Unsupervised Learning Analysis of Human Breast Cancer Cells

Varun Durai

1. Exploratory Data Analysis:

```
fna.data <- "https://bioboot.github.io/bimm143_S20/class-material/WisconsinCancer.csv"
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 will need to omit the diagnosis column from our data frame and set it up as a vector for later.

```
wisc.data <- wisc.df[,-1]
diagnosis  <- wisc.df$diagnosis
```

Q1. How many observations are in this dataset?

We can use `nrow()` to find the number of rows in our data frame, which will tell us the number of observations in the data set.

```
nrow(wisc.data)
```

```
[1] 569
```

This shows us that there are `569` rows, and thus **569 observations in the data set.**

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

We can use the `grep()` function to create a new list containing the indices of the elements of `diagnosis` that have the value `"M"`. Calling the `length()` function on this new list will give us the number of observations with a malignant diagnosis.

```
Mcount <- grep("M", diagnosis)
length(Mcount)
```

```
[1] 212
```

The length of `Mcount` is 212, so **the number of observations that have a malignant diagnosis is 212**

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

```
grep("mean", colnames(wisc.data))
```

```
 [1]  1  2  3  4  5  6  7  8  9 10
```

Using the `grep()` functions on `colnames(wisc.data)` returns a list with 10 elements. Thus, the number of columns with the suffix _mean is **10**.

2. Principal Component Analysis:

