Class 08 Breast Cancer Mini Project BIMM 143

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Class 08 Breast Cancer Mini Project

We are going to be using data from a study from the state of Wisconsin about Breast Cancer.

First we downloaded the data from the lab and put it into the file. We still need to extract the data from the files.

```
# Save your input data file into your Project directory
fna.data <- "WisconsinCancer.csv"

# Complete the following code to input the data and store as wisc.df
wisc.df <- read.csv(fna.data, row.names=1)
# Let's look at just the first 6 rows!
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
```

Next, we want to remove the "diagnosis" column because it will give us all of the answers. We

want to use data to answer the questions instead. So let's remove it.

```
#this code removes it
wisc.data <- wisc.df[,-1]
#we are also going to create a vector for it incase we need it for later
diagnosis <- wisc.df$diagnosis
colors <- rep("black", length(wisc.df$diagnosis))
colors[wisc.df$diagnosis == "M"] <- "red"
#let's look at the first 6 again with the new data set
head(wisc.data)
```

```
        radius_mean texture_mean perimeter_mean area_mean smoothness_mean
842302        17.99        10.38         122.80    1001.0         0.11840
842517        20.57        17.77         132.90    1326.0         0.08474
84300903      19.69        21.25         130.00    1203.0         0.10960
84348301      11.42        20.38          77.58     386.1         0.14250
84358402      20.29        14.34         135.10    1297.0         0.10030
843786        12.45        15.70          82.57     477.1         0.12780
        compactness_mean concavity_mean concave.points_mean symmetry_mean
842302           0.27760         0.3001             0.14710        0.2419
842517           0.07864         0.0869             0.07017        0.1812
84300903         0.15990         0.1974             0.12790        0.2069
84348301         0.28390         0.2414             0.10520        0.2597
84358402         0.13280         0.1980             0.10430        0.1809
843786           0.17000         0.1578             0.08089        0.2087
        fractal_dimension_mean radius_se texture_se perimeter_se area_se
842302                 0.07871    1.0950     0.9053        8.589  153.40
842517                 0.05667    0.5435     0.7339        3.398   74.08
84300903               0.05999    0.7456     0.7869        4.585   94.03
84348301               0.09744    0.4956     1.1560        3.445   27.23
84358402               0.05883    0.7572     0.7813        5.438   94.44
843786                 0.07613    0.3345     0.8902        2.217   27.19
        smoothness_se compactness_se concavity_se concave.points_se
842302       0.006399        0.04904      0.05373           0.01587
842517       0.005225        0.01308      0.01860           0.01340
84300903     0.006150        0.04006      0.03832           0.02058
84348301     0.009110        0.07458      0.05661           0.01867
84358402     0.011490        0.02461      0.05688           0.01885
843786       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
```

```
#look at how it changed!
```

Q1. How many observations are in this dataset?

569 observations.

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

```
malignant_diagnosis <- diagnosis == "M"
sum(malignant_diagnosis)
```

```
[1] 212
```

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

10

2. Principal Component Analysis (PCA)

We are going to check the columns and the standard deviations. It's good that we already removed the wisc.df$diagnosis because those are not numbers.

```
# 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
```

