Class_08_lab

Tessa Sterns PID: 18482353

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##Background

The goal today is to use unsupervised learning and PCA to analize real world data. We will be using data on breast cancer collected through Fine Needle Aspiration. Using these techniques we hope to find trends in the data that pertain to how cell morphology is related to cancer prognosis.

##Data Import

```
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
```

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

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

Questions

Q1. How many observations are in this dataset?

There are `nrow(wisc.data)` observations in this data set.

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

There are `table(diagnosis)` tumors in this data set.

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

There are `length(grep("_mean", colnames(wisc.data)))` variables that have the _mean suffix.

Principal Component Analysis

We want to set 'scale = T' because it scales the pca so that those columns with high variance do not dominate.

```
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
```

```
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)?

PC1 captures 44.27% of the original variance.

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

There needs to be 3 principal componants to capture 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?

There needs to be 7 principle componants to capture 90% of the original variance.

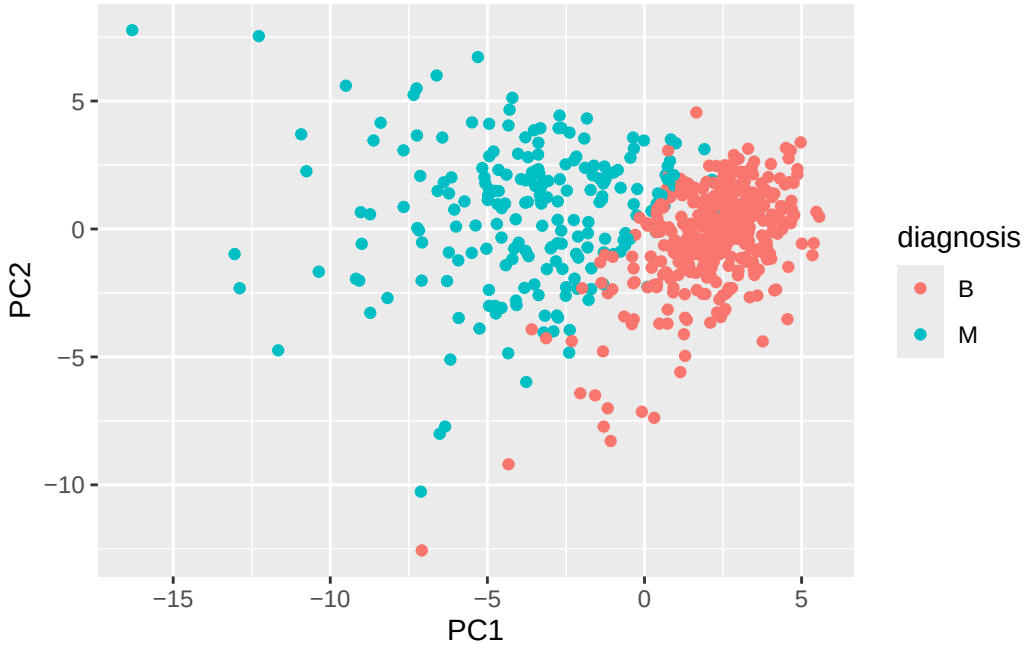
Interpeting PCA Results

The main PC figure is called a "score plot".

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

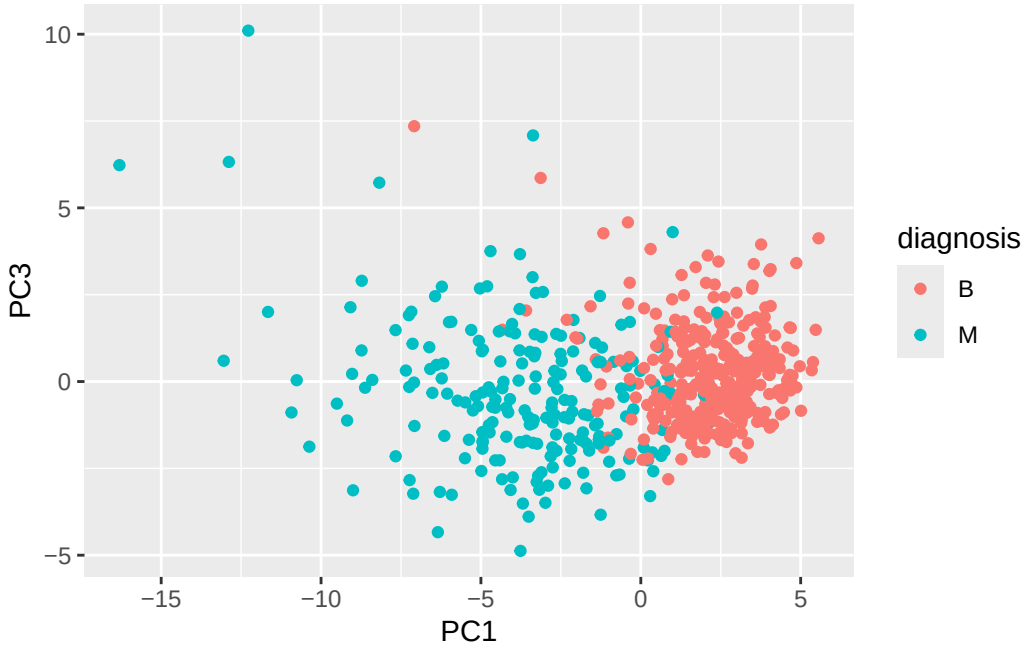
This question is in reference to a `biplot()` which we did not make in class. However looking at the sample biplot including in the lab write up the major drawback is that they are very cluttered and difficult to interpret.

