Class 8 Mini-Project: Unsupervised Learning

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Importing the Data

Here we analyze data from the University of Wisconsin Medical Center on Breast Cancer FNA.

```
#Step 1: Download the Data Set

#Step 2: Place the file in the project folder

# Step 3: Complete the following code to input the data and store as wisc.df
wisc.df <- read.csv("WisconsinCancer.csv", row.names=1)

# Step 4 (optional): Check the file
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
```

The first column, the diagnosis, is not necessary for our analysis. With that in mind, we will make a new data frame that omits this column.

```r
# We can use -1 here to remove the first column
wisc.data <- wisc.df[,-1]
```

Question 1: How many observations are in this dataset?

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

```
## [1] 569
```

Question 2: How many of the observations have a malignant diagnosis (i.e. how many Ms and Bs are there)?

```r
#Number of malignant diagnoses
sum(wisc.df$diagnosis == "M")
```

```
## [1] 212
```

```r
#Number of benign diagnoses
sum(wisc.df$diagnosis == "B")
```

```
## [1] 357
```

Is there another way, easier, way to answer Question 2?

```r
#Create a table of the relevant metrics
table(wisc.df$diagnosis)
```

```
##
##   B   M
## 357 212
```

Question 3: How many variables/features in the data are suffixed with _mean?

```r
#We can use the grep() function, that searches a given data frame for a specified term, in this case th

#We can then use the length() function to arrive at a total
length(grep("_mean", colnames(wisc.df)))
```

```
## [1] 10
```

It will also be helpful to create a "diagnosis" variable for later, made from the diagnosis column of the "wisc.df" data frame. We can store it a factor (using as.factor()) and use it to plot with later.

```r
# Create diagnosis factor for later
diagnosis <- as.factor(wisc.df$diagnosis)
diagnosis
```

```
##   [1] M M M M M M M M M M M M M M M M M M M B B B M M M M M M M M M M M M M M M
##  [38] B M M M M M M M M B M B B B B B M M B M M B B B B M B M M B B B B M B M M
##  [75] B M B M M B B B M M B M M M B B B M B B M M B B B M M B B B B M B B M B B
## [112] B B B B B B M M M B M M B B B M M B M B M M B M M B B M B B M B B B B M B
## [149] B B B B B B B B M B B B B M M B M B B M M B B M M B B B B M B B M M M B M
## [186] B M B B B M B B M M B M M M M B M M M B M B M B B M B M M M M B B M M B B
## [223] B M B B B B B M M B B M B B M M B M B B B B M B B B B B M B M M M M M M M
## [260] M M M M M M M B B B B B B M B M B B M B B M B M M B B B B B B B B B B B B
## [297] B M B B M B M B B B B B B B B B B B B B B M B B B M B M B B B B M M M B B
## [334] B B M B M B M B B B M B B B B B B B M M M B B B B B B B B B B B M M B M M
## [371] M B M M B B B B B M B B B B B M B B B M B B M M B B B B B B M B B B B B B
## [408] B M B B B B B M B B M B B B B B B B B B B B B M B M M B M B B B B B M B B
## [445] M B M B B M B M B B B B B B B B M M B B B B B B M B B B B B B B B B B M B
## [482] B B B B B B M B M B B M B B B B B M M B M B M B B B B B M B B M B M B M M
## [519] B B B M B B B B B B B B B B B M B M M B B B B B B B B B B B B B B B B B B
## [556] B B B B B B B M M M M M M B
## Levels: B M
```

Principle Component Analysis

The main funciton in base R for PCA is "prcomp()". There is an important optional argument called "scale" in this function.

Before we scale, we should check the data to determine if this step is necessary

```
# 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
```

The first line does the principle component analysis (while scaling the data), the second line shows a summary

```
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
```

Question 4: From your results, what proportion of the original variance is captured by the first principal components (PC1)?

44.27%

Question 5: How many principal components (PCs) are required to describe at least 70% of the original variance in the data?

