Class 8

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1.Preparing the data

Data is online here: https://bioboot.github.io/bimm143_S20/class-material/WisconsinCancer.csv

```
fna.data <- "WisconsinCancer.csv"
wisc.df <- read.csv(fna.data, 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
```

Removing the first column (the expert diagnosis)

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

> Q1. How many observations in this dataset?

```
dim(wisc.data)
```

```
[1] 569  30
```

There are 569 observations.

> Q2. How many of the observations hafve a malignant diagnosis

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

```

  B   M 
357 212 
```

There are 212 malignant observations.

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

```
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. How does it work? It searches for matches to argument pattern within each element of a vector.

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

```
[1] 10
```

There are 10 variables in the data suffixed with _mean.

2. Principal Component Analysis

Checking the means and standard deviations to see if we need to scale the data:

```
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
```

Now that we know we need to scale it, lets run the PCA

```
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% of the original variance is captured by the first principal components.

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

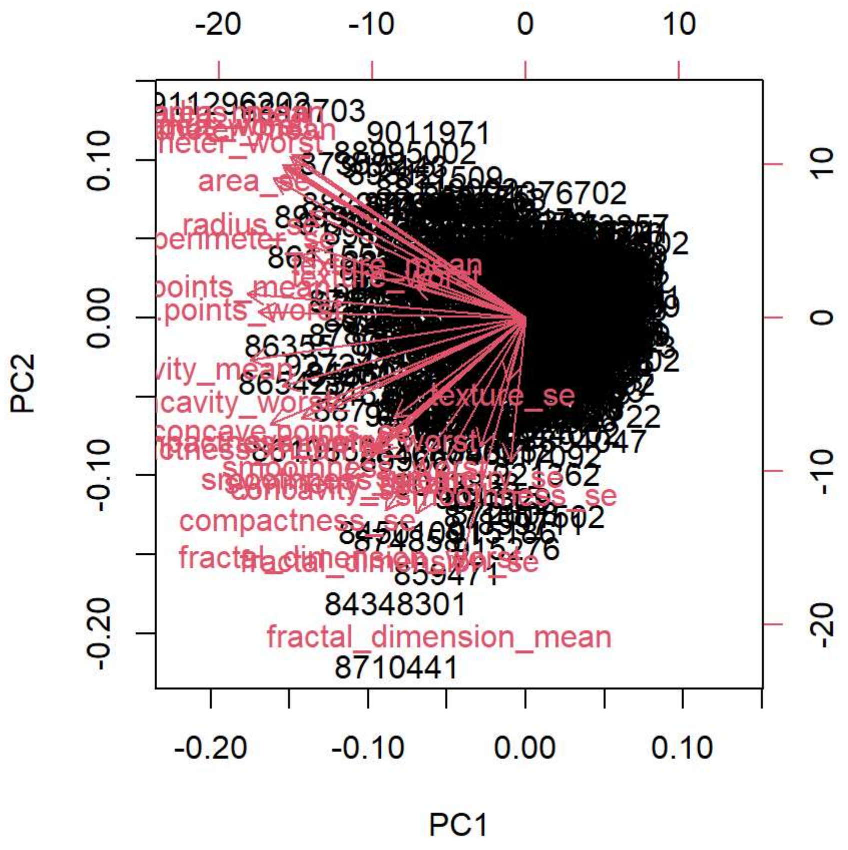
You get more than 70% of the original variance by PCA 3.

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

You get at least 90% of the original variance in the data by PCA 7

Now lets create a simple plot of our pca results:

