Class 08: Machine Learning Mini Project

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Exploratory data analysis

Save your input data file into your Project directory

I downloaded this file and saved it into my 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]
```

Create diagnosis vector for later

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

> Q1. How many observations are in this dataset?

There are 569 observations in this dataset.

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

```
[1] 569
```

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

There are 212 observations that have a malignant diagnosis.

```r
table(diagnosis)
```

```
diagnosis
  B   M 
357 212 
```

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

There are 10 variables/features in the data that are suffixed with _mean.

```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"
```

The function `grep()` could be useful here.

```r
grep("_mean", colnames(wisc.data) )
```

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

```
length(grep("_mean", colnames(wisc.data)))
```

```
[1] 10
```

Principal Component Analysis (PCA)

First we need to consider whether the data needs “scaling” to make our compassionate fair.

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 
```

Perform PCA on wisc.data by completing the following code

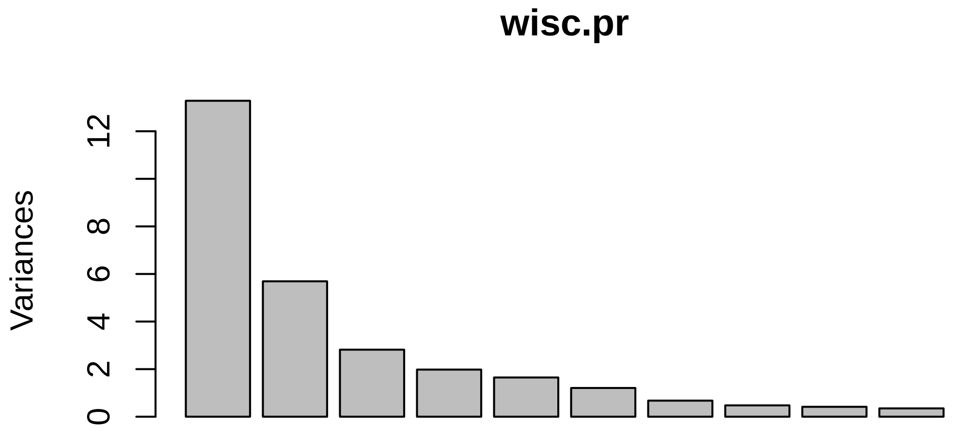
```
wisc.pr <- prcomp( wisc.data, scale = TRUE )
```

```
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
```

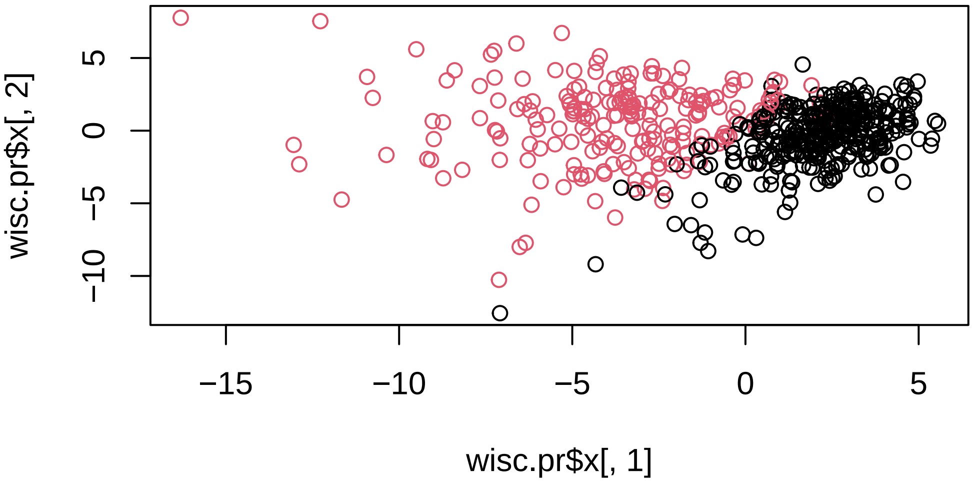
```
Cumulative Proportion  0.98649 0.98915 0.99113 0.99288 0.99453 0.99557 0.9966
                          PC22    PC23   PC24    PC25    PC26    PC27    PC28
Standard deviation     0.16565 0.15602 0.1344 0.12442 0.09043 0.08307 0.03987
Proportion of Variance 0.00091 0.00081 0.0006 0.00052 0.00027 0.00023 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
```