3 PCs

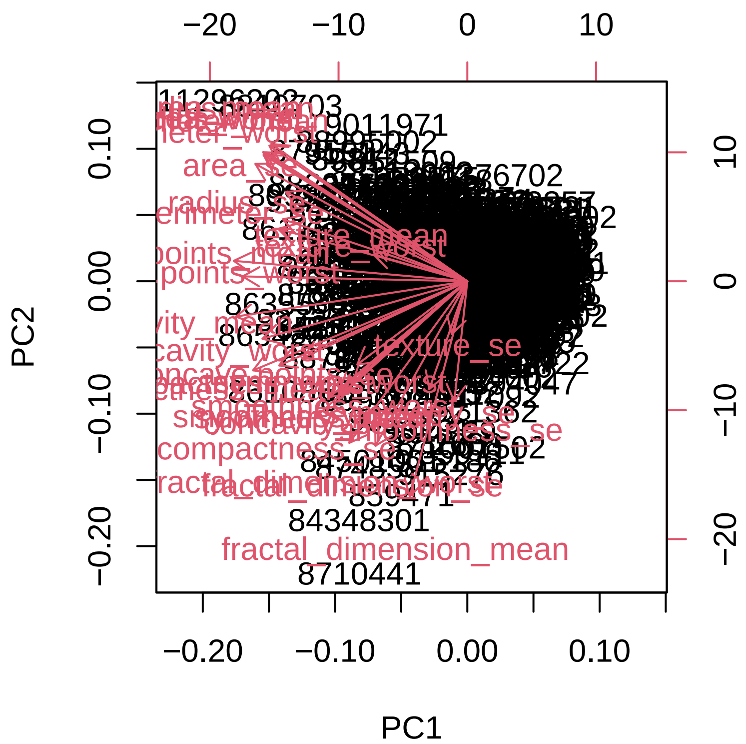
Question 6: How many principal components (PCs) are required to describe at least 90% of the original variance in the data?

7 PCs

The main result of these types of methods is called a PCA plot (a.k.a. score plot. ordination plot)

Question 7: Make a biplot of the PC data

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



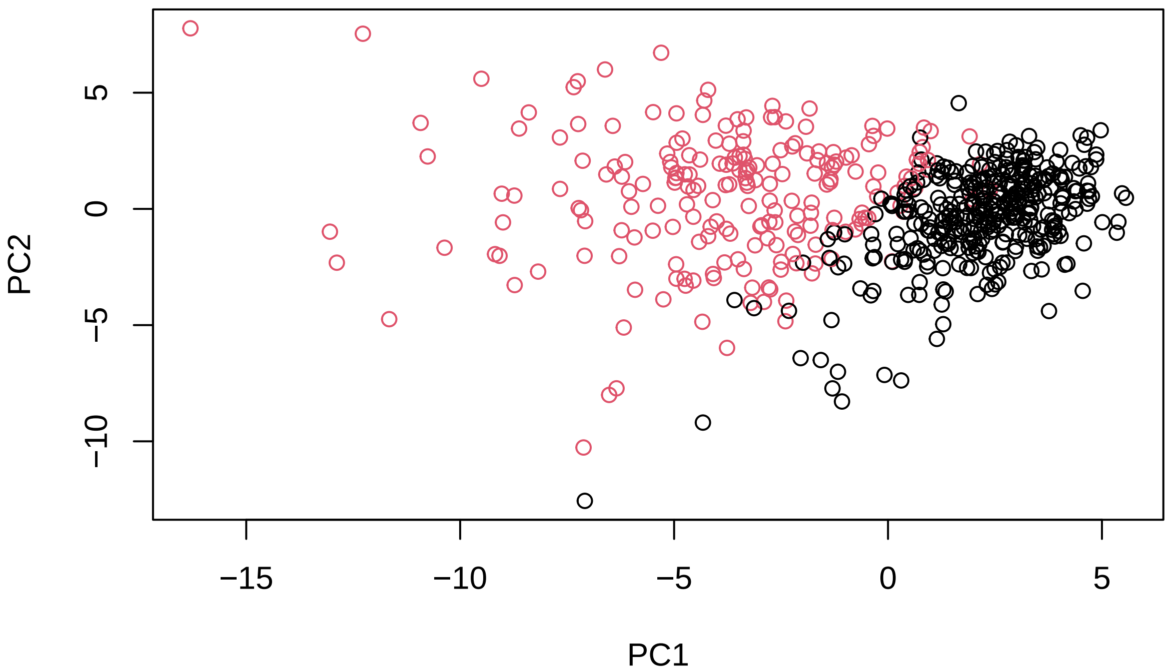

```
#This is a really bad, messy plot
```

