Class 8: Machine Learning Mini Project

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In today's mini-project we will explore a complete analysis using unsupervised learning techniques covered in class (clustering and PCA for now).

The data itself comes from the Wisconsin Breast Cancer Diagnosis Data Set FNA breast biopsy data.

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)
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
```

Remove the diagnosis column and keep it in a separate vector for later # We can use -1 here to remove the first column

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

Exploratory data analysis

The first step of any data analysis, unsupervised or supervised, is to familiarize yourself with the data.

> Q1. How many observations (patients) are in this dataset?

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

```
[1] 569
```

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

```
table(diagnosis)
```

```
diagnosis
  B   M 
357 212 
```

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

First find the column names

```r
colnames(wisc.data)
```

```
 [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"
```

Next I need to search within the column names for the "_mean" pattern. The 'grep()' function might help here.

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

```
[1] 10
```

Q. How many dimensions are in this dataset?

```r
ncol(wisc.data)
```

```
[1] 30
```

Principal Component Analysis

First do we need to scale the data before PCA or not.

Check column means and standard deviations

```
round(apply(wisc.data,2,sd),3)
```

```
            radius_mean            texture_mean          perimeter_mean
                  3.524                   4.301                  24.299
              area_mean         smoothness_mean        compactness_mean
                351.914                   0.014                   0.053
         concavity_mean     concave.points_mean           symmetry_mean
                  0.080                   0.039                   0.027
 fractal_dimension_mean               radius_se              texture_se
                  0.007                   0.277                   0.552
           perimeter_se                 area_se           smoothness_se
                  2.022                  45.491                   0.003
         compactness_se            concavity_se       concave.points_se
                  0.018                   0.030                   0.006
            symmetry_se    fractal_dimension_se            radius_worst
                  0.008                   0.003                   4.833
          texture_worst         perimeter_worst              area_worst
                  6.146                  33.603                 569.357
       smoothness_worst       compactness_worst         concavity_worst
                  0.023                   0.157                   0.209
   concave.points_worst          symmetry_worst fractal_dimension_worst
                  0.066                   0.062                   0.018
```

Looks like we need to scale.

Perform PCA on wisc.data by completing the following code

```
wisc.pr <- prcomp( wisc.data, scale=TRUE)
summary(wisc.pr)
```

```
Importance of components:
                          PC1    PC2     PC3     PC4     PC5     PC6     PC7
Standard deviation     3.6444 2.3857 1.67867 1.40735 1.28403 1.09880 0.82172
Proportion of Variance 0.4427 0.1897 0.09393 0.06602 0.05496 0.04025 0.02251
Cumulative Proportion  0.4427 0.6324 0.72636 0.79239 0.84734 0.88759 0.91010
                           PC8    PC9    PC10   PC11    PC12    PC13    PC14
```

