Class 08: Mini Project Breast Cancer

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Background

In today's class we will be employing all R techniques for data analysis that we have learned thus far - including the machine learning methods of clustering and PCA - to analyze real breast cancer biopsy data.

Data Import

Data from the Wisconsin Cancer CSV file:

```r
fna.data <- "WisconsinCancer.csv"

wisc.df <- read.csv(fna.data, row.names=1)

head(wisc.df, 3)
```

```
         diagnosis radius_mean texture_mean perimeter_mean area_mean
842302           M       17.99        10.38          122.8      1001
842517           M       20.57        17.77          132.9      1326
84300903         M       19.69        21.25          130.0      1203
```

```
         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
         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
         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
         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
         perimeter_worst area_worst smoothness_worst compactness_worst
842302             184.6       2019           0.1622            0.6656
842517             158.8       1956           0.1238            0.1866
84300903           152.5       1709           0.1444            0.4245
         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
         fractal_dimension_worst
842302                   0.11890
842517                   0.08902
84300903                 0.08758
```

Removing the first column from the dataframe as this is the pathologist provided diagnosis which is the answer to if our cell samples are malignant or benign:

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

Creating diagnosis vector from the original dataset:

```
diagnosis <- wisc.df$diagnosis
```

Q1. How many observations are in this dataset?

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

```
[1] 569
```

There are 569 observations in this dataset.

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

```r
count = 0
for (i in 1:nrow(wisc.data)){
  if (diagnosis[i]=="M"){
    count = count + 1
  }
}
count
```

```
[1] 212
```

There are 212 observations with a malignant diagnosis in this dataset.

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

```r
sum(endsWith(colnames(wisc.data), "_mean"))
```

```
[1] 10
```

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

Principal Component Analysis (PCA)

The main function in base R called `prcomp()` we will use the optional argument `scale=TRUE` here as the data columns/features/dimensions are on very different scales in the original dataset.

Perform PCA on wisc.data by completing the following code:

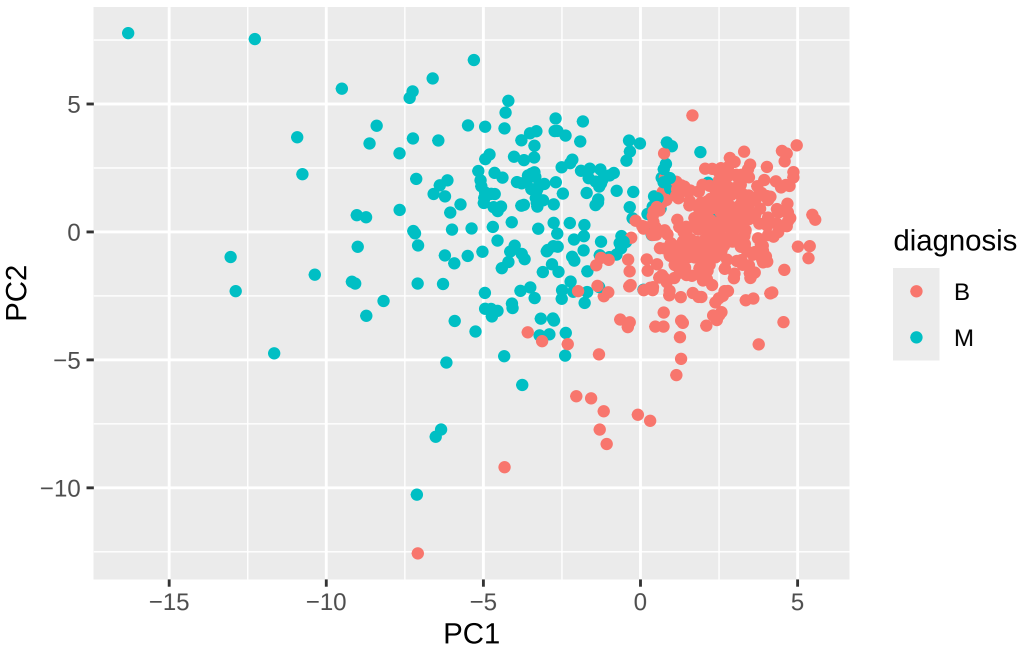
```r
wisc.pr <- prcomp(wisc.data, scale=TRUE)
attributes(wisc.pr)
```

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

$class
[1] "prcomp"
```

```
library(ggplot2)

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



Let's check the mean and standard deviation to see if scaling is necessary:

```
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 
```

View the summary:

```
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 component (PC1)?