A summary of the “x” for wisc.pr

```
#wisc.pr$x
```

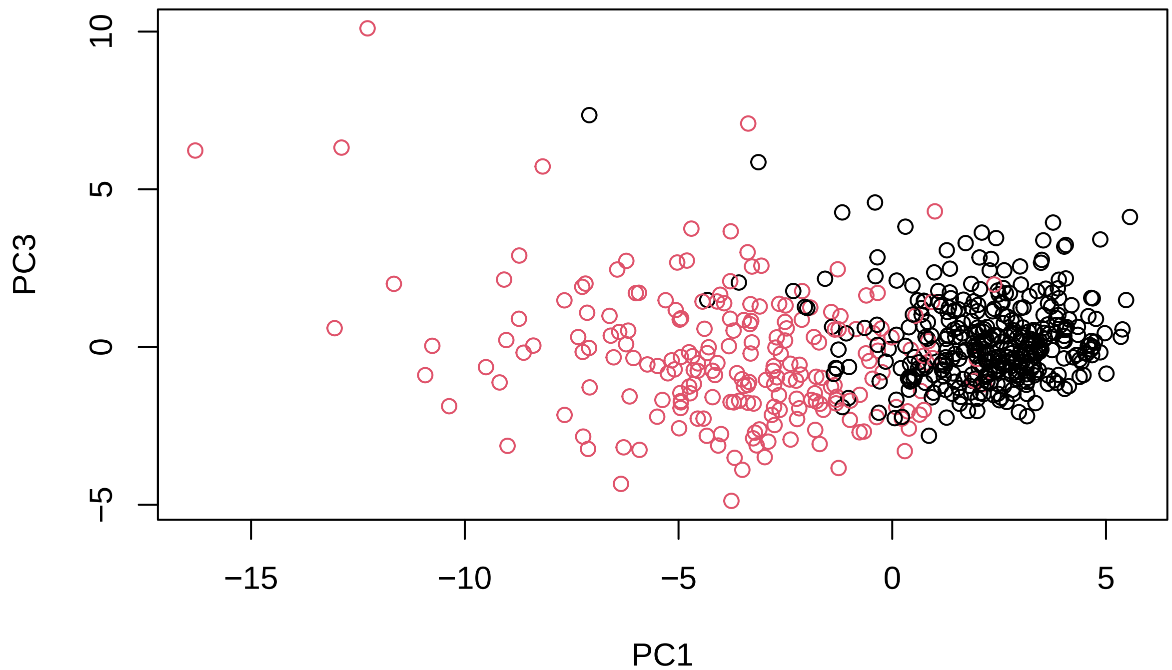
We will now plot PC1 vs. PC2 x values

```
#We can use a simple plot to see how the two compare
plot(wisc.pr$x[,1:2], col = diagnosis)
```



Question 8: Generate a similar plot for principal components 1 and 3. What do you notice about these plots?

```
plot(wisc.pr$x[,c(1,3)], col = diagnosis)
```



This graph has greater overlap between the two groups, as less of the variance can be explained by PC1 + PC3 than PC1 + PC2.

```
#Rotations of the data for PC1
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
```

Question 9: 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?

-0.26085376

Question 10: What is the minimum number of principal components required to explain 80% of the variance of the data?

