Class 8 Breast Cancer Analysis Mini Project

Peyton Chiu (PID:A18145937)

Table of contents

Background

The goal of this mini-project is to explore a complete analysis using the unsupervised learning techniques covered in class.

The data itself comes from the Wisconsin Breast Cancer Diagnostic Data Set first reported by K. P. Benne and O. L. Mangasarian: “Robust Linear Programming Discrimination of Two Linearly Inseparable Sets”.

Values in this data set describe characteristics of the cell nuclei present in digitized images of a fine needle aspiration (FNA) of a breast mass.

Data import

Data was downloaded from the class website as a CSV file

```r
wisc.df <- read.csv("WisconsinCancer.csv", 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
```

The first column "diagnosis" is the expert opinion on the sample (i.e. FNA)

```
wisc.df$diagnosis
```

```
  [1] "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M"
 [19] "M" "B" "B" "B" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M"
 [37] "M" "B" "M" "M" "M" "M" "M" "M" "M" "M" "B" "M" "B" "B" "B" "B" "B" "M"
 [55] "M" "B" "M" "M" "B" "B" "B" "B" "M" "B" "M" "M" "B" "B" "B" "B" "M" "B"
 [73] "M" "M" "B" "M" "B" "M" "M" "B" "B" "B" "M" "M" "B" "M" "M" "M" "B" "B"
 [91] "B" "M" "B" "B" "M" "M" "B" "B" "B" "M" "M" "B" "B" "B" "B" "M" "B" "B"
[109] "M" "B" "B" "B" "B" "B" "B" "B" "B" "M" "M" "M" "B" "M" "M" "B" "B" "B"
[127] "M" "M" "B" "M" "B" "M" "M" "B" "M" "M" "B" "B" "M" "B" "B" "M" "B" "B"
[145] "B" "B" "M" "B" "B" "B" "B" "B" "B" "B" "B" "B" "M" "B" "B" "B" "B" "M"
[163] "M" "B" "M" "B" "B" "M" "M" "B" "B" "M" "M" "B" "B" "B" "B" "M" "B" "B"
[181] "M" "M" "M" "B" "M" "B" "M" "B" "B" "B" "M" "B" "B" "M" "M" "B" "M" "M"
[199] "M" "M" "B" "M" "M" "M" "B" "M" "B" "M" "B" "B" "M" "B" "M" "M" "M" "M"
[217] "B" "B" "M" "M" "B" "B" "B" "M" "B" "B" "B" "B" "B" "M" "M" "B" "B" "M"
[235] "B" "B" "M" "M" "B" "M" "B" "B" "B" "B" "M" "B" "B" "B" "B" "B" "M" "B"
[253] "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "B" "B" "B" "B"
[271] "B" "B" "M" "B" "M" "B" "B" "M" "B" "B" "M" "B" "M" "M" "B" "B" "B" "B"
[289] "B" "B" "B" "B" "B" "B" "B" "B" "B" "M" "B" "B" "M" "B" "M" "B" "B" "B"
[307] "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "M" "B" "B" "B" "M" "B" "M"
[325] "B" "B" "B" "B" "M" "M" "M" "B" "B" "B" "B" "M" "B" "M" "B" "M" "B" "B"
[343] "B" "M" "B" "B" "B" "B" "B" "B" "B" "M" "M" "M" "B" "B" "B" "B" "B" "B"
[361] "B" "B" "B" "B" "B" "M" "M" "B" "M" "M" "M" "B" "M" "M" "B" "B" "B" "B"
[379] "B" "M" "B" "B" "B" "B" "B" "M" "B" "B" "B" "M" "B" "B" "M" "M" "B" "B"
[397] "B" "B" "B" "B" "M" "B" "B" "B" "B" "B" "B" "B" "M" "B" "B" "B" "B" "B"
[415] "M" "B" "B" "M" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "M" "B"
```

```
[433] "M" "M" "B" "M" "B" "B" "B" "B" "B" "M" "B" "B" "M" "B" "M" "B" "B" "M"
[451] "B" "M" "B" "B" "B" "B" "B" "B" "B" "B" "M" "M" "B" "B" "B" "B" "B" "B"
[469] "M" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "M" "B" "B" "B" "B" "B" "B"
[487] "B" "M" "B" "M" "B" "B" "M" "B" "B" "B" "B" "B" "M" "M" "B" "M" "B" "M"
[505] "B" "B" "B" "B" "B" "M" "B" "B" "M" "B" "M" "B" "M" "M" "B" "B" "B" "M"
[523] "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "M" "B" "M" "M" "B" "B" "B"
[541] "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B"
[559] "B" "B" "B" "B" "M" "M" "M" "M" "M" "M" "B"
```

