Breast Cancer Mini Project

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Background

In today's class, we will apply the methods and techniques of clustering and PCA to help make sense if a real world breast cancer fine needle aspiration (FNA) biopsy data set.

Data Import

We start by importing our data. It is a CSV file, so we will use the `read.csv` function.

```r
fna.data <- "WisconsinCancer.csv"

wisc.df <- read.csv(fna.data, row.names = 1)
head(wisc.df, 4)
```

```
         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
         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
         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
         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
         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
         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
         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
         fractal_dimension_worst
842302                   0.11890
842517                   0.08902
84300903                 0.08758
84348301                 0.17300
```

```r
# Removing the pathologist diagnosis so that we can do it ourselves
wisc.data <- wisc.df[,-1]

#Setting up a diagnosis vector for later
diagnosis <- wisc.df$diagnosis
```

> Q1. How many observations are in this dataset?

```r
dim(wisc.data)
```

```
[1] 569  30
```

There are 569 observations

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

```r
table(diagnosis)
```

```
diagnosis
  B   M
357 212
```

There are 212 observations that have a malignant diagnosis

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

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

```
[1] 10
```

There are 10 variables/features in the data suffixed with "_mean"

Principal Component Analysis

The next step in your analysis is to perform principal component analysis (PCA) on wisc.data.

```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, scale = T)
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 component (PC1)?

44.2% of the original data is captured by PCA1.

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

Three PCAs are needed to record the original caruance if the data.

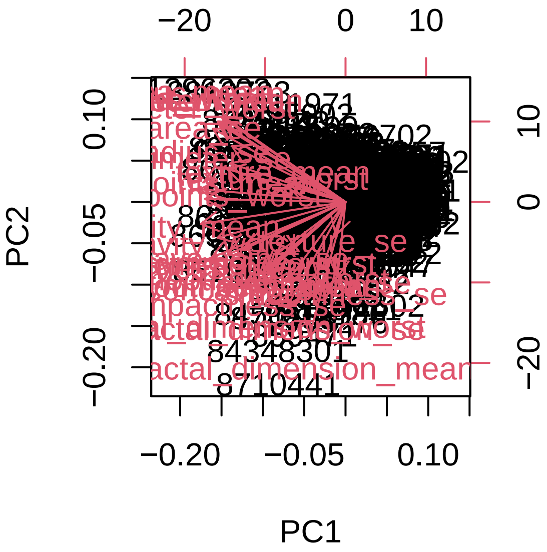
> Q6. How many principal components (PCs) are required to describe at least 90% of the original variance in the data?

To record 90% of the original variance, 7 PCAs are needed.

Interpreting PCA results

Now you will use some visualizations to better understand your PCA model. A common visualization for PCA results is the so-called biplot.

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



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

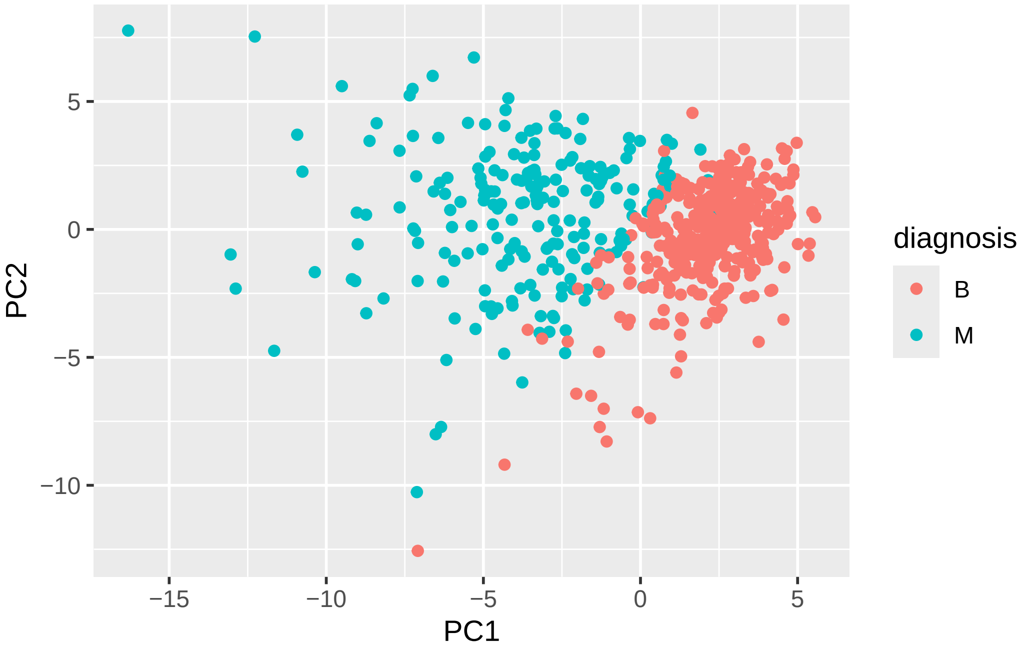
This graph is not easy to understand, there is a lot of overlapping text in similar colors that makes individual components hard to determine.

Let's Use ggplot instead

