Class 08: Breast Cancer Analysis Mini Project

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Background

The goal of this mini-project is for you to explore a complete analysis using the unsupervised learning techniques covered in class. You'll extend what you've learned by combining PCA as a preprocessing step to clustering using data that consist of measurements of cell nuclei of human breast masses. This expands on our RNA-Seq analysis from last day.

The data itself comes from the Wisconsin Breast Cancer Diagnostic Data Set first reported by K. P. Benne and O. L. Mangasarian: "Robust Linear Programming Discrimination of Two Linearly Inseparable Sets".

Values in this data set describe characteristics of the cell nuclei present in digitized images of a fine needle aspiration (FNA) of a breast mass.

Data Import

Input data file is saved into my Project directory as a CSV

```r
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
```

The first column `diagnosis` is the expert opinion on the sample (i.e. patient FNA)

```
wisc.df$diagnosis
```

```
  [1] "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M"
 [19] "M" "B" "B" "B" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M"
 [37] "M" "B" "M" "M" "M" "M" "M" "M" "M" "M" "B" "M" "B" "B" "B" "B" "B" "M"
 [55] "M" "B" "M" "M" "B" "B" "B" "B" "M" "B" "M" "M" "B" "B" "B" "B" "M" "B"
 [73] "M" "M" "B" "M" "B" "M" "M" "B" "B" "B" "M" "M" "B" "M" "M" "M" "B" "B"
 [91] "B" "M" "B" "B" "M" "M" "B" "B" "B" "M" "M" "B" "B" "B" "B" "M" "B" "B"
[109] "M" "B" "B" "B" "B" "B" "B" "B" "B" "M" "M" "M" "B" "M" "M" "B" "B" "B"
[127] "M" "M" "B" "M" "B" "M" "M" "B" "M" "M" "B" "B" "M" "B" "B" "M" "B" "B"
[145] "B" "B" "M" "B" "B" "B" "B" "B" "B" "B" "B" "B" "M" "B" "B" "B" "B" "M"
[163] "M" "B" "M" "B" "B" "M" "M" "B" "B" "M" "M" "B" "B" "B" "B" "M" "B" "B"
[181] "M" "M" "M" "B" "M" "B" "M" "B" "B" "B" "M" "B" "B" "M" "M" "B" "M" "M"
[199] "M" "M" "B" "M" "M" "M" "B" "M" "B" "M" "B" "B" "M" "B" "M" "M" "M" "M"
[217] "B" "B" "M" "M" "B" "B" "B" "M" "B" "B" "B" "B" "B" "M" "M" "B" "B" "M"
[235] "B" "B" "M" "M" "B" "M" "B" "B" "B" "B" "M" "B" "B" "B" "B" "B" "M" "B"
[253] "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "B" "B" "B" "B"
[271] "B" "B" "M" "B" "M" "B" "B" "M" "B" "B" "M" "B" "M" "M" "B" "B" "B" "B"
[289] "B" "B" "B" "B" "B" "B" "B" "B" "B" "M" "B" "B" "M" "B" "M" "B" "B" "B"
[307] "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "M" "B" "B" "B" "M" "B" "M"
[325] "B" "B" "B" "B" "M" "M" "M" "B" "B" "B" "B" "M" "B" "M" "B" "M" "B" "B"
[343] "B" "M" "B" "B" "B" "B" "B" "B" "B" "M" "M" "M" "B" "B" "B" "B" "B" "B"
```

```
[361] "B" "B" "B" "B" "B" "M" "M" "B" "M" "M" "M" "B" "M" "M" "B" "B" "B" "B"
[379] "B" "M" "B" "B" "B" "B" "B" "M" "B" "B" "B" "M" "B" "B" "M" "M" "B" "B"
[397] "B" "B" "B" "B" "M" "B" "B" "B" "B" "B" "B" "B" "M" "B" "B" "B" "B" "B"
[415] "M" "B" "B" "M" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "M" "B"
[433] "M" "M" "B" "M" "B" "B" "B" "B" "B" "M" "B" "B" "M" "B" "M" "B" "B" "M"
[451] "B" "M" "B" "B" "B" "B" "B" "B" "B" "B" "M" "M" "B" "B" "B" "B" "B" "B"
[469] "M" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "M" "B" "B" "B" "B" "B" "B"
[487] "B" "M" "B" "M" "B" "B" "M" "B" "B" "B" "B" "B" "M" "M" "B" "M" "B" "M"
[505] "B" "B" "B" "B" "B" "M" "B" "B" "M" "B" "M" "B" "M" "M" "B" "B" "B" "M"
[523] "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "M" "B" "M" "M" "B" "B" "B"
[541] "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B"
[559] "B" "B" "B" "B" "M" "M" "M" "M" "M" "M" "B"
```