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

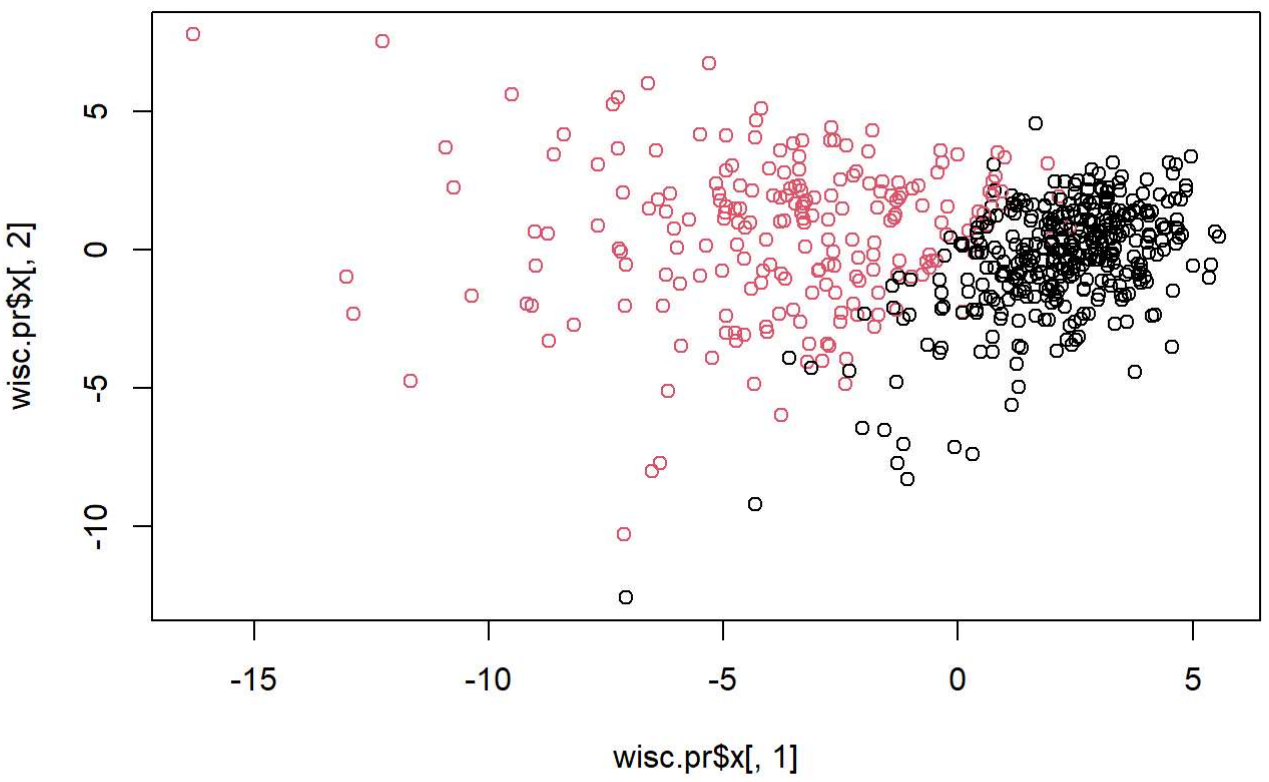


Ew > Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?

This plot is ugly as sin. It’s difficult to understand because everything is piled on top of one another and you can’t distinguish any individual points from anything else. It just looks like noise.

