Class 08: Mini Project

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This is a mini project on data analysis of cancer cells. Data is collected from FNA on breast masses. Types of variables include: - radius - texture - smoothness - diagnosis (benign or malignant)

Download and Familiarize ourselves with the Dataset

First, we read in our data and view for errors:

```
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
```

We will now remove the diagnosis column as it is the professional diagnosis and the "answer" to which cells are malignant or benign and will not be in our analysis.

```
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
```

Now we will create a diagnosis vector for comparison later.

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

Q1. How many observations are in this dataset?

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

```
[1] 569
```

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

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

```
  B   M
357 212
```

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

First find the column names

```
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 "_mean" pattern. The 'grep()' function will help here. The 'length()' function can tell us how many that 'grep()' returned.

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

length(inds)
```

```
[1] 10
```

how many dimensions are in this dataset?

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

```
[1] 30
```

30 things were measured.

Principal Component. Analysis

First we need to scale the data. It would need to be scaled if the input data have significantly different variances or different units of measurement.

First we need to find the sd.

```
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
```

```r
# 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% is captured by PC1 (see proportion of variance)

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

3 PC's are required to describe at least 70% of the original variance. (see cumulative proportion)

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

7 PC's are required to describe at least 90% of the original variance (see cumulative proportion).

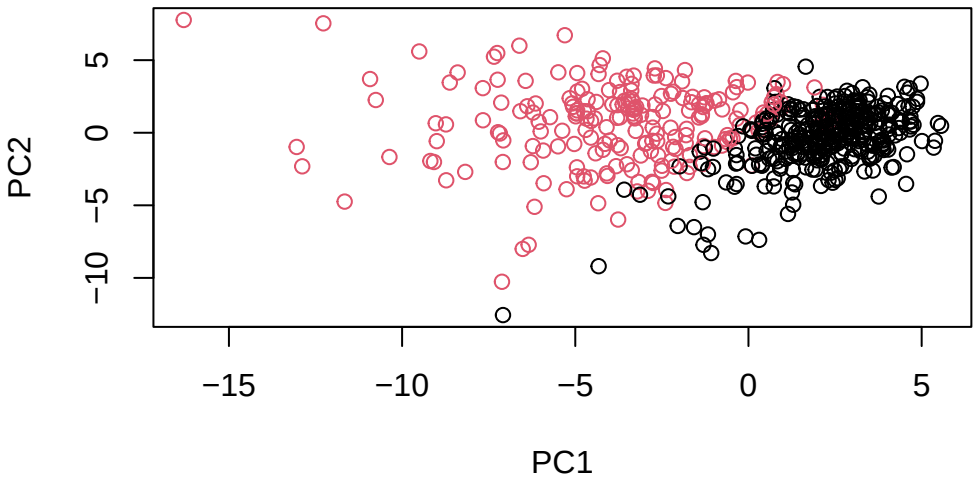
> Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?

This plot is impossible to understand. It is a huge mess. We cannot distinguish the malignant from the benign patients.

We need to make our plot of PC1 vs PC2 (aka score plot). The main result of our PCA:

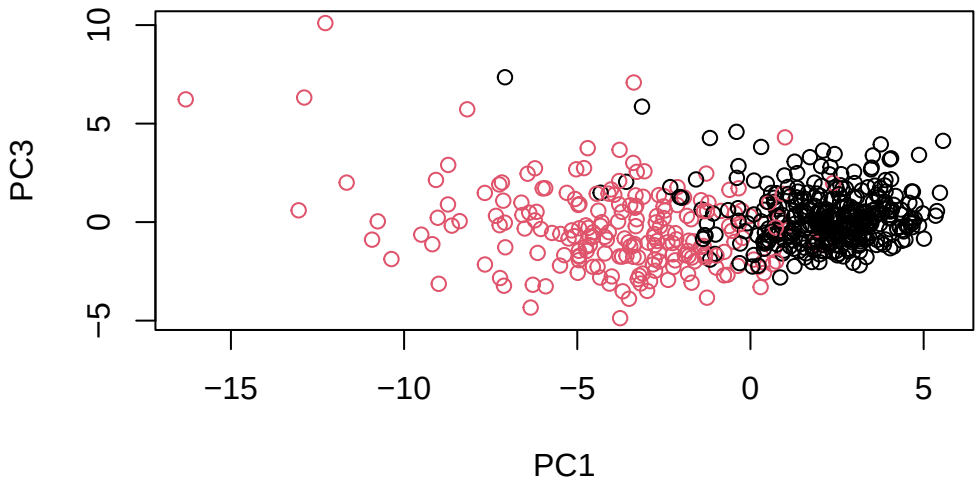
```
# Scatter plot observations by components 1 and 2

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?

