Class 08: Mini Project

Lena (A16420052)

Outline

Today we will apply the machine learning methods we introduced in the last class on breast cancer biopsy data from fine needle aspiration (FNA)

Data input

The data is supplied in CSV format

```
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
```

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

```r
#set diagnosis as a factor
diagnosis <- as.factor(wisc.df$diagnosis)
head(diagnosis)
```

```
[1] M M M M M M
Levels: B M
```

> Q1. How many observations are in the dataset?

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

```
[1] 569
```

```r
#dim(wisc.data) also works!
```

There are 569 observations in the dataset

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

```r
sum(diagnosis== "M")
```

```
[1] 212
```

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

```

  B   M 
357 212 
```

There are 212 observations with a malignant diagnosis.

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

```r
#colnames(wisc.data)
#grep searches first argument inside of second factor
length(grep("_mean", colnames(wisc.data)))
```

```
[1] 10
```

There are 10 variables/features with the suffix _mean.

Principle Component Analysis

We need to scale our input data before PCA as some of the columns are measures in terms of very different units with different means and different variances. The upshot here is we set `scale=TRUE` argument to `prcomp()`

```
# 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
```

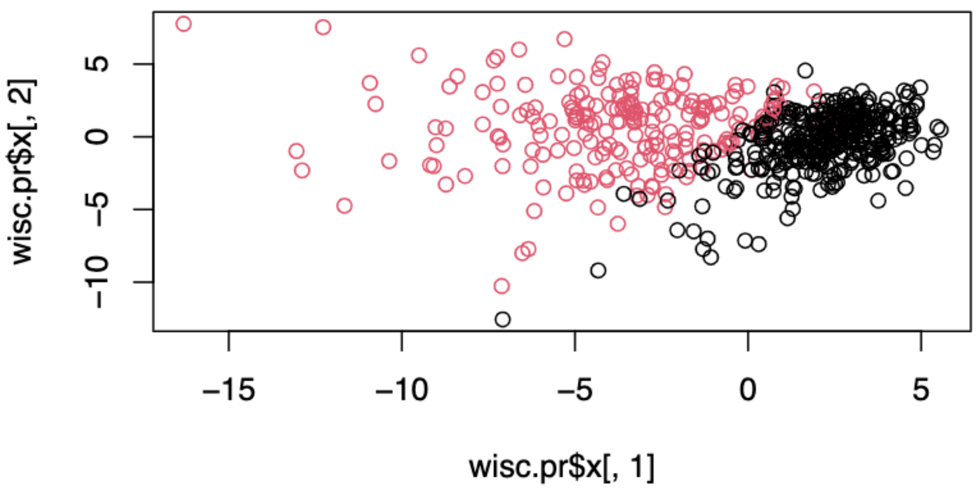
```
# Perform PCA on wisc.data by completing the following code
wisc.pr <- prcomp(wisc.data, scale=TRUE)
```

```
# Look at summary of results
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
```

Generate one of our main results figures- the PC plot (a.k.a "score plot", "orientation plot", "PC1 vs PC2 plot", "PC plot", "projection plot", etc.) It is known by different names in different fields.

```
#can use xlab, ylab arguments to name axis in 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)?

```
wisc.pr$sdev[1]^2/sum(wisc.pr$sdev^2)
```

```
[1] 0.4427203
```

```
#wisc.pr$sdev[1] gives you the stdev for PC1 ([1])
#sum(wisc.pr$sdev^2) gives you total for the proportion
```

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

```r
#cumsum() cumulative sum
var_PCs <- cumsum(wisc.pr$sdev^2/sum(wisc.pr$sdev^2))
which(var_PCs >= 0.7)[1]
```