```
Standard deviation     0.69037 0.6457 0.59219 0.5421 0.51104 0.49128 0.39624
Proportion of Variance 0.01589 0.0139 0.01169 0.0098 0.00871 0.00805 0.00523
Cumulative Proportion  0.92598 0.9399 0.95157 0.9614 0.97007 0.97812 0.98335
                          PC15    PC16    PC17    PC18    PC19    PC20   PC21
Standard deviation     0.30681 0.28260 0.24372 0.22939 0.22244 0.17652 0.1731
Proportion of Variance 0.00314 0.00266 0.00198 0.00175 0.00165 0.00104 0.0010
Cumulative Proportion  0.98649 0.98915 0.99113 0.99288 0.99453 0.99557 0.9966
                          PC22    PC23   PC24    PC25    PC26    PC27    PC28
Standard deviation     0.16565 0.15602 0.1344 0.12442 0.09043 0.08307 0.03987
Proportion of Variance 0.00091 0.00081 0.0006 0.00052 0.00027 0.00023 0.00005
Cumulative Proportion  0.99749 0.99830 0.9989 0.99942 0.99969 0.99992 0.99997
                          PC29    PC30
Standard deviation     0.02736 0.01153
Proportion of Variance 0.00002 0.00000
Cumulative Proportion  1.00000 1.00000
```

> Q4. From your results, what proportion of the original variance is captured by the first principal components (PC1)?

44.27%

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

3 PCs capture 72%

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

7 PCs capture 91%

Interpreting PCA results

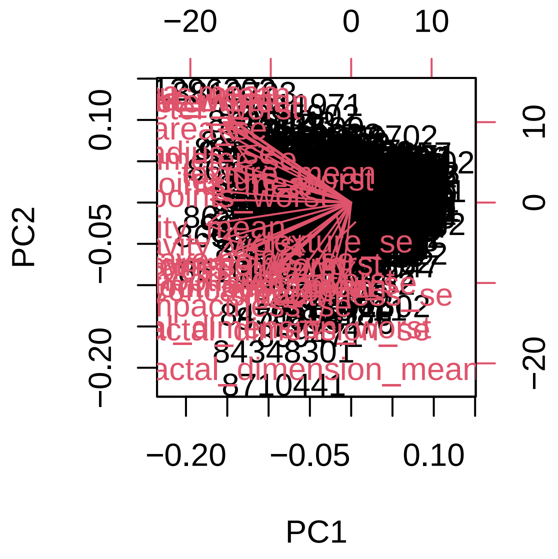
> Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?

There is a distinct difference between 2 sets of data. We need to better organize the data to make sense of it.

PC Plot

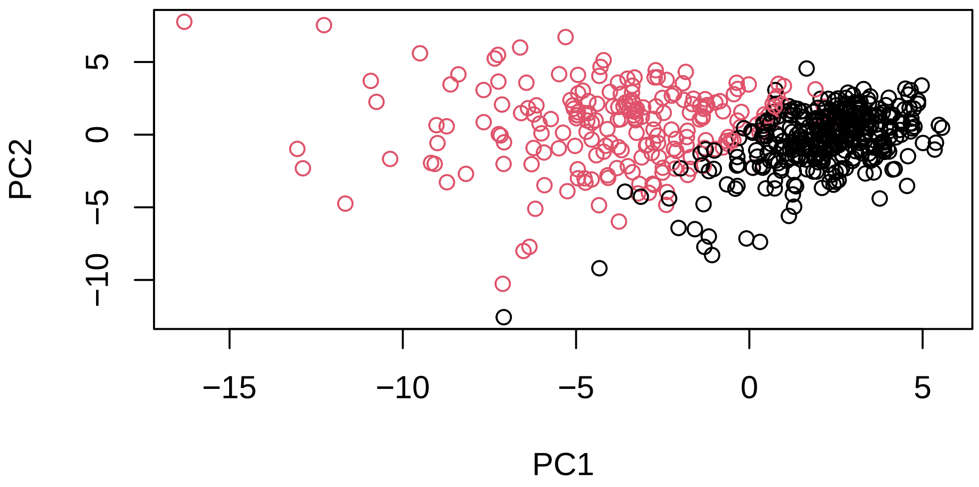
We need to make out plot of PC1 vs PC2 (aka score plot, PC-plot, etc.) The main results of PCA…

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



Scatter plot observations by components 1 and 2

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

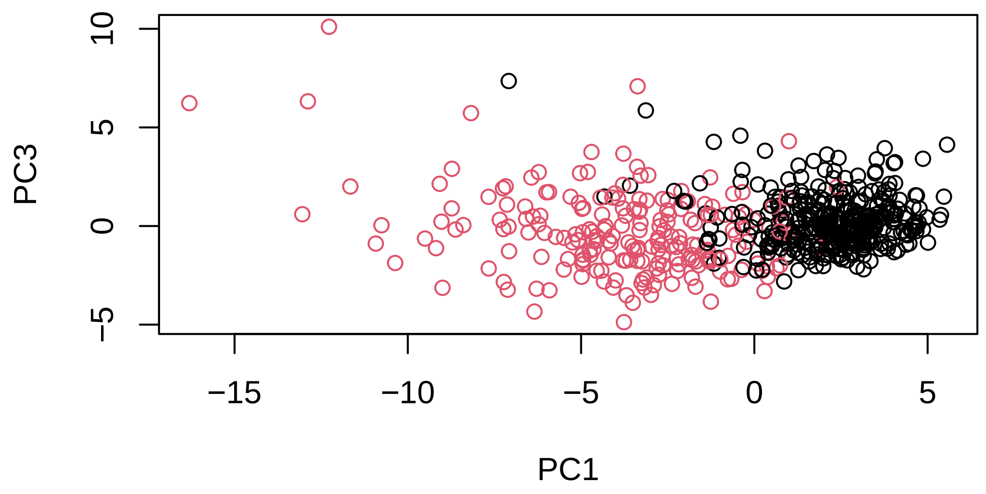


> Q8. Generate a similar plot for principal components 1 and 3. What do you notice about these plots?

The red and the black localization of points are around the same areas on the graph. The majority of the red dots is on the left of the majority of the black dots.

Repeat for components 1 and 3

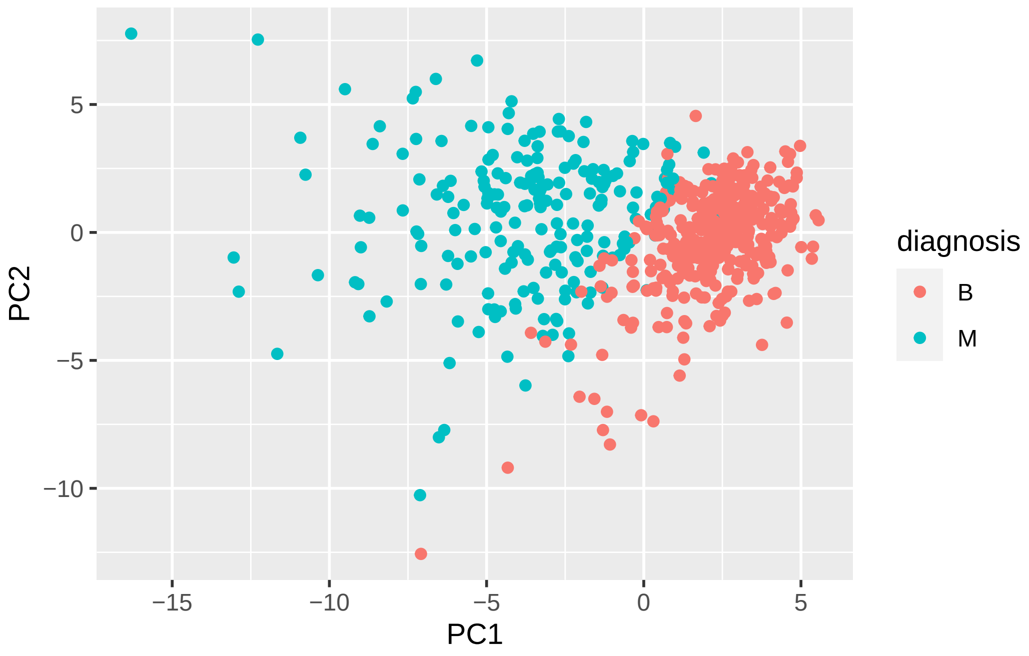
```r
plot(wisc.pr$x[,1], wisc.pr$x[,3], col = diagnosis,
     xlab = "PC1", ylab = "PC3")
```