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

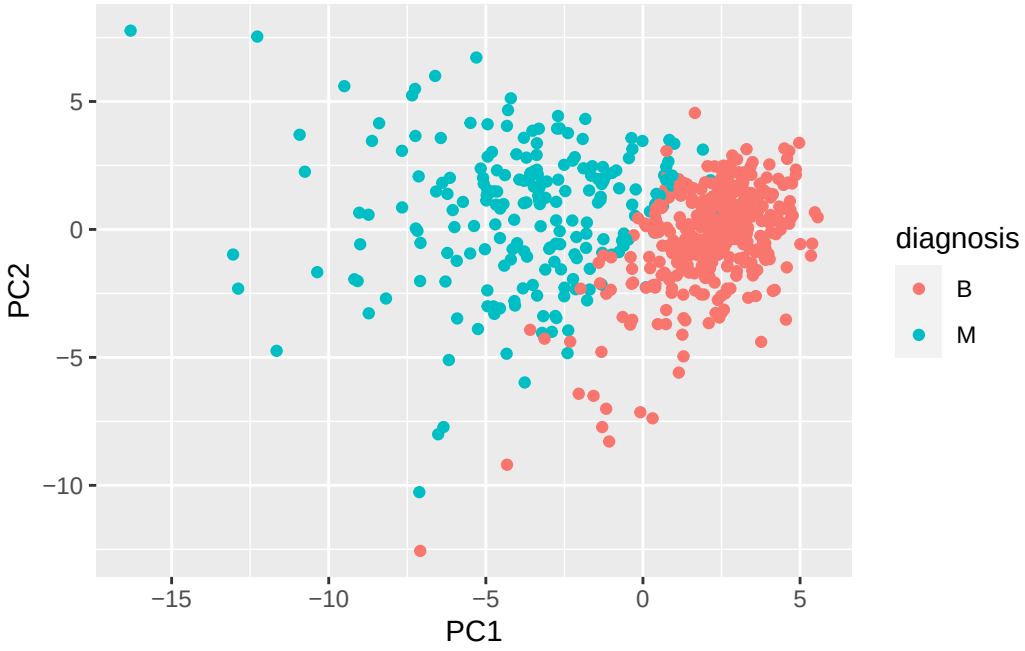


Let's make the same plot with ggplot:

```
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 component
pr.var <- wisc.pr$sdev^2

head(pr.var)
```

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

```
summary(wisc.pr)
```

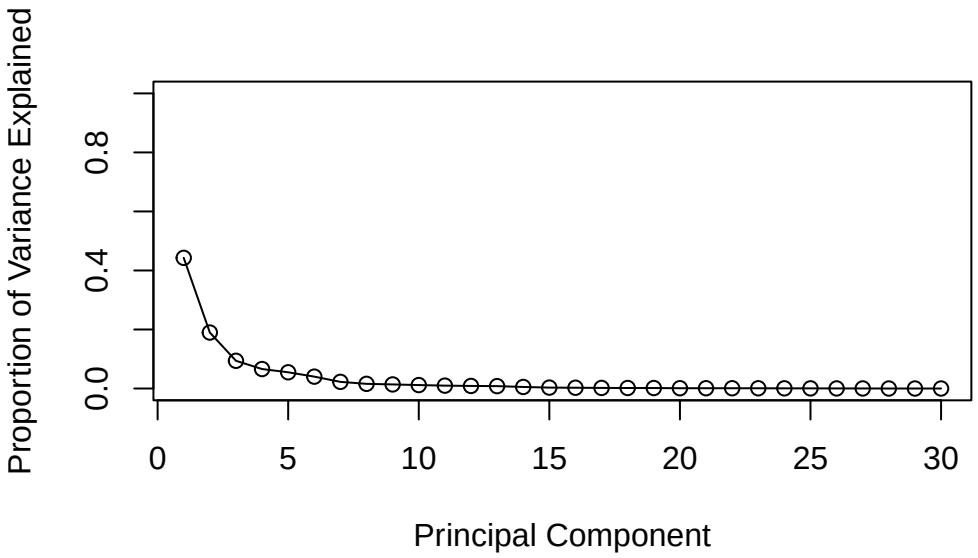
```
Importance of components:
                          PC1    PC2     PC3     PC4     PC5     PC6     PC7
Standard deviation     3.6444 2.3857 1.67867 1.40735 1.28403 1.09880 0.82172
Proportion of Variance 0.4427 0.1897 0.09393 0.06602 0.05496 0.04025 0.02251
Cumulative Proportion  0.4427 0.6324 0.72636 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
```

