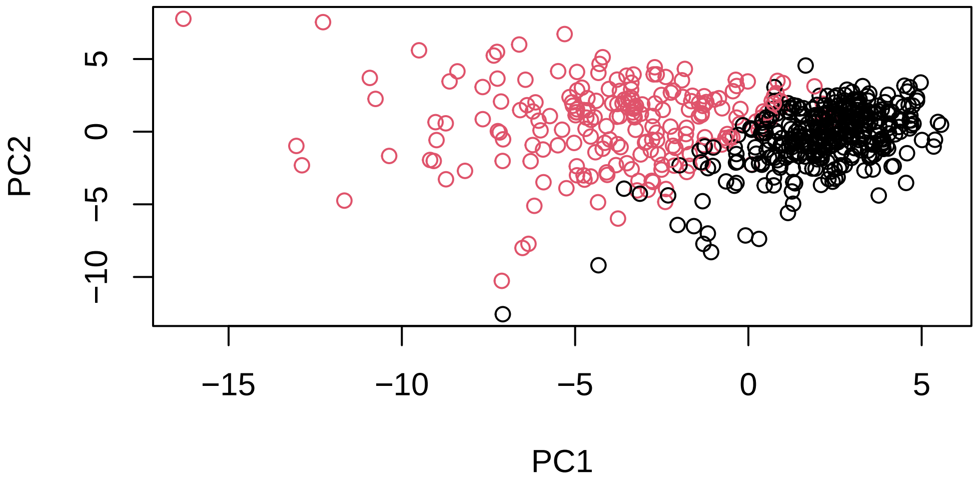
```
table(grps, diagnosis)
```

```
    diagnosis
grps   B   M
   1  20 164
   2 337  48
```

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



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



Q13. This method doesn't work well with four clusters.

```
d <- dist(wisc.pr$x[, 1:7], method = "euclidean")
wisc.pr.hclust <- hclust(d, method="ward.D2")
wisc.pr.hclust.clusters.2 <- cutree(wisc.pr.hclust, k=2)
table(wisc.pr.hclust.clusters.2, diagnosis)
```

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

```
wisc.pr.hclust <- hclust(d, method="ward.D2")
wisc.pr.hclust.clusters.4 <- cutree(wisc.pr.hclust, k=4)
table(wisc.pr.hclust.clusters.4, diagnosis)
```

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

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

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

```
table(wisc.pr.hclust.clusters.2, diagnosis)
```

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

```r
table(wisc.pr.hclust.clusters.4, diagnosis)
```

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

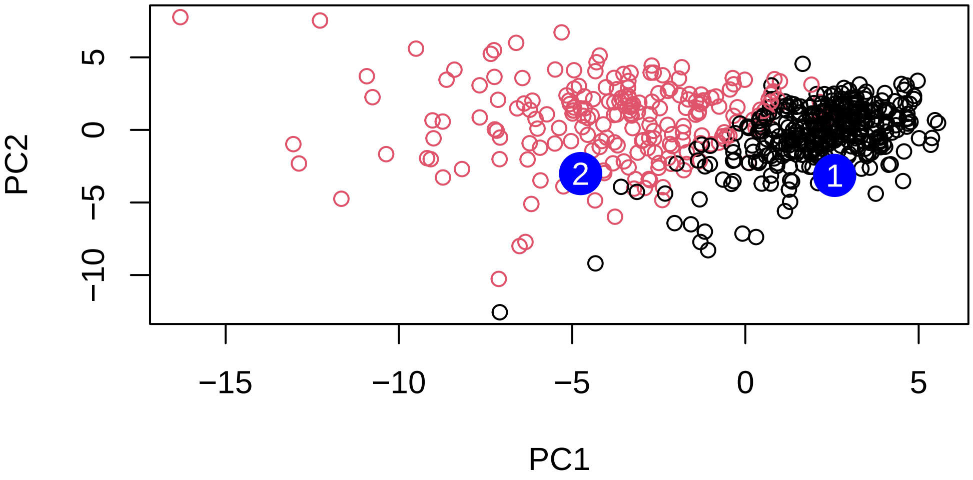
Q14. I think the hierchial cluster performed with ward.D2 method and 2 clusters is the best, as it identifies most of the malignant tumors correctly while keeping a low number of benign tumors misclassified.

Prediction

```r
#url <- "new_samples.csv"
url <- "https://tinyurl.com/new-samples-CSV"
new <- read.csv(url)
npc <- predict(wisc.pr, newdata=new)
npc
```

```
           PC1       PC2        PC3        PC4       PC5        PC6        PC7
[1,]  2.576616 -3.135913  1.3990492 -0.7631950  2.781648 -0.8150185 -0.3959098
[2,] -4.754928 -3.009033 -0.1660946 -0.6052952 -1.140698 -1.2189945  0.8193031
            PC8       PC9       PC10      PC11      PC12      PC13     PC14
[1,] -0.2307350 0.1029569 -0.9272861 0.3411457  0.375921 0.1610764 1.187882
[2,] -0.3307423 0.5281896 -0.4855301 0.7173233 -1.185917 0.5893856 0.303029
          PC15       PC16        PC17        PC18        PC19       PC20
[1,] 0.3216974 -0.1743616 -0.07875393 -0.11207028 -0.08802955 -0.2495216
[2,] 0.1299153  0.1448061 -0.40509706  0.06565549  0.25591230 -0.4289500
           PC21       PC22       PC23       PC24        PC25         PC26
[1,]  0.1228233 0.09358453 0.08347651  0.1223396  0.02124121  0.078884581
[2,] -0.1224776 0.01732146 0.06316631 -0.2338618 -0.20755948 -0.009833238
             PC27        PC28         PC29         PC30
[1,]  0.220199544 -0.02946023 -0.015620933  0.005269029
[2,] -0.001134152  0.09638361  0.002795349 -0.019015820
```

```
plot(wisc.pr$x[,1:2], col = diagnosis ,
     xlab = "PC1", ylab = "PC2")
points(npc[,1], npc[,2], col="blue", pch=16, cex=3)
text(npc[,1], npc[,2], c(1,2), col="white")
```



Q16. Patient 2 might need a prioritized check-up as it is clustered with malignant tumors, indicating the possibility of a malignant tumor for this patient.