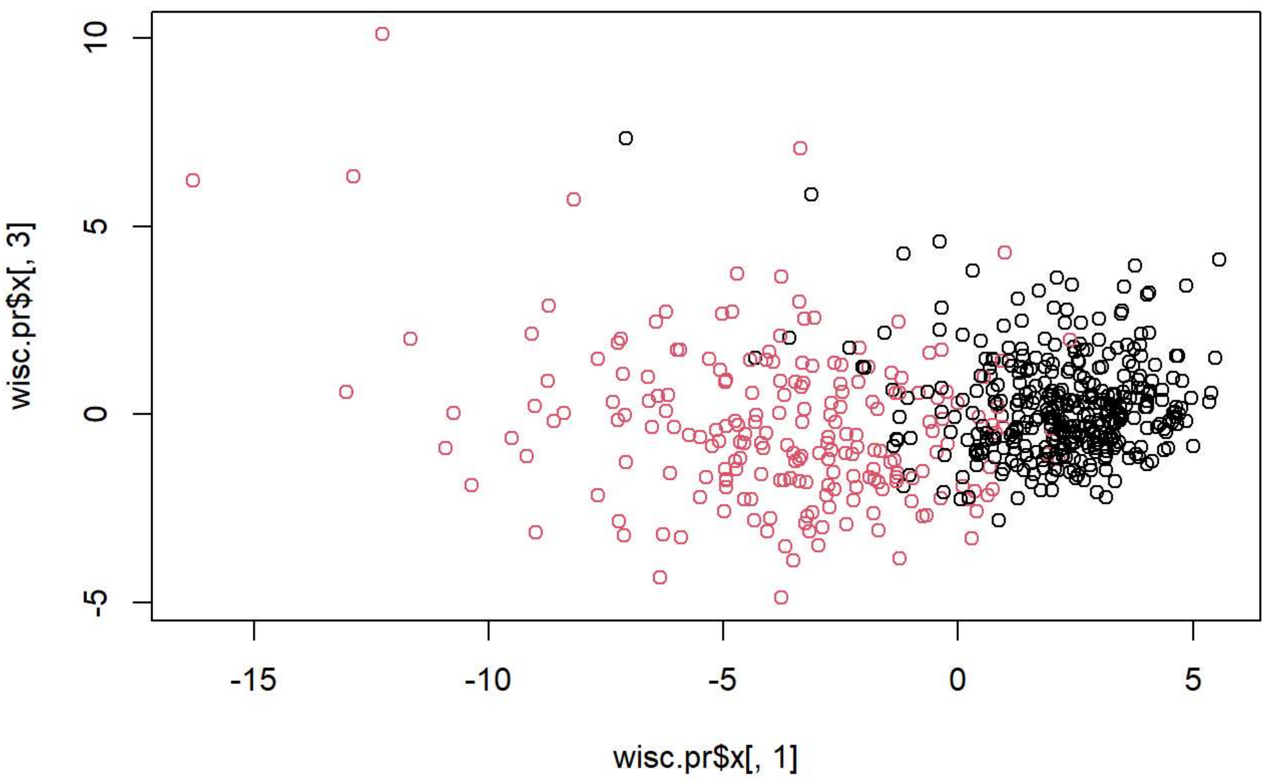
Lets make a better plot

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



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

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



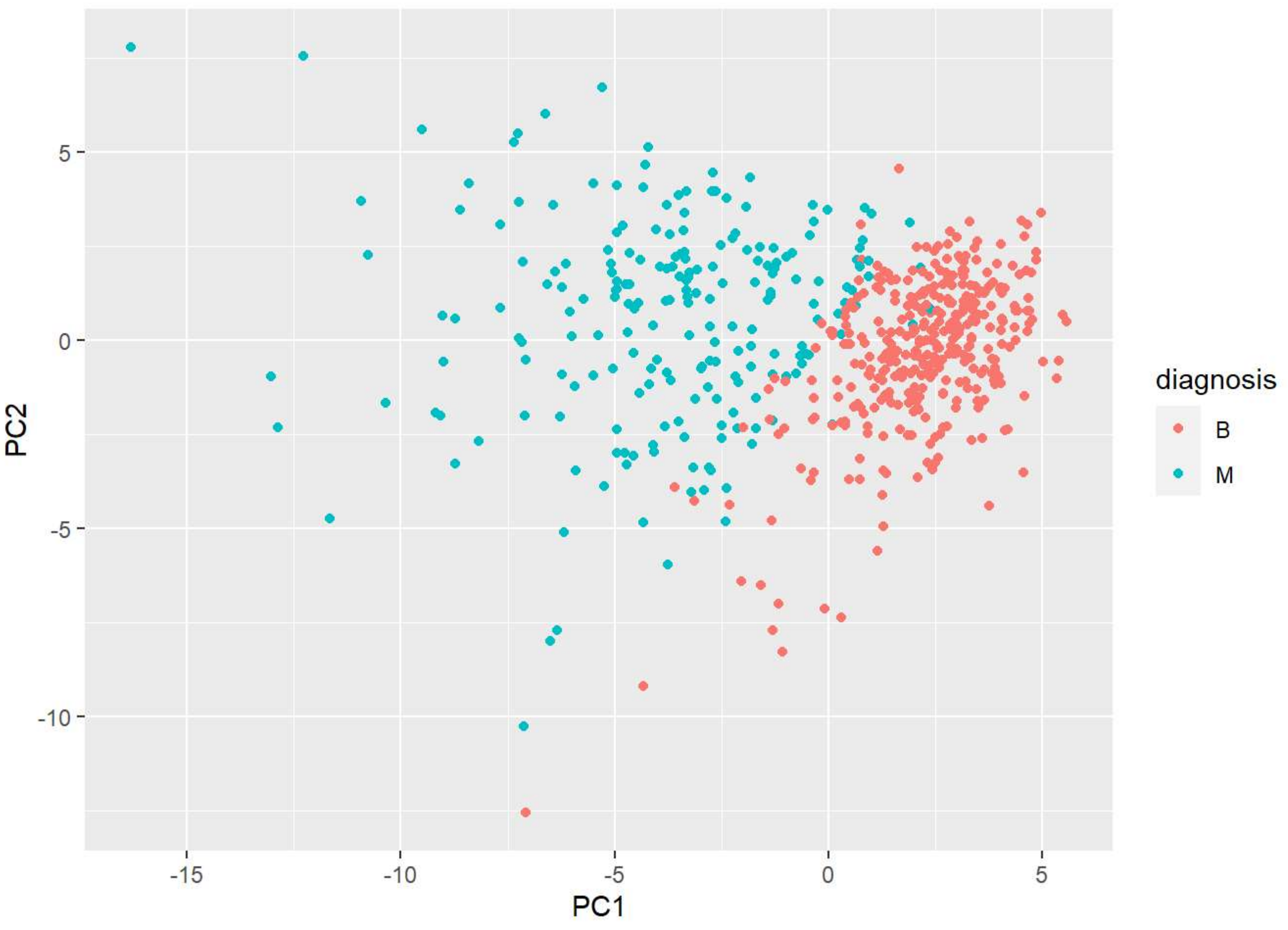
I notice that benign and malignant are slightly less separate than they were in PCA1 vs PCA2.