```
# 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
```

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

From the output above, we can see that the proportion of the original variance captured by PC1 is **0.4427 or 44.27%**.

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

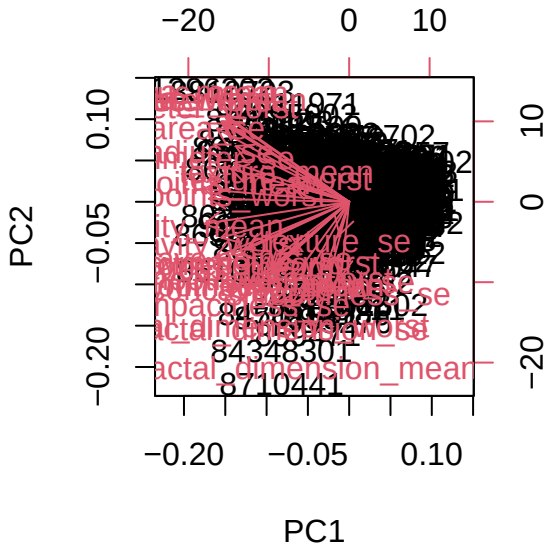
3 principal components (PC3) are required to descrive at least 70% of the original variance in the data.

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

7 principal components (PC7) are required to descrive at least 70% of the original variance in the data.

Interpreting PCA results

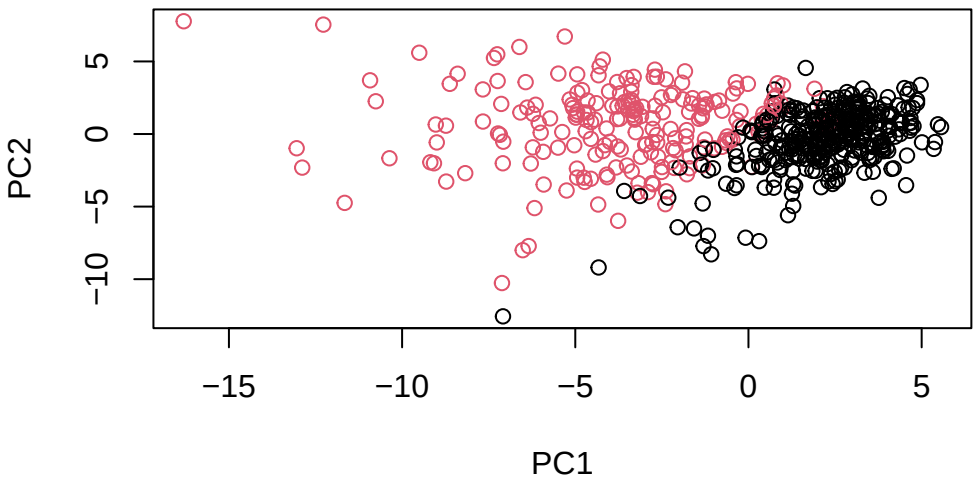
```
biplot(wisc.pr)
```



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

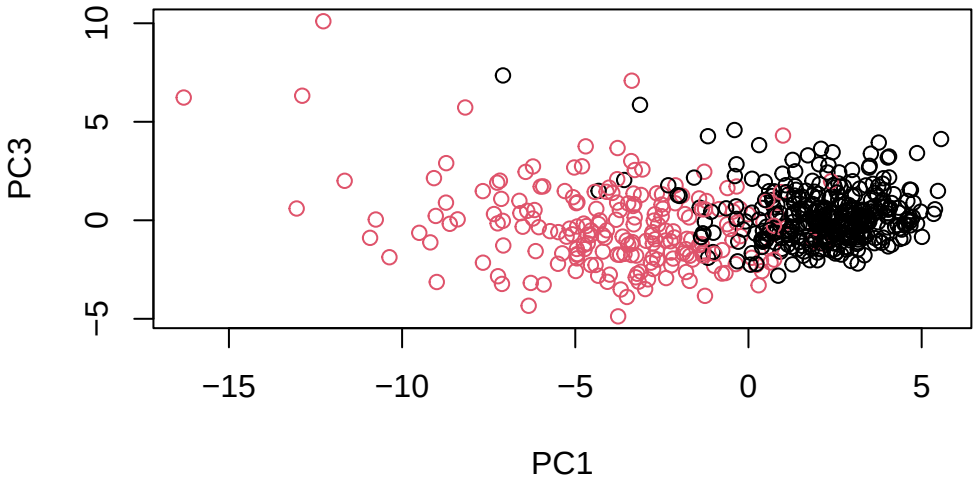
This plot is impossible to understand since it all of the information is clustered together and it does not give us a clear understanding of the data that we have produced

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



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

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

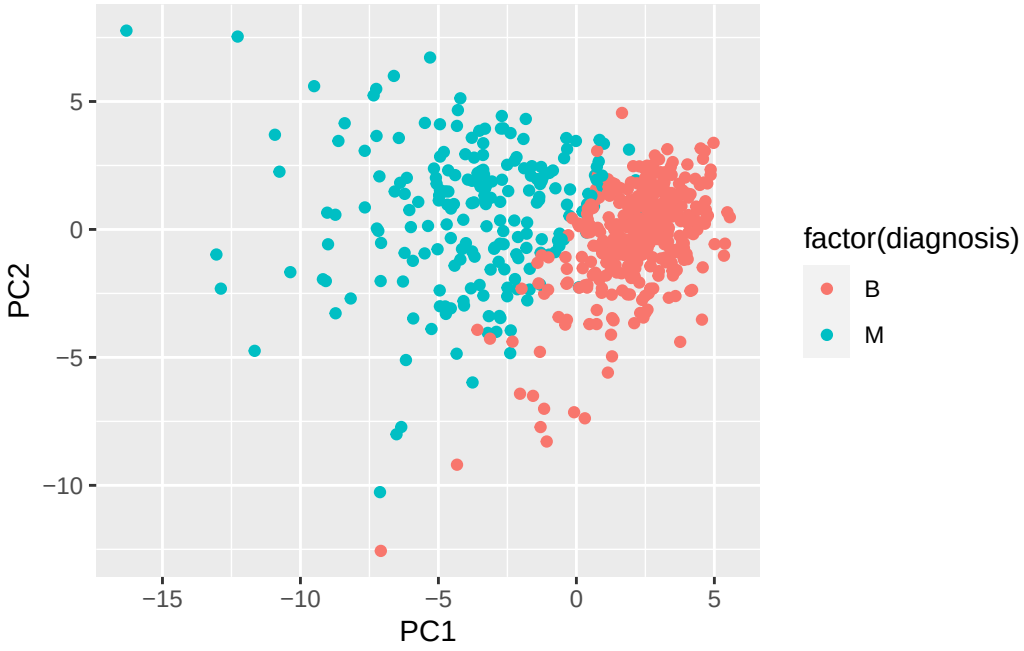


While the plots are very similar, there seems to be more overlap between the malignant and non-malignant data points in the comparison with PC3 when compared to the comparison with PC2.