```
library(ggplot2)
```

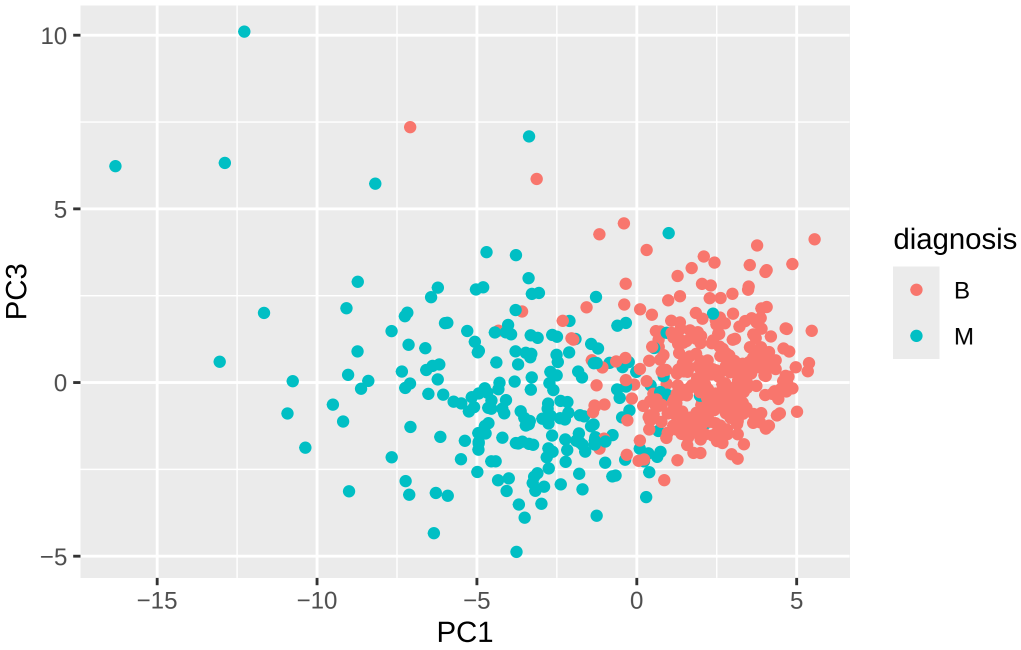
```
Warning: package 'ggplot2' was built under R version 4.4.3
```

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



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

```
library(ggplot2)

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



The variance displayed in the points is less in the second plot. The points are scattered more in the first graph. Another difference is that the y axis values change, decreasing in the secind plot

Variance explained

We will now use a scree plot to show how much variance each PC captures.

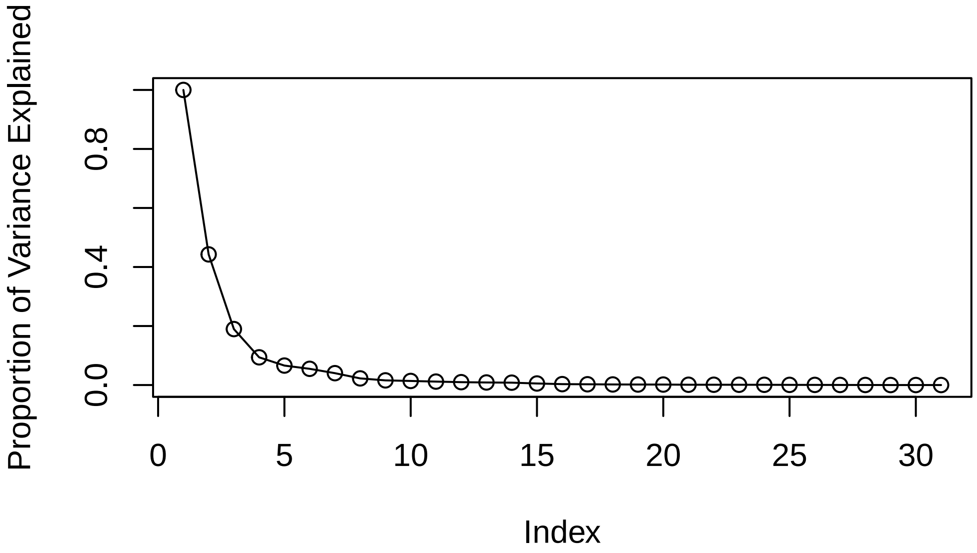
We will calculate variance by squaring the `sdev` component of `wisc.pr`