Now we are going to the PCA

```
# Perform PCA on wisc.data by completing the following code
wisc.pr <- prcomp(wisc.data, scale=TRUE)
#Let's check the summary too!
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)?

44.27%

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

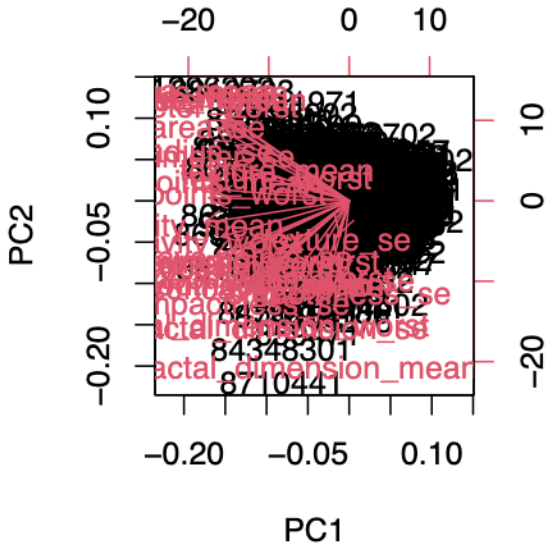
3 PCs (we reach 72.636% in PC3)

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

7 PCs (we reach 91.010% in PC7)

We are going to create a biplot using the `biplot()` function.

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

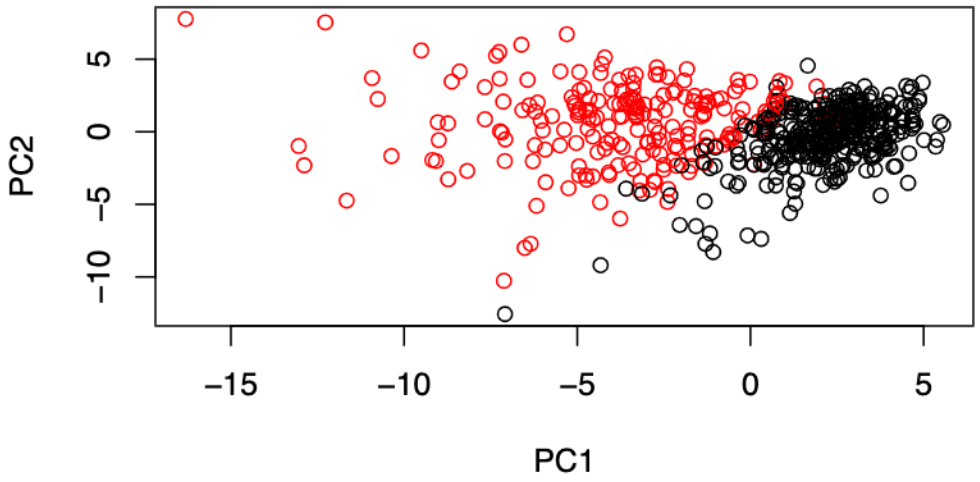


> Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?

This is terrible. It is a jumbled mess of labels and plot points. We need to just to PC1 and PC2 in order to condense the data!

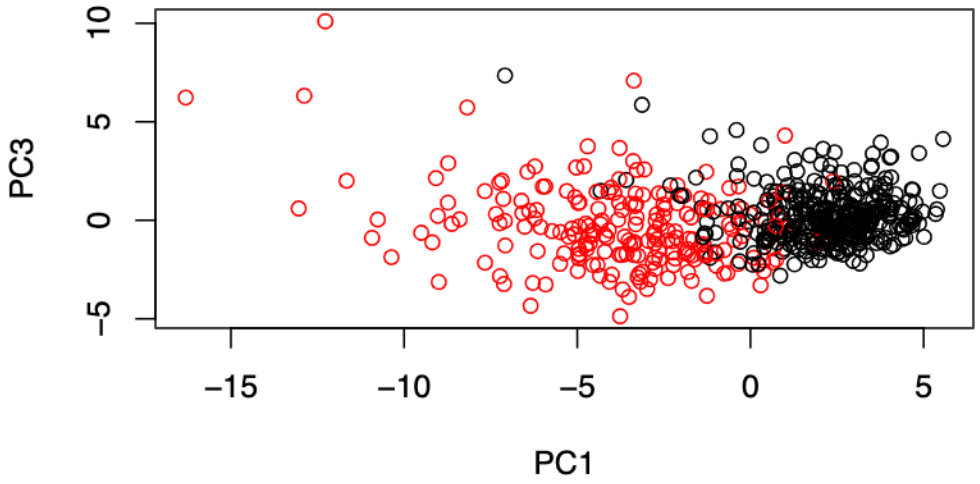
We are going to fix this by only using PC1 and PC2.

```
# Scatter plot observations by components 1 and 2
plot(wisc.pr$x, col=colors, xlab = "PC1", ylab = "PC2")
```



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

```
# Repeat for components 1 and 3
plot(wisc.pr$x[,c(1,3)], col = colors,
     xlab = "PC1", ylab = "PC3")
```



I noticed that the plots are similar but the fist plot is a lot cleaner. But both the plots are capturing a separation in the data between the benign (black) and malignant (red).

Now we are going to visulize using `ggplot()`!