Remove the diagnosis from the data for subsequent analysis

```
wisc.data <- wisc.df[,-1]
dim(wisc.data)
```

```
[1] 569  30
```

Store the diagnosis as a vector to use later when we compare our results to those from experts in the field

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

> Q1. How many observations are in this dataset?

There are 569 observations/patients in the data set

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

```
table(wisc.df$diagnosis)
```

```

  B   M 
357 212 
```

212 of the observations have a malignant diagnosis

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

```
#colnames(wisc.data)

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

```
[1] 10
```

There are 10 variables in the data suffixed with _mean

Principal Component Analysis

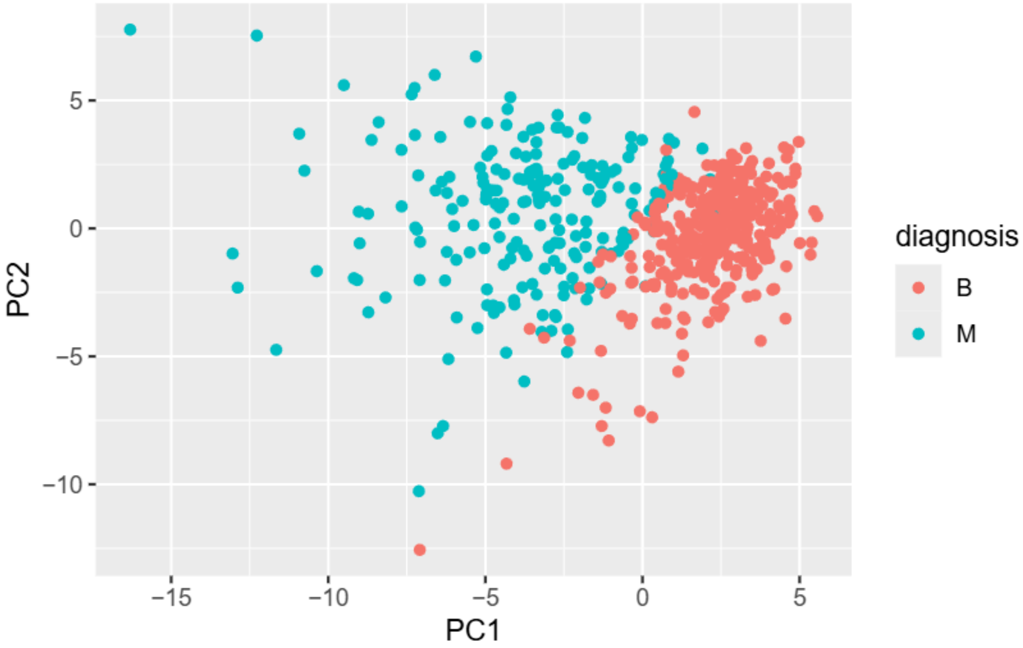
The prcomp function to do PCA has scale=False default. In general we nearly always want to set this to TRUE so our analysis is dominated by columns/variables in our dataset that have high standard deviation and mean when compared to others for instance because of differences in scale

```r
wisc.pr <- prcomp(wisc.data, 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
```

The main PC result figure is called a “score plot” or “PC plot” or “ordination plot”