```r
library(ggplot2)

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

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



Variance Explained

Calculate the variance of each principal component by squaring the sdev component of wisc.pr (i.e. wisc.pr$sdev^2). Save the result as an object called pr.var.

Calculate variance of each component

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

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

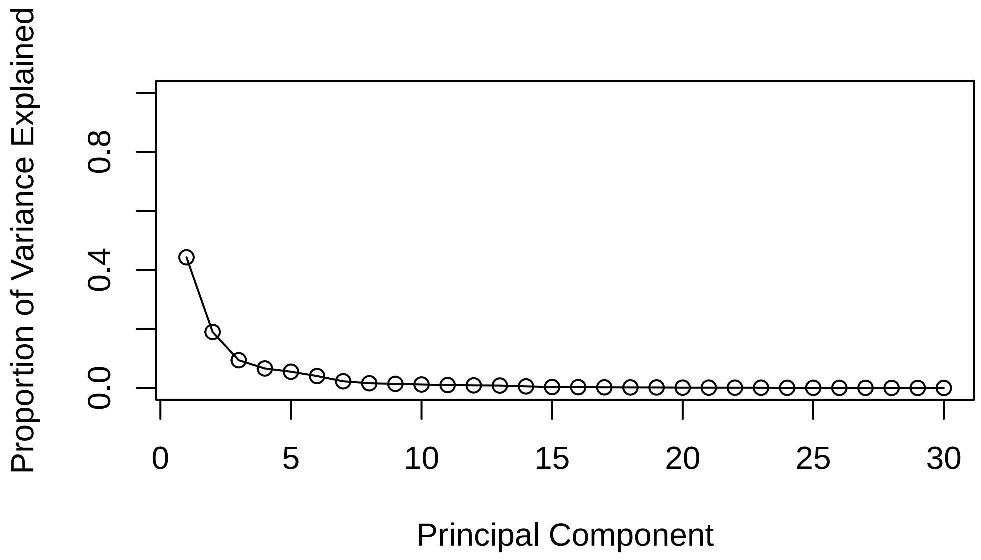
Calculate the variance explained by each principal component by dividing by the total variance explained of all principal components. Assign this to a variable called pve and create a plot of variance explained for each principal component.