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



Let’s make a PC plot (a.k.a. “score plot” or “PC1 vs PC2” etc. plot)

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



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

The proportion of the original variance that is captured by the first principal components (PC1) is 44.27%.

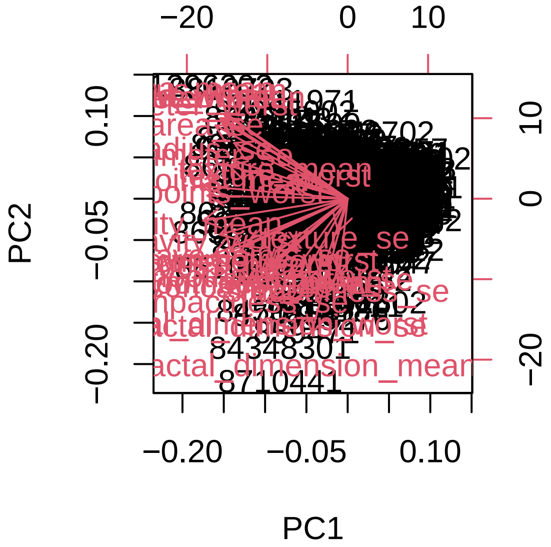
> Q5. How many principal components (PCs) are required to describe at least 70% of the original variance in the data?

Three principal components (PCs) are required to described at least 70% of the original variance in the data. This information can be found by looking at the cumulative proportion of PC3 (72.636%).

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

There are seve principal components that are required to describe at least 90% of the original variance in the data. This information can be found by looking at the cumulative proportion of PC7 (91.010%).

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

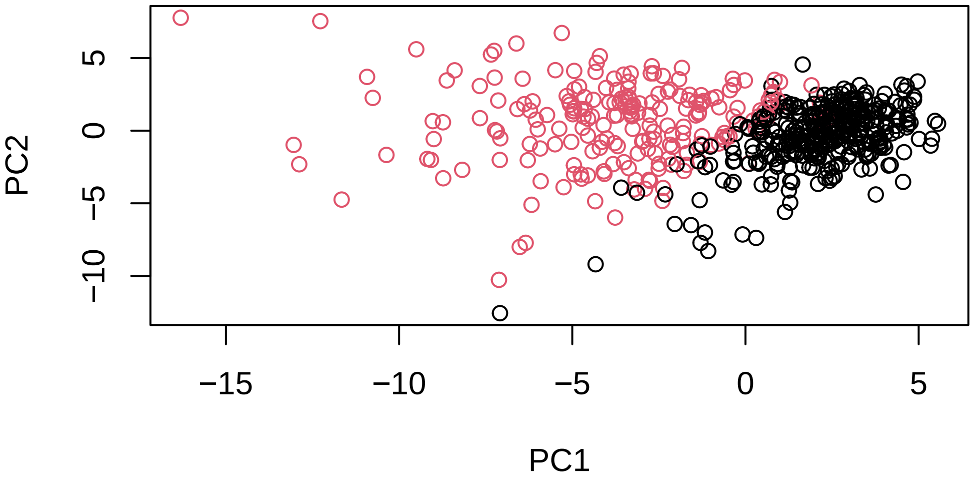


Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?

What stands out to me about this plot is that all of the data is very compact and difficult to analyze. I can tell that there are data labels and numerical values within the plot, but they are very hard to decipher, and therefore hard to understand.