-1 is used to remove the diagnosis column, which is not needed right now, but needed later as a vector

```r
wisc.data <- wisc.df[,-1]
diagnosis <- wisc.df[,1]
```

Lastly, explore and get familiar

Q1. Q1. How many observations are in this dataset?

There are 569 observations/patients in the dataset.

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

There are 212 observations that have a malignant diagnosis.

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

```

  B   M 
357 212 
```

Q3. How many variables/features in the data 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"
```

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

```
[1] 10
```

Principal Coordinate Analysis

The `prcomp()` function to do PCA has a `scale=FALSE`default. In general we nearly always want to set this to TRUE so our analysis is not dominated by columns/variables in our data set that have high standard deviation and mean when compared to others just because the units of measurement are on different scales

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

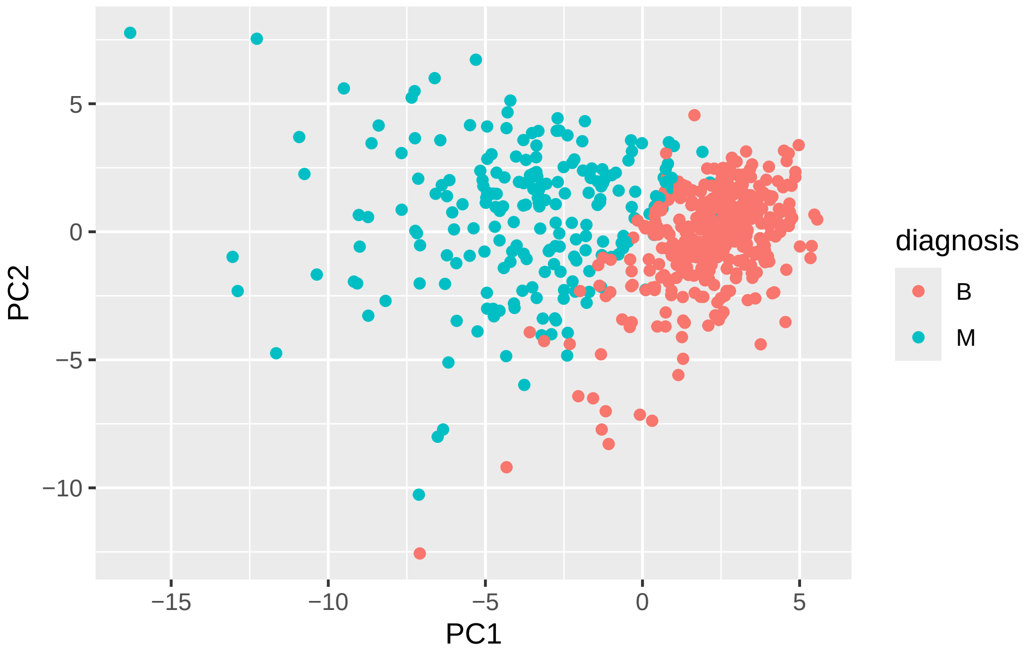
```
Importance of components:
                          PC1    PC2     PC3     PC4     PC5     PC6     PC7
Standard deviation     3.6444 2.3857 1.67867 1.40735 1.28403 1.09880 0.82172
Proportion of Variance 0.4427 0.1897 0.09393 0.06602 0.05496 0.04025 0.02251
Cumulative Proportion  0.4427 0.6324 0.72636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