```r
library(ggplot2)
ggplot(wisc.pr$x) +
  aes(PC1, PC2, col=diagnosis) +
        geom_point()
```



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

44.27% of the original variance is captured by PC1

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

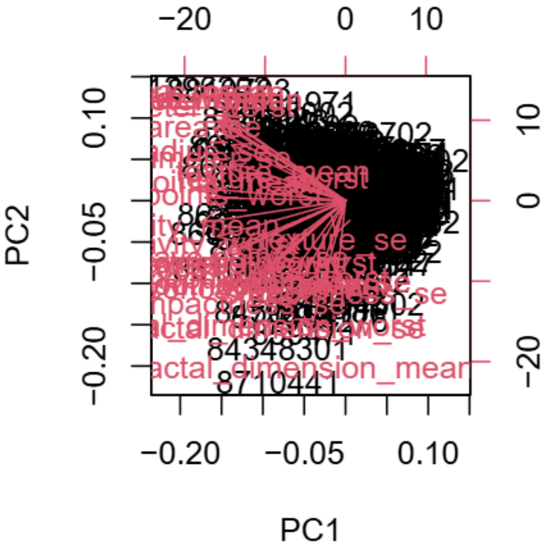
You need 3 PCs to describe at least 70% of the original variance

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

You need at least 7 PCs to describe at least 90% of the original variance

Interpreting PCA results

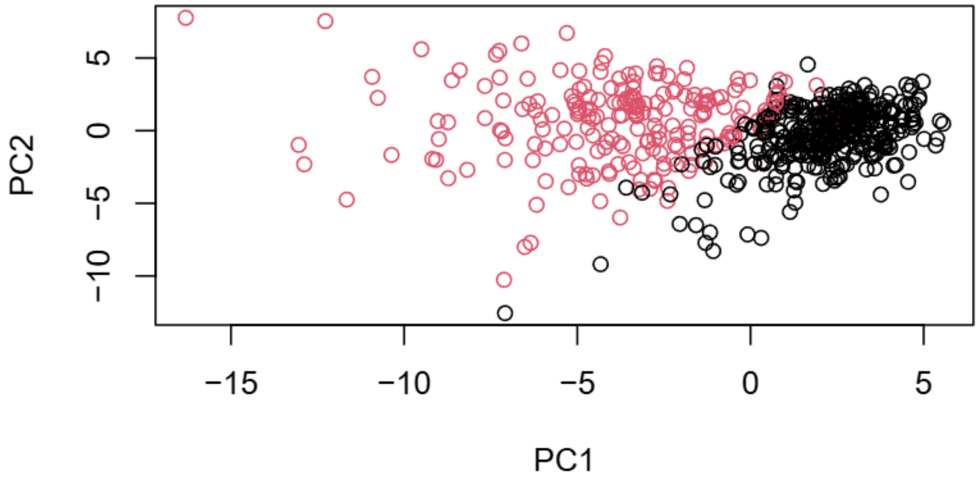
```
biplot(wisc.pr)
```



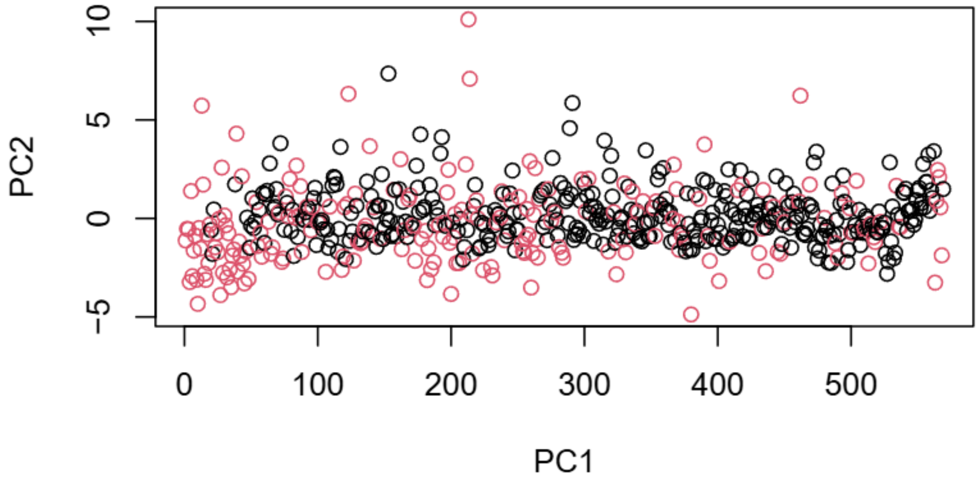
Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?

The data is all clustered together with all the text overlapping each other. The graph is hard to understand because of this.