```r
var_explained <- wisc.pr$sdev^2/sum(wisc.pr$sdev^2)
var_explained[1]
```

```
[1] 0.4427203
```

The first principal component captures 44.27% of the original variance.

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

```r
var_explained <- wisc.pr$sdev^2 / sum(wisc.pr$sdev^2)
cumulative <- cumsum(var_explained)
which(cumulative >= 0.70)[1]
```

```
[1] 3
```

Three principal components 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?

```r
var_explained <- wisc.pr$sdev^2 / sum(wisc.pr$sdev^2)
cumulative <- cumsum(var_explained)
which(cumulative >= 0.90)[1]
```

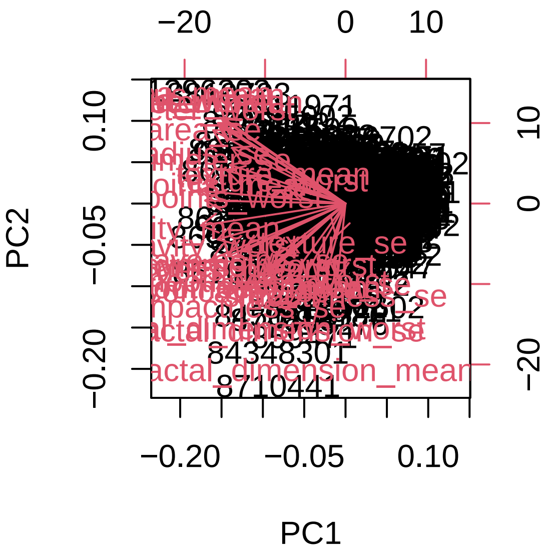
```
[1] 7
```

Seven principal components 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?

A quick bioplot of the principal components:

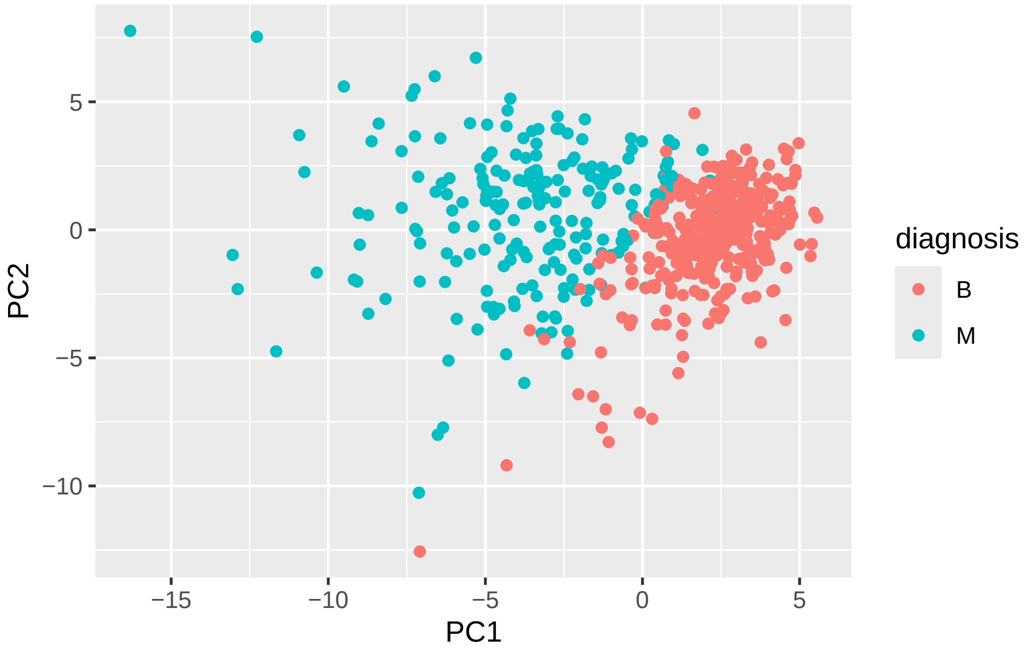
```r
biplot(wisc.pr)
```



This plot shows a lot of features, dimensions, and a lot of numbers from the 2 principal components. Plotting PC1 vs PC2:

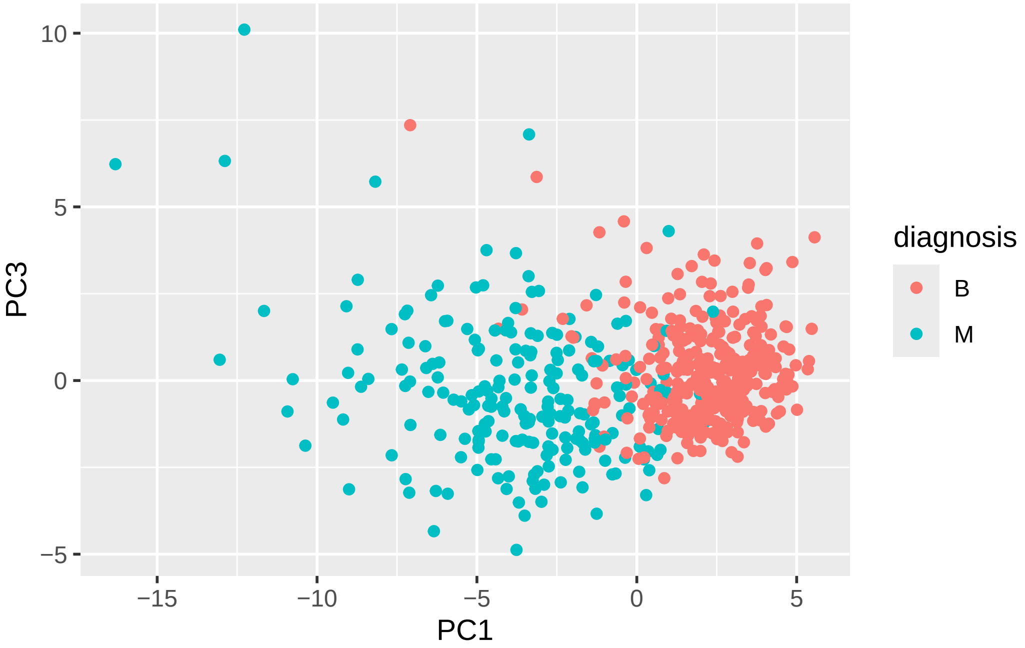
```
library(ggplot2)

