Class 08 Mini-project

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##Unsupervised Learning Analysis of Human Breast Cancer Cells

#Data Import Save the file to you computer in the Class 08 BIMM143 folder

```
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
```

Create a new df without the expert diagnosis so you don't have the "answer" to whether the cells are malignant or benign

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

Store the diagnosis values as a factor vector

```
diagnosis <- factor(wisc.df[,1])
head(diagnosis)

[1] M M M M M M
Levels: B M
```

Get familiar with the data set: Q1) How many observations are in this dataset? ie. How many people?

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

```
[1] 569
```

There are 569 different people/ observations in this data set

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

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

```
  B   M 
357 212 
```

There are 212 malignant diagnosis

Q3) How many variables/features in the data are suffixed with _mean? Use `colnames()` to find the column names

```
colname <- colnames(wisc.data)
colname
```

```
 [1] "radius_mean"             "texture_mean"           
 [3] "perimeter_mean"          "area_mean"              
 [5] "smoothness_mean"         "compactness_mean"       
 [7] "concavity_mean"          "concave.points_mean"    
 [9] "symmetry_mean"           "fractal_dimension_mean" 
[11] "radius_se"               "texture_se"             
[13] "perimeter_se"            "area_se"                
[15] "smoothness_se"           "compactness_se"         
[17] "concavity_se"            "concave.points_se"      
[19] "symmetry_se"             "fractal_dimension_se"   
[21] "radius_worst"            "texture_worst"          
[23] "perimeter_worst"         "area_worst"             
[25] "smoothness_worst"        "compactness_worst"      
[27] "concavity_worst"         "concave.points_worst"   
[29] "symmetry_worst"          "fractal_dimension_worst"
```

Then you search for "_mean" pattern using the `grep()` function

```
grep("_mean",colname)
```

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

To find how many times we found them you can use the `length()` function

```
length(grep("_mean",colname))
```

```
[1] 10
```

There are 10 variables/features that end with "_mean"

How many dimensions are in this data set?

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

```
[1] 569  30
```

569 rows and 30 columns

#Principal Component Analysis

First we need to see if the data needs to be scaled. We start by checking the column means `colMeans()` and apply it to find the standard deviations for each component

```
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 
```

```
round(apply(wisc.data,2,sd),2)
```

```
            radius_mean            texture_mean          perimeter_mean 
                   3.52                    4.30                   24.30 
              area_mean         smoothness_mean        compactness_mean 
                351.91                    0.01                    0.05 
         concavity_mean     concave.points_mean           symmetry_mean 
                   0.08                    0.04                    0.03 
 fractal_dimension_mean               radius_se              texture_se 
                   0.01                    0.28                    0.55 
           perimeter_se                 area_se           smoothness_se 
                   2.02                   45.49                    0.00 
         compactness_se            concavity_se       concave.points_se 
                   0.02                    0.03                    0.01 
            symmetry_se    fractal_dimension_se            radius_worst 
                   0.01                    0.00                    4.83 
          texture_worst         perimeter_worst              area_worst 
```

```
                  6.15                   33.60                  569.36
      smoothness_worst       compactness_worst         concavity_worst
                  0.02                    0.16                    0.21
  concave.points_worst          symmetry_worst fractal_dimension_worst
                  0.07                    0.06                    0.02
```

You can see that the sd for each variable is quite different so the data is measured with different units and therefore should be scaled.

How we can try `prcomp()` with scaling

```
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
```

We captured 100% of the variance after 29 principal component analysis iterations

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?

You need at least 3 PCs

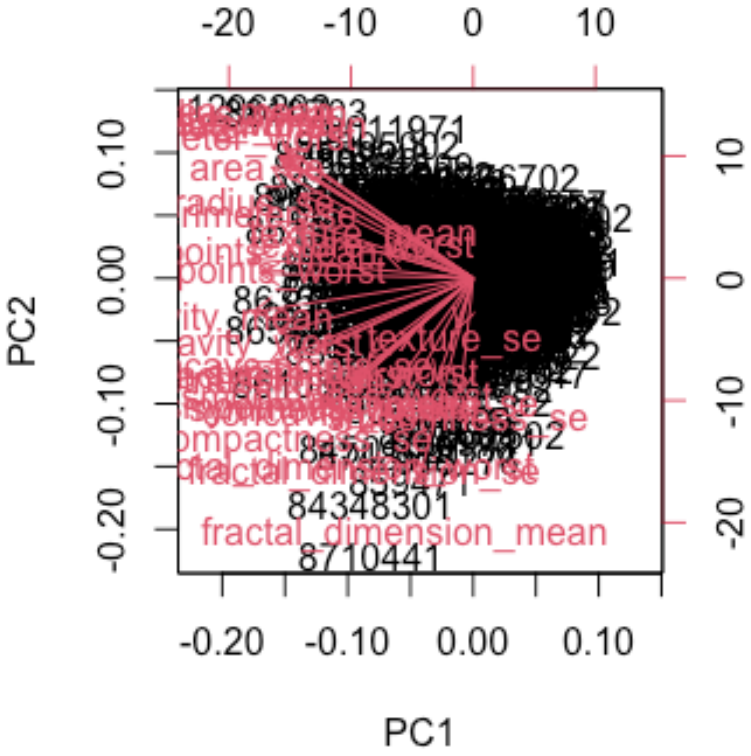
Q6) How many principal components (PCs) are required to describe at least 90% of the original variance in the data?