The main PC result figure is called a “score plot” or a “PC polt” or “ordination plot”...

```r
library(ggplot2)

ggplot(wisc.pr$x)+
  aes(PC1, PC2, col=diagnosis) +
  geom_point()
```



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

44.27% of the original variance is captured by PC1

```
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
```

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

3 principal components are required to describe at least 70% of the data

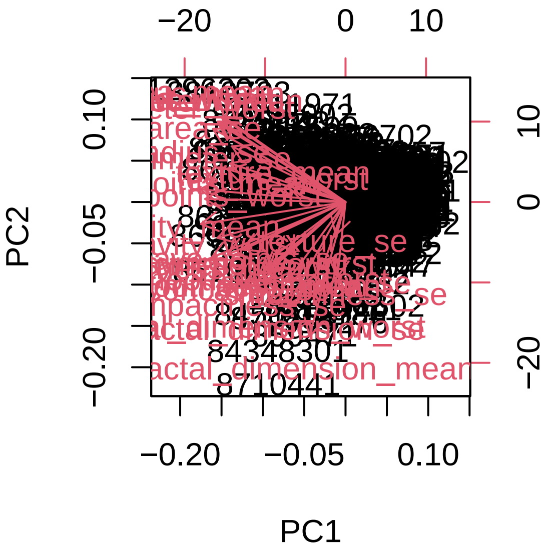
> Q6. How many principal components (PCs) are required to describe at least 90% of the original variance in the data?

About 8 principal components are requied to describe at least 90% of the original variance in the data

Interpreting PCA Results

Create a biplot of the `wisc.pr` using the `biplot()` function

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



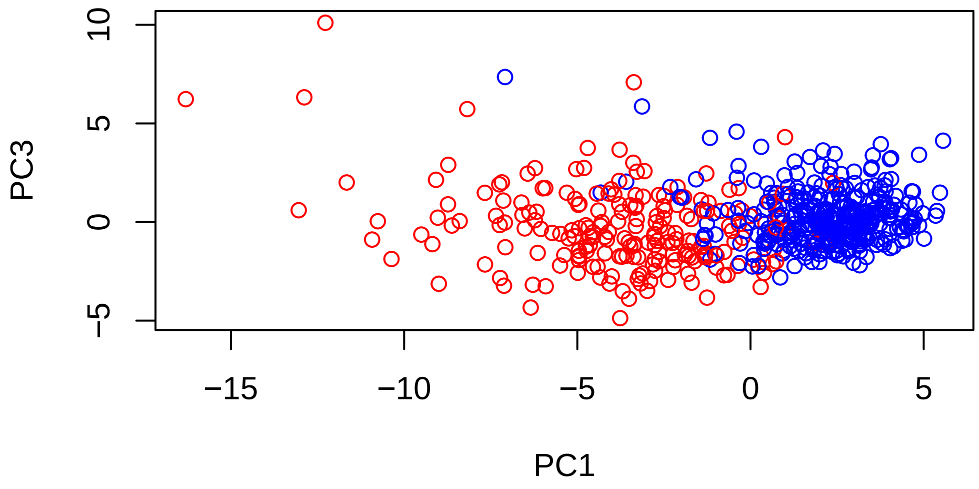
Q7. What stand out to you about this plot? Is it easy or difficult to understand and why?

There are too many plots on this plot, there is no scaling of values to remove this noise.