Now lets make a nice version of this plot in ggplot 2!

```
df <- as.data.frame(wisc.pr$x)
df$diagnosis <- diagnosis
library(ggplot2)
```

```
Warning: package 'ggplot2' was built under R version 4.1.3
```

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



> 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[,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 
```

The component loading loading vector for concave.points.mean is -0.26

> 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 is 4 PC's. You can see this via

```
y <- summary(wisc.pr)
attributes(y)
```

```
$names
[1] "sdev"       "rotation"   "center"     "scale"      "x"         
[6] "importance"

$class
[1] "summary.prcomp"
```

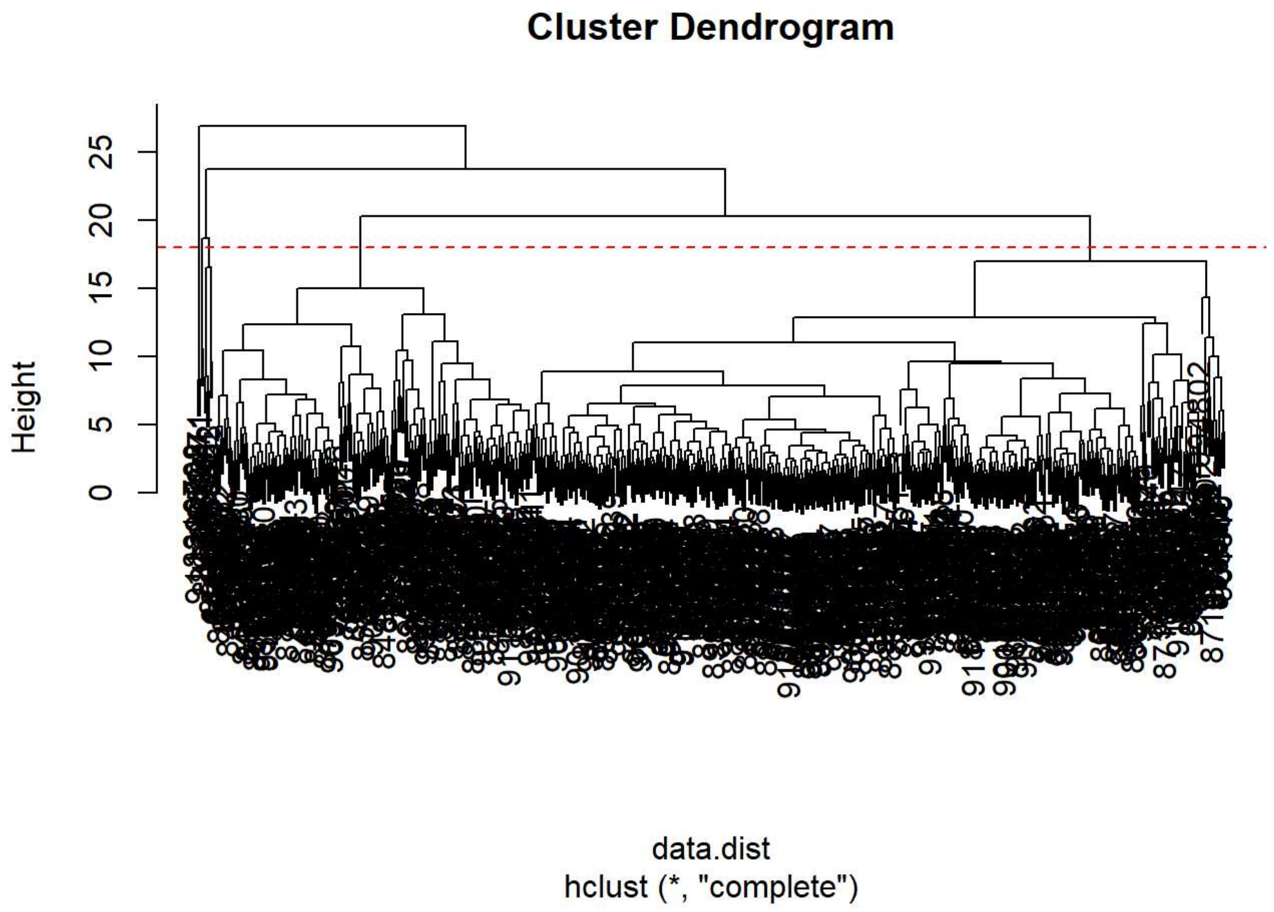
```
sum(y$importance[3,]<=0.8)
```

