Class 8: Unsupervised Mini Project

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It is important to consider scaling your dataset

```
head(mtcars)
```

```
                   mpg cyl disp  hp drat    wt  qsec vs am gear carb
Mazda RX4         21.0   6  160 110 3.90 2.620 16.46  0  1    4    4
Mazda RX4 Wag     21.0   6  160 110 3.90 2.875 17.02  0  1    4    4
Datsun 710        22.8   4  108  93 3.85 2.320 18.61  1  1    4    1
Hornet 4 Drive    21.4   6  258 110 3.08 3.215 19.44  1  0    3    1
Hornet Sportabout 18.7   8  360 175 3.15 3.440 17.02  0  0    3    2
Valiant           18.1   6  225 105 2.76 3.460 20.22  1  0    3    1
```

```
colMeans(mtcars)
```

```
       mpg        cyl       disp         hp       drat         wt       qsec 
 20.090625   6.187500 230.721875 146.687500   3.596563   3.217250  17.848750 
        vs         am       gear       carb 
  0.437500   0.406250   3.687500   2.812500 
```

```
apply(mtcars, 2, sd)
```

```
       mpg        cyl       disp         hp       drat         wt 
 6.0269481  1.7859216 123.9386938  68.5628685  0.5346787  0.9784574 
      qsec         vs         am       gear       carb 
 1.7869432  0.5040161  0.4989909  0.7378041  1.6152000 
```

```
x<- scale(mtcars)
head(x)
```

```
                           mpg        cyl        disp         hp       drat
Mazda RX4           0.1508848 -0.1049878 -0.57061982 -0.5350928  0.5675137
Mazda RX4 Wag       0.1508848 -0.1049878 -0.57061982 -0.5350928  0.5675137
Datsun 710          0.4495434 -1.2248578 -0.99018209 -0.7830405  0.4739996
Hornet 4 Drive      0.2172534 -0.1049878  0.22009369 -0.5350928 -0.9661175
Hornet Sportabout -0.2307345  1.0148821  1.04308123  0.4129422 -0.8351978
Valiant           -0.3302874 -0.1049878 -0.04616698 -0.6080186 -1.5646078
                           wt       qsec         vs         am       gear
Mazda RX4         -0.610399567 -0.7771651 -0.8680278  1.1899014  0.4235542
Mazda RX4 Wag     -0.349785269 -0.4637808 -0.8680278  1.1899014  0.4235542
Datsun 710        -0.917004624  0.4260068  1.1160357  1.1899014  0.4235542
Hornet 4 Drive    -0.002299538  0.8904872  1.1160357 -0.8141431 -0.9318192
Hornet Sportabout  0.227654255 -0.4637808 -0.8680278 -0.8141431 -0.9318192
Valiant            0.248094592  1.3269868  1.1160357 -0.8141431 -0.9318192
                          carb
Mazda RX4          0.7352031
Mazda RX4 Wag      0.7352031
Datsun 710        -1.1221521
Hornet 4 Drive    -1.1221521
Hornet Sportabout -0.5030337
Valiant           -1.1221521
```

```r
round(colMeans(x),2)
```

```
 mpg  cyl disp   hp drat   wt qsec   vs   am gear carb
   0    0    0    0    0    0    0    0    0    0    0
```

```r
apply(x,2,sd)
```

```
 mpg  cyl disp   hp drat   wt qsec   vs   am gear carb
   1    1    1    1    1    1    1    1    1    1    1
```

Key point: It is always a good idea to scale your data before to PCA

Breast Cancer Bioposy Analysis

```r
# 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)
# We can use -1 here to remove the first column
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
```

```
# Create diagnosis vector for later
diagnosis<- wisc.df[,1]
head(diagnosis)
```

```
[1] "M" "M" "M" "M" "M" "M"
```

We remove the first diagnosis column as it is essentially the "answer" and we do not want it to affect our analysis results.

Q1. How many observations are in this dataset?

```
dim(wisc.df)
```

```
[1] 569  31
```

The `dim()` function helps to compute a total of 569 observations in this data frame.