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

These plots show a distinct difference in clustering between the two colors.

```r
col <- ifelse(diagnosis == "M", "red", "blue")
plot(wisc.pr$x[,c(1,3)], col = col ,
     xlab = "PC1", ylab = "PC3")
```



PCA Scree-plot

A plot of how much variance each PC captures. We can get this from `wisc.pr$sdev` or from the output of `summary(wisc.pr)`

```
var.tbl <- summary(wisc.pr)
head(var.tbl$importance)
```

```
                            PC1      PC2      PC3      PC4      PC5      PC6
Standard deviation     3.644394 2.385656 1.678675 1.407352 1.284029 1.098798
Proportion of Variance 0.442720 0.189710 0.093930 0.066020 0.054960 0.040250
Cumulative Proportion  0.442720 0.632430 0.726360 0.792390 0.847340 0.887590
                             PC7       PC8       PC9      PC10      PC11
Standard deviation     0.8217178 0.6903746 0.6456739 0.5921938 0.5421399
Proportion of Variance 0.0225100 0.0158900 0.0139000 0.0116900 0.0098000
Cumulative Proportion  0.9101000 0.9259800 0.9398800 0.9515700 0.9613700
                            PC12      PC13      PC14      PC15      PC16
Standard deviation     0.5110395 0.4912815 0.3962445 0.3068142 0.2826001
Proportion of Variance 0.0087100 0.0080500 0.0052300 0.0031400 0.0026600
Cumulative Proportion  0.9700700 0.9781200 0.9833500 0.9864900 0.9891500
                            PC17      PC18      PC19      PC20      PC21
Standard deviation     0.2437192 0.2293878 0.2224356 0.1765203 0.1731268
```

```
Proportion of Variance 0.0019800 0.0017500 0.0016500 0.0010400 0.0010000
Cumulative Proportion  0.9911300 0.9928800 0.9945300 0.9955700 0.9965700
                            PC22      PC23      PC24      PC25      PC26
Standard deviation     0.1656484 0.1560155 0.1343689 0.1244238 0.0904303
Proportion of Variance 0.0009100 0.0008100 0.0006000 0.0005200 0.0002700
Cumulative Proportion  0.9974900 0.9983000 0.9989000 0.9994200 0.9996900
                             PC27      PC28       PC29       PC30
Standard deviation     0.08306903 0.0398665 0.02736427 0.01153451
Proportion of Variance 0.00023000 0.0000500 0.00002000 0.00000000
Cumulative Proportion  0.99992000 0.9999700 1.00000000 1.00000000
```

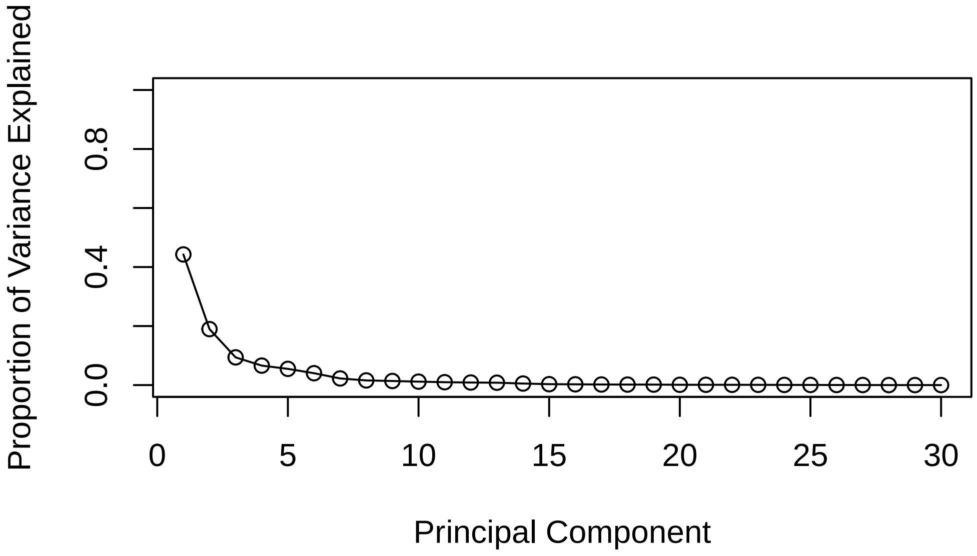
```
pr.var <- wisc.pr$sdev^2
head(pr.var)
```