```
[1] 3
```

```r
var_PCs[3]
```

```
[1] 0.7263637
```

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

```r
var_PCs <- cumsum(wisc.pr$sdev^2/sum(wisc.pr$sdev^2))
which(var_PCs >= 0.9)[1]
```

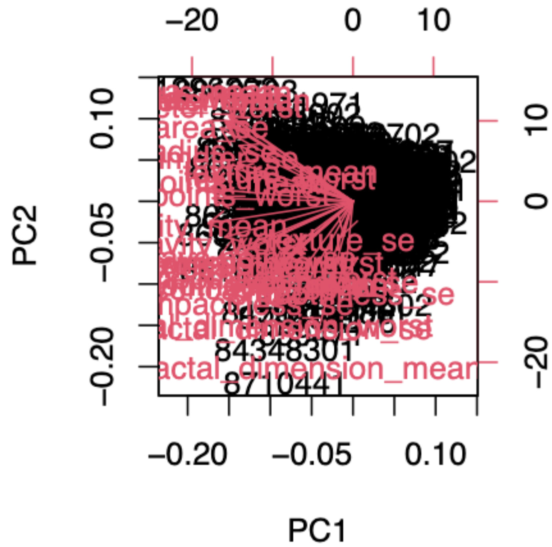
```
[1] 7
```

```r
var_PCs[7]
```

```
[1] 0.9100953
```

Interpreting PCA results

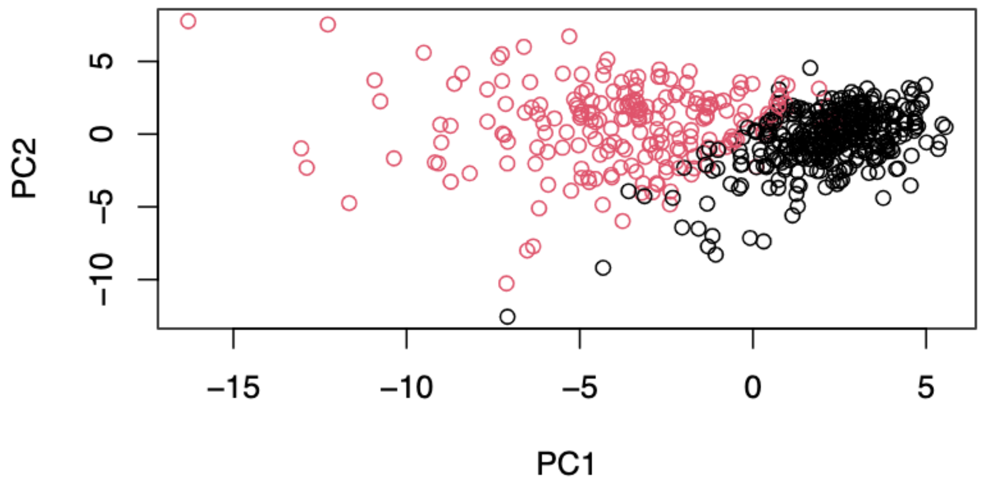
```r
biplot(wisc.pr)
```



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

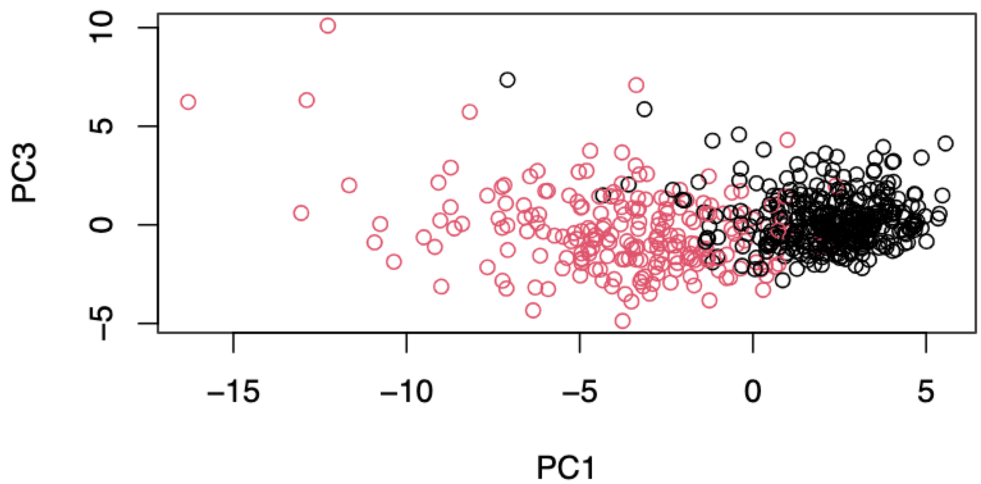
This plot is very difficult to interpret and understand because the points are overlapping.