```
# 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()
```

Next we are going to calculate the variance!

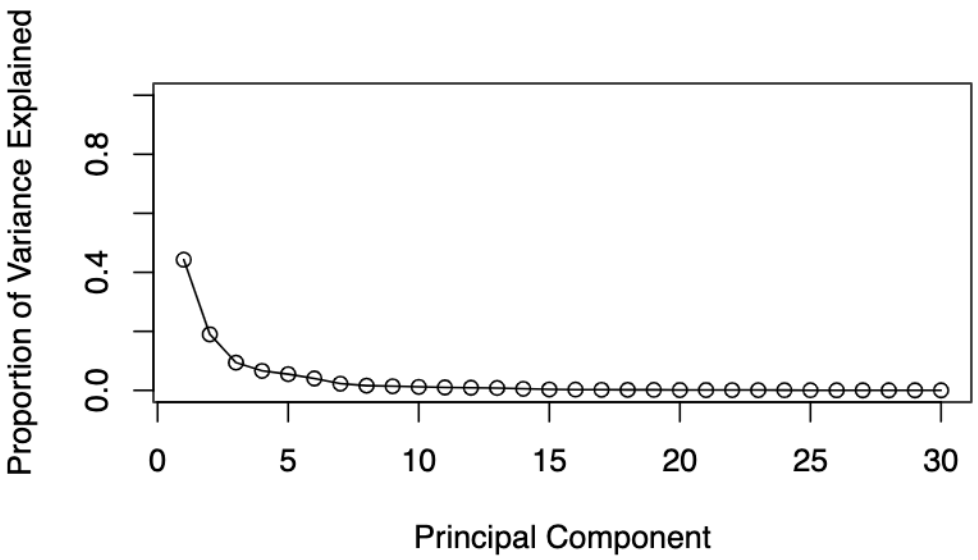
```
# Calculate variance of each component
pr.var <- wisc.pr$sdev^2
head(pr.var)
```

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

Next we are going to calculate the variance explained by each principal component. Then we are going to plot it!

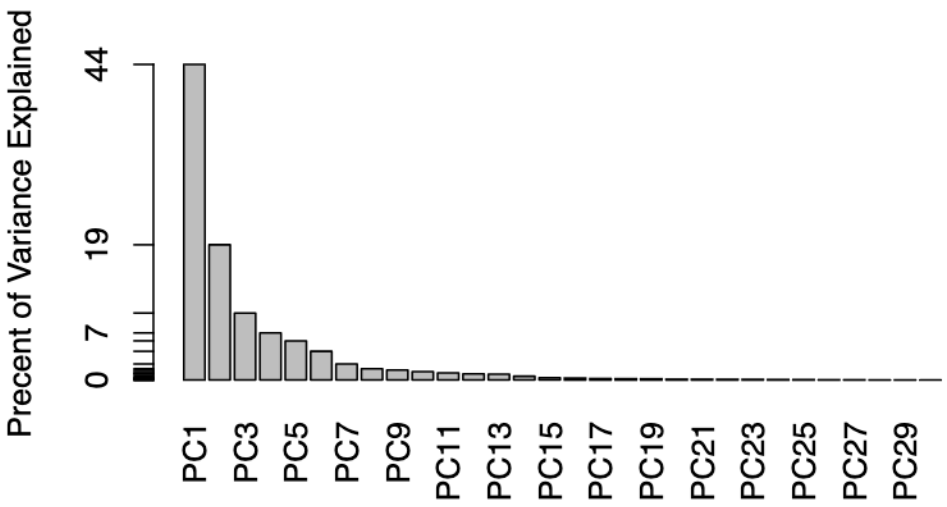
```
# Variance explained by each principal component: pve
pve <- pr.var / sum(pr.var)

# Plot variance explained for each principal component
plot(pve, xlab = "Principal Component",
     ylab = "Proportion of Variance Explained",
     ylim = c(0, 1), type = "o")
```



Here is an alternative to visualize the same data.