```
library(ggplot2)

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



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

```
ggplot(wisc.pr$x) +
  aes(x = PC1, y = PC3, col = diagnosis) +
  geom_point()
```

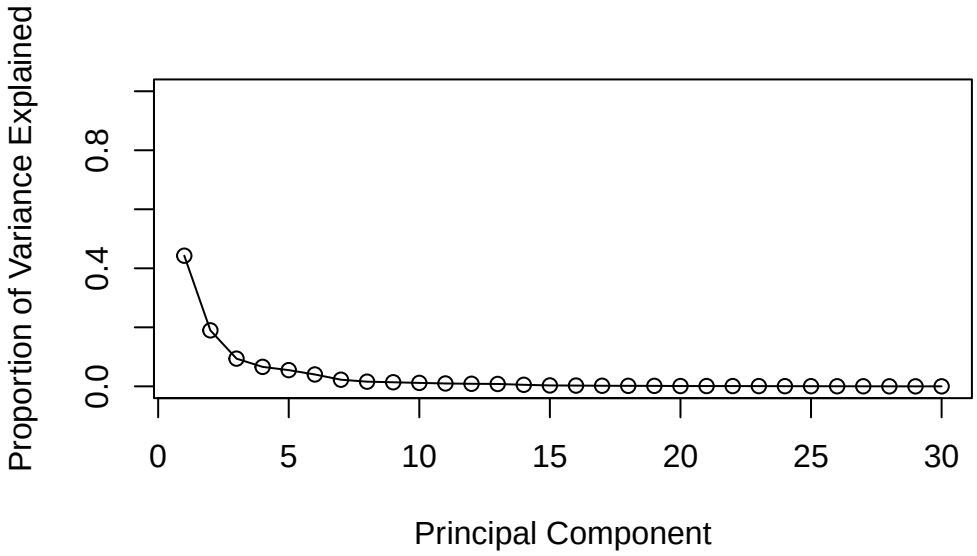


Both of these plots are very similar, the second one with PC3 mostly looks like the y-axis is shifted down. They both show that PC1 shows the most variance in the data with benign tumors apearing on the positive side of the x-axis and malignent tumors showing on the negative side of the x-axis.

```
# 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")
```



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?

The loading vector is `wisc.pr$rotation["concave.points_mean", "PC1"]`.