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

Variance explained by each principal component: pve

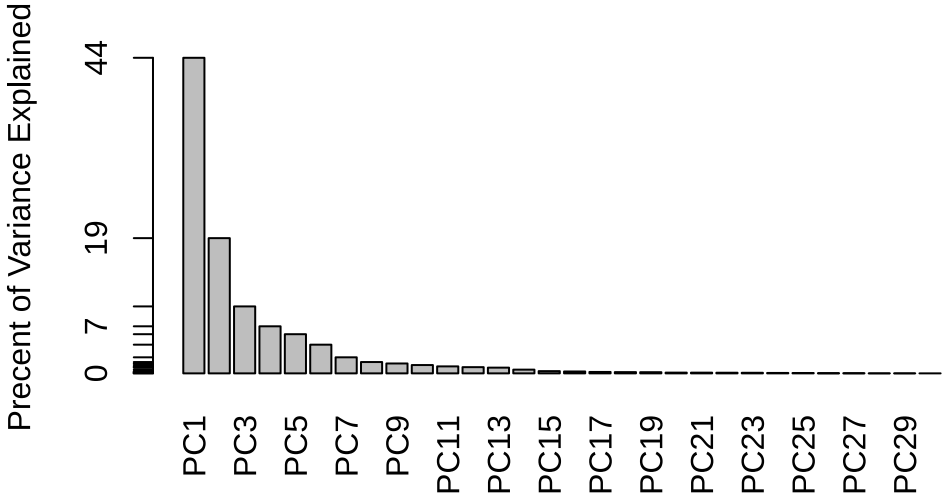
```
pve <- pr.var / sum(pr.var)
```

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



An alternative scree plot can be made

```r
screeplot <- 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`?

```r
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?

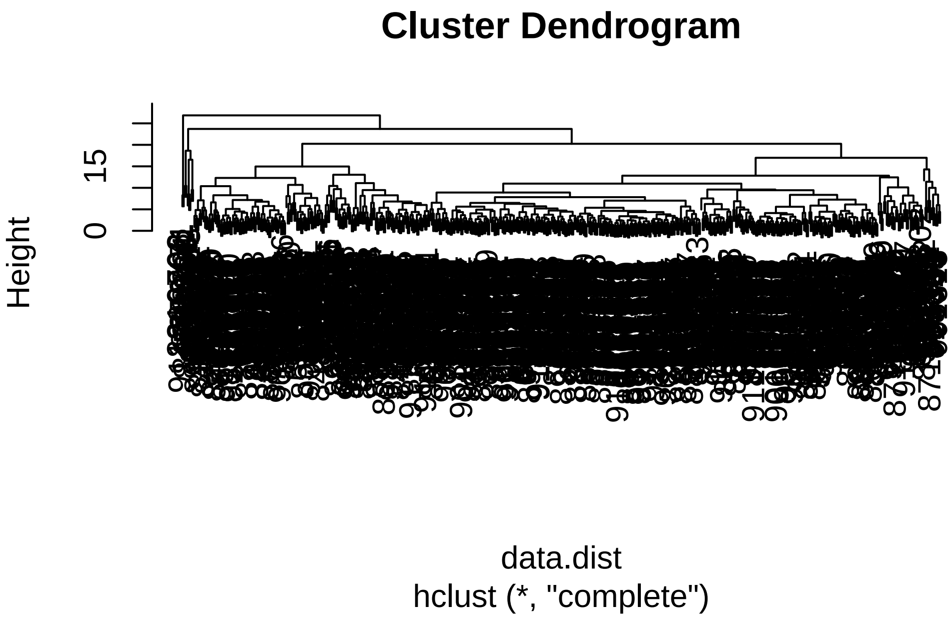
5 principal components are required to explain 80% of the variance of the data