5 PCs

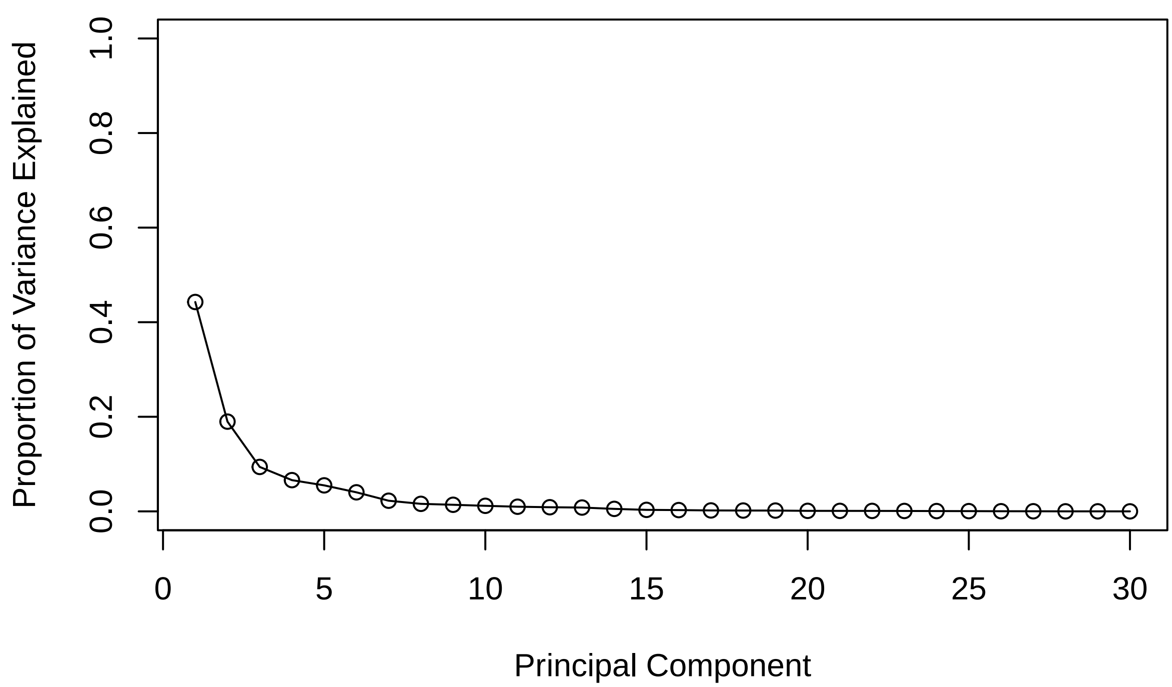
These plots describe the percentage of variance that can be explained by each PC

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

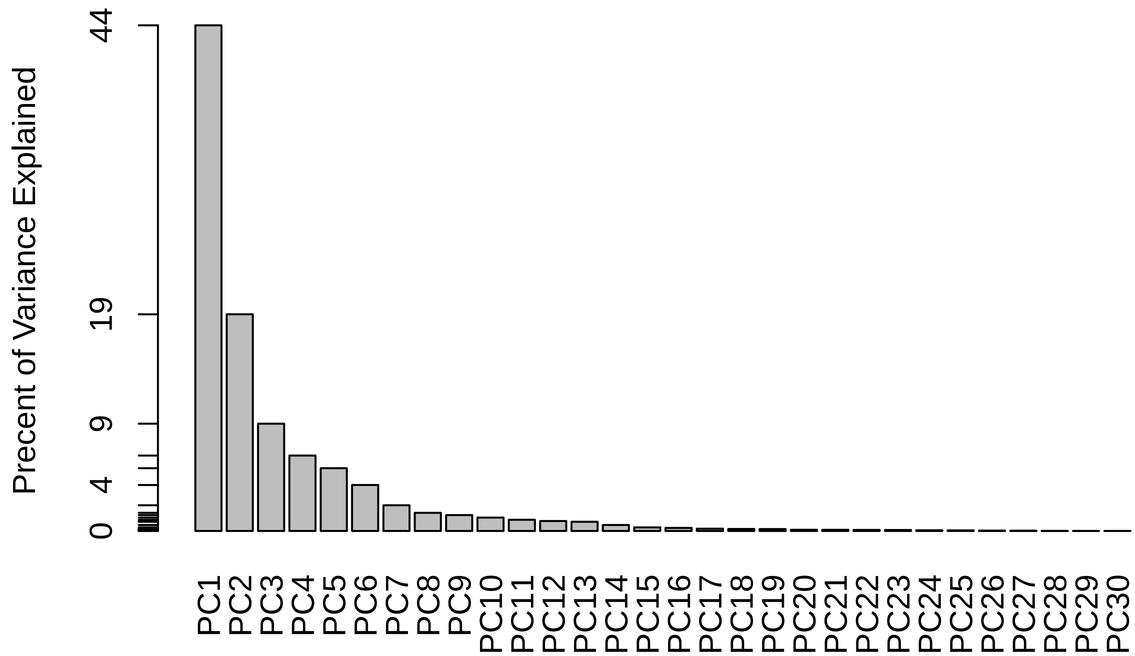
```
## [1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