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



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

```
ggplot(as.data.frame(wisc.pr$x)) +
  aes(PC1, PC3, col=diagnosis) +
  geom_point()
```



In these two plots, the principal component analysis shows that the principal components are identifying divisions in the data. In the above plot, the points are lower and more clustered towards the bottom.

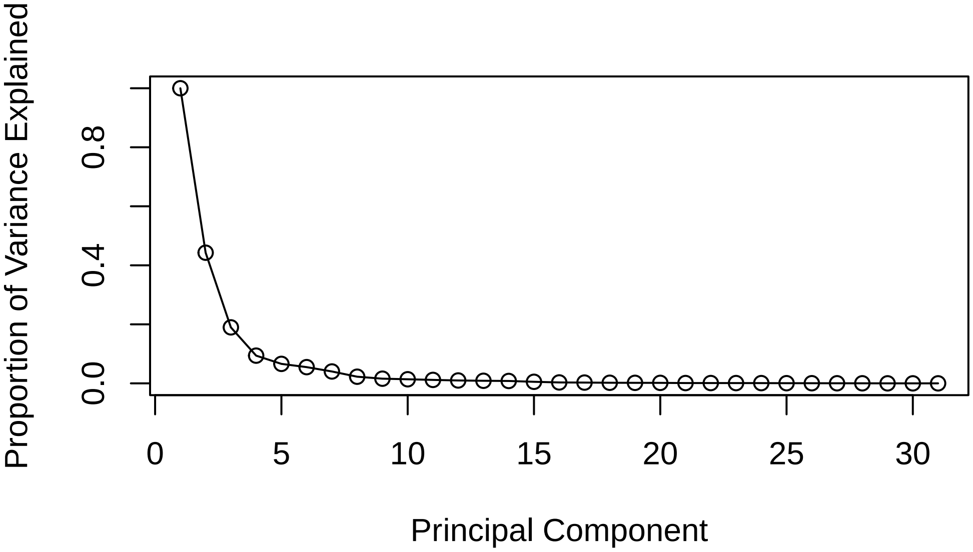
```
pr.var <- wisc.pr$sdev^2

head(pr.var)
```