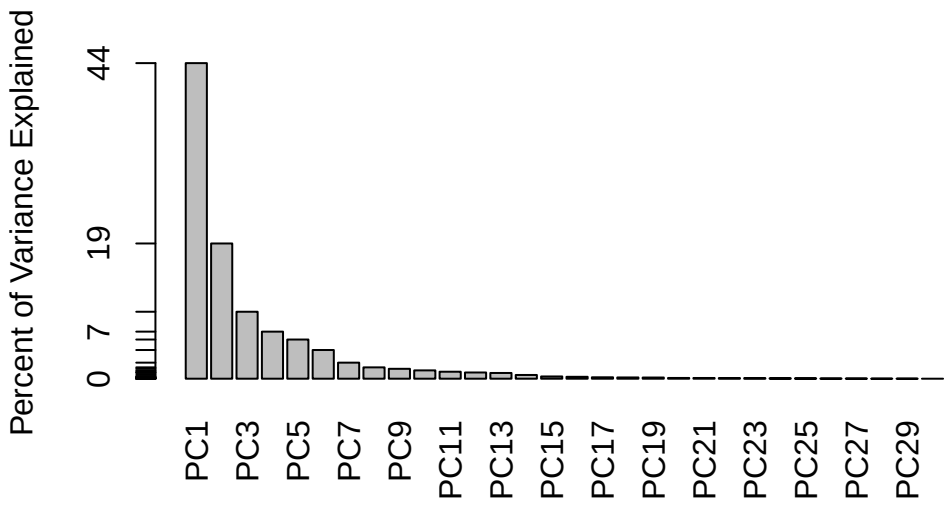
```r
#variance explained by each principal component:pve

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

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



```
#alternative scree plot of the same data, note data. driven y-axis
barplot(pve, ylab = "Percent of Variance Explained", names.arg = paste0("PC", 1:length(pve
axis(2, at=pve, labels = round(pve,2)*100)
```



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["concave.points_mean",1]
```

```
[1] -0.2608538
```

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

```
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
```

The minimum number of principal components required to explain at least 80% of the data is 5.

Hierarchical Clustering

```r
#scale the wisc.data using the 'scale()' function

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

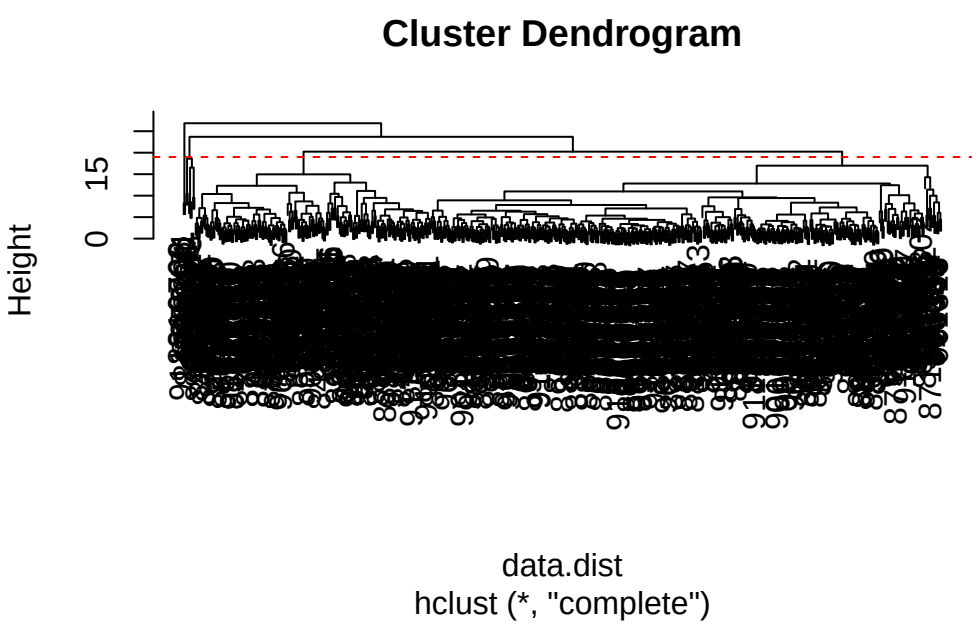
```r
#calculate the euclidean distance
data.dist <- dist(data.scaled)
```