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

```
table(diagnosis)
```

```
diagnosis
  B   M
357 212
```

The `table()` function shows us that there are a total of 212 malignant diagnosis in the data set

Remove the first diagnosis column as it is essentially the "answer" and we do not want it to affect our analysis results.

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

```
q3 <- sum(grepl("_mean$", names(wisc.df)))
q3
```

```
[1] 10
```

There are 10 variables/features that are suffixed with _mean

Performing PCA

```
# Check column means and standard deviations
colMeans(wisc.data)
```

```
            radius_mean            texture_mean          perimeter_mean
           1.412729e+01            1.928965e+01            9.196903e+01
              area_mean         smoothness_mean        compactness_mean
           6.548891e+02            9.636028e-02            1.043410e-01
         concavity_mean     concave.points_mean          symmetry_mean
           8.879932e-02            4.891915e-02            1.811619e-01
 fractal_dimension_mean               radius_se              texture_se
           6.279761e-02            4.051721e-01            1.216853e+00
           perimeter_se                 area_se           smoothness_se
           2.866059e+00            4.033708e+01            7.040979e-03
         compactness_se            concavity_se       concave.points_se
           2.547814e-02            3.189372e-02            1.179614e-02
            symmetry_se    fractal_dimension_se            radius_worst
```

```
          2.054230e-02            3.794904e-03            1.626919e+01
         texture_worst         perimeter_worst              area_worst
          2.567722e+01            1.072612e+02            8.805831e+02
     smoothness_worst       compactness_worst         concavity_worst
          1.323686e-01            2.542650e-01            2.721885e-01
 concave.points_worst          symmetry_worst fractal_dimension_worst
          1.146062e-01            2.900756e-01            8.394582e-02
```

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

```
           radius_mean            texture_mean          perimeter_mean
          3.524049e+00            4.301036e+00            2.429898e+01
             area_mean         smoothness_mean        compactness_mean
          3.519141e+02            1.406413e-02            5.281276e-02
        concavity_mean     concave.points_mean          symmetry_mean
          7.971981e-02            3.880284e-02            2.741428e-02
 fractal_dimension_mean               radius_se              texture_se
          7.060363e-03            2.773127e-01            5.516484e-01
          perimeter_se                 area_se          smoothness_se
          2.021855e+00            4.549101e+01            3.002518e-03
        compactness_se            concavity_se       concave.points_se
          1.790818e-02            3.018606e-02            6.170285e-03
           symmetry_se    fractal_dimension_se            radius_worst
          8.266372e-03            2.646071e-03            4.833242e+00
         texture_worst         perimeter_worst              area_worst
          6.146258e+00            3.360254e+01            5.693570e+02
     smoothness_worst       compactness_worst         concavity_worst
          2.283243e-02            1.573365e-01            2.086243e-01
 concave.points_worst          symmetry_worst fractal_dimension_worst
          6.573234e-02            6.186747e-02            1.806127e-02
```