Hierarchical clustering

Just clusting the original data is not very informative or helpful

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

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



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

```

  1   2   3   4 
177   7 383   2 
```

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

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

Combining methods (PCA and Clustering)

Clustering the original data was not very productive. The PCA results looked promising. Here we combined these methods by clustering from our PCA results. In other words "clustering in PC space"

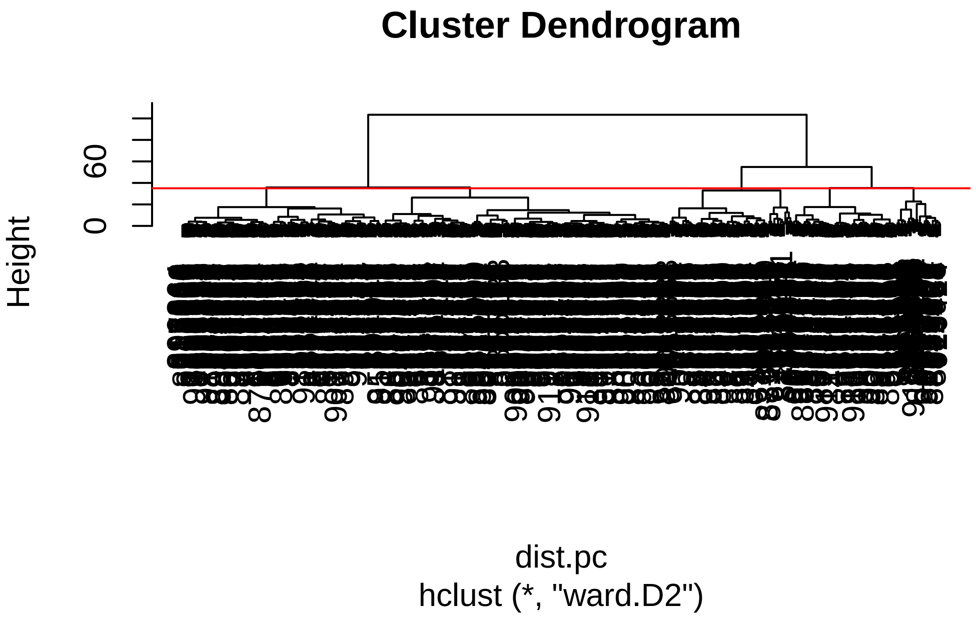
```
dist.pc <- dist(wisc.pr$x[,1:3])
wisc.pr.hclust <- hclust(dist.pc, method = "ward.D2")
```

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

height=35 is when the clustering model of `wisc.pr.hclust` has four clusters.

View the tree…

```
plot(wisc.pr.hclust)
abline(h=35, col="red")
```



To get out clustering membership vector (i.e. out main clustering result) we "cut" the tree at a desired height or to yield a desired number of "k"

```
grps <- cutree(wisc.pr.hclust, h=70)
table(grps)
```

```
grps
  1   2 
203 366 
```

How does this clustering grps compare to the expert diagnosis

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

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

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

Yes, because there is less split of the data. When there is two clusters there is a split in data where there is a majority of M in one and B in the other.