```
# Scatter plot observations by components 1 and 2
plot(wisc.pr$x[,1], wisc.pr$x[, 2], col = diagnosis ,
     xlab = "PC1", ylab = "PC2")
```



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

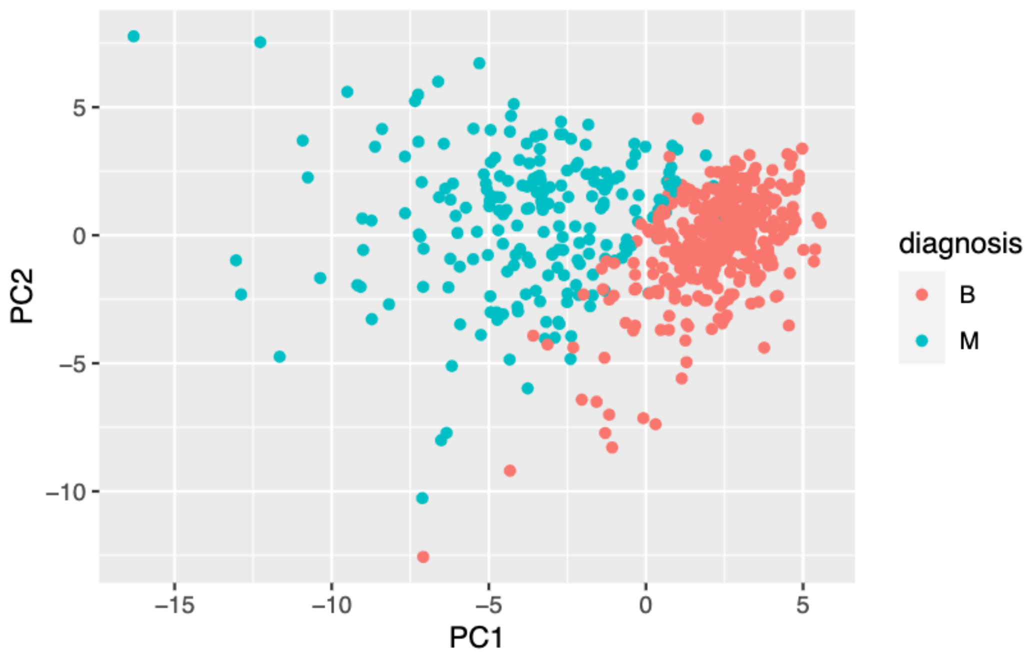
```
plot(wisc.pr$x[,1], wisc.pr$x[, 3], col = diagnosis ,
     xlab = "PC1", ylab = "PC3")
```



Each point represents observations variance for PC1 VS PC3 instead of a point for each observation for every PC.

Using ggplot2 to visualize data

```
# 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()
```

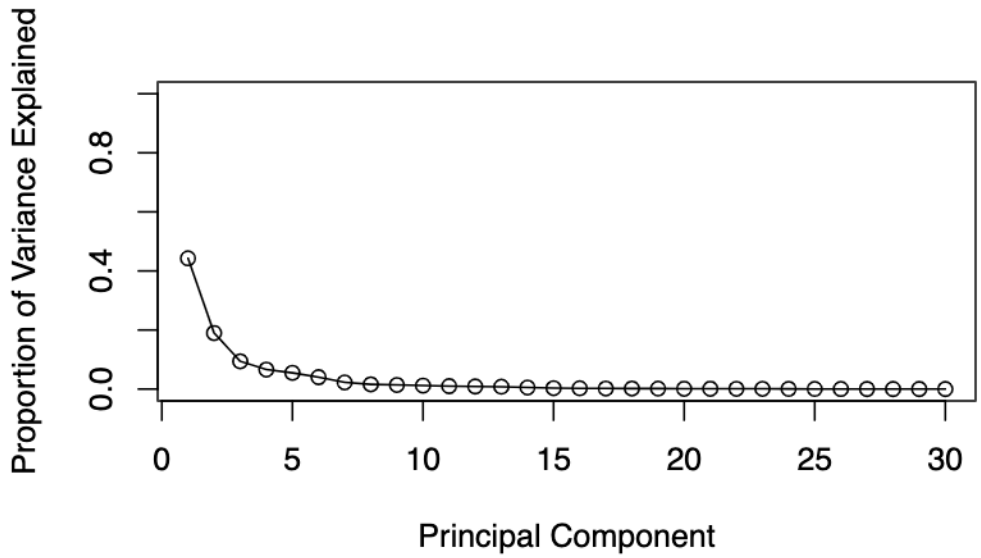


Variance Explained