Need to scale data before conducting PCA because means and standard deviation all exhibit a very broad range and are on different scales

```
# Perform PCA on wisc.data by completing the following code
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 components (PC1)?

According to PC1, 44.3% of the original variance is captured

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

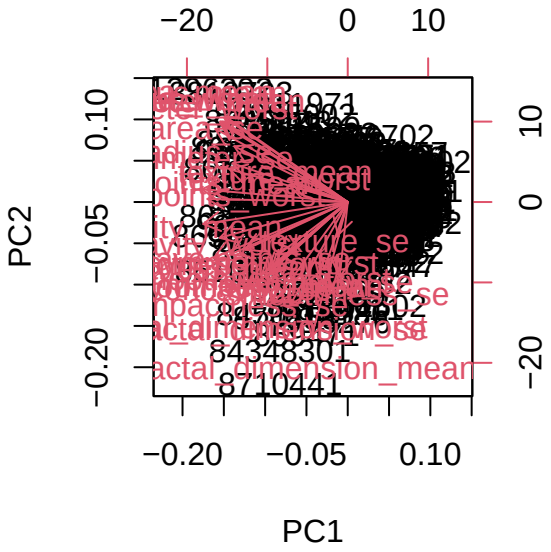
3 PCs are required to describe at least 70% of the original variance in the data

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

7 PCs are required to describe at least 90% of the original variance in the data

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

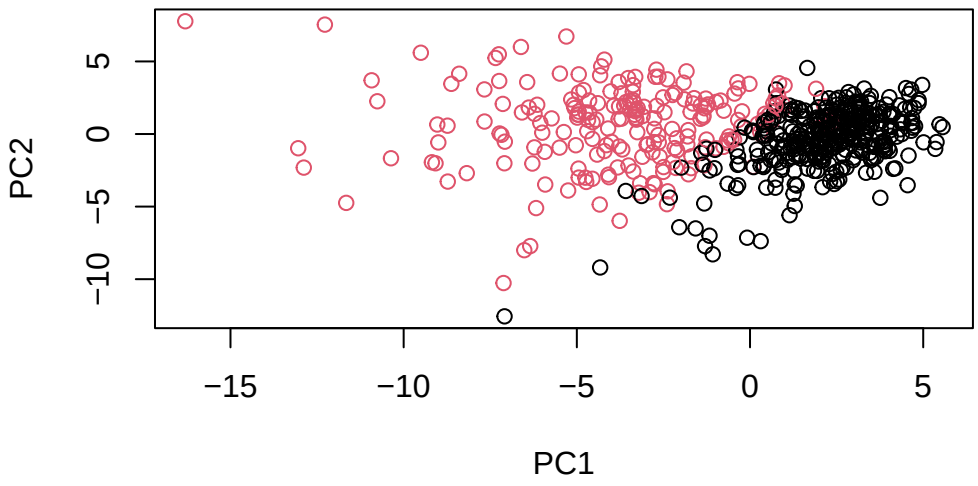
```
biplot(wisc.pr)
```



This plot stands out as very crowded and dense, with almost too much information provided on the plot to the extent in which it is very difficult to draw any conclusions. Furthermore they are four dimensions on this plot which may be better represented with a different plot type of method.

Main "PC score plot"

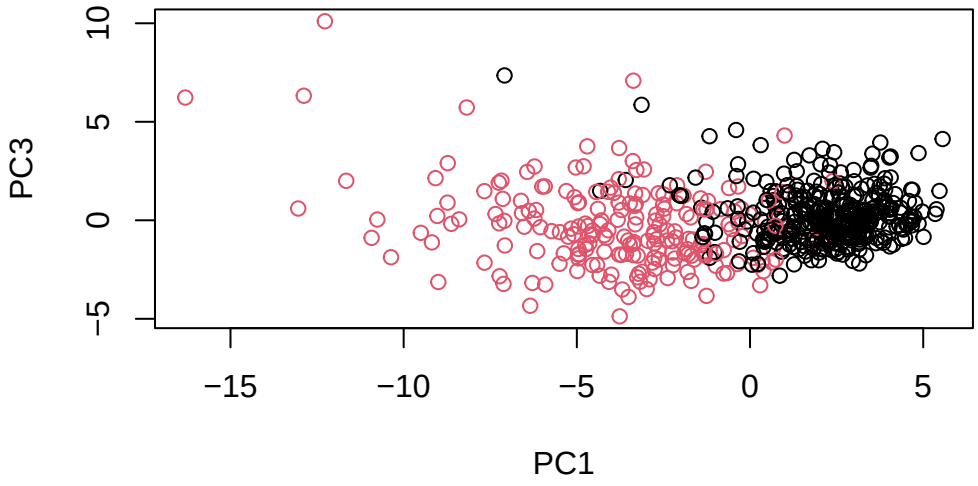
```
plot(wisc.pr$x[,1],wisc.pr$x[,2], col=as.factor(diagnosis),  xlab = "PC1", ylab = "PC2")
```



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

These plots do a much better job and cleaning up the data and grouping the patients by malignant and benign, showing the clear distinction between the diagnosis based on the location and color of the points. There is a clear separation between diagnosis and this can lead to many groundbreaking hypothesis and conclusions for these given patient subgroups based on the data-set.

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



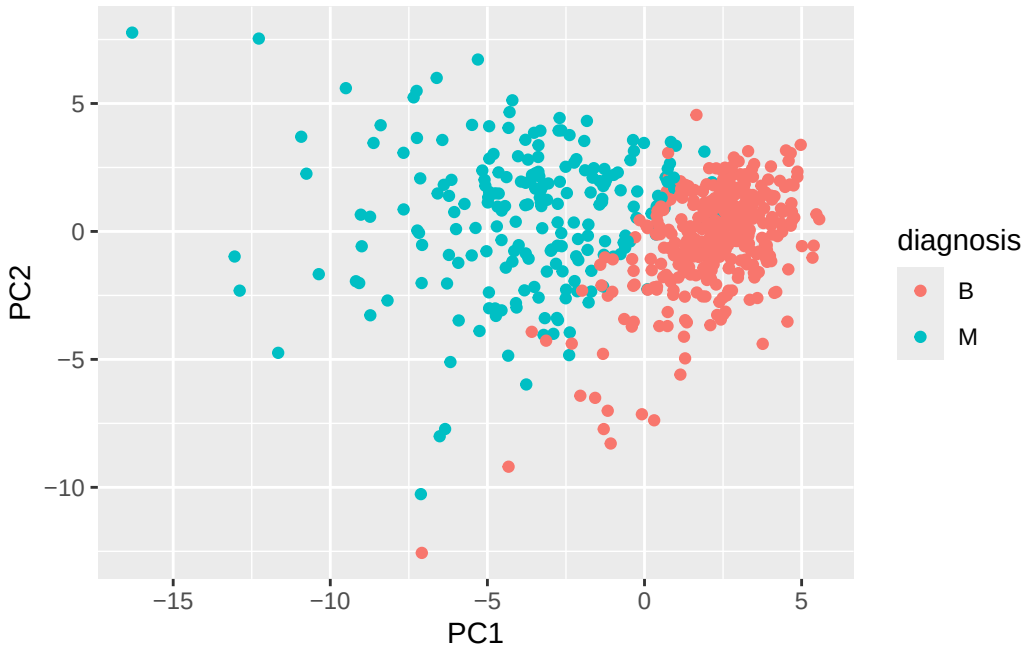
Making plot using ggplot function