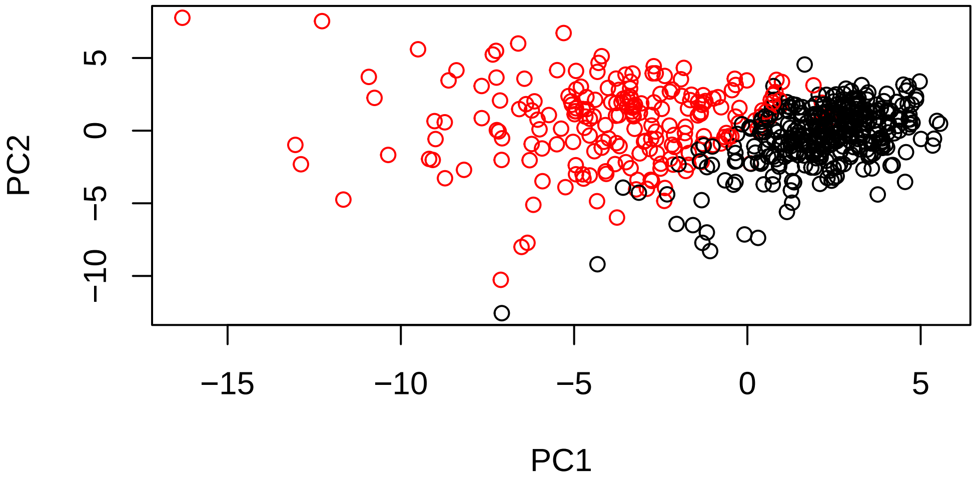
> Q13. Which method gives your favorite results for the same data.dist dataset? Explain your reasoning.

Using `ward.D2` provides a clear separation between M and B samples that were both balanced. Overall, M and B were accurately grouped and a strong alignment in each cluster can be observed.

Combining Methods

Create a graph of PC1 and PC2

```
col <- ifelse(diagnosis == "M", "red", "black")
plot(wisc.pr$x[,1:2], col=col)
```



Re-order the factor and re plot

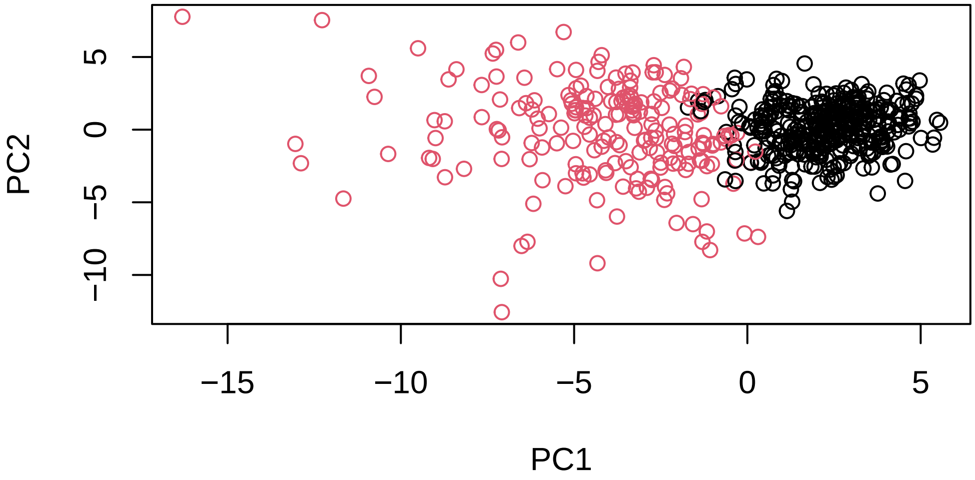
```
g <- as.factor(grps)
levels(g)
```

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

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

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

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



Cut this model into two clusters and assign to `wisc.pr.hclust.clusters`

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

```
                       diagnosis
wisc.pr.hclust.clusters   B   M
                      1  24 179
                      2 333  33
```

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

There is a distinct and balaned separation of the four clusters. Cluster 1 consist of majority M samples and cluster 2 consists of majority B samples.

> 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 k means model separates the diagnoses well however there is some overlap. The heiarchical model shows a distinct separation but with four clusters instead of 2, thus fragmenting the separation.

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

Hierarchical clustering is both higher in sensitivity and specificity than the k means model. This was concluded as there were greater benign and malignant samples that were correctly grouped.

Sensitivity: TP/(TP+FN) Specificity: TN/(TN+FN)

7. Prediction

We can use out PCA model for prediction with new input patient samples.

```
#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
```

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

We should prioritize patient 2 due to closer clusering associated with a malignant disease diagnosis. They are a higher risk group for malignant disease.