Scatter plot observations by components 1 and 2

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

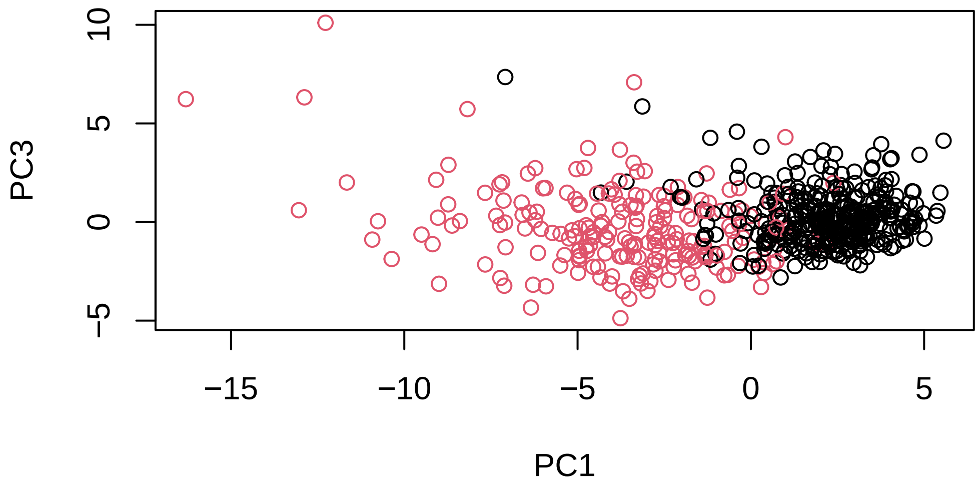


Repeat for components 1 and 3

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

The scatterplots for PC1 vs PC2 and PC1 vs PC3 are much easier to analyze and comprehend compared to the biplot made previously. The graph effectively shows the differeces in clutering bewteen the two diagnosis groups.

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



Create a data.frame for ggplot

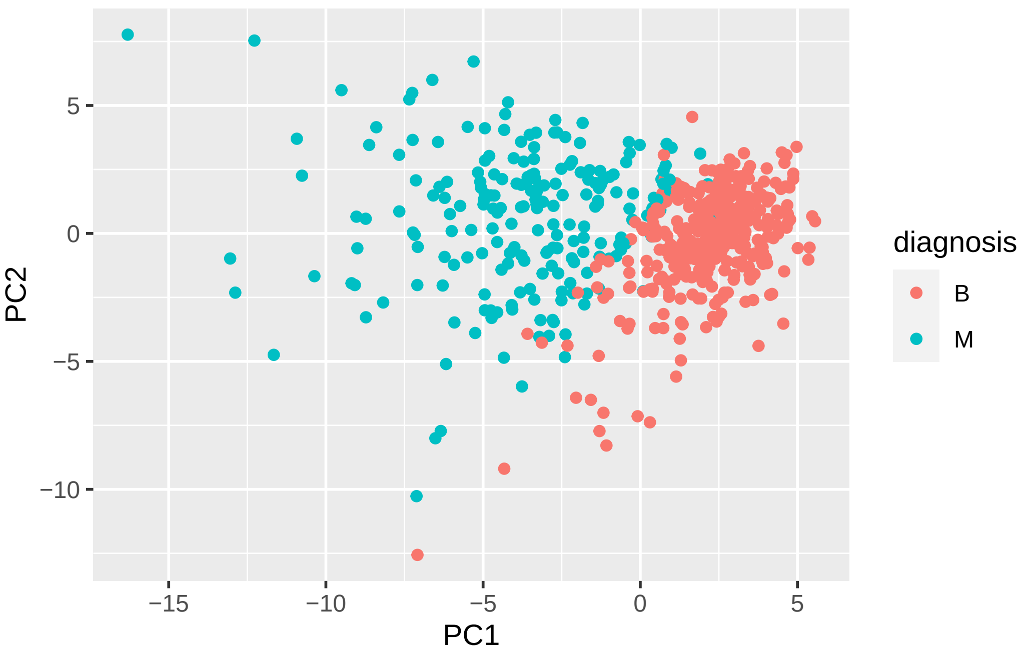
```
df <- as.data.frame(wisc.pr$x)
df$diagnosis <- diagnosis
```