```
# Create a data.frame for ggplot
df <- as.data.frame(wisc.pr$x)
df$diagnosis <- diagnosis

# Load the ggplot2 package
library(ggplot2)
```

```
Warning: package 'ggplot2' was built under R version 4.3.3
```

```
# Make a scatter plot colored by diagnosis
ggplot(df) +
  aes(PC1, PC2, col= diagnosis) +
  geom_point()
```



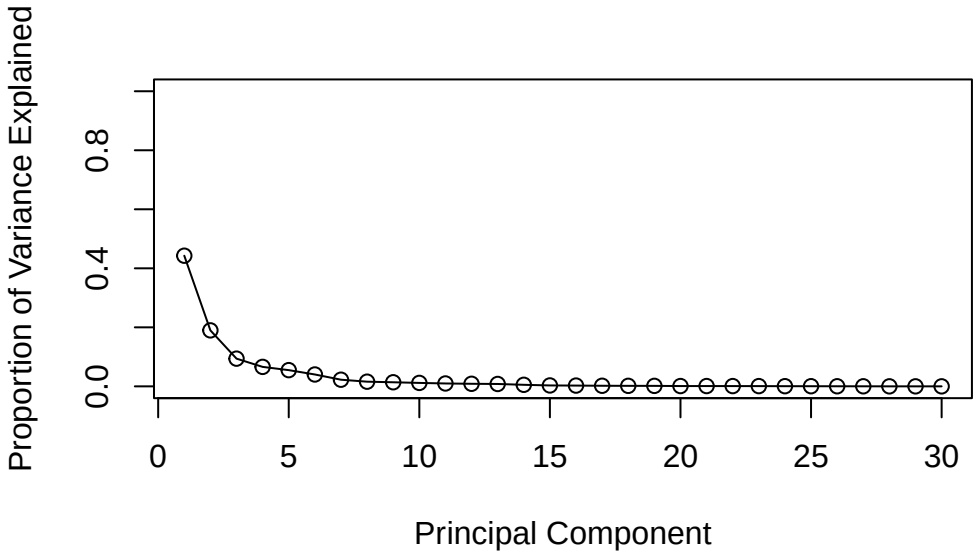
Calculating the Variance

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

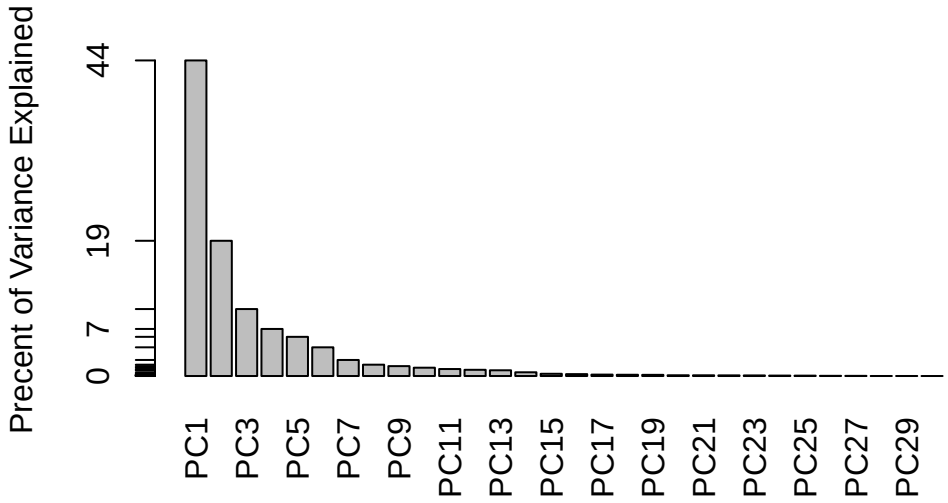
```
[1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

```
# 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 )
```