```
# 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")
```



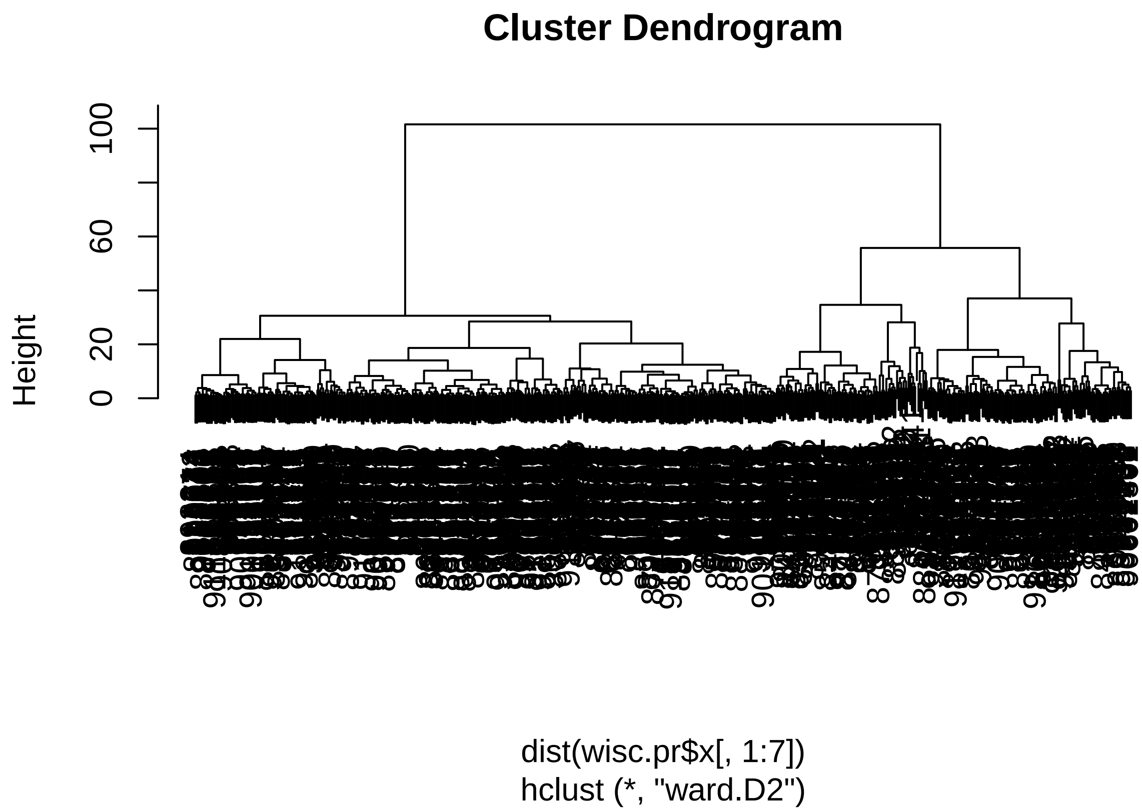
```r
# Alternative scree plot of the same data, note data driven y-axis
barplot(pve, ylab = "Precent of Variance Explained",
     names.arg=paste0("PC",1:length(pve)), las=2, axes = FALSE)
axis(2, at=pve, labels=round(pve,2)*100 )
```