```
# 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")
```



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?

```
load_vec <- wisc.pr$rotation[,1]
load_vec["concave.points_mean"]
```

```
concave.points_mean
         -0.2608538
```

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

```
pr.var_PC <- cumsum(pve)
which(pr.var_PC >= 0.8)[1]
```

```
[1] 5
```

```
pr.var_PC[5]
```

```
[1] 0.8473427
```

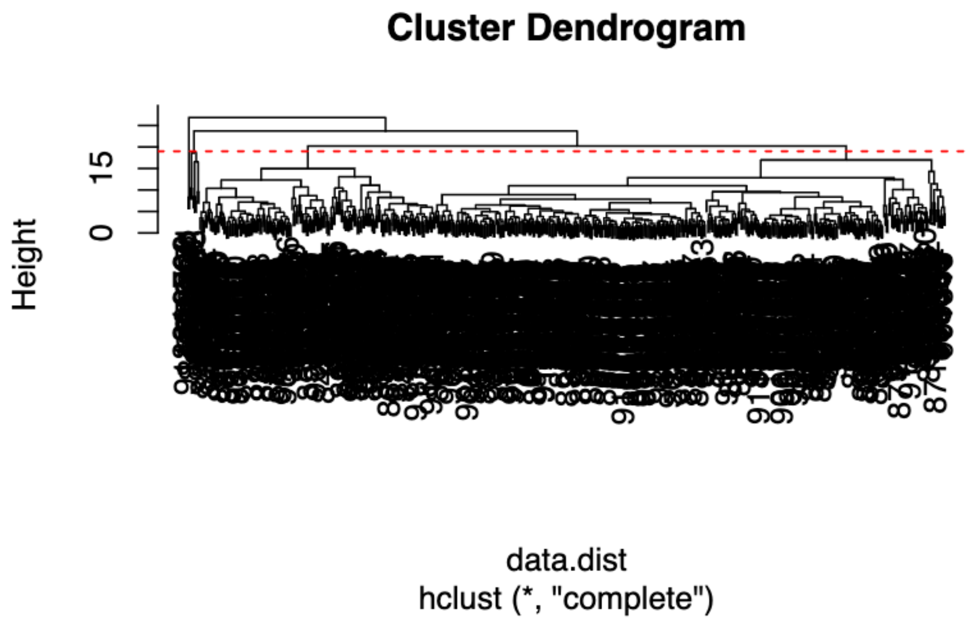
Hierarchical clustering

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

```
Call:
hclust(d = data.dist, method = "complete")

Cluster method   : complete
Distance         : euclidean
Number of objects: 569
```

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

```r
plot(wisc.hclust)
abline(h=19, col="red", lty=2)
```



From analyzing the dendrogram, h=19 is where the clustering model has 4 clusters.

Selecting number of clusters

Generate 2 cluster groups from this hclust object.