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?

```
q9<- wisc.pr$rotation["concave.points_mean",1]
q9
```

```
[1] -0.2608538
```

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

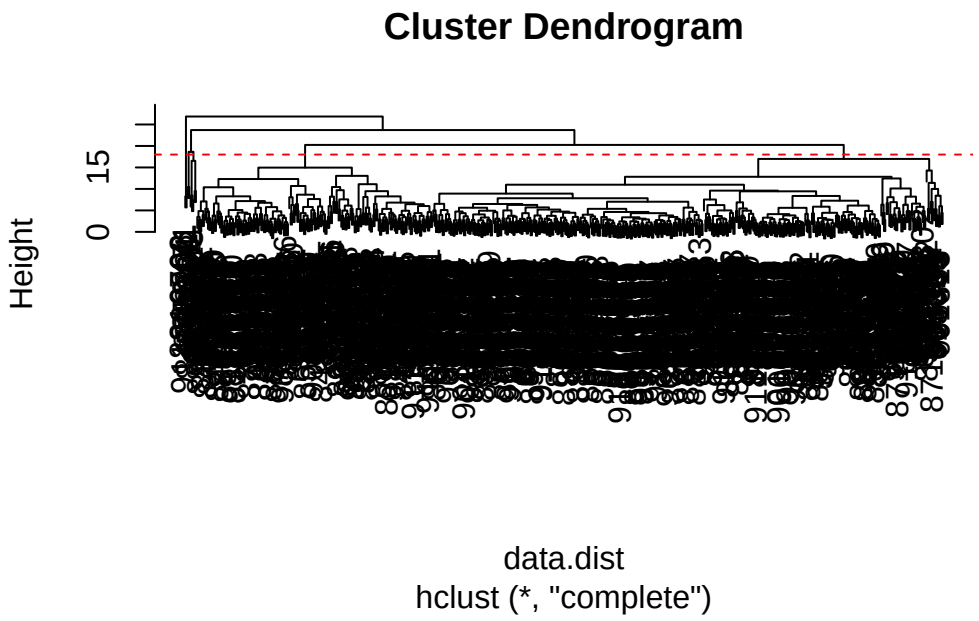
5 PCs is the minimum number of principal components required to explain 80% of the variance of the data

Heirachical Clustering

```
# Scale the wisc.data data using the "scale()" function
data.scaled <- scale(wisc.data)
data.dist <- dist(data.scaled)
wisc.hclust <- hclust(data.dist, "complete")
```

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

```
plot(wisc.hclust)
abline(h=18, col="red", lty=2)
```



Height of 18 allows us to see 4 distinct clusters in the dendrogam.