You need 7 PCs

#Interpreting PCA results

Lets try interpreting PCA results using `biplot()`

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

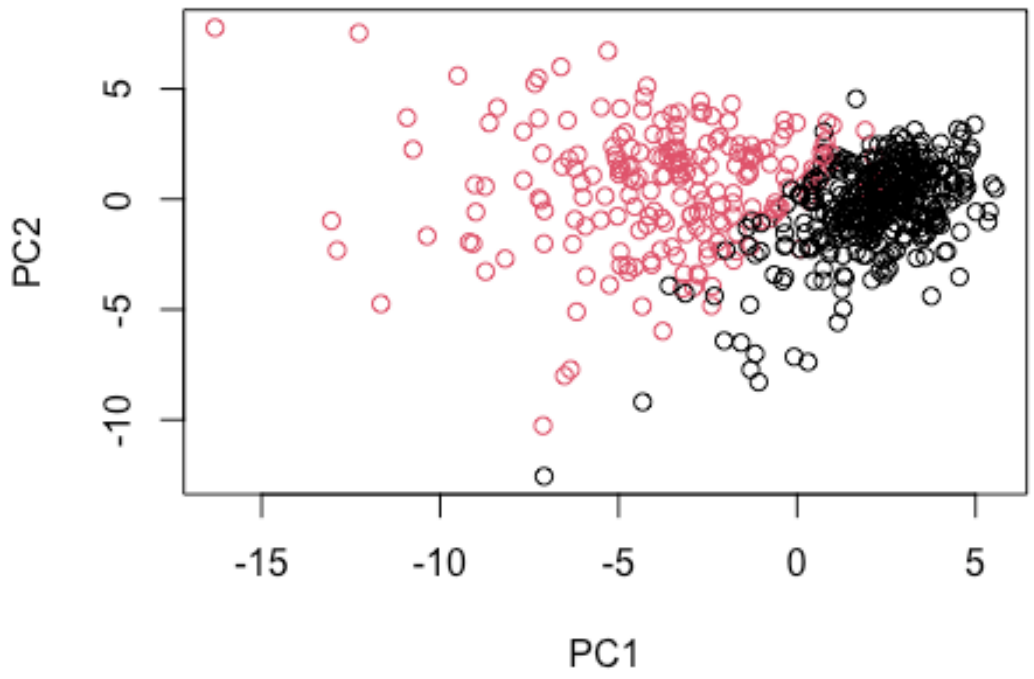


Q7) What stands out to you about this plot? Is it easy or difficult to understand? Why?

This plot is dogwater. Rubbish.

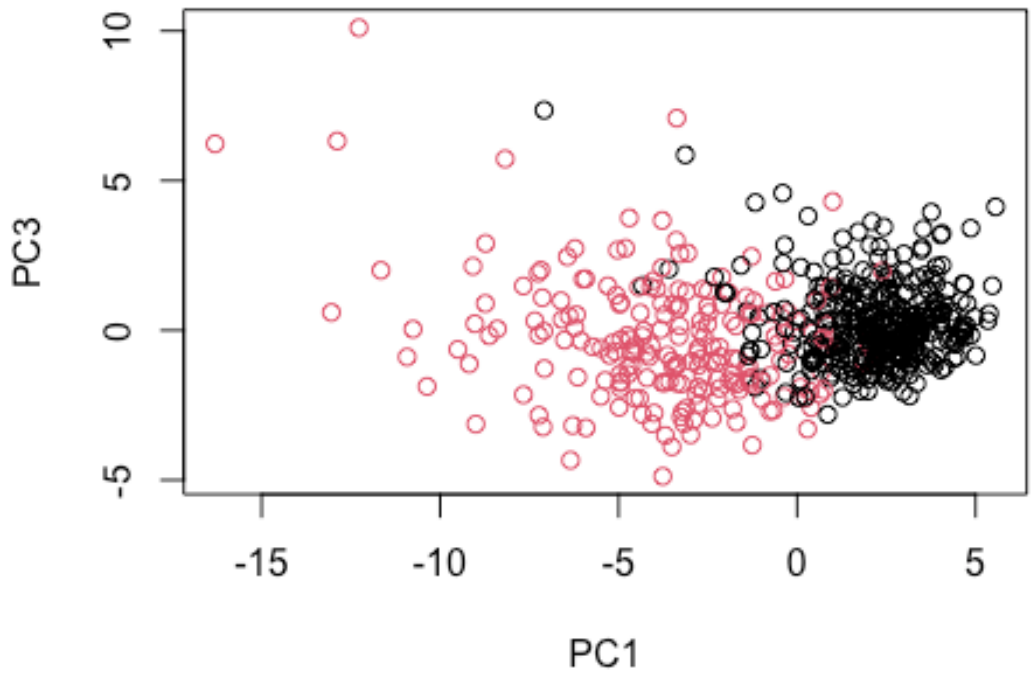
Lets try plotting it with a regular scatter plot colored by diagnosis

```
plot(wisc.pr$x[,1], wisc.pr$x[,2], col=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 = diagnosis,
     xlab = "PC1", ylab = "PC3")
```