Load the ggplot2 package

```
library(ggplot2)
```

Make a scatter plot colored by diagnosis

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



Variance explained

Calculate variance of each component

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

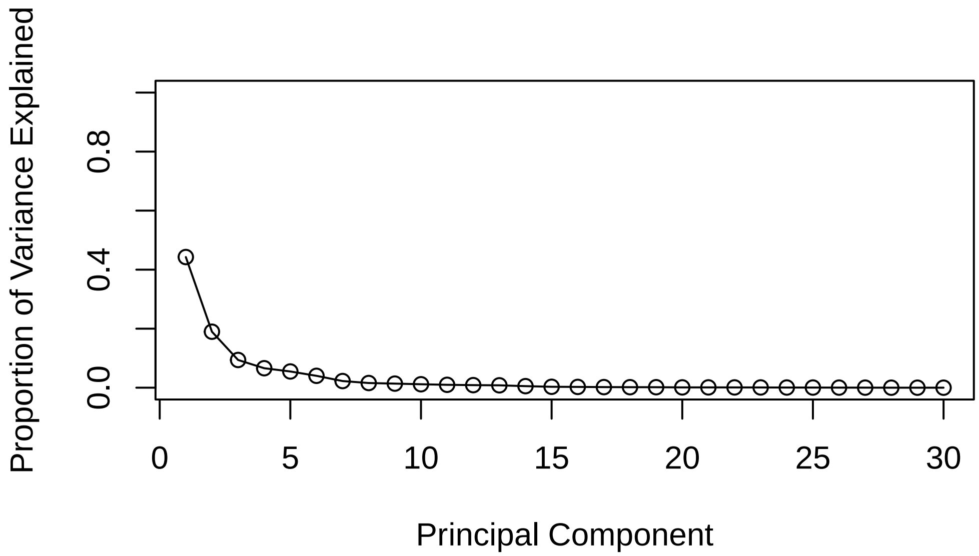
```
[1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

Variance explained by each principal component: pve

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

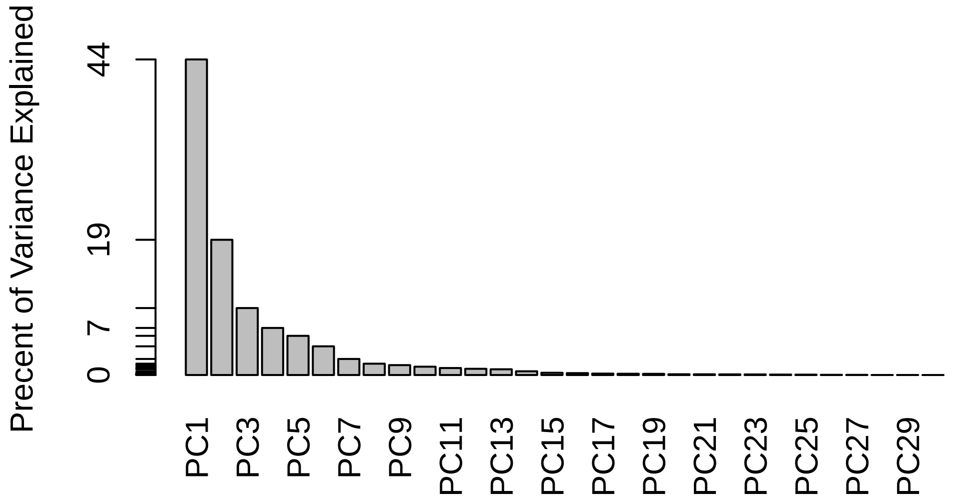
Plot variance explained for each principal component

```
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 )
```



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?

For the first principal component, the component of the loading vector for the feature 'concave.points_mean' is -0.26085376.