```
# 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 )
```



I am going to skip the optional part of exploring extra graphs.

> 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?

We need to find the loading vector for the feature `concave.points_mean`

```
loading_vector_pc1 <- wisc.pr$rotation[, 1]
loading_value_concave_points_mean <- loading_vector_pc1['concave.points_mean']
loading_value_concave_points_mean
```

```
concave.points_mean
         -0.2608538
```

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

at PC5 or you need 5 PC's to explain 80% of the data

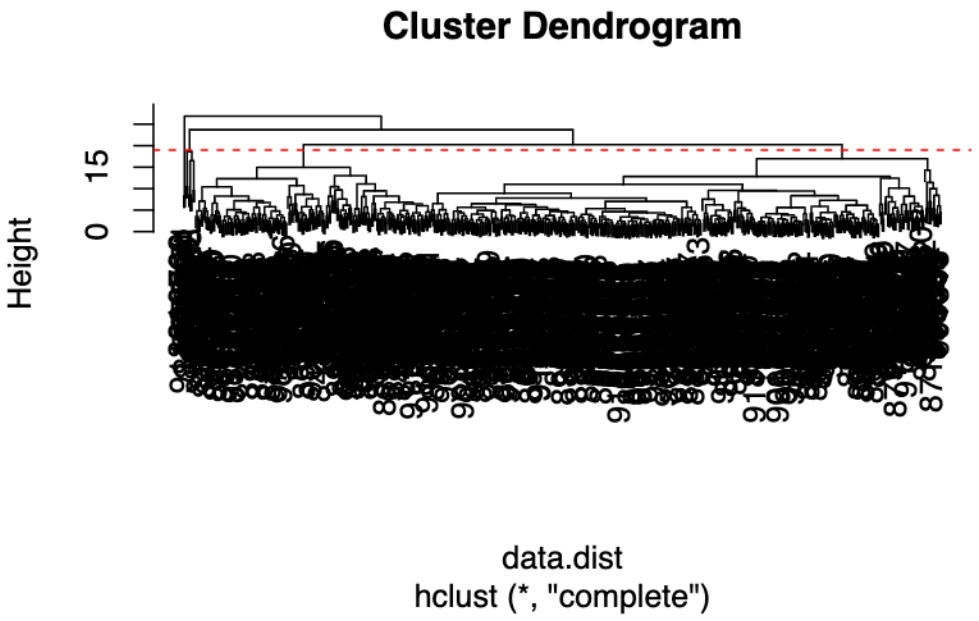
Hierarchical Clustering

We are going to be using hierarchical clustering!

```
# Scale the wisc.data data using the "scale()" function
data.scaled <- scale(wisc.data)
#now calculate the distances
data.dist <- dist(data.scaled)
#now put them into clusters
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=19, col="red", lty=2)
```



The height would have to be 19!

We are going to cut up the clusters so there are 4!

```
wisc.hclust.clusters <- cutree(wisc.hclust, h=19)
#let's table it!
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.clusters2 <- cutree(wisc.hclust, h=13)
#let's table it!
table(wisc.hclust.clusters2, diagnosis)
```