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?

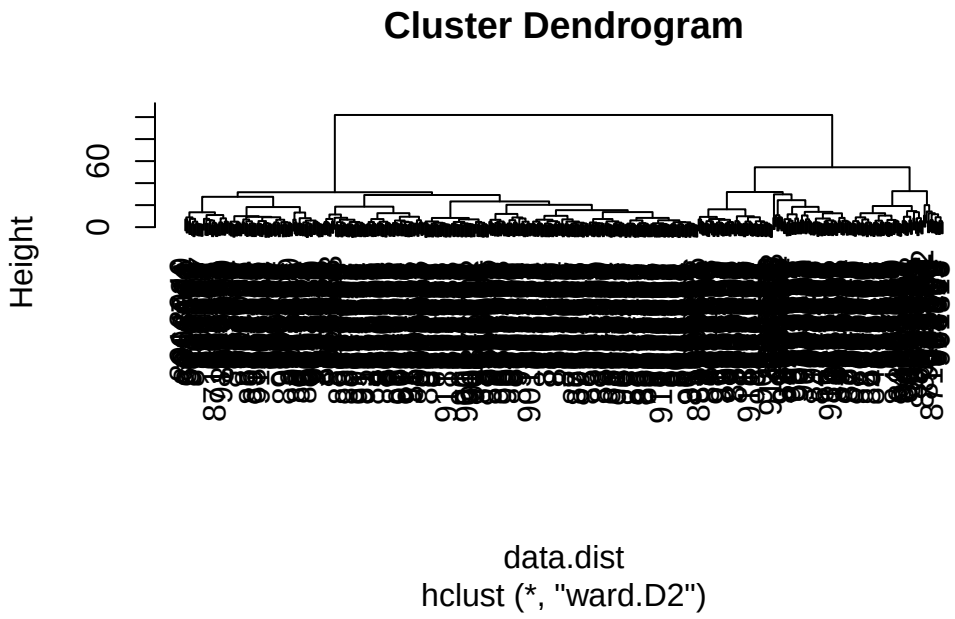
```
wisc.hclust.clusters <- cutree(wisc.hclust, k=6)
table(wisc.hclust.clusters, diagnosis)
```

```
                    diagnosis
wisc.hclust.clusters   B   M
                   1  12 165
                   2   0   5
                   3 331  39
                   4   2   0
                   5  12   1
                   6   0   2
```

No I could not find a better clustering scheme as going greater than 4 clusters created groupings that were no more specific for malignant and benign, and did not reduce the likelihood of false positives/negatives, making the extra grouping not helpful and just less representative overall. When decreasing the grouping to less than 3, the groups would then overlap and you will begin to get crossover between malignant and benign diagnosis which is not useful as well.

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

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



I very much prefer the `ward.D2` method of clustering this makes a plot that clearly shows two defined and representative groups of benign and malignant, without too much excess or crowding of information of groups that does not add to the overall story of the data. Other methods tend to create too many different groups and subgroups which can be tedious to work through to simply reach the same end goal of two main subgroup populations.

##Optional: K-means Clustering

```
wisc.km <- kmeans(scale(wisc.data), centers= 2, nstart= 20)
table(wisc.km$cluster, diagnosis)
```

```
   diagnosis
      B   M
  1 343  37
  2  14 175
```