```
wisc.hclust.clusters <- cutree(wisc.hclust, k=2)
#if you do h do 18
table(wisc.hclust.clusters, diagnosis)
```

```
                    diagnosis
wisc.hclust.clusters   B   M
                   1 357 210
                   2   0   2
```

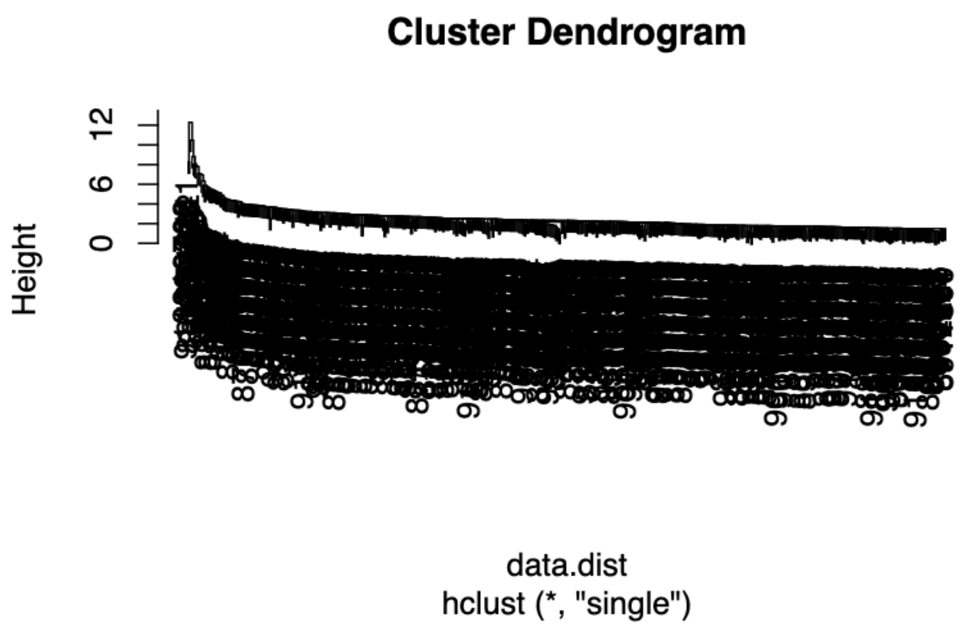
> Q12. Can you find a better cluster vs diagnoses match by cutting into a different number of clusters between 2 and 10?

No I cannot find a better cluster vs diagnoses match than k=4. All other number of clusters result in low separation for cluster vs diagnosis match.

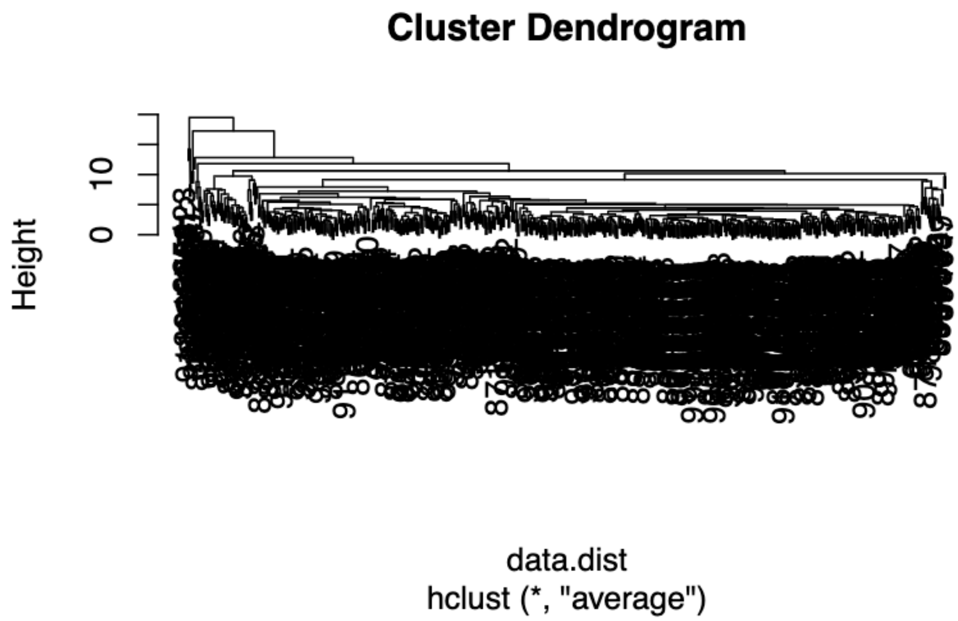
Q13. Which method gives your favorite results for the same data.dist dataset? Explain your reasoning.

Method= ward.D2 because it separates clusters sooner at a lower height.

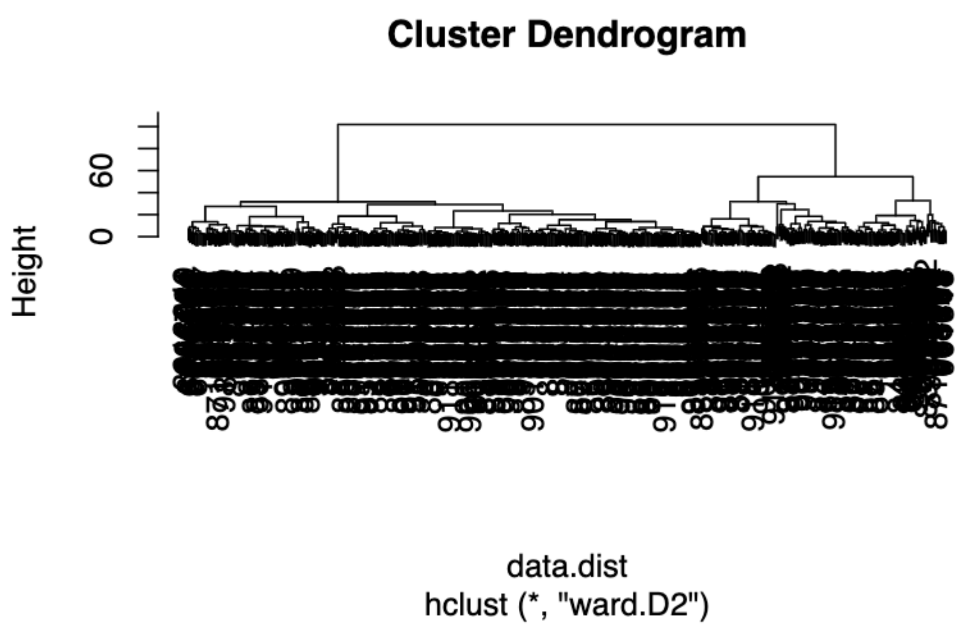
```
single <- hclust(data.dist, method="single")
average <- hclust(data.dist, method="average")
ward.D2 <- hclust(data.dist, method="ward.D2")