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

Plotting the variance explained by each principal component:

```
pve <- pr.var / sum(pr.var)
plot(c(1,pve), xlab = "Principal Component",
     ylab = "Proportion of Variance Explained",
     ylim = c(0, 1), type = "o")
```



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? This tells us how much this original feature contributes to the first PC. Are there any features with larger contributions than this one?

```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 concave points means, which is acomponent of the loading vector, contributes the most to the `wisc.pr` data set in the first column. There are not any functions that are higher than the concave.points_mean.

4. Hierarchial Clustering

The goal of this section is to do hierarchical clustering of the original data to see if there is any obvious grouping into malignant and benign clusters.

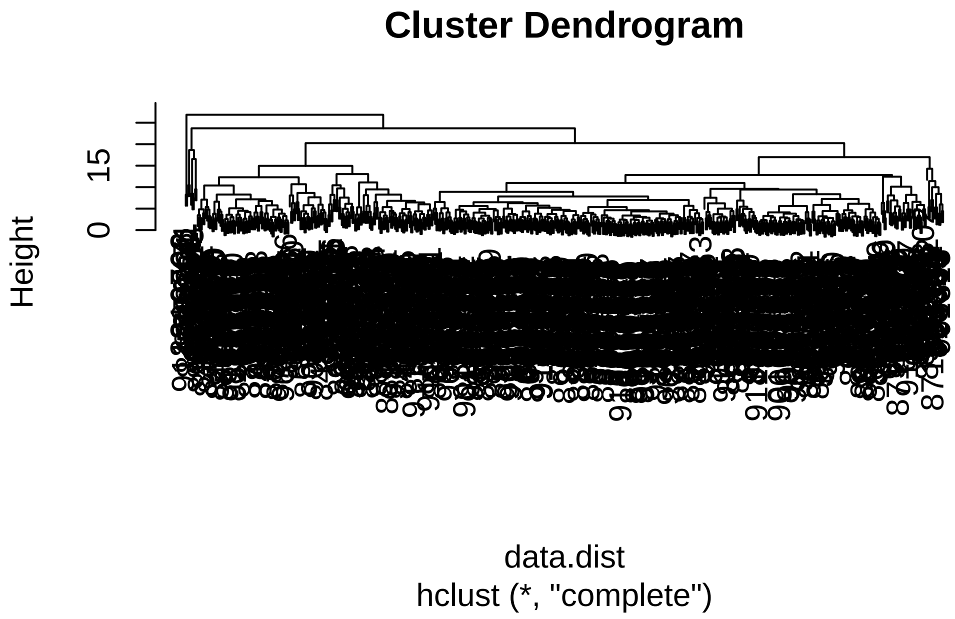
```r
data.scaled <- scale(wisc.data)
data.dist <- dist(data.scaled, method = "euclidian")
wisc.hclust <- hclust(data.dist, method = "complete")
```

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