```
# 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=factor(diagnosis)) +
  geom_point()
```



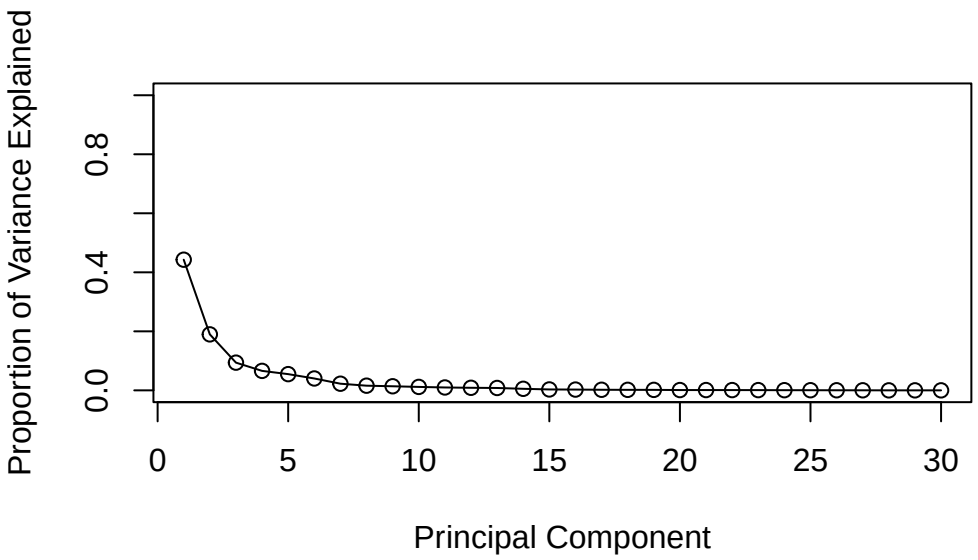
Variance Explained

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

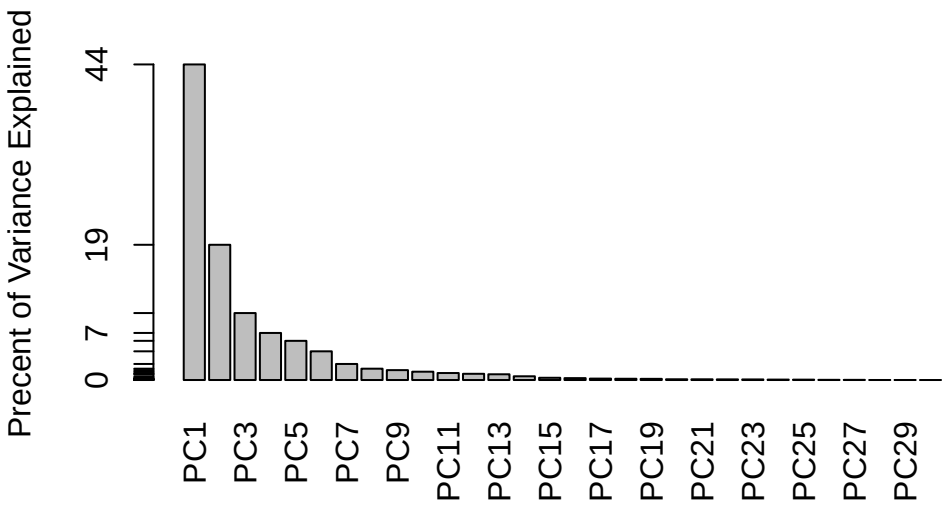
```
[1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

```
# 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 = "Precent of Variance Explained",
     names.arg=paste0("PC",1:length(pve)), las=2, axes = FALSE)
axis(2, at=pve, labels=round(pve,2)*100 )
```



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?

```
wisc.pr$rotation[8,1]
```

```
[1] -0.2608538
```