```r
#We can create an even more descriptive graph
#library(ggplot2)
#install.packages("factoextra")
#library(factoextra)
#fviz_eig(wisc.pr, addlabels = TRUE)
```

Hierarchical clustering of raw data is not very helpful

```r
#Using the minimum number of principal components required to describe at least 90% of the variability
wisc.pr.hclust <- hclust(dist(wisc.pr$x[,1:7]), method = "ward.D2")
plot(wisc.pr.hclust)
```

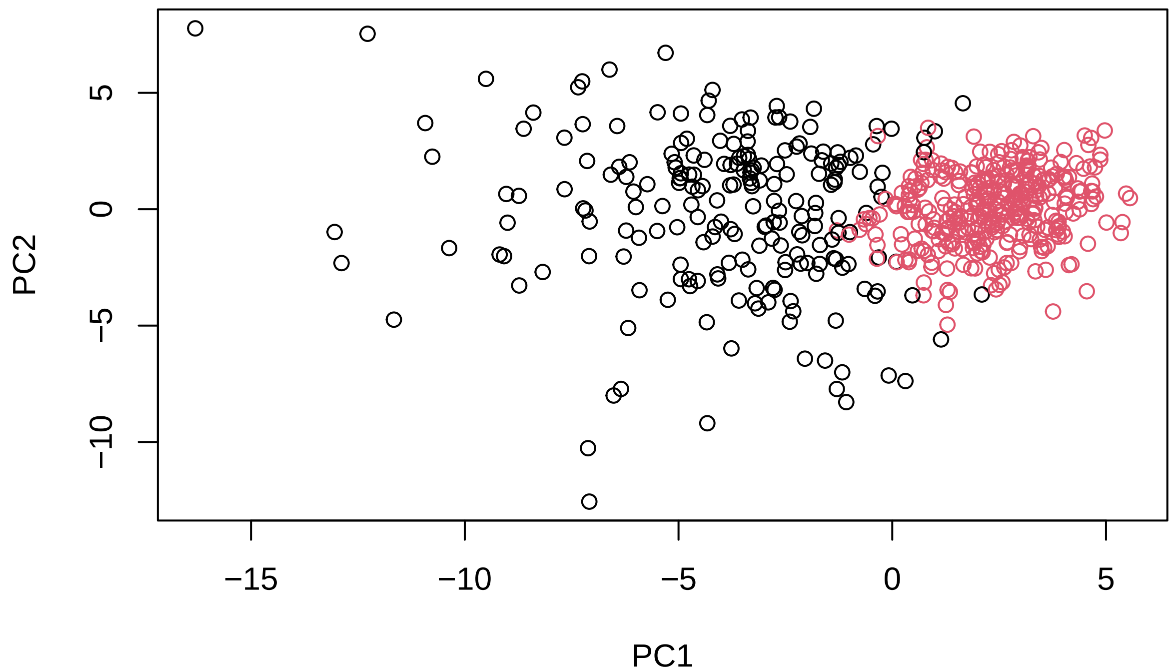


It looks as though the data divides into two groups, which could map onto the "benign" and "malignant" categories. Let's find out. Using the cutree() function, we can sort the clusters into two membership groups.

```
#We can first ask how many data points are in each of the two groups
grps <- cutree(wisc.pr.hclust, k=2)
table(grps)
```

```
## grps
##   1   2
## 216 353
```

```
#We can plot PC1 vs. PC2 again, coloring by grps to see how it compares to coloring by diagnosis
plot(wisc.pr$x[,1:2], col = grps)
```




```
#Next, we can use our diagnosis factor to see how many of each diagnosis are in each of these two groups
table(grps, diagnosis)
```

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