```
                     diagnosis
wisc.hclust.clusters2   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
```

If you cut at 13 you will get 10 clusters and if you cut at 24, you will get 2 clusters. Looking more at these you could explore how different clusters could effect the data.

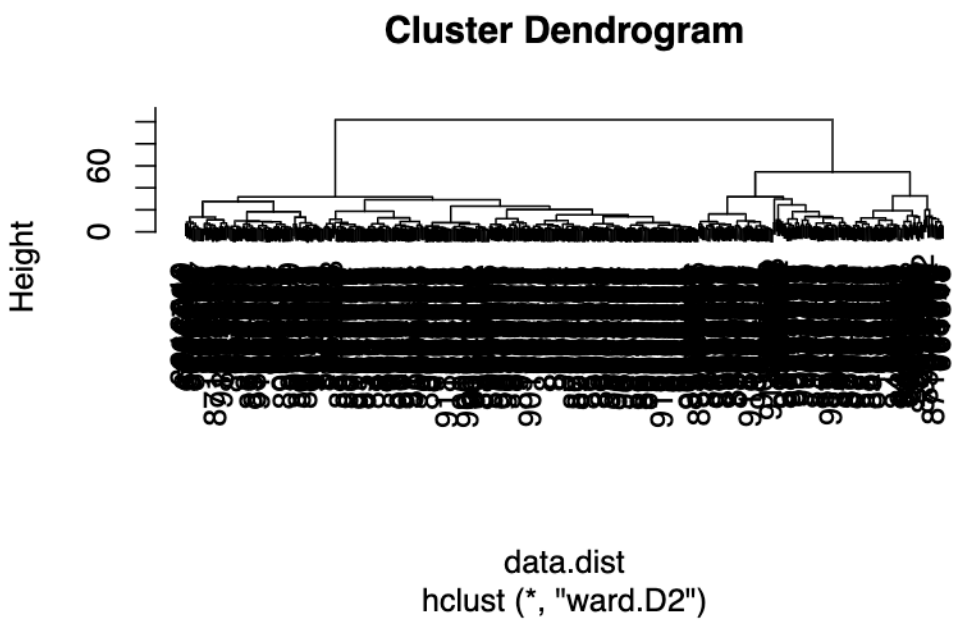
Q13. Which method gives your favorite results for the same data.dist dataset? Explain your reasoning!

I like ward.D2 the best because it provides tends to produce compact, well-separated clusters, which is preferable.

Combining Methods

We are going to redo the plot. Instead of using the complete method, we are going to use ward.D2

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



This is a lot more promising. Next we are going to figure if those two main branches are malignant or benign!

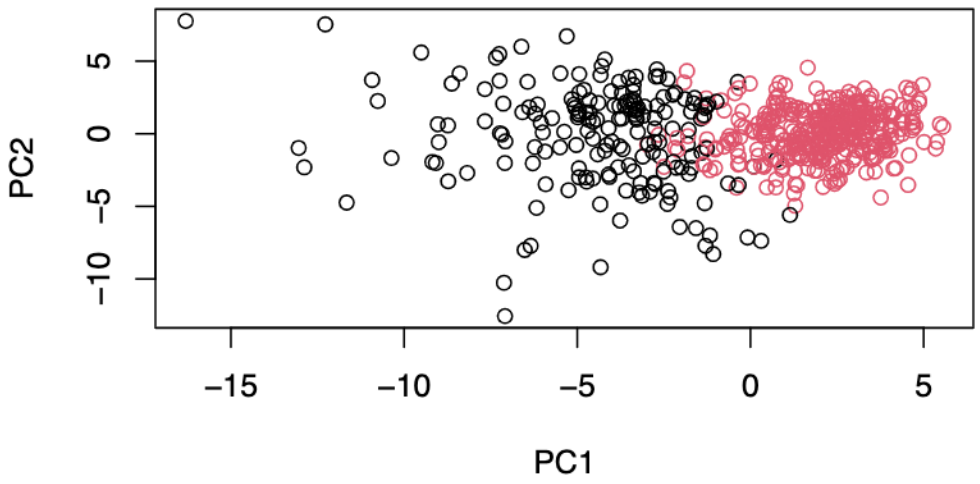
```
grps <- cutree(wisc.hclust.ward, k=2)
table(grps)
```

```
grps
  1   2
184 385
```

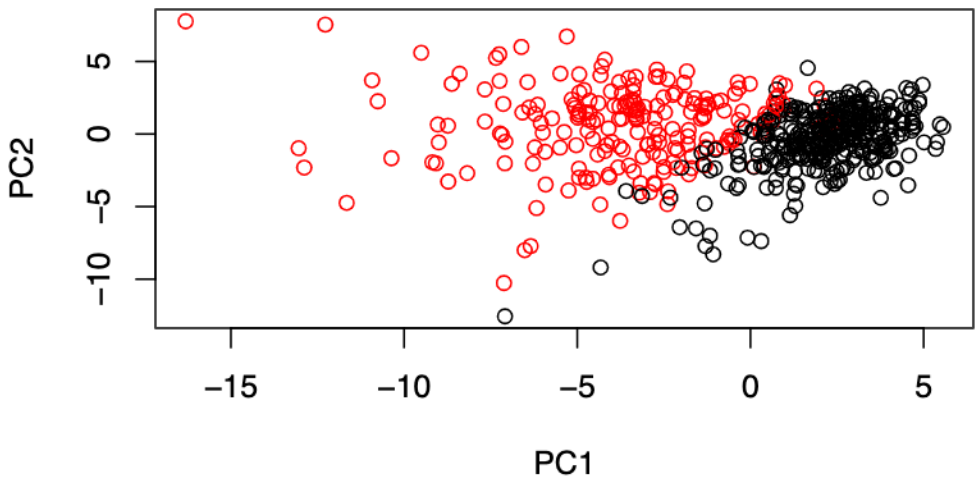
```
table(grps, diagnosis)
```