```
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
```

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

The minimum number of principal components required to explain 80% of the variance of the data is 5. This information can be found by looking at the cumulative proportion for PC5 (84.734%).

```r
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
```

Hierarchical Clustering

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

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

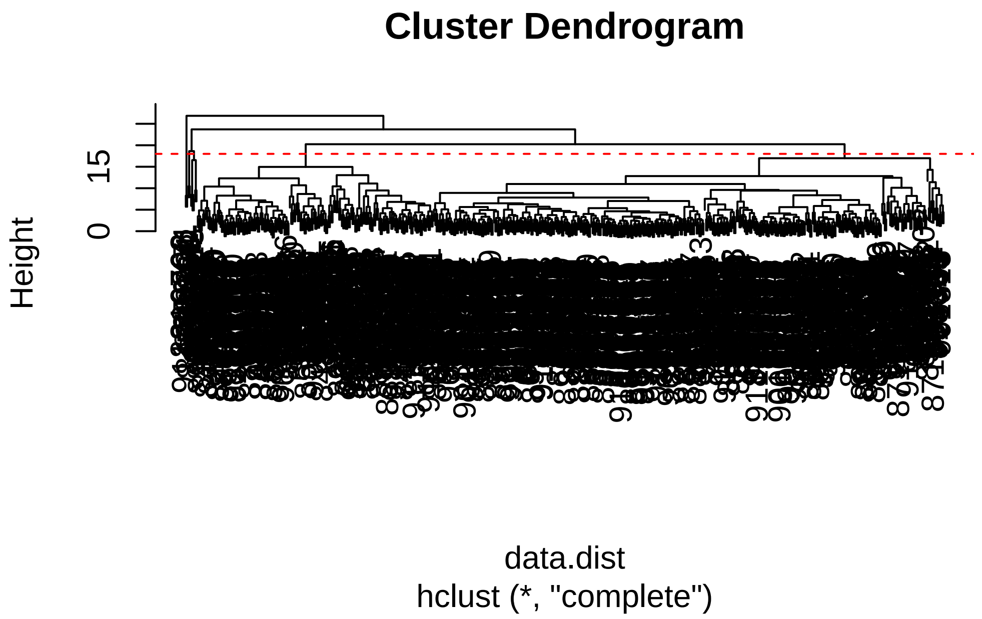
```
data.dist <- dist(data.scaled)
```

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

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

The height at which the clustering model has four clusters is 18.

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



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

```r
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?

There is not a better cluster than four because the two diagnoses (benign and malignant) there is a very clear distinction bewtween these values.

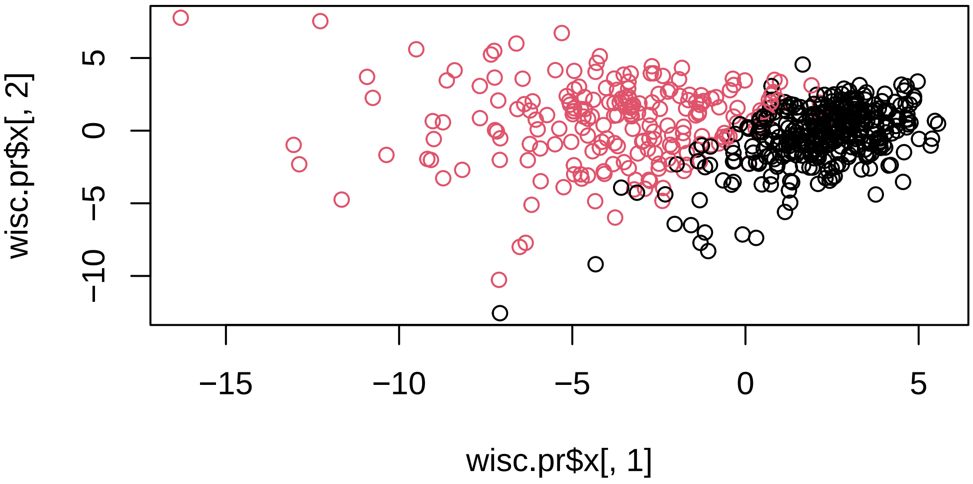
> Q13. Which method gives your favorite results for the same data.dist dataset? Explain your reasoning.