plot(single)
```




```
plot(average)
```




```r
plot(ward.D2)
```



Combining methods

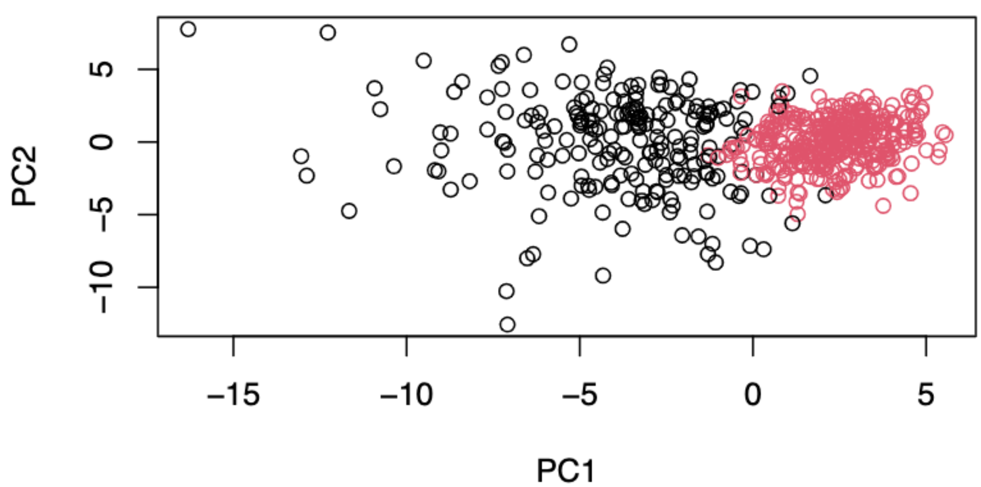
```
#it is [7] because that is what we solved in Q6
d <- dist(wisc.pr$x[, 1:7])
wisc.hclust.pr <- hclust(d, method= "ward.D2")
grps <- cutree(wisc.hclust.pr, k=2)
table(grps)
```