```
[1] 4
```

3. Hierarchical Clustering

Lets make a cluster dendrogram that shows our results from the initial table

```
data.scaled <- scale(wisc.data)
data.dist <- dist(data.scaled, method = "euclidian")
wisc.hclust <- hclust(data.dist, method = "complete")
plot(wisc.hclust)
abline(h=18, col = "red" ,lty =2)
```



At height 18, there are 4 clusters below it.

```r
wisc.hclust.clusters <- cutree(wisc.hclust, k = 10)
table(wisc.hclust.clusters, diagnosis)
```

```
                    diagnosis
wisc.hclust.clusters   B   M
                  1   12  86
                  2    0  59
                  3    0   3
                  4  331  39
                  5    0  20
                  6    2   0
                  7   12   0
                  8    0   2
                  9    0   2
                  10   0   1
```

> Q.12 Can you find a better cluster vs diagnoses match by cutting into a different number of clusters between 2 and 10?

You can find other matches by changing the parameters, but it is hard to tell if the matches are "better" or not.

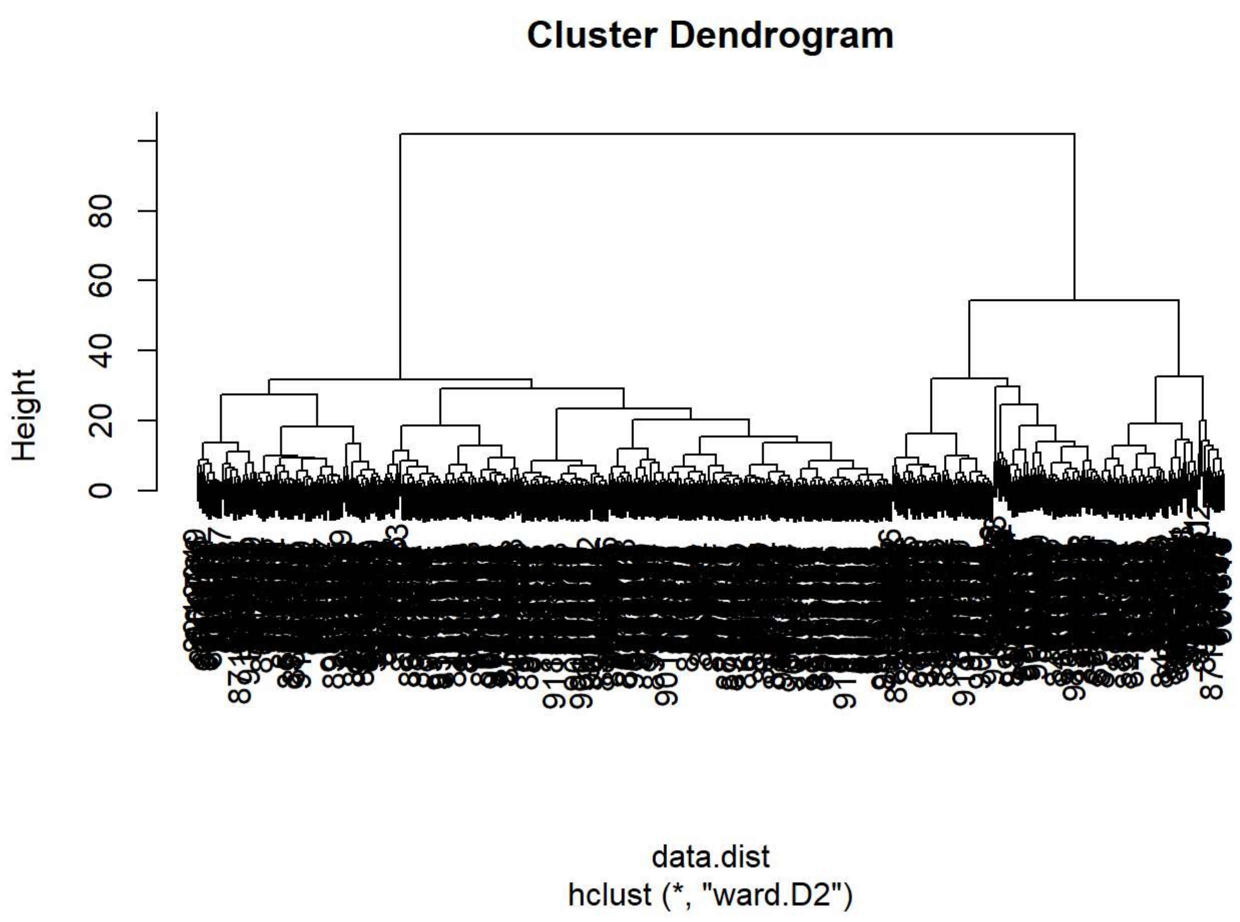
> Q13. Which method gives your favorite results for the same data.dist dataset? Explain your reasoning.

In this case, ward.D2 is my favorite method because it minimizes the variance within clusters.

5. Combining methods

We need to create a model that is a dendrogram of the PCA results.

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



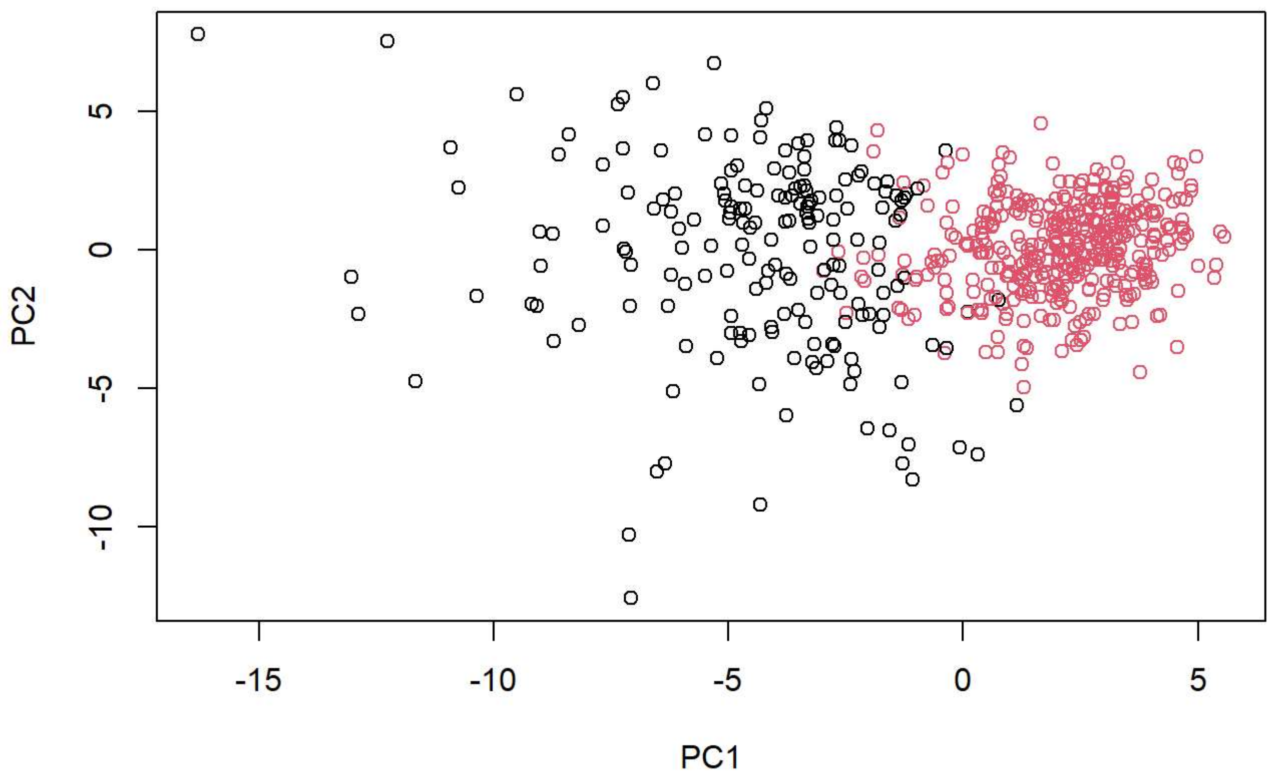
```
grps <- cutree(wisc.pr.hclust, k=2)
table(grps)
```