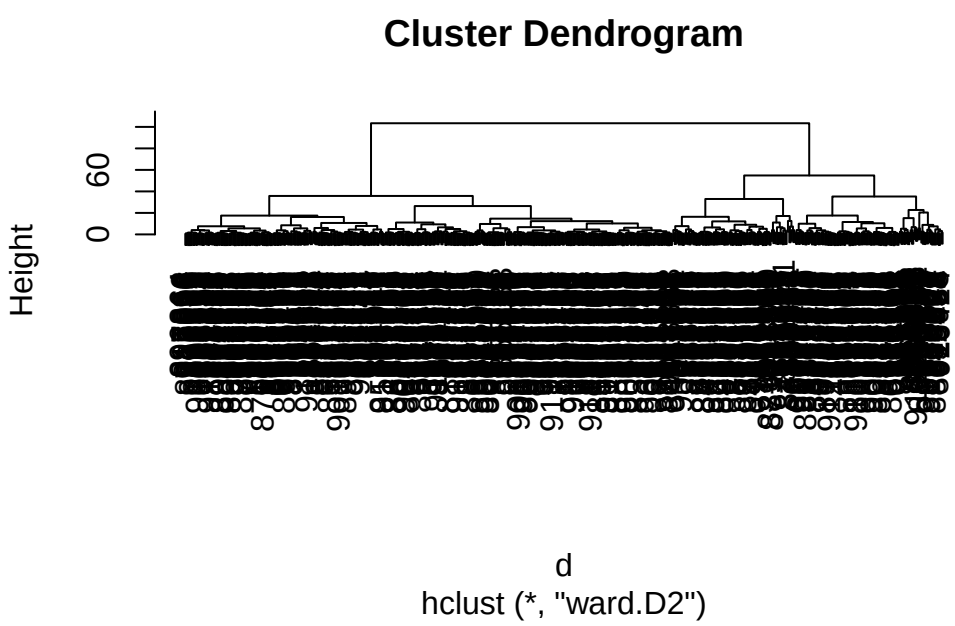
> Q14. How well does k-means separate the two diagnoses? How does it compare to your hclust results?

I believe that k-means does a relatively good job and separating the two groups as it clearly defines the malignant and benign groupings with very similar size to the hclust method, albeit with slightly larger grouping in the malignant group with an increase of 10 from hclust, however benign grouping was the same between both. There were also no extra/small groupings made, therefore k-means does seem fairly effective at separating the two diagnosis in relation to hclust.

Combine PCA and clustering

Our PCA results were `wisc.pr$x`

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



Cut tree into two groups/branches/clusters

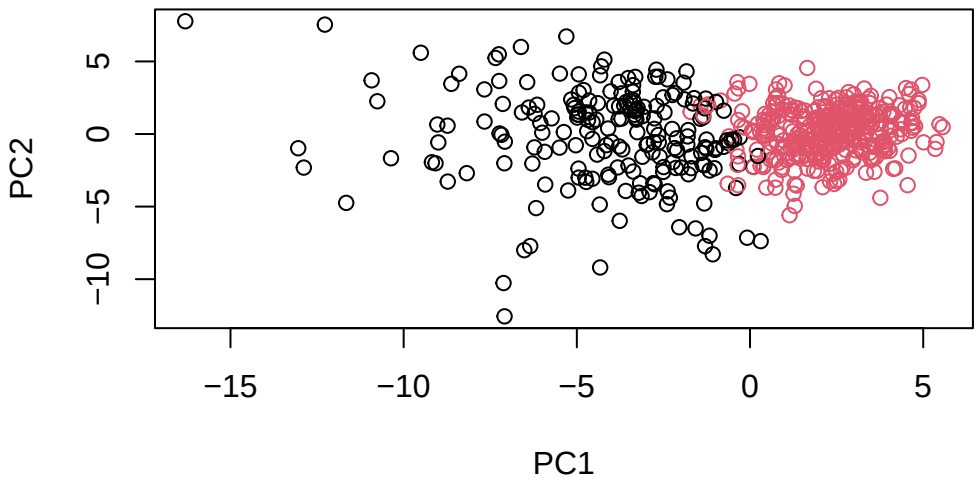
```
grps<- cutree(hc, k=2)
table(grps)
```

```
grps
  1   2
203 366
```

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

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

```
plot(wisc.pr$x,col=grps)
```




```
##library(rgl)
##plot3d(wisc.pr$x[,1:3], xlab="PC 1", ylab="PC 2", zlab="PC 3", cex=1.5, size=1, type="s",
##rglwidget(width=400, height=400)
##Code runs properly, just can't be rendered into PDF form
```

```
wisc.pr.hclust <- hclust(dist(wisc.pr$x[,1:7]), method="ward.D2")
wisc.pr.hclust.clusters <- cutree(wisc.pr.hclust, k=2)
table(wisc.pr.hclust.clusters)
```

```
wisc.pr.hclust.clusters
  1   2
216 353
```

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

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

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

This new model best separates and defines the malignant group out of all other models as we have the greatest number of malignant diagnosis in cluster 1 (188) with the highest sensitivity of 88.7%, yet in cluster 2 it does not define the benign grouping as well, for 329 diagnosis of benign is slightly lower than both previous methods with lower specificity at ~92%. The other models are collecting around 340-50 benign diagnosis with similar false positive rates.