Variance explained by each principal component: pve

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

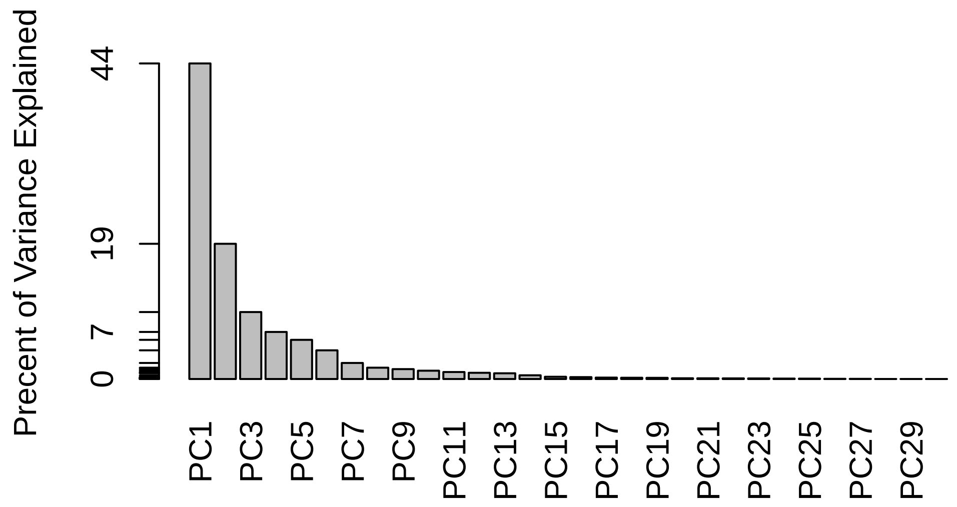
Plot variance explained for each principal component

```
plot(pve, xlab = "Principal Component",
     ylab = "Proportion of Variance Explained",
     ylim = c(0, 1), type = "o")
```



Alternative scree plot of the same data, note data driven y-axis

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



Communicating PCA results

> Q9. For the first principal component, what is the component of the loading vector (i.e. wisc.pr$rotation[,1]) for the feature concave.points_mean?

How much do the original variables contribute to the new PCs that we have calculated? To get at this data we can look at the '$rotation' component of the returned PCA object

```
head(wisc.pr$rotation[,1:3])
```

```
                        PC1         PC2          PC3
radius_mean      -0.2189024  0.23385713 -0.008531243
texture_mean     -0.1037246  0.05970609  0.064549903
perimeter_mean   -0.2275373  0.21518136 -0.009314220
area_mean        -0.2209950  0.23107671  0.028699526
smoothness_mean  -0.1425897 -0.18611302 -0.104291904
compactness_mean -0.2392854 -0.15189161 -0.074091571
```

Focus in on PC1

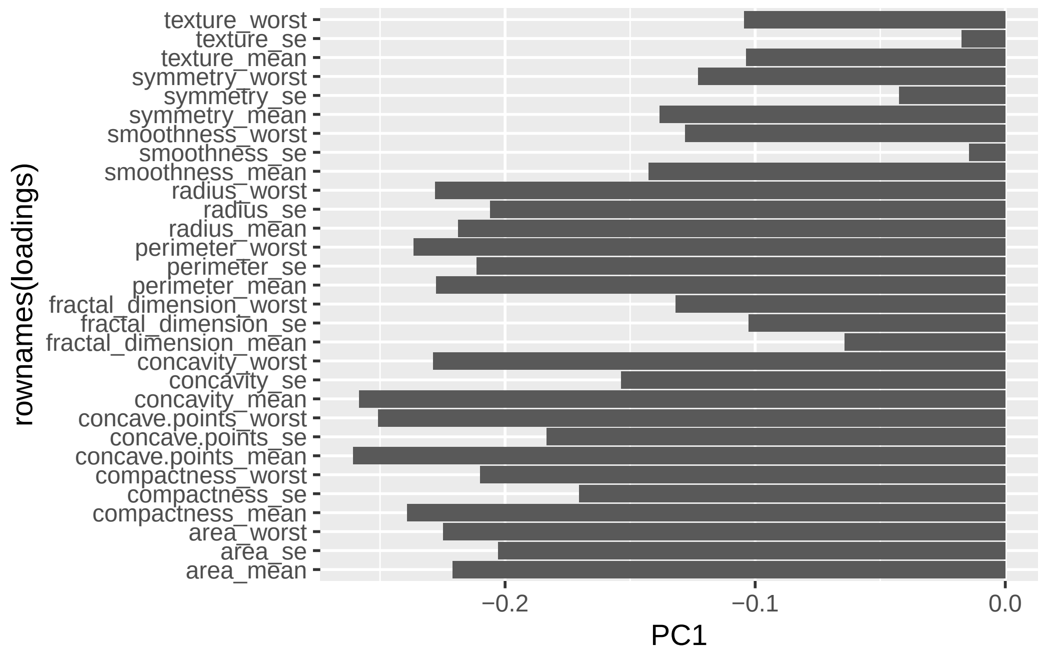
```
wisc.pr$rotation["concave.points_mean",1]
```

```
[1] -0.2608538
```