```
grps
  1   2
184 385
```

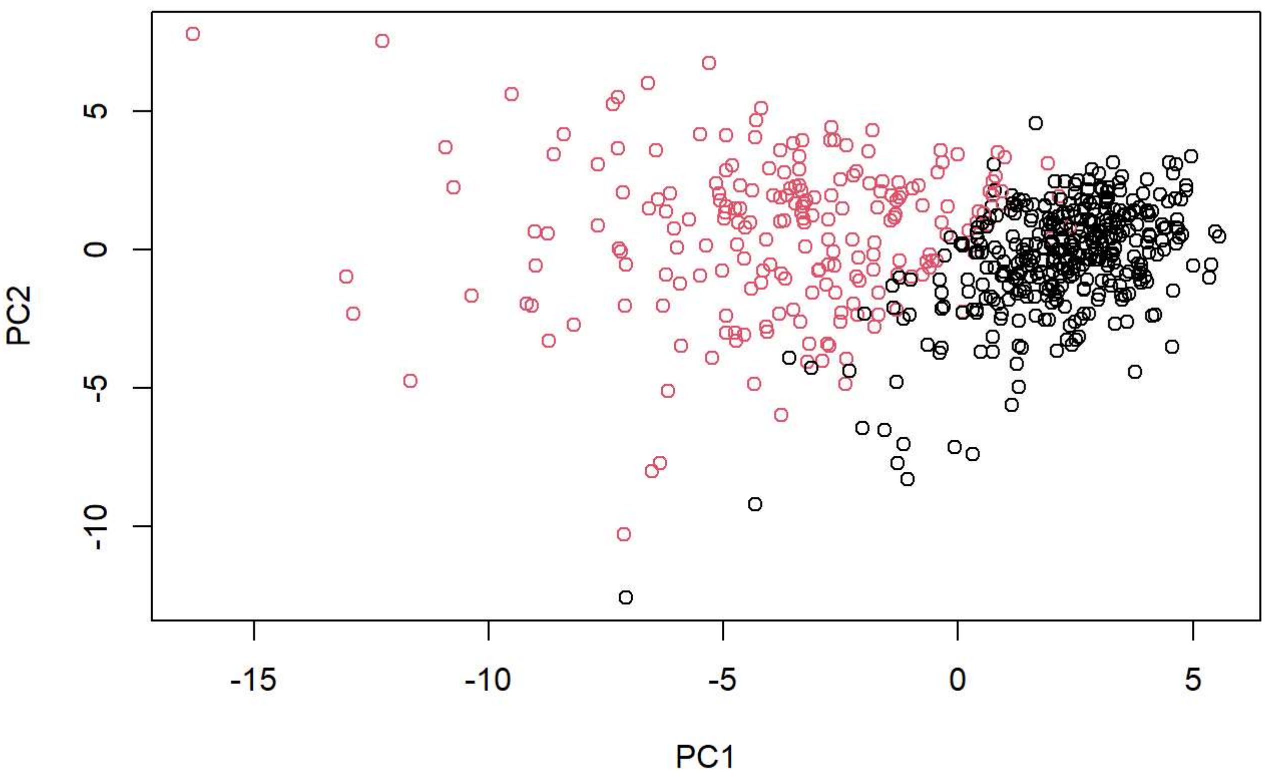
```
table(grps, diagnosis)
```