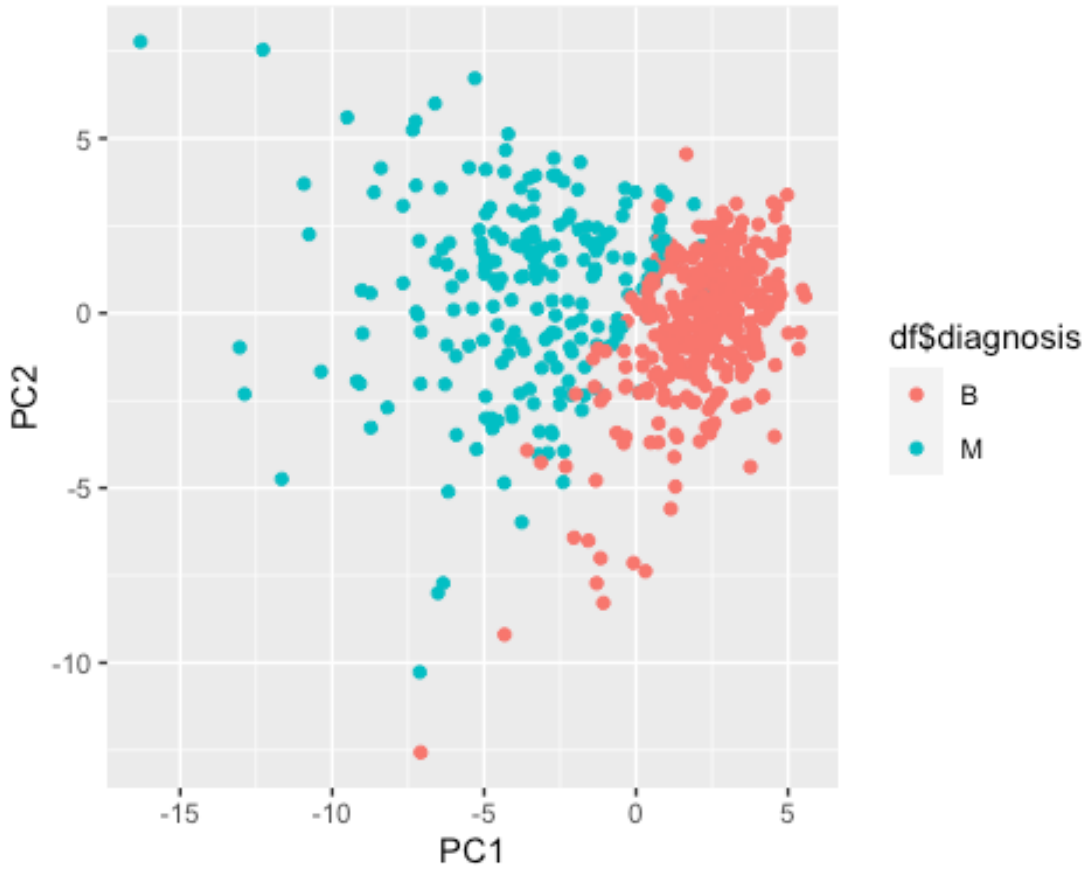
These plots are easier to see some sort of pattern with regards to the diagnosis. The plot with PC2 looks a little cleaner cut and seems to separate the 2 diagnosis variables a little better. Also because the difference is seen among the x axis, it shows that PC1 is capturing the diagnosis variation

#Lets try and look at this on ggplot

```
df <- as.data.frame(wisc.pr$x)
df$diagnosis <- diagnosis

library(ggplot2)

ggplot(df) + aes(PC1, PC2, col=df$diagnosis) + geom_point()
```



#Variance explained

get the standard deviations from the wisc.pr output

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

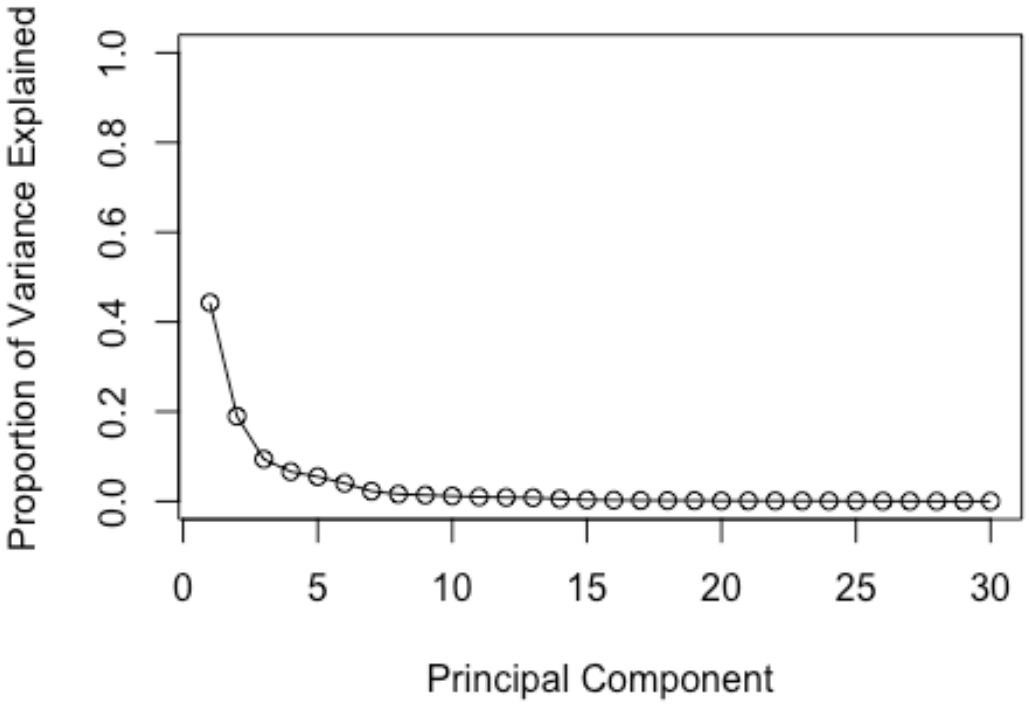
```
[1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

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