There is complicated mix of variables that go together to make up PC1 i.e. there are many of the original variables that together contribute highly to PC1.

```
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 for 85%

Hierarchical clustering

The goal of this section is to do hierarchical clustering of the original data.

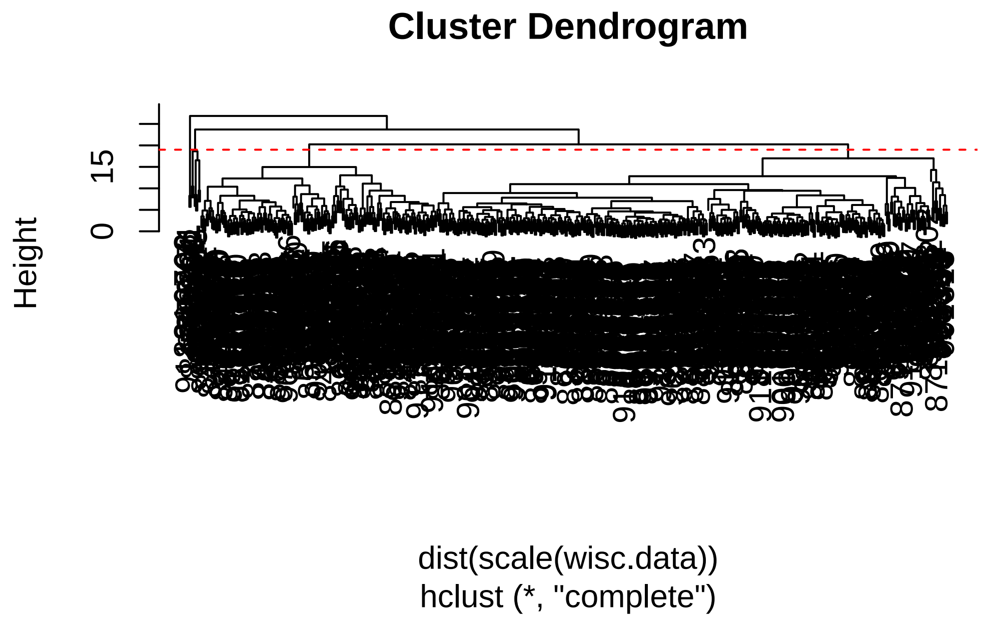
First we will scale the data, then distance matrix, then hclust

```r
data.scaled <- scale(wisc.data)
data.dist <- dist(data.scaled)
wisc.hclust <- hclust(dist(scale(wisc.data)))
```

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

Height 19

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



Cut this tree to yield cluster membership vector with 'cutree()' function. How well do the two clusters separate the M and B diagnoses?

```r
wisc.hclust.clusters <- cutree(wisc.hclust, h=19)
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?

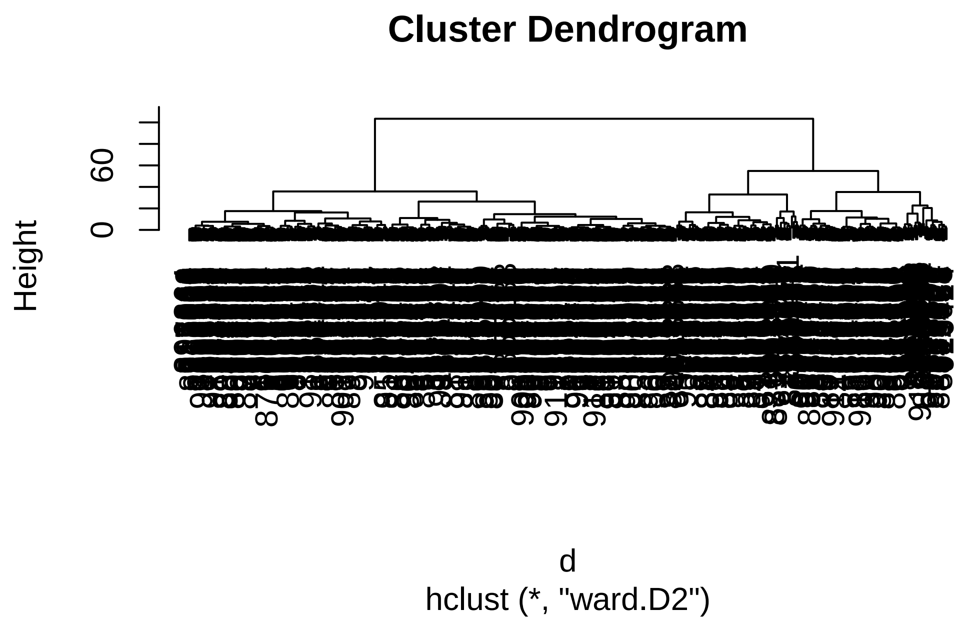
I think a better cluster vs diagnoses match would be at 10 since there is a bigger distinction between benign and malignant data points.