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

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

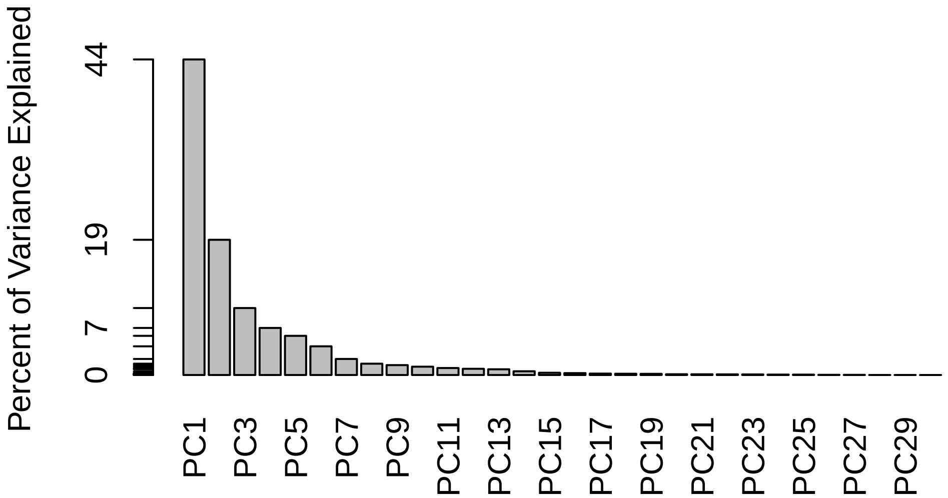
We will now calculate the variance of each principle component by dividing by the variance of all principle components.

```
pve <- pr.var / sum( pr.var )

plot(c(1,pve), xlav = "Principal Component", ylab = "Proportion of Variance Explained", ylim
Warning in plot.window(...): "xlav" is not a graphical parameter

Warning in plot.xy(xy, type, ...): "xlav" is not a graphical parameter

Warning in axis(side = side, at = at, labels = labels, ...): "xlav" is not a
graphical parameter
Warning in axis(side = side, at = at, labels = labels, ...): "xlav" is not a
graphical parameter

Warning in box(...): "xlav" is not a graphical parameter

Warning in title(...): "xlav" is not a graphical parameter
```



Let's create an alternate scree plot of the data using `barplot()`

```
barplot(pve, ylab = "Percent 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

In this section we will check your understanding of the PCA results, in particular the "loadings" and "variance explained".

> 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? This tells us how much this original feature contributes to the first PC. Are there any features with larger contributions than this one?

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