```
[1] 0.44272026 0.18971182 0.09393163 0.06602135 0.05495768 0.04024522
```

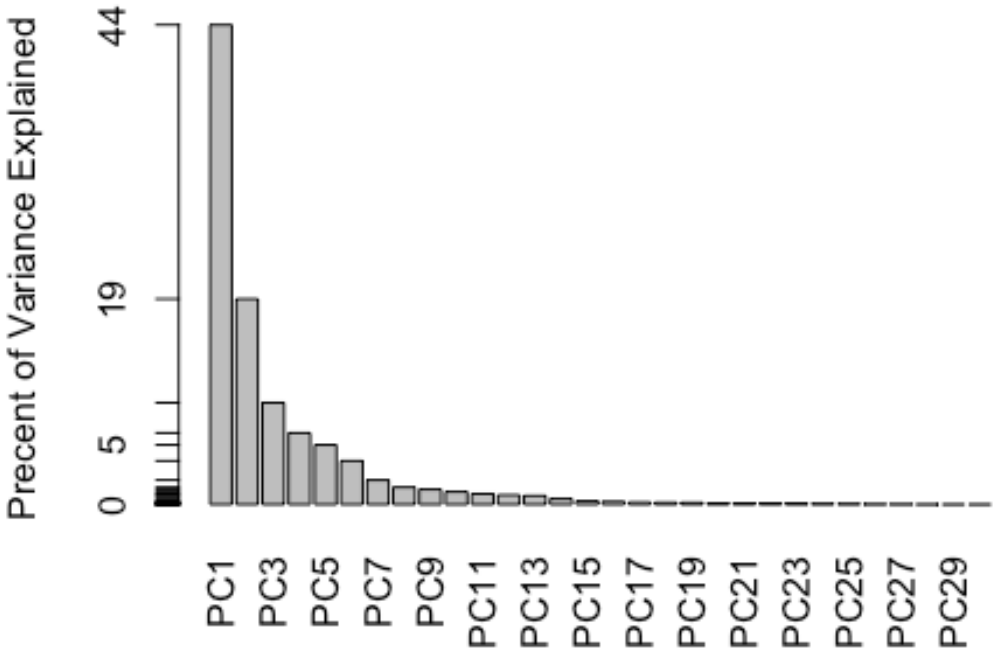
Plot variance explained for each principal component

```
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[,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 
 fractal_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 
```

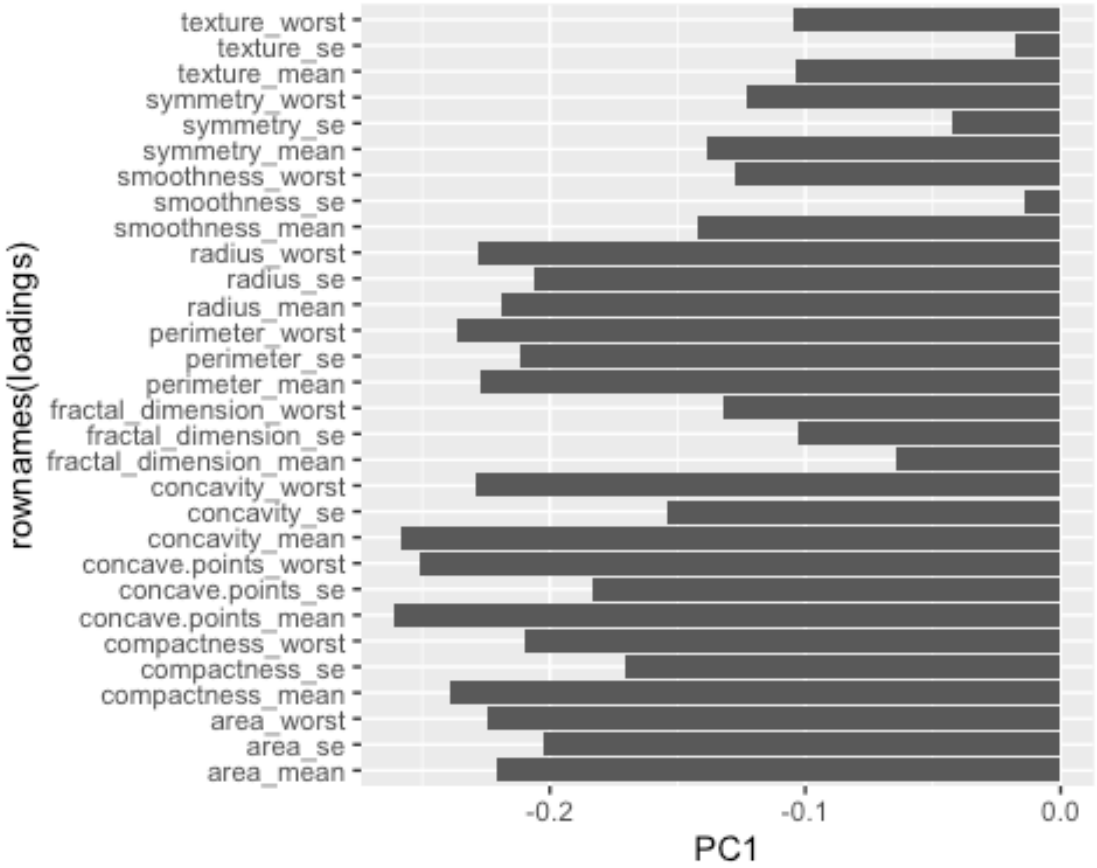
```
            -0.10446933             -0.23663968             -0.22487053
      smoothness_worst       compactness_worst         concavity_worst
            -0.12795256             -0.21009588             -0.22876753
   concave.points_worst          symmetry_worst fractal_dimension_worst
            -0.25088597             -0.12290456             -0.13178394
```

Using `concave.points_mean` you get:

```
wisc.pr$rotation["concave.points_mean",1]

[1] -0.2608538

loadings <- as.data.frame(wisc.pr$rotation)
ggplot(loadings)+ aes(PC1, rownames(loadings))+ geom_col()
```



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

5 PCs

Hierarchical clustering

Scale the wisc.data data using the "scale()" function

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

Calculate the (Euclidean) distances between all pairs of observations in the new scaled dataset

```
data.dist <- dist(data.scaled)
```

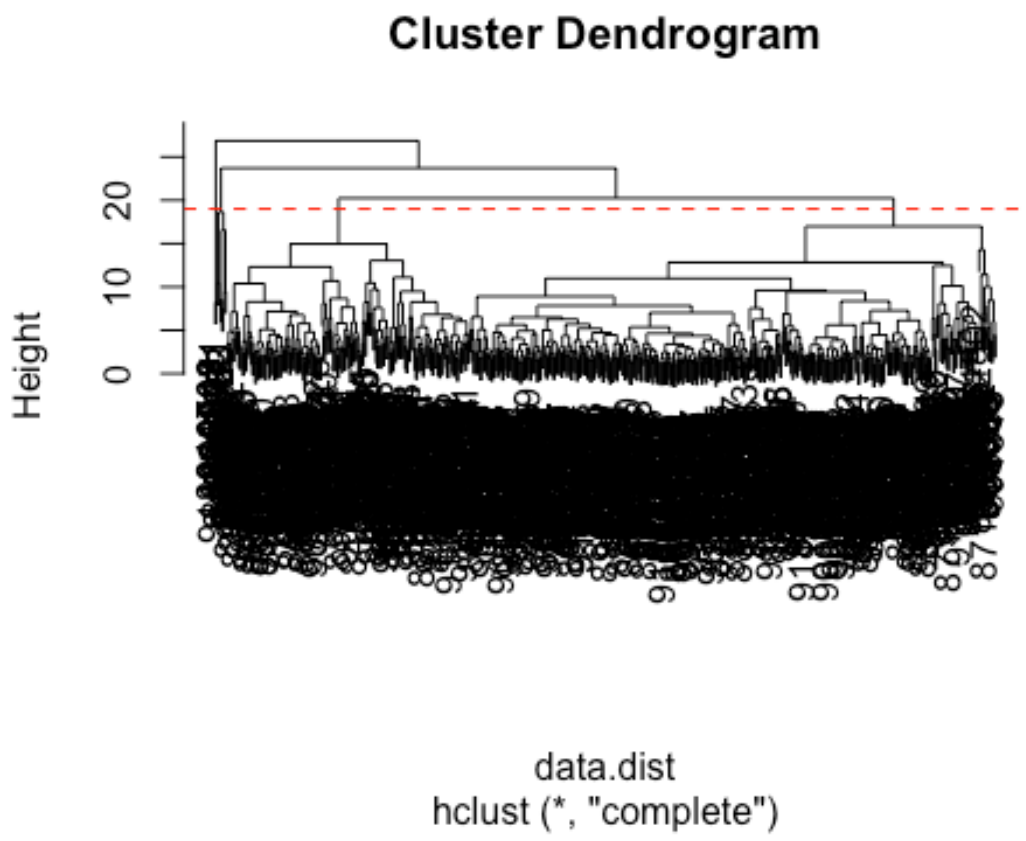
Create a hierarchical clustering model using complete linkage. Manually specify the method argument to hclust()