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

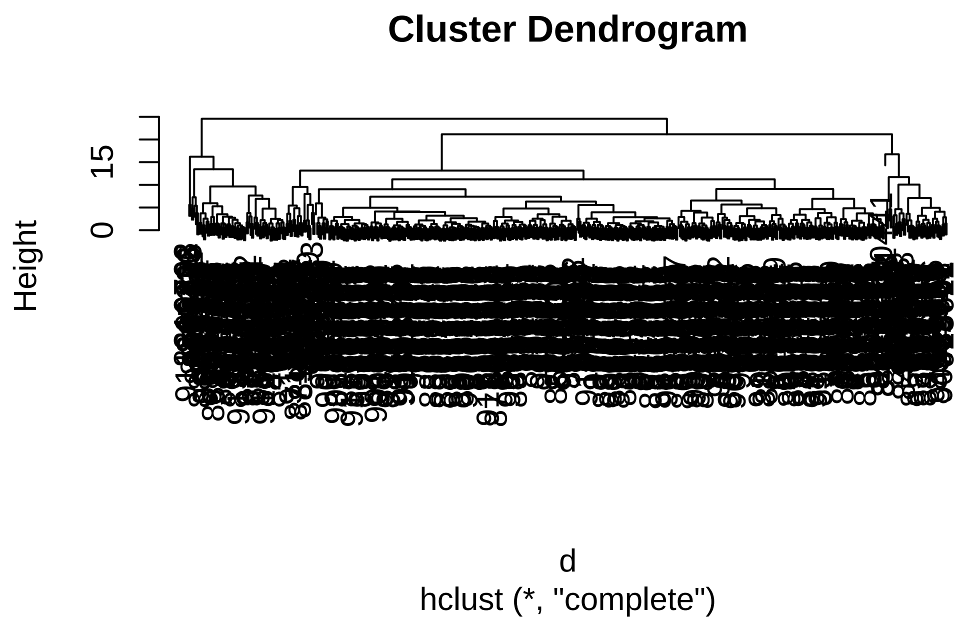
```
                    diagnosis
wisc.hclust.clusters   B   M
                  1   12  86
                  2    0  59
                  3    0   3
                  4  331  39
                  5    0  20
                  6    2   0
                  7   12   0
                  8    0   2
                  9    0   2
                  10   0   1
```

Try clustering in 3 PCs, that is PC1, PC2, and PC3 as input

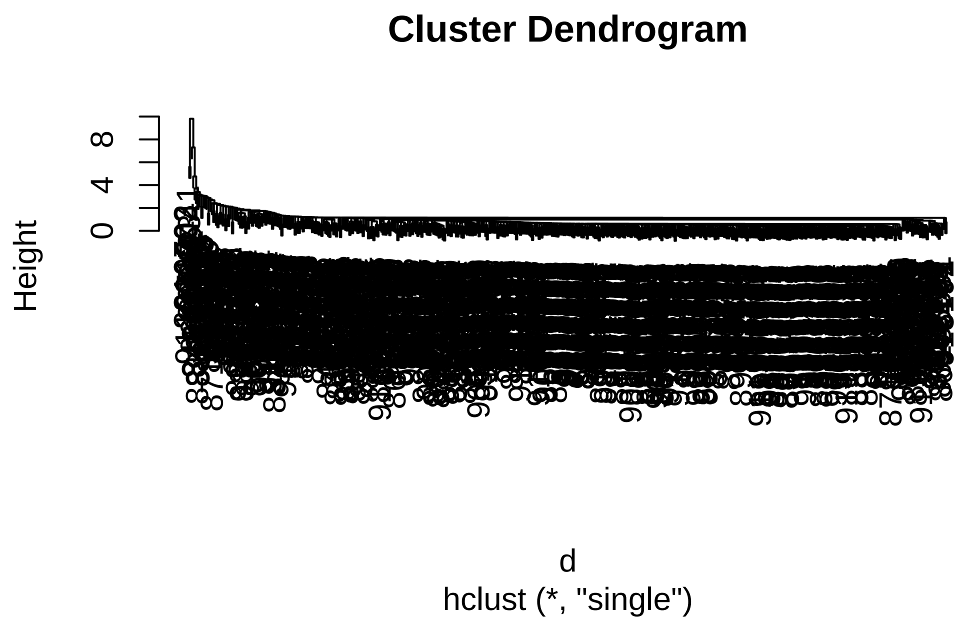
```
d <- dist(wisc.pr$x[,1:3])
wisc.pr.hclust <- hclust(d, method="ward.D2")
plot(wisc.pr.hclust)
```