```
              radius_mean              texture_mean            perimeter_mean 
              -0.21890244               -0.10372458               -0.22753729 
                area_mean           smoothness_mean          compactness_mean 
              -0.22099499               -0.14258969               -0.23928535 
           concavity_mean       concave.points_mean             symmetry_mean 
              -0.25840048               -0.26085376               -0.13816696 
fractional_dimension_mean                 radius_se                texture_se 
              -0.06436335               -0.20597878               -0.01742803 
             perimeter_se                   area_se             smoothness_se 
              -0.21132592               -0.20286964               -0.01453145 
```

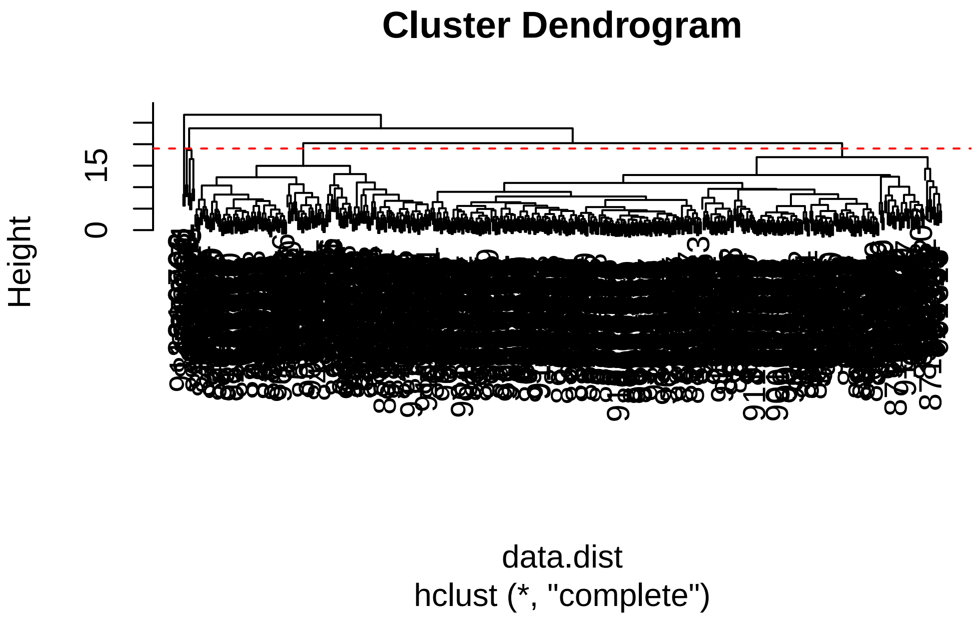
```
         compactness_se            concavity_se       concave.points_se 
            -0.17039345             -0.15358979             -0.18341740 
            symmetry_se    fractal_dimension_se            radius_worst 
            -0.04249842             -0.10256832             -0.22799663 
          texture_worst         perimeter_worst              area_worst 
            -0.10446933             -0.23663968             -0.22487053 
       smoothness_worst       compactness_worst         concavity_worst 
            -0.12795256             -0.21009588             -0.22876753 
   concave.points_worst          symmetry_worst fractal_dimension_worst 
            -0.25088597             -0.12290456             -0.13178394 
```

The `concave.points_mean` principle component is -0.26085376. There are not any components with larger contributions. The negative number represents how the feature varies relative to the PC axis.

Hierarchical clustering

> Q.10 Using the `plot` and `abline()` functions, what is the height at which the clustering model has 4 clusters?

```r
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)
```



The height neccessary to create a model with 4 clusters is 19. Although there are other possible heights that would meet the same outcome, 19 was chosen

Selecting number of clusters

```r
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
```

> Q11. OPTIONAL: Can you find a better cluster vs diagnoses match by cutting into a different number of clusters between 2 and 6? How do you judge the quality of your result in each case?

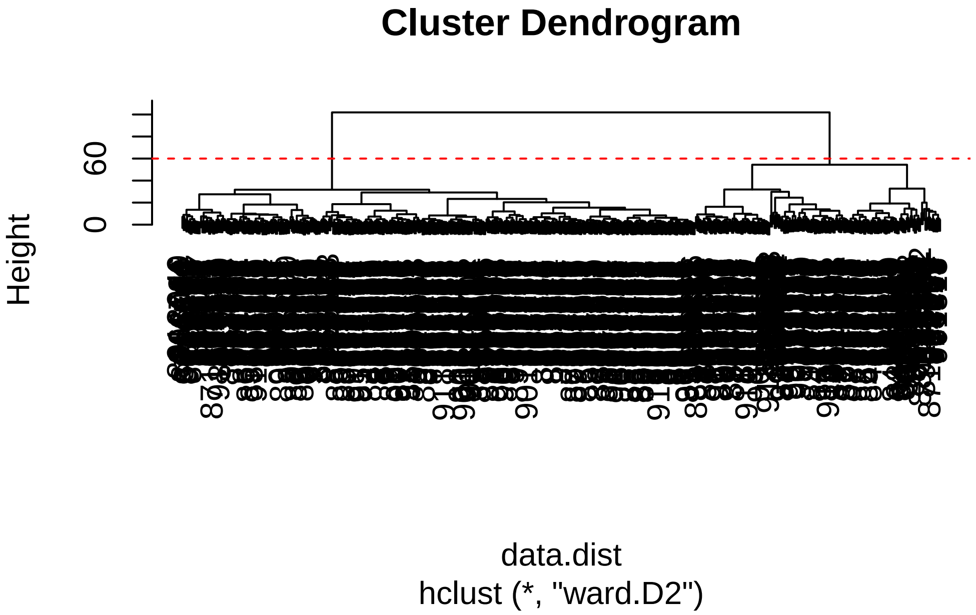
I could not find a better cluster vs diagnosis match by changing the number of clusters. There was not a greater separation between malignant and benign that I could determine using clusters between 2 and 6.

Using different methods

There are number of different “methods” we can use to combine points during the hierarchical clustering procedure. These include `single`, `complete`, `average` and (my favorite) `ward.D2`.

> Q12. Which method gives your favorite results for the same data.dist dataset? Explain your reasoning.

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

plot(wisc.hclustdiffmethod)
abline(h=60, col = "red", lty=2)
```



```r
wisc.hclust.clustersdiffmethod <- cutree(wisc.hclustdiffmethod, k = 4)
table(wisc.hclust.clustersdiffmethod, diagnosis)
```