```
wisc.hclust <- hclust(data.dist)
```

Now we can plot this data Q11) Using the plot() and abline() functions, what is the height at which the clustering model has 4 clusters?

h=19 gives 4 clusters

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



#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?

Cutting into clusters that are higher than 2, doesn't help our case because ideally we want 2 clusters, one that matches B and one that matches M.

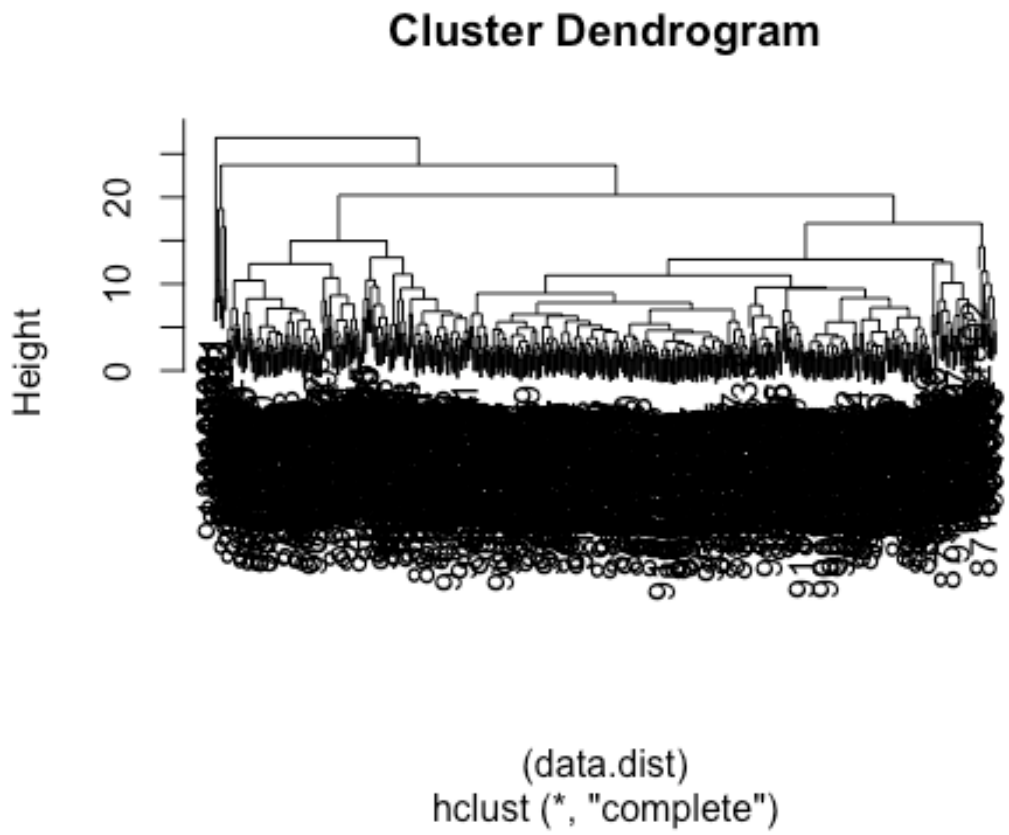
```
wisc.hclust.clusters <- cutree(wisc.hclust, k=10)
table(wisc.hclust.clusters, diagnosis)
```

```
                    diagnosis
wisc.hclust.clusters   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
```

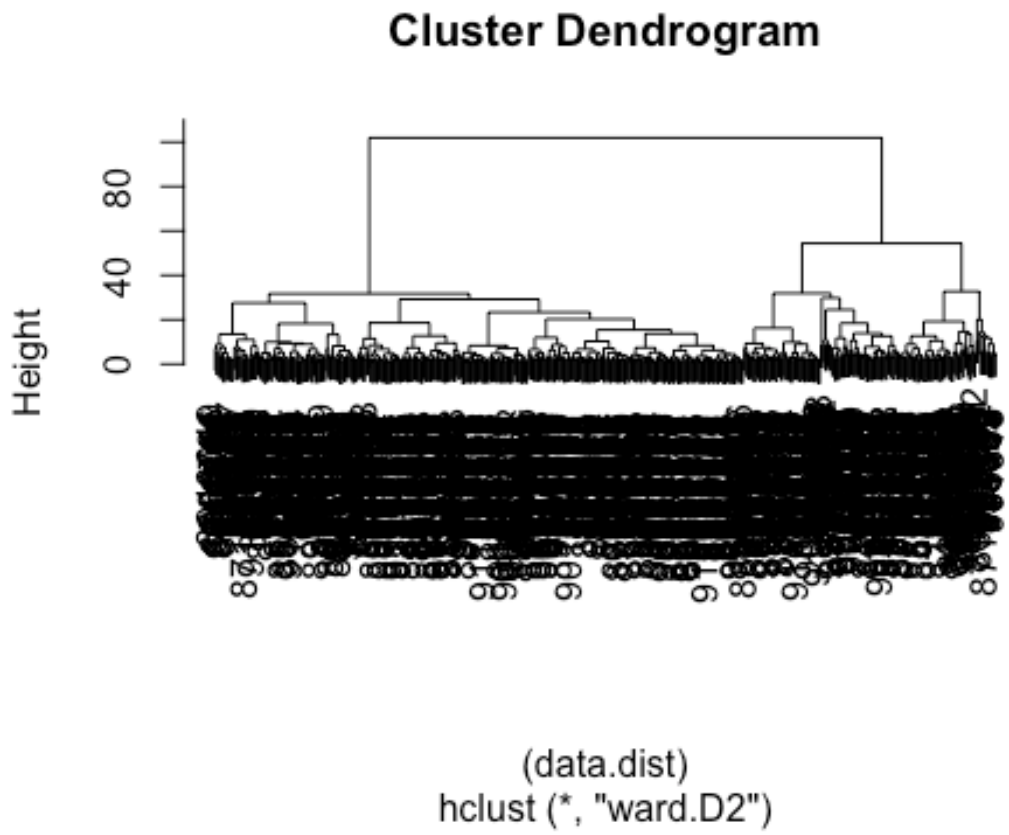
#Combine Methods

Q13. Which method gives your favorite results for the same data.dist dataset? Explain your reasoning. Lets try out some methods and see which one looks best:

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




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

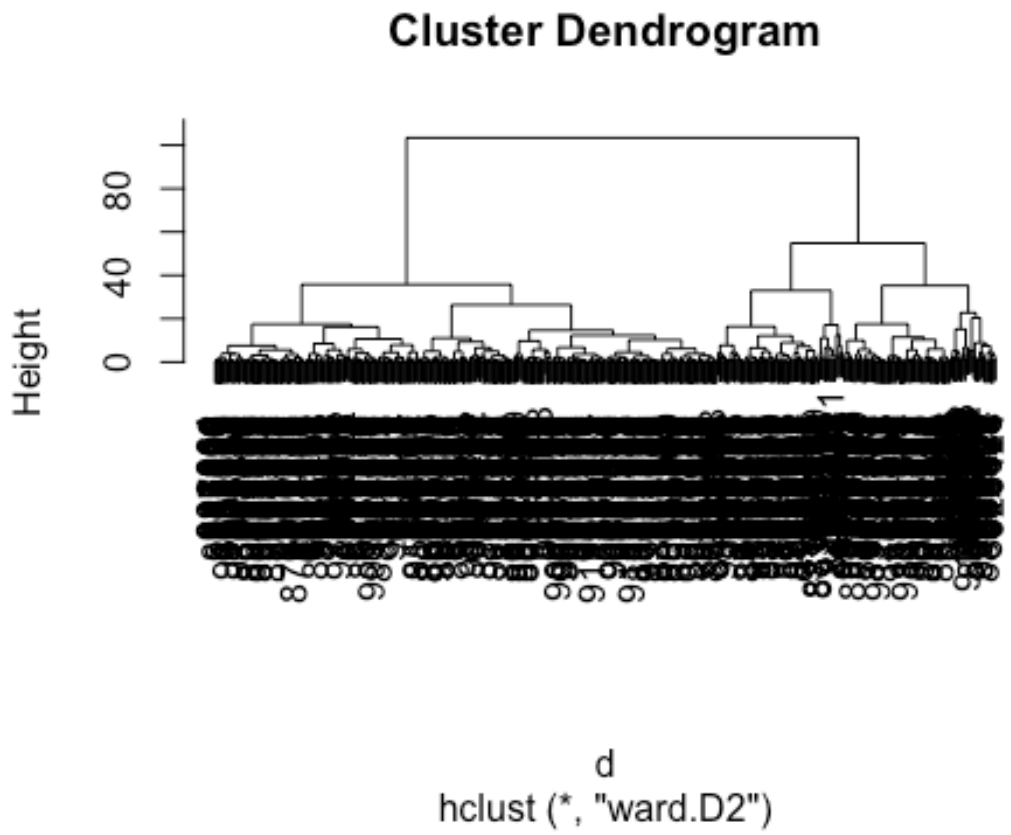


I like the `ward.D2` because it gives me the biggest goal posts and more separation between clusters.

My PCA results were interesting as they showed a separation of M and B samples along PC1

I want to cluster my PCA results - that is use the `wisc.pr$x` as input to my `hclust()` You can try just taking the first 3 PCs because those are encompassing a lot of the variance. Also you can use method="ward.D2"