```
    diagnosis
grps   B   M
   1  20 164
   2 337  48
```

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



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



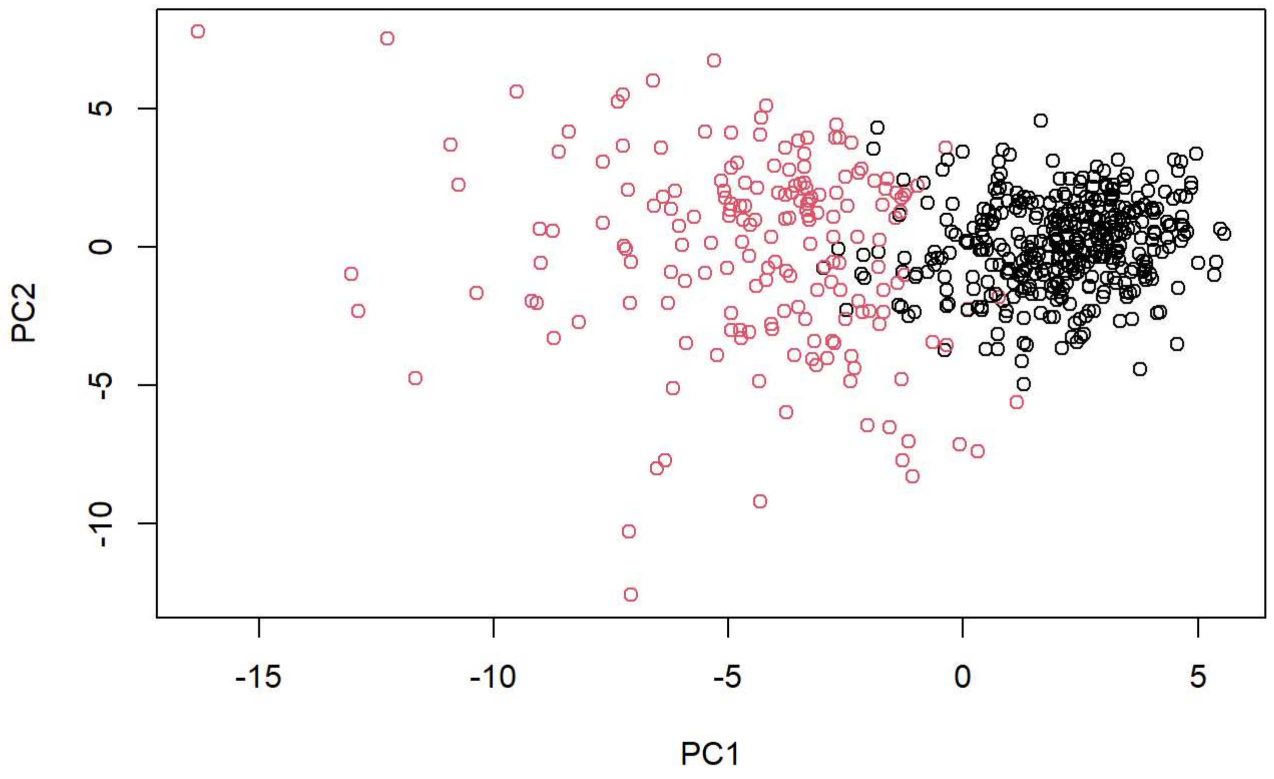
```
g <- as.factor(grps)
levels(g)
```

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

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

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

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



```
wisc.pr.hclust <- hclust(dist(wisc.pr$x[,1:7]), method="ward.D2")
wisc.pr.hclust.clusters <- cutree(wisc.pr.hclust, k=4)
table(wisc.pr.hclust.clusters, diagnosis)
```

```
                       diagnosis
wisc.pr.hclust.clusters   B   M
                      1   0  45
                      2   2  77
                      3  26  66
                      4 329  24
```

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

Four clusters does not split out particularly well because of group “3” which kind of has a lot in both categories. I liked the model with two groups better because it was simpler and easier to generalize as the mostly benign group and mostly malignant group.

> 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.

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

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

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

```
                    diagnosis
wisc.hclust.clusters   B   M
                  1   12  86
                  2    0  59
                  3    0   3
                  4  331  39
                  5    0  20
                  6    2   0
                  7   12   0
                  8    0   2
                  9    0   2
                  10   0   1
```

It seems like they separated the diagnoses well, with the wisc.km cluster seemingly doing better than the PCA model because there is more separation between benign and malignant.

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

```r
# For the kmeans method:
175/(175+37)
```

```
[1] 0.8254717
```

```r
343/(343+37)
```

```
[1] 0.9026316
```

```r
# For the PCA method
188/(188+24)
```

```
[1] 0.8867925
```

```r
329/(329+24)
```

```
[1] 0.9320113
```

Overall, it seems like PCA method resulted in better of both specificity and sensitivity.