```r
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?

```r
plot(wisc.hclust)

abline(h =19, col = "red", lty = 2)
```



19 is the height where we get 4 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
```

The data points.

> Q12. Can you find a better cluster vs diagnoses match by cutting into a different number of clusters between 2 and 10?

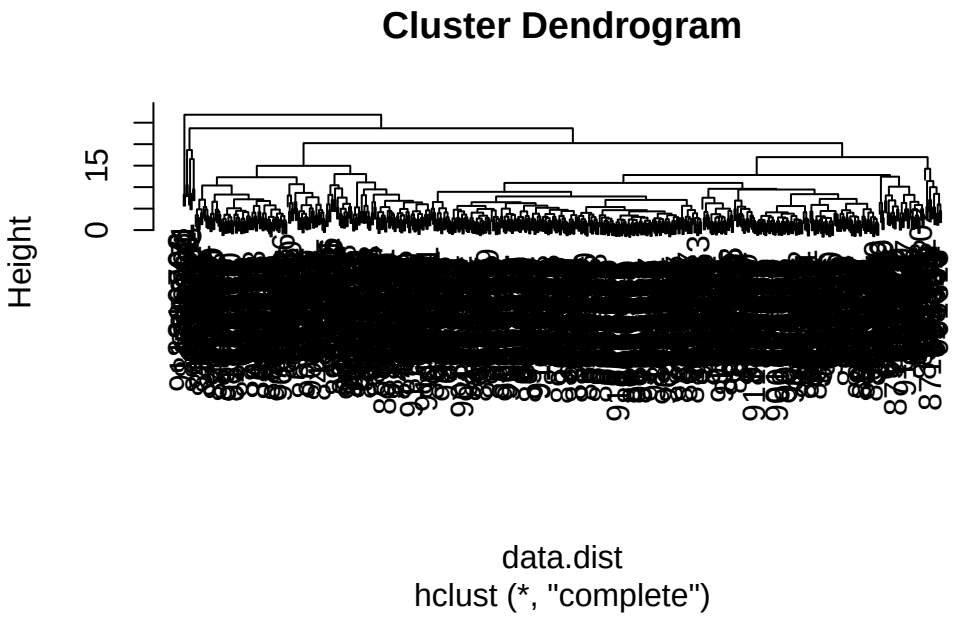
```
table(cutree(wisc.hclust, k =9), diagnosis)
```