```
d <- dist(wisc.pr$x[,1:3])
wisc.pr.hclust <- hclust(d,method="ward.D2")
plot(wisc.pr.hclust)
```



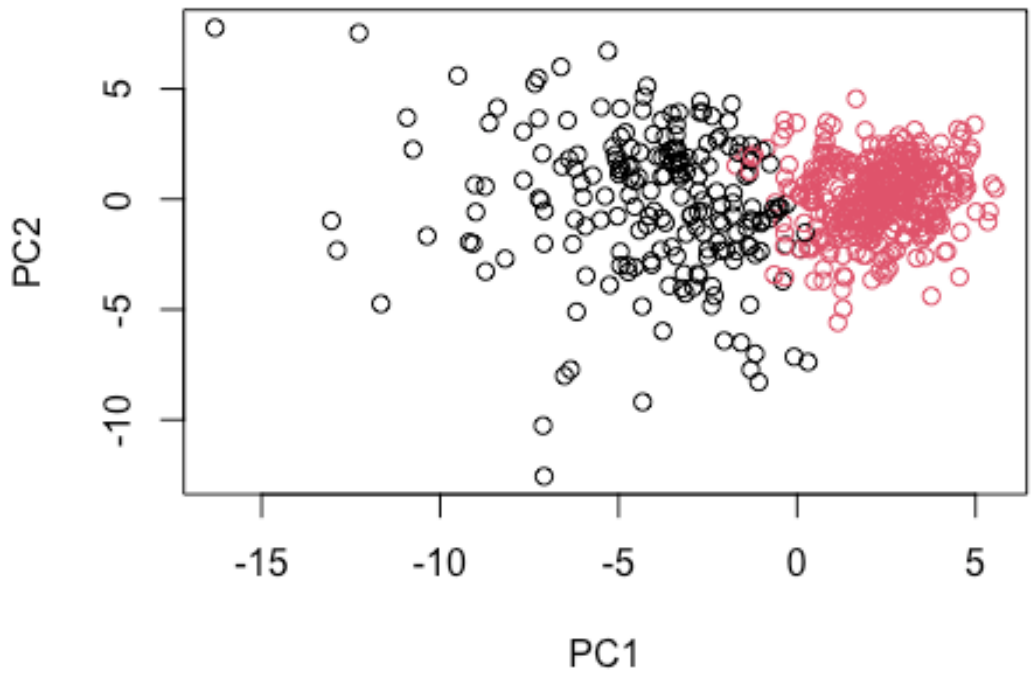
Lets cut into 2 groups/clusters

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