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

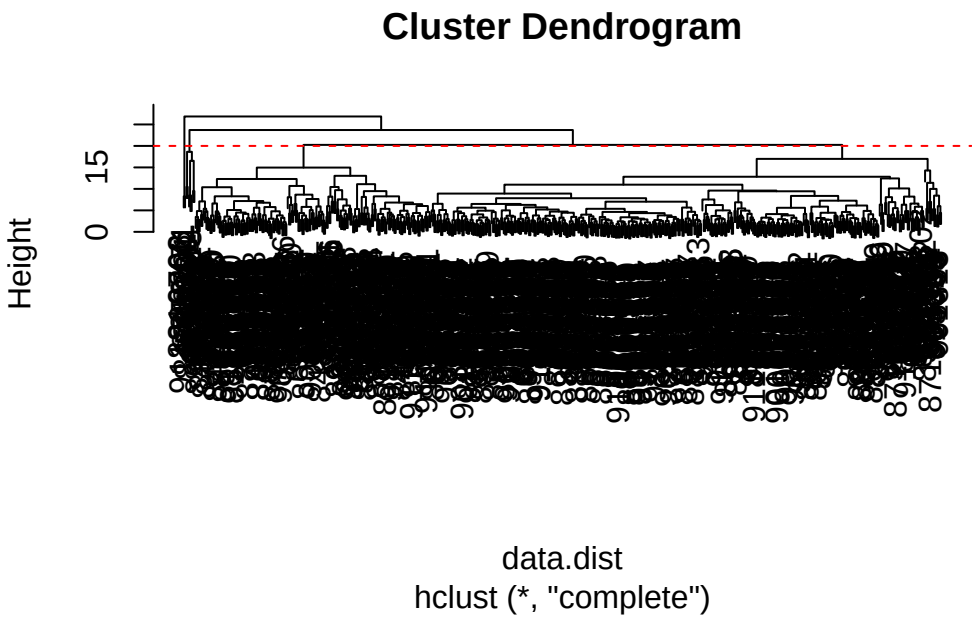
5 principal components (PC5) are required to explain 90% of the variance of the data.

3. Heirarchical clustering

```
data.scaled <- scale(wisc.data)
data.dist <- dist(data.scaled)
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?

```
plot(wisc.hclust)
abline(h = 20, col="red", lty=2)
```



The height at which the clustering model has 4 clusters is **20**.

Selecting number of clusters

```
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 = 8)
table(wisc.hclust.clusters, diagnosis)
```