```
plot( wisc.pr$x, col = diagnosis ,
     xlab = "PC1", ylab = "PC2")
```



```r
plot( wisc.pr$x[,3], col = diagnosis ,
     xlab = "PC1", ylab = "PC2")
```



PCA Screen -plot

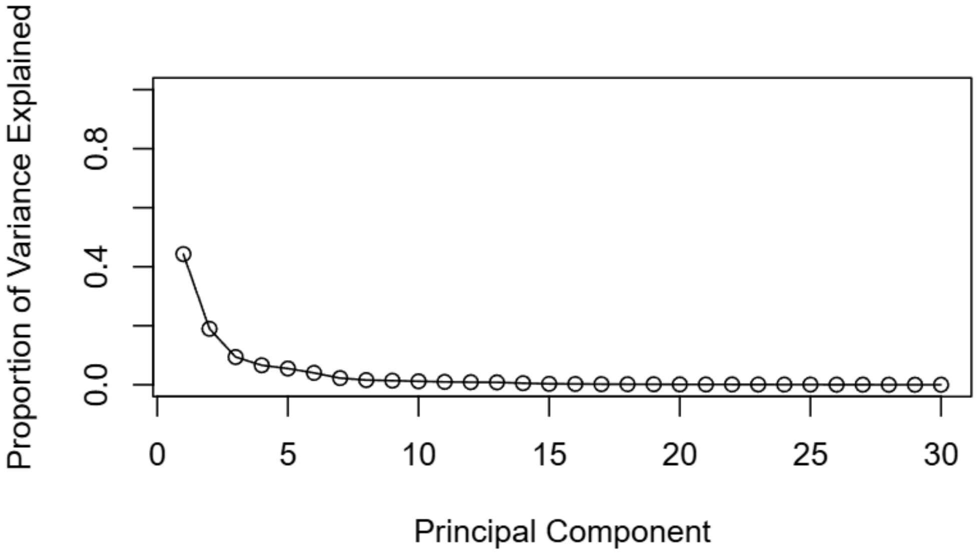
A plot of how much variance each PC captures. We can get this from `wisc.pr$sdev` or from the output of `summary(wisc.pr)`

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

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

```
pve <-  (wisc.pr$sdev^2) / sum(wisc.pr$sdev^2)

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



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", "PC1"]
```

```
[1] -0.2608538
```

The loading is -0.2608538

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

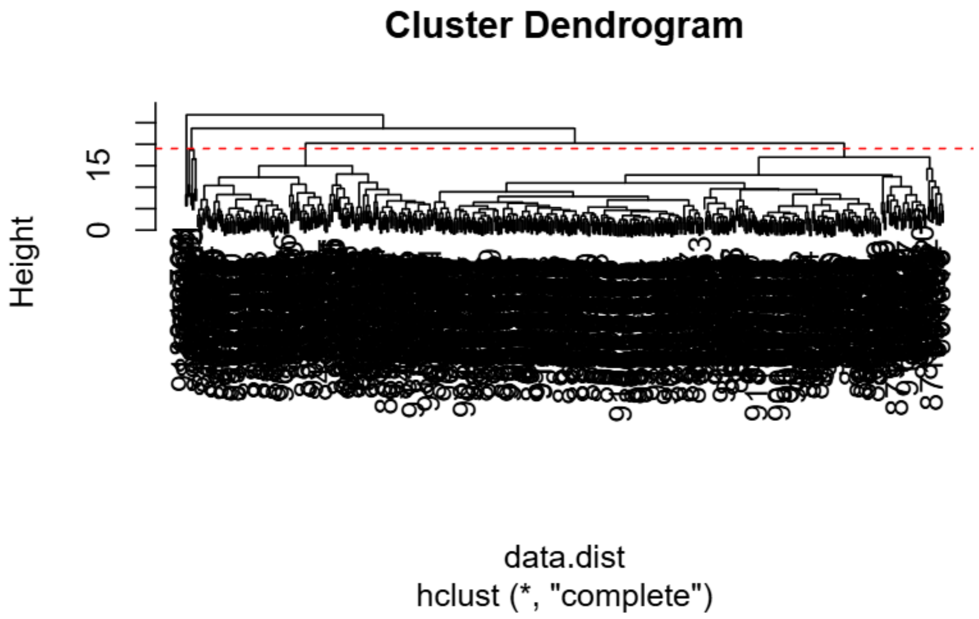
You need at least 5 PCs to explain 80% of the variance

Hierarchial Clustering

Just clustering the original data is not very informative or helpful

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

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



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

The height at which the clustering model has 4 clusters is 19