```
    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=colors)
```



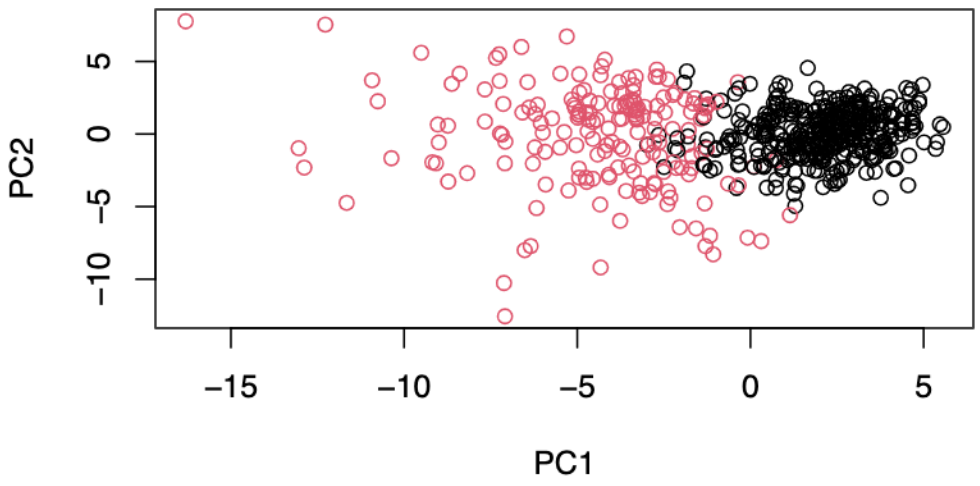

```
g <- as.factor(grps)
levels(g)
```

```
[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)
```




```
## Use the distance along the first 7 PCs for clustering i.e. wisc.pr$x[, 1:7]
wisc.pr.hclust <- hclust(data.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  20 164
                      2 337  48
```

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

They are split up in the same exact way!

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.

I don't have the wisc.km$cluster because I skipped the optional section. But looking at the table of wisc.hclust.clusters, we can see that they are cut up and split more.

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

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

Sensitivity/Specificity

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

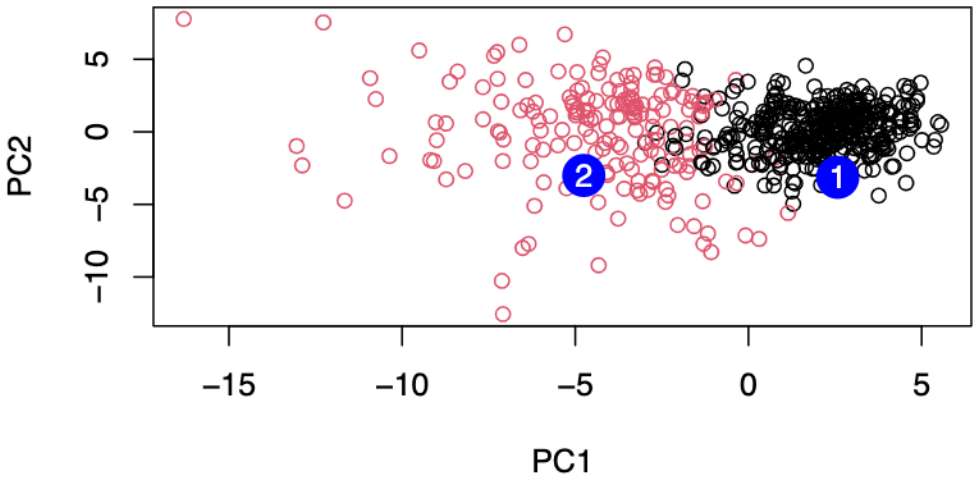
The best sensitivity would be the flipped data set because you can more easily detect the unhealthy patients. The best for specificity would be the regular data set.

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=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?

We should look at patient number 2 because they most like have a lump that is actually cancerous!