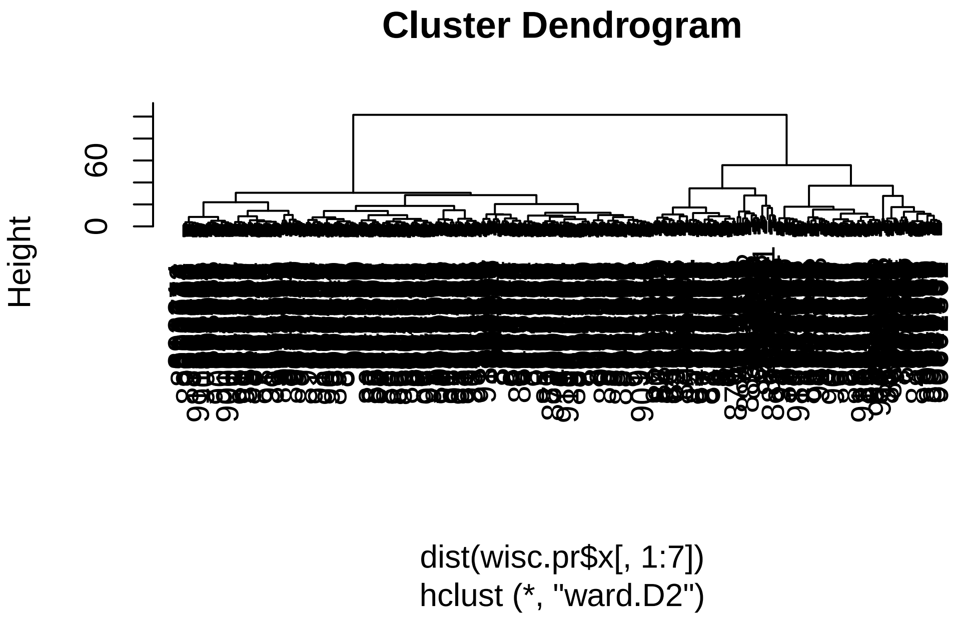
```
                              diagnosis
wisc.hclust.clustersdiffmethod   B   M
                             1   0 115
                             2   6  48
                             3 337  48
                             4  14   1
```

I like the `ward.D2` because it gives much more discernable "goalposts", and the clustering with k = 4 presented a much more distinguishable difference between benign and malignant samples.

Combining methods

We have tried PCA and hierarchical clustering separately. Now let's combine them: cluster on the PC scores instead of the original 30 features.

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



Note the two main branches of our dendrogram indicating two main clusters - maybe these are malignant and benign. Let's find out!

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

```
grps
  1   2 
216 353 
```

I want to know how the clusterinf in `grps` with values 1 or 2 correspond to the expert `diagnosis`