"ward.d2" is my preferred method for giving results for the same data.dist dataset. This is because the "ward.d2" function allows for the clusters to be more organized in more sepecific ways. Within each cluster, there is less variance.

Combining Methods

I want to cluster in "PC sapce."

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



The `hclust()` function wants a distance matrix as input…

```
d <- dist(wisc.pr$x[, 1:7])
wisc.pr.hclust <-hclust(d, method="ward.D2")
```

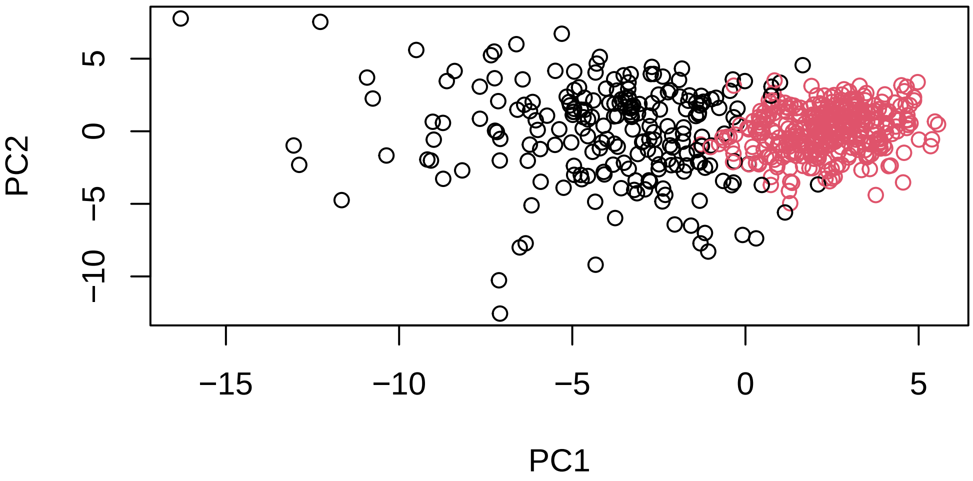
```
grps <- cutree(wisc.pr.hclust, k=2)
table(grps)
```

```
grps
  1   2
216 353
```