> Q16. How well do the k-means and hierarchical clustering models you created in previous sections (i.e. before PCA) do in terms of separating the diagnoses? Again, use the table() function to compare the output of each model (wisc.km$cluster and wisc.hclust.clusters) with the vector containing the actual diagnoses.

```
table(wisc.km$cluster,diagnosis)
```

```
   diagnosis
      B   M
  1 343  37
  2  14 175
```

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

```
                    diagnosis
wisc.hclust.clusters   B   M
                   1  12 165
                   2   0   5
                   3 331  39
                   4   2   0
                   5  12   1
                   6   0   2
```

The km clustering model, like the others, does a fairly good job and separating the two groups. It remains very consist with the other models in terms of separating out the benign group with 343 diagnosis, which is in line with the other models and of high specificity, however the malignant group is slightly less specific with 175 true diagnosis or ~82% sensitivity. The hclust method is only slightly less specific for both groups compared to km with 337 for benign and 164 for malignant which are both very close yet not the best method for clustering as we want as much specificity and sensitivity as possible to make the correct diagnosis.

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

K-means and wisc.hclust clustering resulted in a model with the best specificity as 343 true benign diagnosis (correctly rejecting healthy patients) accounts for the highest specificity of all models at 96.1% while the wisc.pr hclust model accounts for the highest sensitivity (correctly identifying unhealthy patients) as it identified 188 malignant patients, eliciting 88.7% sensitivity, which was greatest out of all models.

**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
```

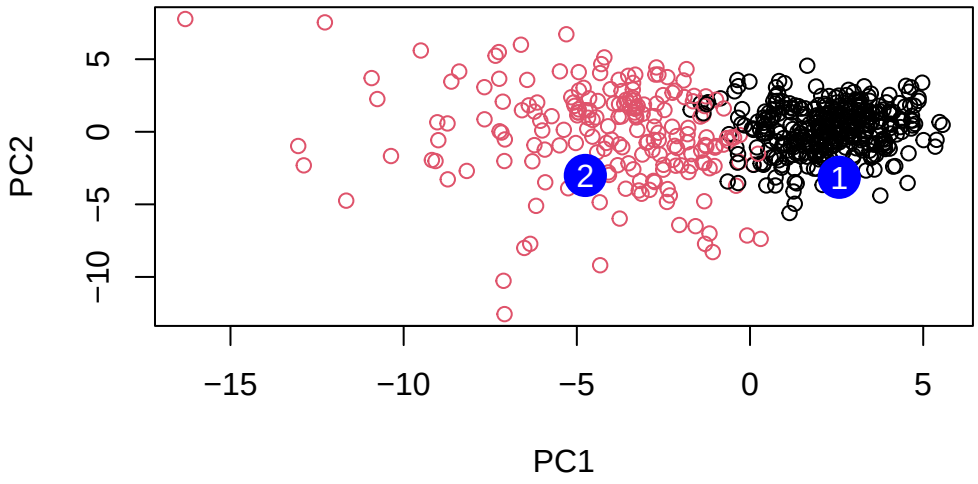
```
g<-as.factor(grps)
levels(g)
```

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

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

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

```
plot(wisc.pr$x[,1:2], col=g)
points(npc[,1], npc[,2], col="blue", pch=16, cex=3)
text(npc[,1], npc[,2], c(1,2), col="white")
```



Q18. Which of these new patients should we prioritize for follow up based on your results?

We should prioritize patient 2 as they lie within the red "malignant" grouping of the data set and therefore should follow up in order to confirm and determine the extent of the diagnosis of malignancy. If they fell in the black, they would be considered benign and healthy, which they are not and require more follow ups accordingly.