```
grps
  1   2
203 366
```

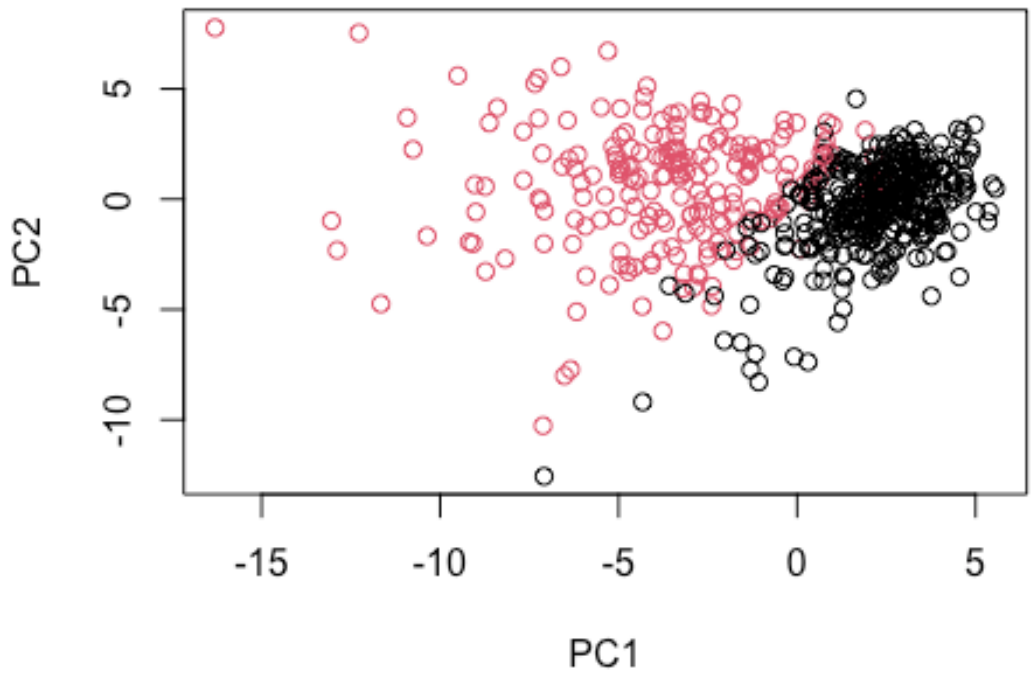
Now we can plot using this grps variable

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



Now compare to the plot we made before

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



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

Lets relevel the B and M for groups though so black is malignant and red is benign

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

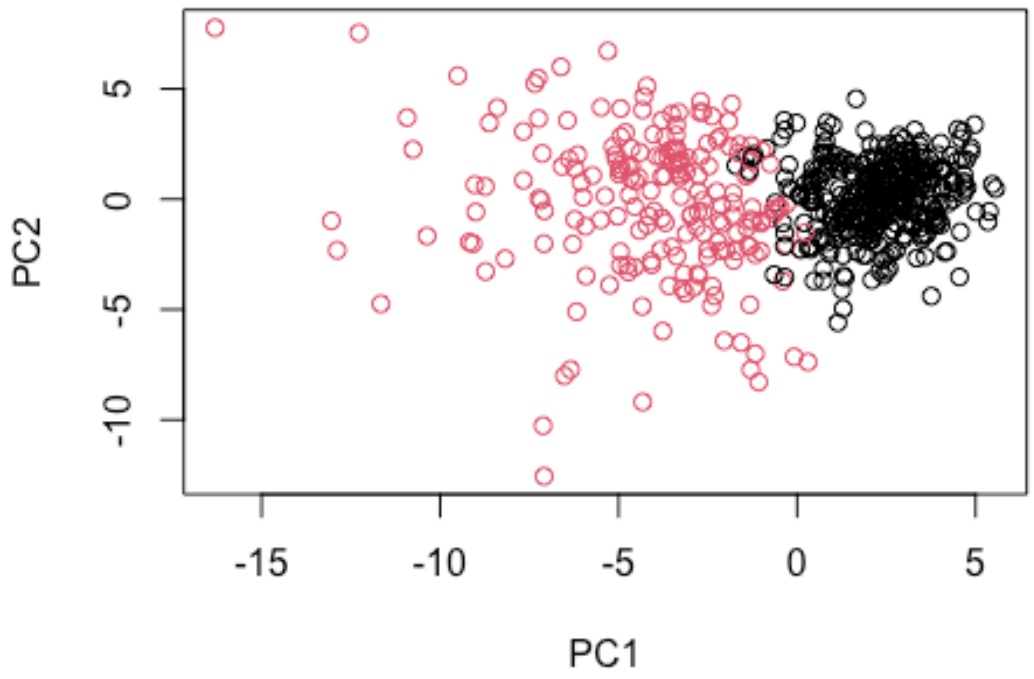
```
[1] "1" "2"
```

```
g <- relevel(g,2)
levels(g)
```

```
[1] "2" "1"
```

Now we can replot

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



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

```
table(g, diagnosis)
```

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

We can text the accuracy by checking for false positive Malignant cases you get: For our prediction we get in group 2 (Benign) 33 cases that were actually scored as Malignant by the experts so there is a 6.4% chance of giving a false positive.

```
33/(333+179)
```

```
[1] 0.06445312
```