```
  diagnosis
     B   M
1   12  86
2    0  79
3    0   3
4  331  39
5    2   0
6   12   0
7    0   2
8    0   2
9    0   1
```

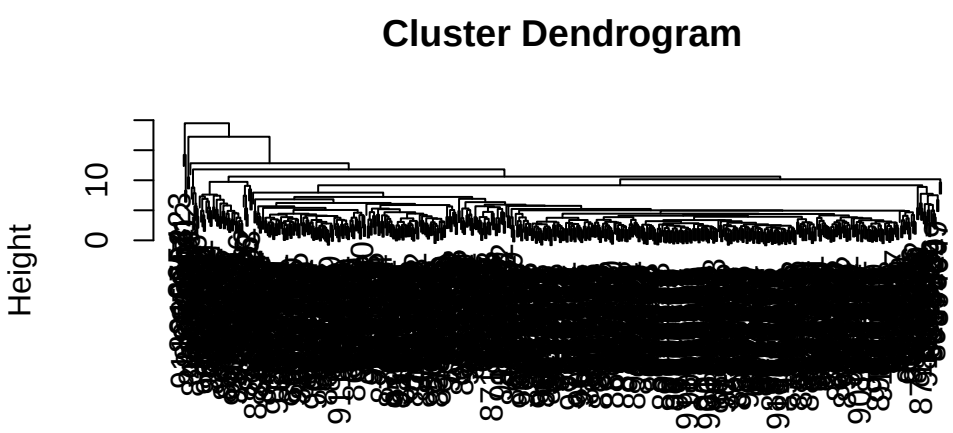
I could not find a number of clusters that would result in a better diagnoses match than 4.

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

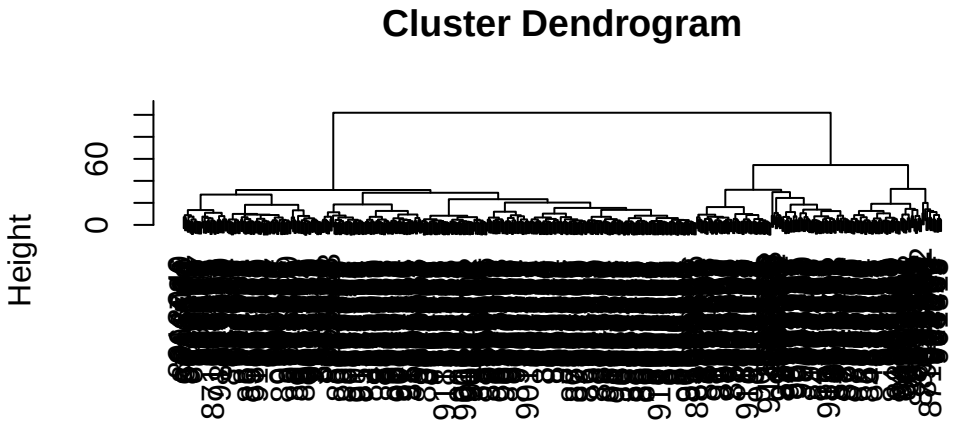
```
plot(hclust(data.dist, method = "complete"))
```




```
plot(hclust(data.dist, method = "average"))
```




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



My favorite method is the ward.D2 because it uses a bottom-up strategy and the resulting dendogram looks much clearer to me.

Combine Results: PCA and HCLUST

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

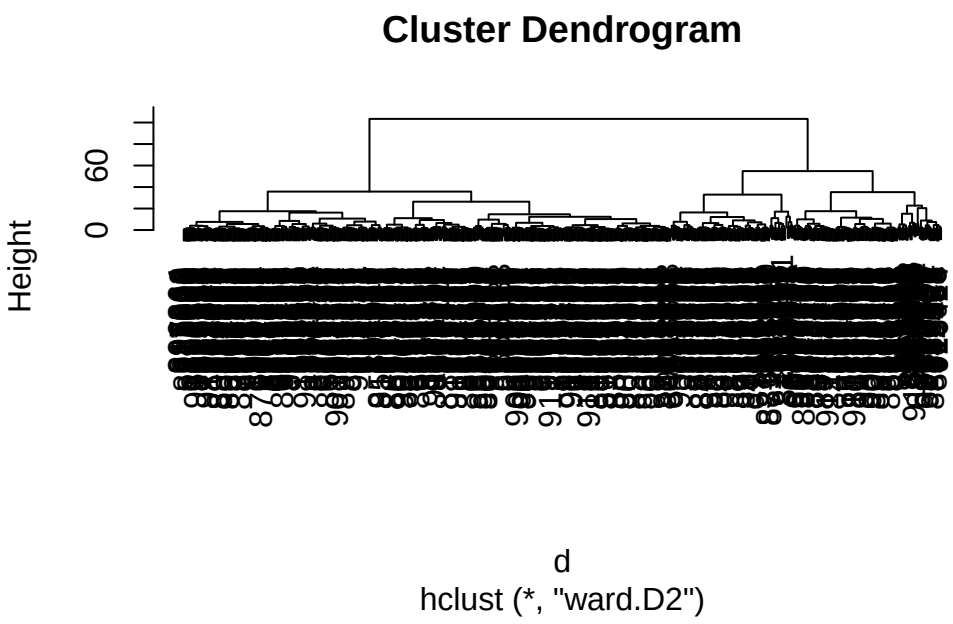
I want to cluster my PCA results - that is use 'wisc.pr$x' as input to hclust().

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)
```