```
wisc.hclust.clusters
  1   2 
567   2 
```

> Q10. Using the plot() and abline() functions, what is the height at which the clustering model has 4 clusters?

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



The clustering model has 4 clusters at the height of 20.

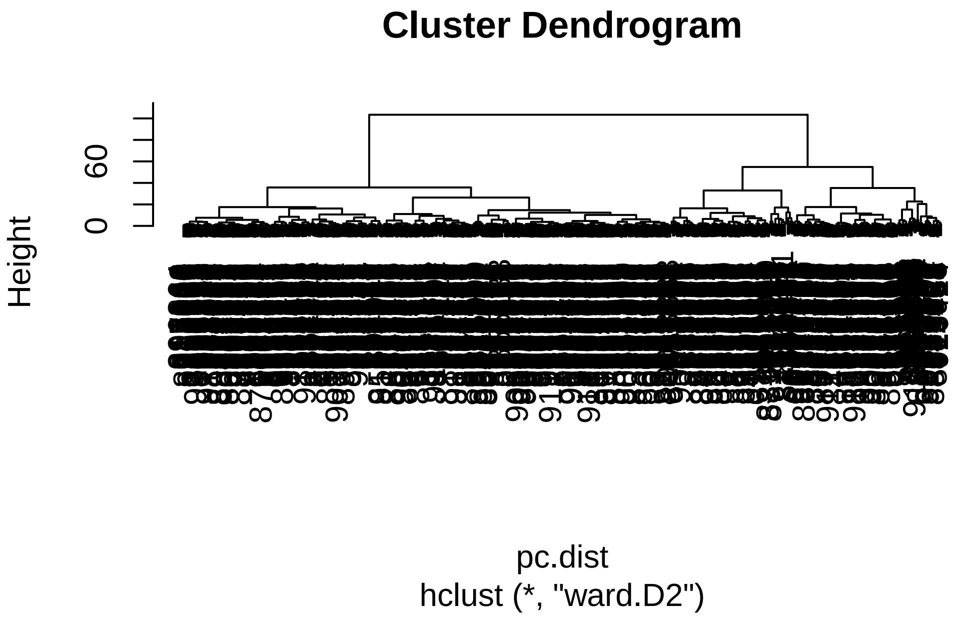
> Q12. Which method gives your favorite results for the same data.dist dataset? Explain your reasoning.

I prefer the cluster dendrogram as is more detailed towards the original nodes of the dataset and also it best visualizes accuracy and variance in the dataset.

Combining Methods

The idea here is that I can take my new variables (the PCs) that are better descriptors of the dataset than the original features (i.e. the 30 columns in wisc.data) and use these as a basis for clustering

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



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

```
grps
  1   2 
203 366 
```

I can now run `table()` with both my clustering `grps` and the expert `diagnosis`

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

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

> Q13. How well does the newly created hclust model with two clusters separate out the two "M" and "B" diagnoses?

The newly created hclust model with two cluster separates the two "M" and "B" diagnoses pretty well as demonstrated in more closed form dendrogram. The dendrogram is also much simpler.

Our cluster “1” has 179 “M” diagnosis Our cluster “2” has 333 “B” diagnosis 179 TP 24 FP 333 TN 24 FN Sensitivity: TP/(TP + FN)

```
179/(179+33)
```

```
[1] 0.8443396
```

Specificity: TN/(TN+FP)

```
333/(333+24)
```

```
[1] 0.9327731
```

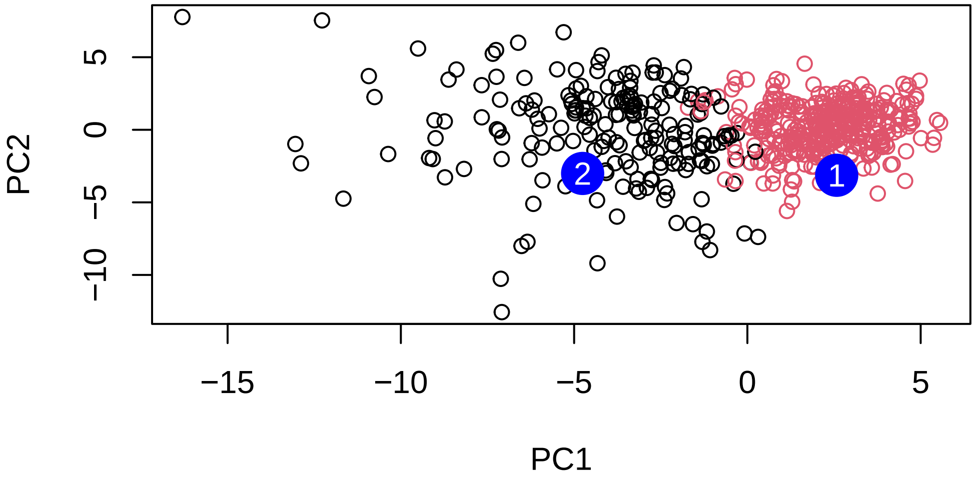
Prediction

We can use our PCA model for prediction of new un-seen cases.

```
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
```

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



Q16. Which of these new patients should we prioritize for follow up based on your results?

Since there is a tighter cluster around patient 1, this is the patient we should prioritize for a follow up based on the results as there is a large variation or spread around patient 2.