```
grps
  1   2
216 353
```

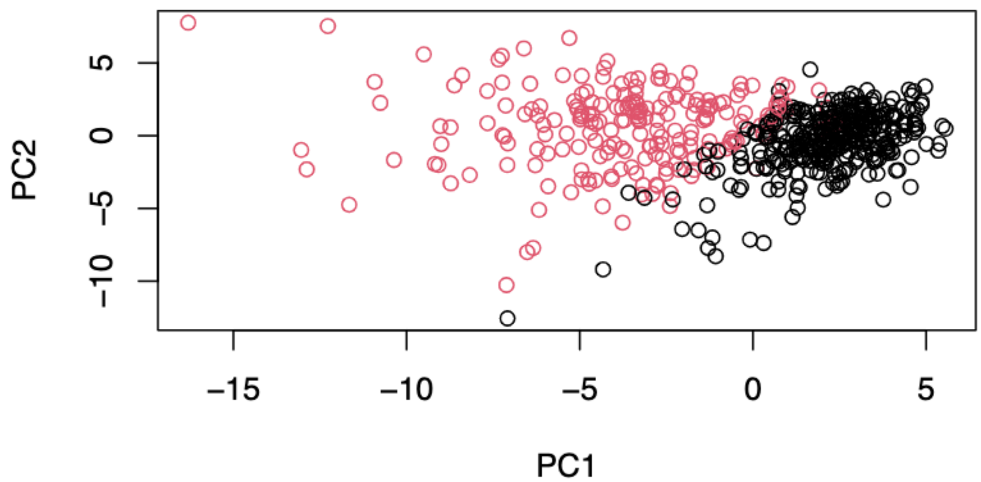
```
table(grps, diagnosis)
```

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

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



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



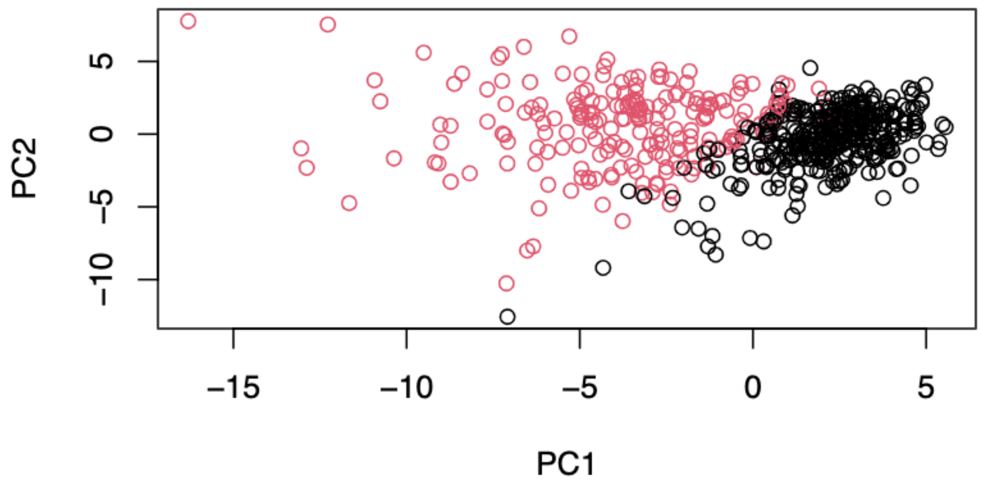
> Q15. How well does the newly created model with four clusters separate out the two diagnoses?

The newly created model with four clusters separates better.

```
# Compare to actual diagnoses
wisc.pr.hclust <- hclust(dist(wisc.pr$x[, 1:7]), method="ward.D2")
wisc.pr.hclust.clusters <- cutree(wisc.pr.hclust, k=2)
table(wisc.pr.hclust.clusters, diagnosis)
```

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

```
plot(wisc.pr$x[,1:7], col=diagnosis)
```




```
#wisc.pr$x is pulling PCs
```