```
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?

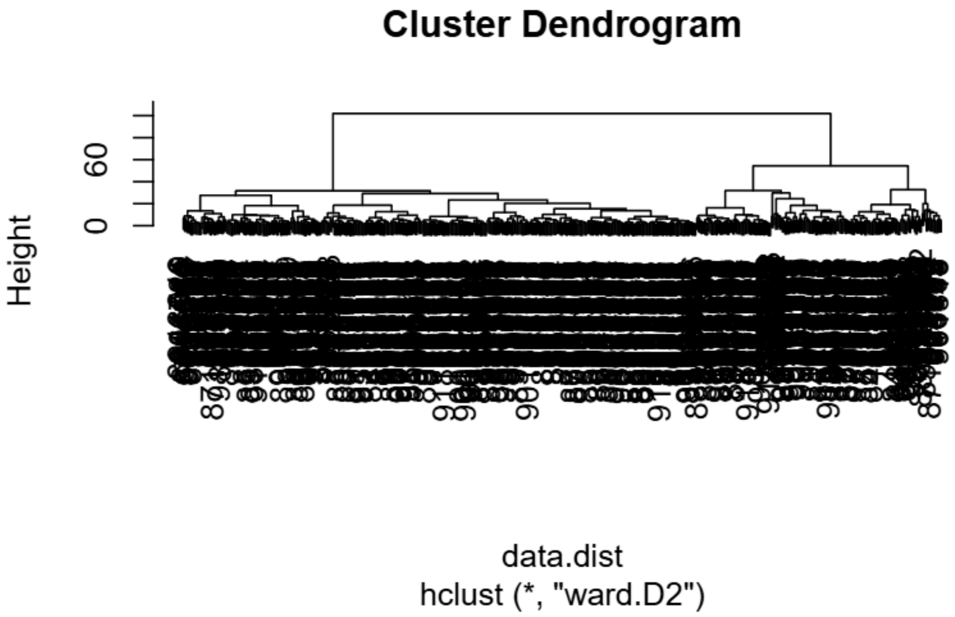
```
wisc.hclust.clusters <- (cutree(wisc.hclust, k=5))
table(wisc.hclust.clusters, diagnosis)
```

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

Yes, cutting the tree into 5 clusters results in a better match as the clusters are more pure than if there were cut into 4 clusters.

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

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



After looking through all the different methods for hclustering I feel that "ward.D2" gives my favorite results. This is because the output looked most like a tree with there being clear hierarchies that seem relatively well structured and logical compared to the other methods

Kmeans clustering

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

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

Combining Methods (Clustering and PCA)

Clustering the original data was not very effective. The PCA results looked promising. Here we combine these methods by clustering from our PCA results. In other words ‘clustering in PC space’