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

There needs to be five PC components to explain at least 80% of the variance.

```
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
```

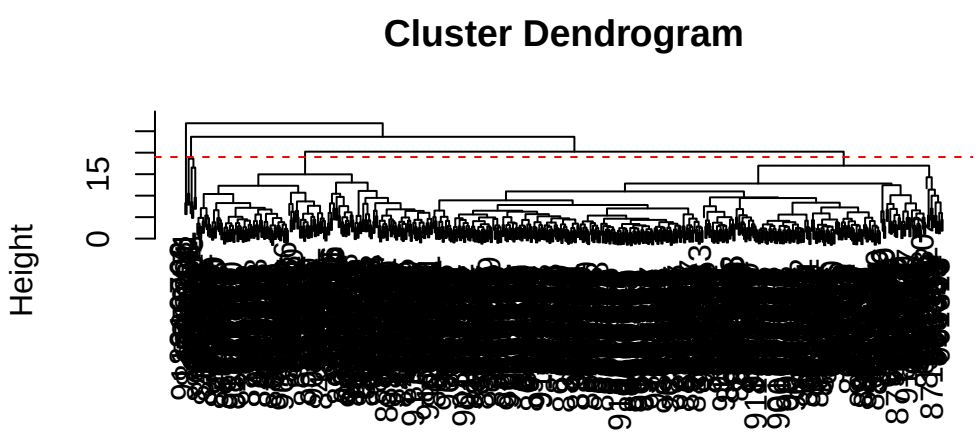
Hierarchal Clustering

```
# Scale the wisc.data data using the "scale()" function
data.scaled <- scale(wisc.data)

data.dist <- dist(data.scaled)

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

```
Call:
hclust(d = data.dist, method = "complete")

Cluster method   : complete
Distance         : euclidean
Number of objects: 569
```

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

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




```
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?

No the data is still ugly.

```
wisc.hclust.clusters2<- cutree(wisc.hclust, k=2)

table(wisc.hclust.clusters2, diagnosis)
```

```
                    diagnosis
wisc.hclust.clusters2   B   M
```

```
  1 357 210
  2   0   2
```

```
wisc.hclust.clusters10<- cutree(wisc.hclust, k=10)

table(wisc.hclust.clusters10, diagnosis)
```

```
                    diagnosis
wisc.hclust.clusters10   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
```

Using different methods

```
single.clus <- hclust(data.dist, method = "single")
single.clus.cut <- cutree(single.clus, k =2)
table(single.clus.cut, diagnosis)
```

```
              diagnosis
single.clus.cut   B   M
              1 357 210
              2   0   2
```

```
# Not a big fan as this method as it produced a single cluster that contained both benign and

av.clus <- hclust(data.dist, method = "average")
av.clus.cut <- cutree(av.clus, k = 2)
table(av.clus.cut, diagnosis)
```

```
          diagnosis
av.clus.cut   B   M
```

```
  1 357 209
  2   0   3
```

```
# This method also seemed to produce a single cluster that contained both types of tumors.

wD2.clus <- hclust(data.dist, method = "ward.D2")
wD2.clus.cut <- cutree(wD2.clus, k = 2)
table(wD2.clus.cut, diagnosis)
```

```
            diagnosis
wD2.clus.cut   B   M
           1  20 164
           2 337  48
```

```
# made two distinct groups though some false positive and negatives still occured.
```