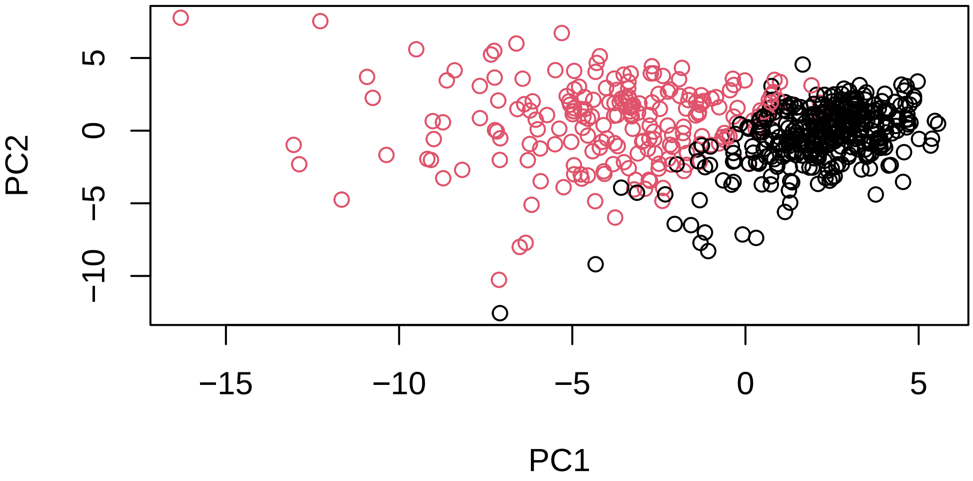
```
table(grps, diagnosis)
```

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

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



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



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

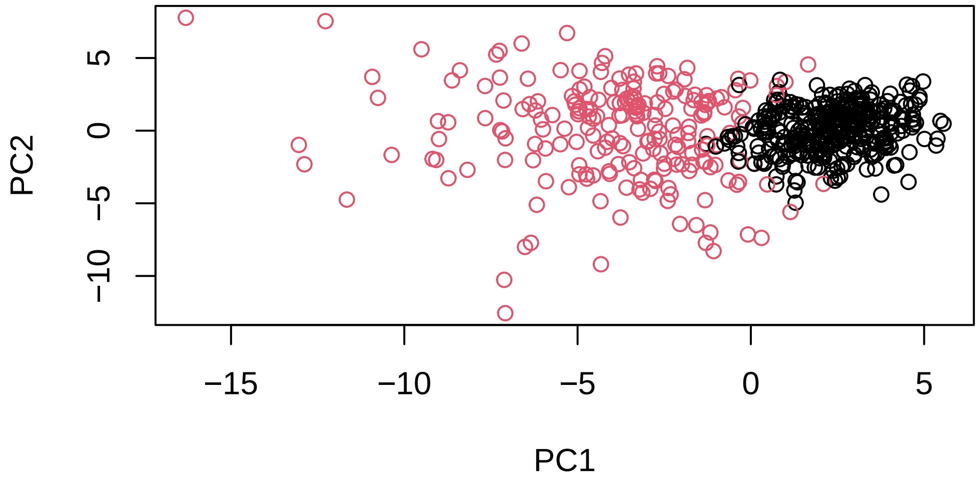
```
[1] "1" "2"
```

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

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

Plot using our re-ordered factor

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



Use the distance along the first 7 PCs for clustering i.e. wisc.pr$x[, 1:7]

```
wisc.pr.hclust <- hclust(d, method="ward.D2")
```

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

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

The newly created model with two clusters separates out the two diagnoses works much better than the model with four clusters. This is due to the fact that the two cluster model creates a much clearer distinction between the malignant and benign diagnoses.

Compare to actual diagnoses

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

```
                       diagnosis
```

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

> 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.

The `wisc.hclust.clusters` method seems to be better because it separates the benign and malignant diagnoses in a more distinct way.

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

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

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

```
                    diagnosis
wisc.hclust.clusters   B   M
                   1  12 165
                   2   2   5
                   3 343  40
                   4   0   2
```

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

`wisc.hclust.clusters` has a the best sensitivity because it has a higher sensitivity than `wisc.pr.hclust.clusters`. `wisc.hclust.clusters` has a the best specificity because it has a higher specificity than `wisc.pr.hclust.clusters`. This result shows that the `wisc.hclust.clusters` method is more sensitive and specific.

FN TP TN FP

Sensitivity TP/(TP+FN)

For `wisc.pr.hclust.clusters`

```r
188/(188+28)
```

```
[1] 0.8703704
```

For `wisc.hclust.clusters`

```r
165/(165+12)
```

```
[1] 0.9322034
```

Specificity TN/(TN+FN)

For `wisc.pr.hclust.clusters`

```r
329/(329+28)
```

```
[1] 0.9215686
```

For `wisc.hclust.clusters`

```r
343/(343+12)
```

```
[1] 0.9661972
```