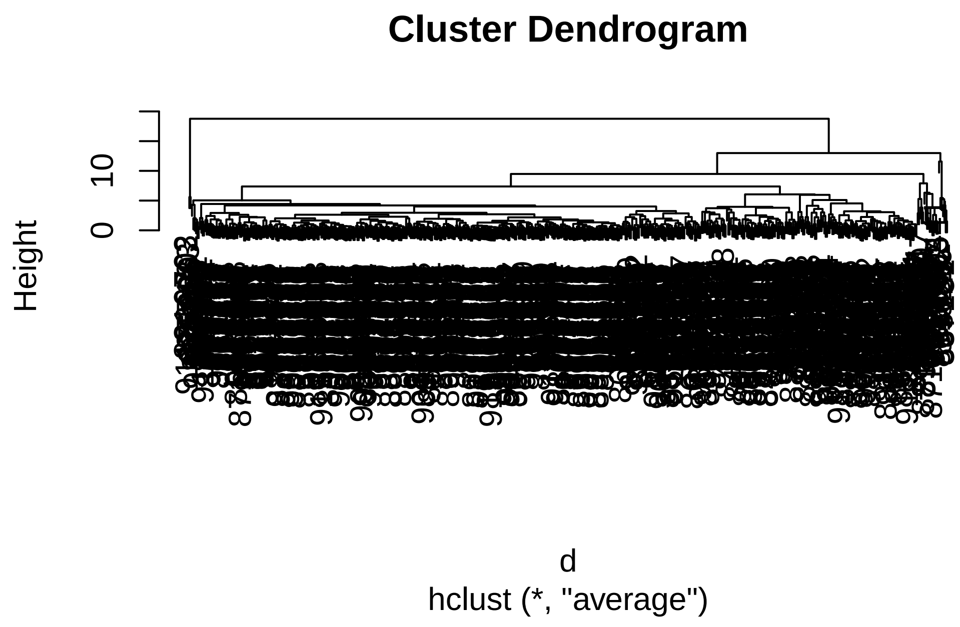
```r
d <- dist(wisc.pr$x[,1:3])
wisc.pr.hclust <- hclust(d, method="complete")
plot(wisc.pr.hclust)
```



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



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



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

My favorite method is the 'complete' because it distributes the branches more evenly and is easier to see the different branches.

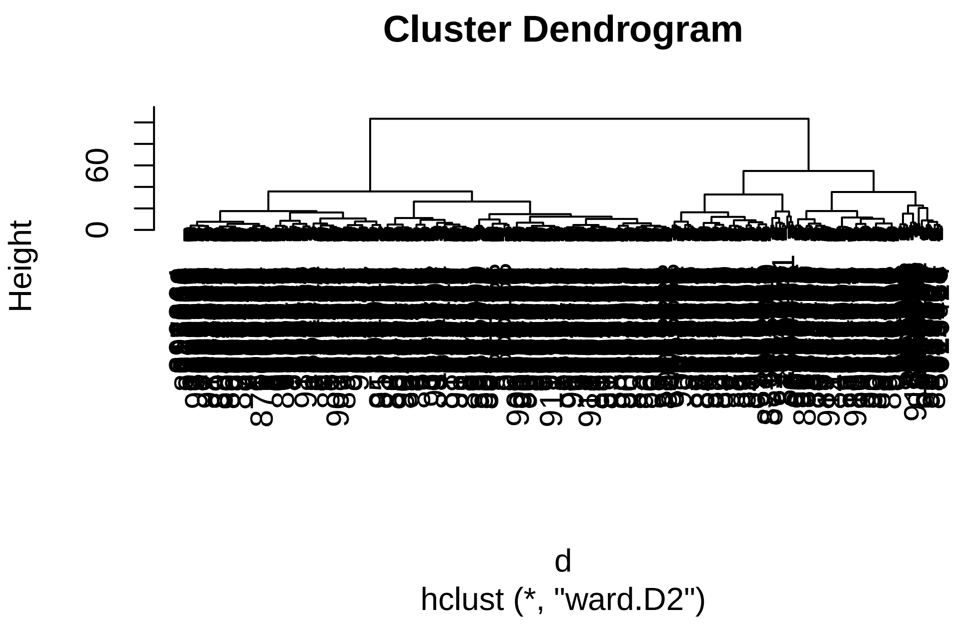
> Q15. How well does the newly created model with four clusters separate out the two diagnoses?

The newly created model with the four cluster separated out the points visually with the plot in different colors, but the table does not make a clear distinction between the patients with malignant and benign conditions.

#Combine methods: PCA and HCLUST My PCA results were interesting as they showed a separation of M and B samples along PC1.

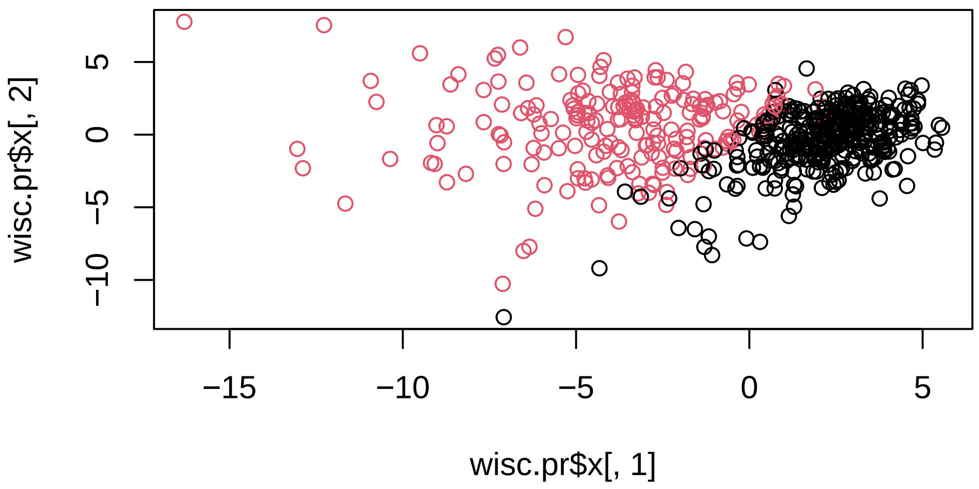
Let's cut this tree into four groups/clusters