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

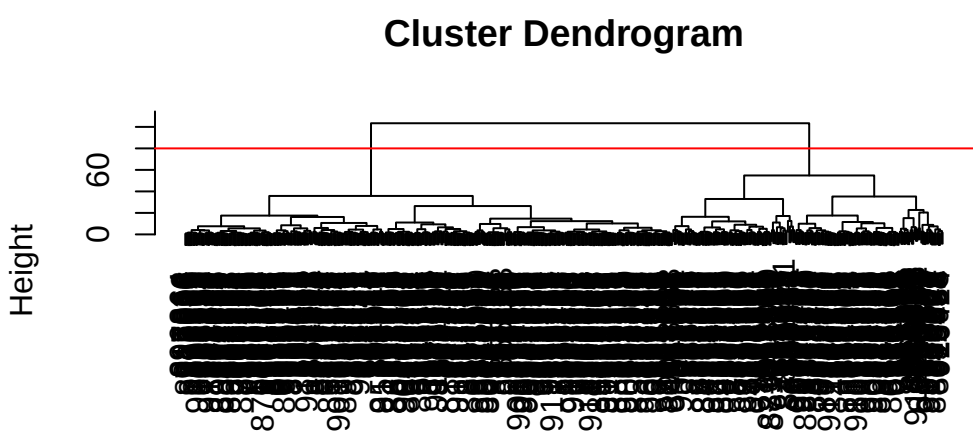
Without combing PCA with clustering I think that the ward.D2 is my favorite method. Even from a pure math standpoint I think that limiting variance within a given group is a good way to determine group membership. The other methods produced a lot of dirty data that was hard to determine biological signifigance from.

Combining methods

Since first 3 PCA's contain most of the variance we can cluster off of them.

Behold a better tree

```
dist.pc <- dist(wisc.pr$x[,1:3])

wisc.pr.hclust<- hclust(dist.pc, method = "ward.D2")

plot(wisc.pr.hclust)
abline(h = 80, col="red")
```



To arive at the clustering memborship vector we can cut the tree at a desired hight.

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

table(grps)
```

```
grps
  1   2
203 366
```

Comparing the clustering groups to expert diagnosis.

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

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

```
## Use the distance along the first 7 PCs for clustering i.e. wisc.pr$x[, 1:7]
d2 <- dist(wisc.pr$x[,1:7])
wisc.pr.hclust2 <- hclust(d2, method="ward.D2")

wisc.pr.hclust.clusters <- cutree(wisc.pr.hclust2, k=2)
```

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

Overall this method does fairly well, as good as performing clusters on PCA first. `table(wisc.pr.hclust.clusters, diagnosis)`

> 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.

```
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, diagnosis)
```

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

Using the PCA then clustering method reduced the number of false negatives we had while also increasing the number of false positives. While they both yielded fairly similar results overall using PCA had cleaner data in the end.

Sensitivity and Specificity

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

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

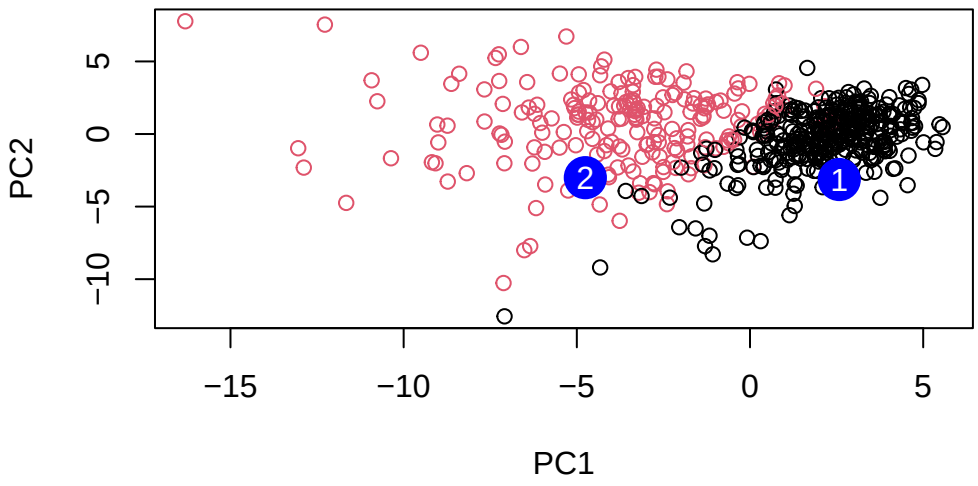
Because performing PCA before clustering resulted in fewer false negatives the PCA followed by a clustering using ward.D2 was both specific and sensitive.

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
```

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

I would prioritize patient 2, their results align with the cluster of malignent tumors whereas patient 1 is more likely benign.