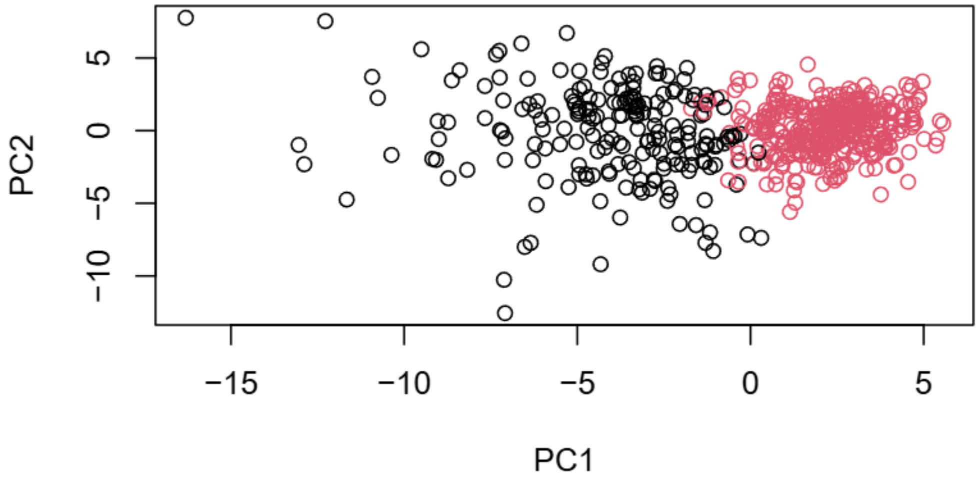
```r
dist.pc<- dist(wisc.pr$x[,1:3])
wisc.pr.hclust <-hclust(dist.pc, method = "ward.D2")
grps <- cutree(wisc.pr.hclust, k=2)
table(grps)
```

```
grps
  1   2 
203 366 
```

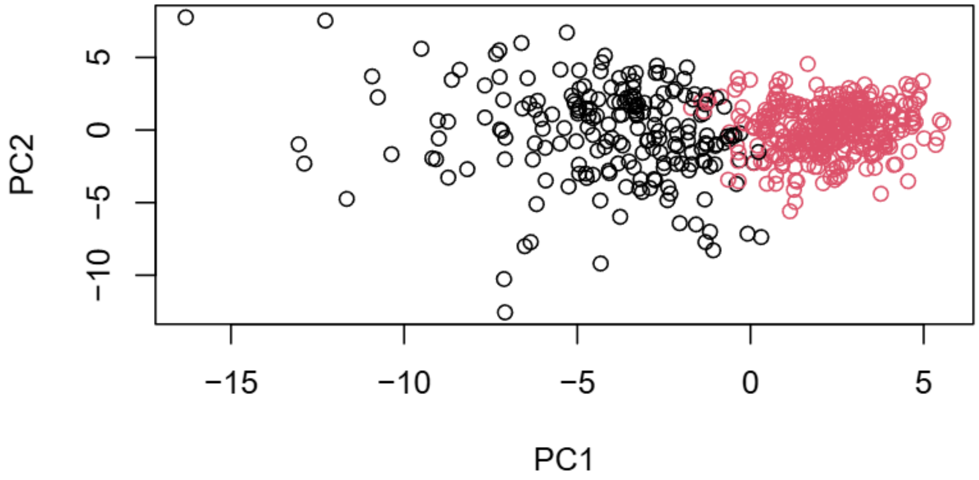
```r
table(grps, diagnosis)
```

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

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



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



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

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

The newly created model does well with most cluster containing a majority of type of cell. While clusters 1 and 2 are very pure cluster 4 and especially 3 are noticeably less. Overall the clusters for the most part contain one type of cell.