```
                   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
```

While 4 clusters seems to split the diagnoses into malignant and non-malignant optimally, 8 clusters creats what seems to be another significant cluster of malignant tumors. This cluster could possibly be better.

Using different methods

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

Complete produces my favorite results since the graphical data is easily readable. It produces clusters with clear groups, so I am confident that the method is reliable.

K-means

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

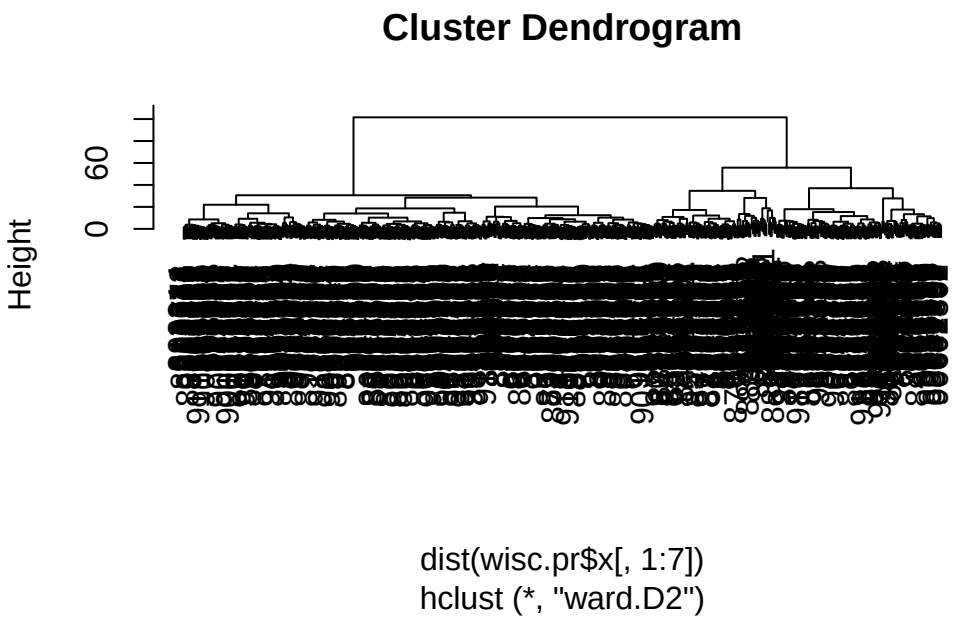
```
  diagnosis
     B   M
  1 356  82
  2   1 130
```

Q14. How well does k-means separate the two diagnoses? How does it compare to your hclust results?

Some minor overlap exists between the two clusters, which seems to be greater than the overlap present in the hclust results.

5. Combining Methods

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



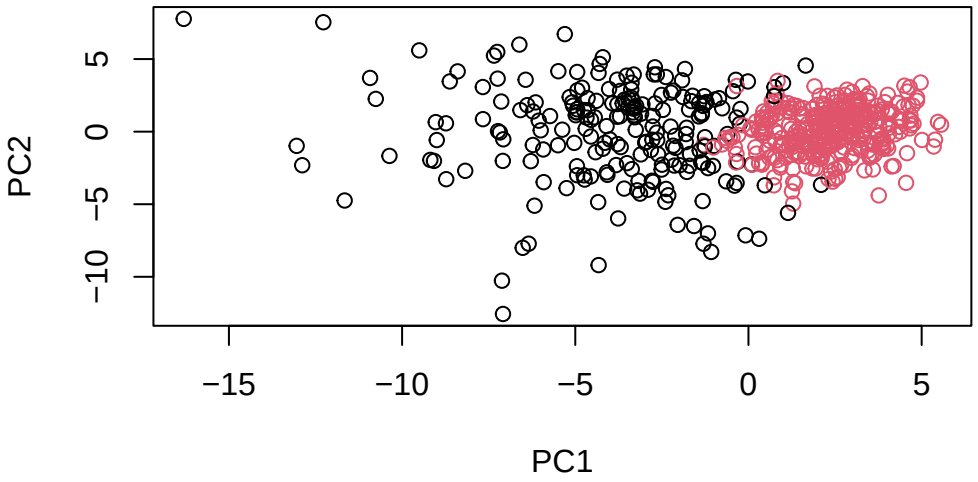