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



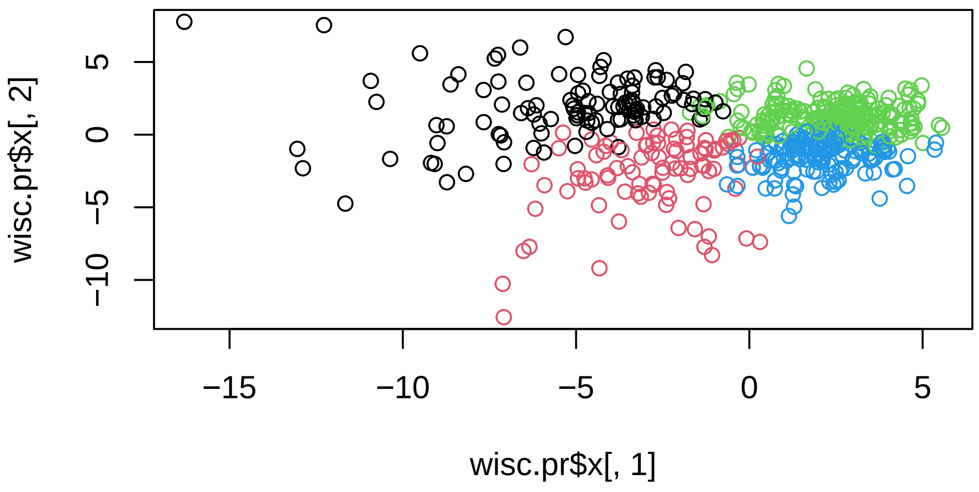
```
grps2 <- cutree(wisc.pr.hclust, k=4)
```

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



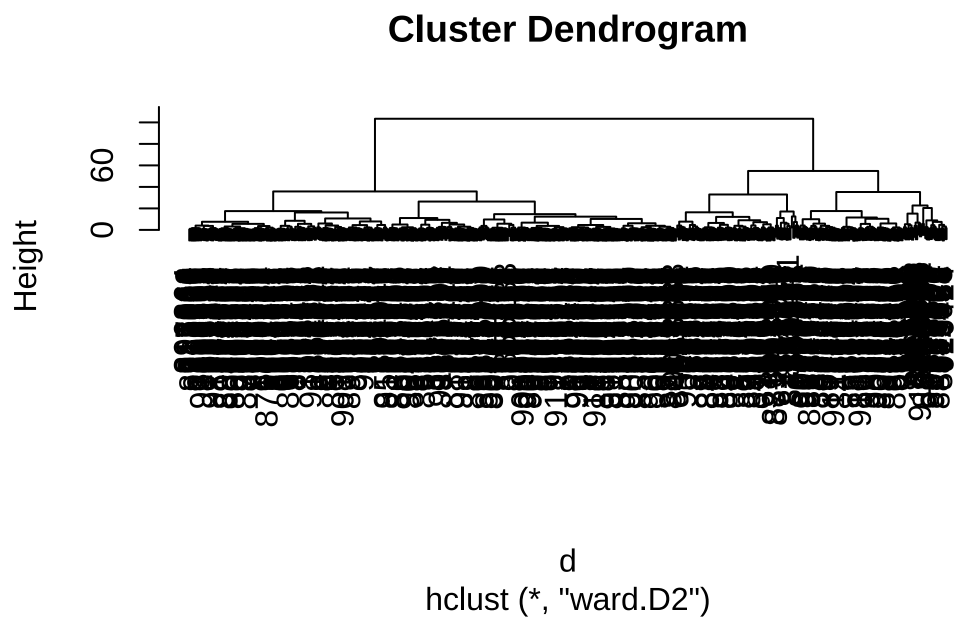
I want to cluster my PCA results - that is use 'wisc.pr$x' as input 'hclust()'

```
plot(wisc.pr$x[,1], wisc.pr$x[,2], col=grps2)
```



And my tree result figure

```
plot(wisc.pr.hclust)
```



Compare to actual diagnoses

```r
table(grps2, diagnosis)
```

```
     diagnosis
grps2   B   M
    1   0 111
    2  24  68
    3 184  32
    4 149   1
```

```r
(179+333)/nrow(wisc.data)
```

```
[1] 0.8998243
```