> 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.hclust.clusters, diagnosis)
```

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

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

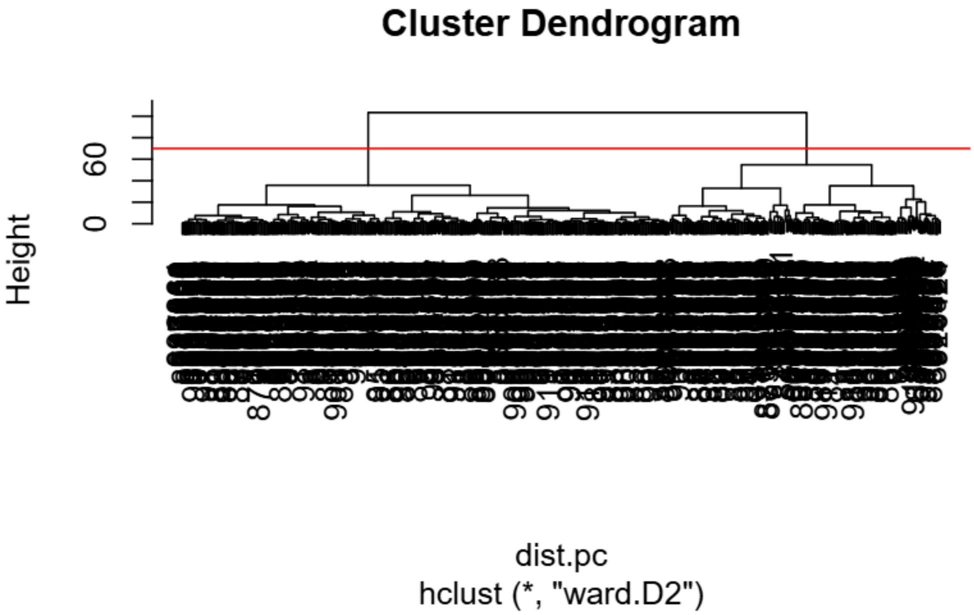
```
   diagnosis
      B   M
  1  14 175
  2 343  37
```

Looking at the k-means and hierarchical clustering models they do a decent job at separating the diagnosis.For both of them the cluster are relatively pure having one a clear majority of one type of diagnosis. While there is some mixing present as a whole both models seperate the diagnosis well.

```
## Take the first 3 PCs
dist.pc<- dist(wisc.pr$x[,1:3])
wisc.pr.hclust <-hclust(dist.pc, method = "ward.D2")
```

View the tree

```
plot(wisc.pr.hclust)
abline(h=70, col ="red")
```



To get our clustering membership vector (i.e. our main clustering results) we "cut" the tree at a desired height or to yield a desired height or to yield a desired number of "k" groups

```
grps <- cutree(wisc.pr.hclust, h=70)
table(grps)
```

```
grps
  1   2
203 366
```

How does this clustering grps compare to the expert

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

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

Sensitivity/Specificity

Sensitivity is TP/(TP+FN) Specificity is TN/(TN +FN)

```
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
```

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

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

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

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

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

For best specificity the analysis procedure that gave the best model was using the combination PCA+ Hierarchical clustering. The best procedure for specificity was the the original hclustering.

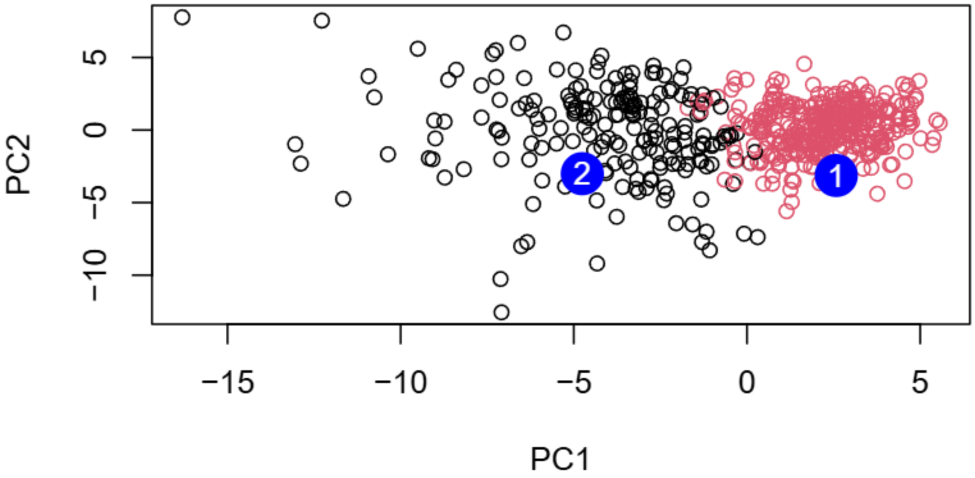
7. Prediction

We can use our PCA model for prediction with new input patient samples

```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
```

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

Based on the my results you should prioritize patient 1 for follow up as the cluster it is strongly associated with malignant cases. In contrast the cluster where patient 2 is in is not.