```
grps <- cutree(wisc.pr.hclust, k=2)
table(grps)
```

```
grps
  1   2
216 353
```

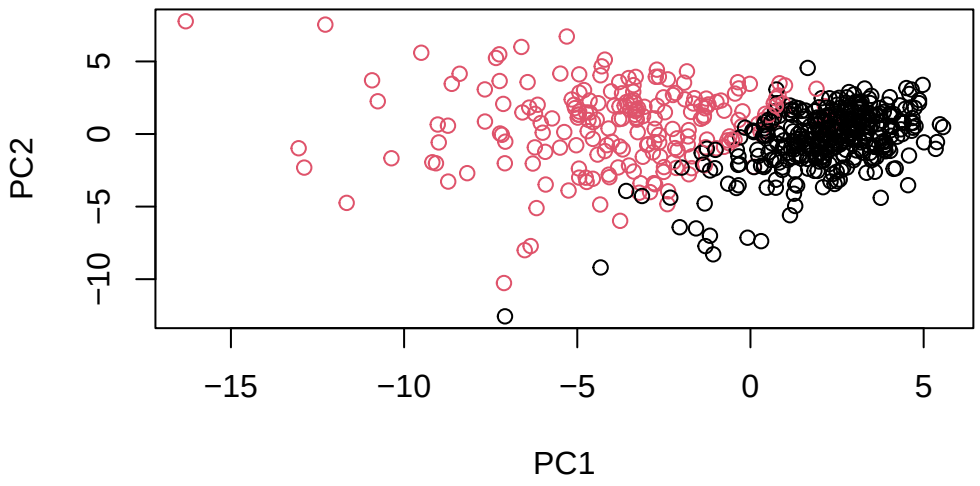
```
table(grps, diagnosis)
```

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

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




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



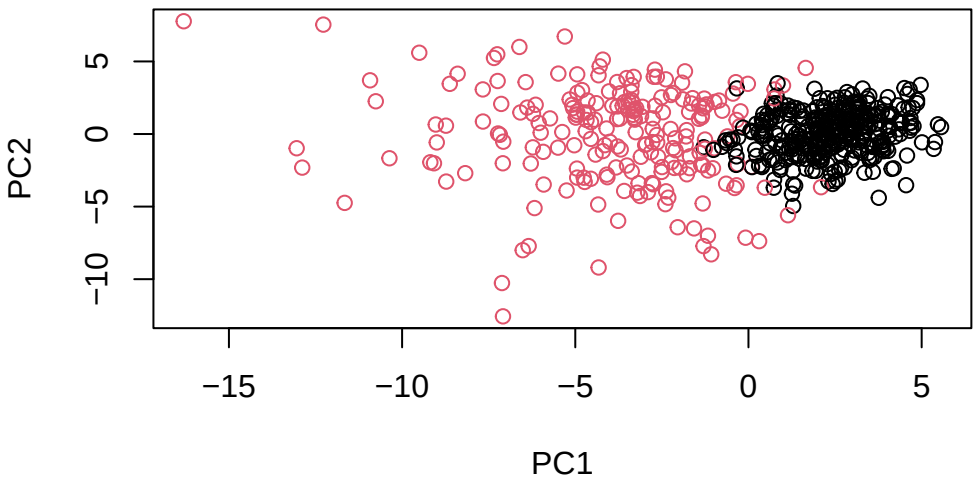

```
g <- as.factor(grps)
levels(g)
```

```
[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)
```




```
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?

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

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

The two diagnoses are seperated from each other with minor overlap between the clusters as observalbe from the table.

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.

```
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
```

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

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

The hierarchical clustering model contains lower overlap between the two diagnoses in its clusters and contains a higher number of clusters while the K-means cluster has higher overlap, but this could be a result of a lower number of clusters.

6. Sensitivity/Specificity

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

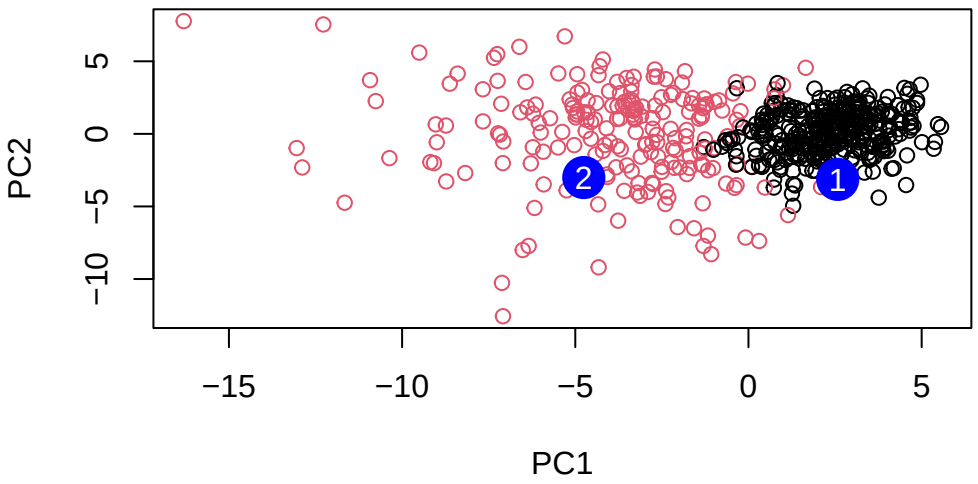
The combining models has higher sensitivity since it contains the highest number of malignant tumors in a single cluster. On the other hand, the K-means clustering model will have the highest specificity since it countains the highest number of benign tumors in a cluster.

7. 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
```

```r
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?

Based on our results, individuals in cluster 2 should be prioritized.