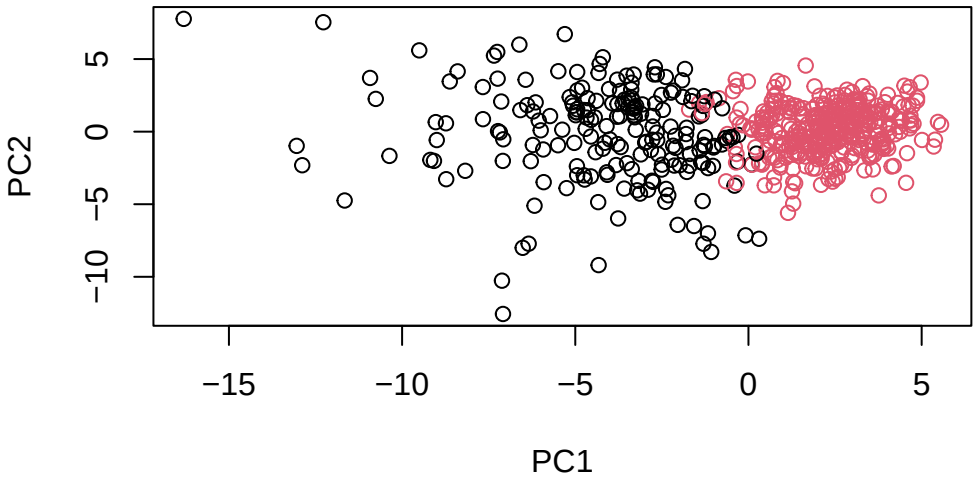


Let's cut this tree into two groups/clusters

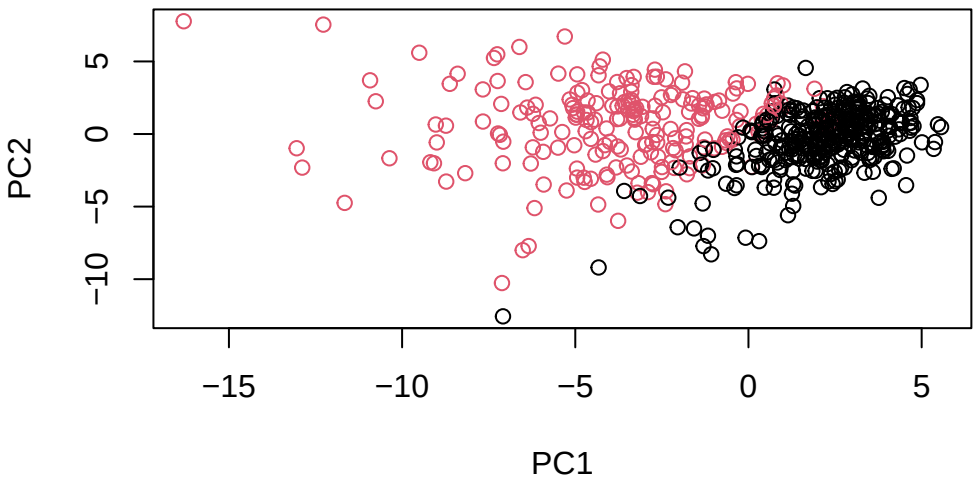
```
grps <- cutree(wisc.pr.hclust, k=2)
table(grps, diagnosis)
```

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

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




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



The HCLUST produced a very similar graph to that of the diagnoses.

How well do the two clusters separate the M and B diagnoses?

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

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

There are 33 false positives - 33 people whose lives are changed by a wrong diagnosis.

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

```
[1] 0.8998243
```

This is ~90% accuracy from this HCLUST diagram.

This is exploratory and we can revise and perhaps get better accuracy.

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

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

```
(188+329)/(nrow(wisc.data))
```

```
[1] 0.9086116
```

They separate out the two diagnoses with approximately 91% accuracy.