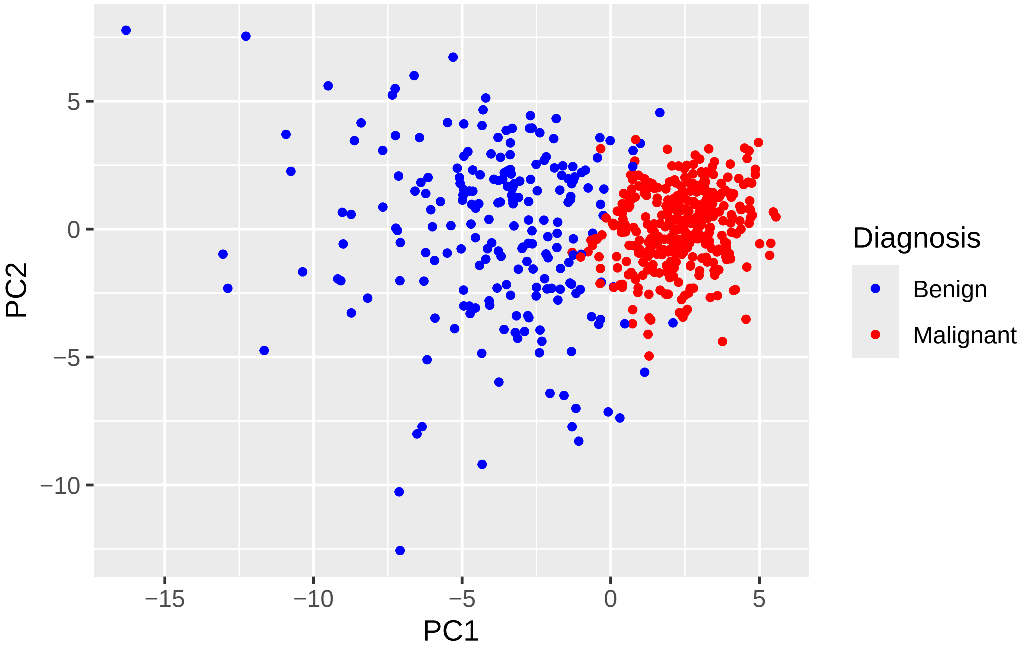
```
table(grps, diagnosis)
```

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

Sensitivity/Specificity

FP: 28 TP: 188 TN: 329 FN: 24 Sensitivity: TP/(TP + FN) Specificity: TN/(TN+FP)

```
ggplot(wisc.pr$x) +
  aes(PC1, PC2, color = factor(grps)) +
  geom_point(size = 1) +
  scale_color_manual(
    values = c("1" = "blue", "2" = "red"), labels = c("Benign", "Malignant")) +
  labs(color = "Diagnosis")
```



> Q13. How well does the newly created hclust model with two clusters separate out the two “M” and “B” diagnoses?

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

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

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

There is no significant difference between the two clusters model and the 4 cluster model

> Q14. How well do the hierarchical clustering models you created in the previous sections (i.e. without first doing PCA) do in terms of separating the diagnoses? Again, use the table() function to compare the output of each model (wisc.hclust.clusters and wisc.pr.hclust.clusters) with the vector containing the actual diagnoses.

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

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

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

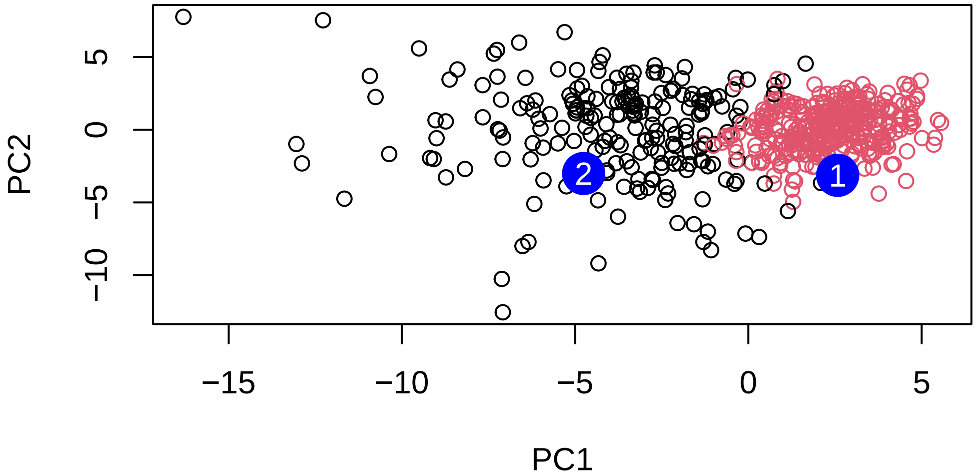
Only the ward method separate out the data properly with 2 clusters, complete also worked but it needed 4 clusters

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=grps)
points(npc[,1], npc[,2], col="blue", pch=16, cex=3)
text(npc[,1], npc[,2], c(1,2), col="white")
```



Q16. Which of these new patients should we prioritize for follow up based on your results?

I would prioritize treatments for patient 1 because they are more closely seen in the malignant side.