Class 08: Breast Cancer Analysis Project

Shazreh Hassan (PID: A13743949)

Table of contents

Background

The goal of this mini-project is to explore a complete analysis using the unsupervised learning techniques covered in class. We'll extend what we've learned by combining PCA as a pre-processing step to clustering using data that consist of measurements of cell nuclei of human breast masses.

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

```r
fna.data <- "https://bioboot.github.io/bimm143_S20/class-material/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
```

We used row.names=1 so that patient id would not be included. We also want to remove diagnosis column:

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

```
[1] 569  30
```

```r
head(wisc.data)
```

```
         radius_mean texture_mean perimeter_mean area_mean smoothness_mean
842302         17.99        10.38         122.80    1001.0         0.11840
842517         20.57        17.77         132.90    1326.0         0.08474
84300903       19.69        21.25         130.00    1203.0         0.10960
84348301       11.42        20.38          77.58     386.1         0.14250
84358402       20.29        14.34         135.10    1297.0         0.10030
843786         12.45        15.70          82.57     477.1         0.12780
         compactness_mean concavity_mean concave.points_mean symmetry_mean
842302            0.27760         0.3001             0.14710        0.2419
842517            0.07864         0.0869             0.07017        0.1812
```

84300903	0.15990	0.1974	0.12790	0.2069
84348301	0.28390	0.2414	0.10520	0.2597
84358402	0.13280	0.1980	0.10430	0.1809
843786	0.17000	0.1578	0.08089	0.2087

	fractal_dimension_mean	radius_se	texture_se	perimeter_se	area_se
842302	0.07871	1.0950	0.9053	8.589	153.40
842517	0.05667	0.5435	0.7339	3.398	74.08
84300903	0.05999	0.7456	0.7869	4.585	94.03
84348301	0.09744	0.4956	1.1560	3.445	27.23
84358402	0.05883	0.7572	0.7813	5.438	94.44
843786	0.07613	0.3345	0.8902	2.217	27.19

	smoothness_se	compactness_se	concavity_se	concave.points_se
842302	0.006399	0.04904	0.05373	0.01587
842517	0.005225	0.01308	0.01860	0.01340
84300903	0.006150	0.04006	0.03832	0.02058
84348301	0.009110	0.07458	0.05661	0.01867
84358402	0.011490	0.02461	0.05688	0.01885
843786	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
```

Exploratory data analysis

> Q1. How many observations are in the dataset?

There are 569 observations

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

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

```

  B   M 
357 212 
```

There are 212 malignant diagnoses

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

```r
#colnames(wisc.data)

grep("_mean", colnames(wisc.data))  #returns column indices
```

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

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

```
[1] 10
```

Principal component analysis

The main function covered in base R for PCA is called `prcomp()`. We want to **scale and center** our data before PCA to make sure each feature is contributing equally to the analysis, preventing variables with larger variance from taking over in analysis. The optional argument `scale` should almost always be switched to `scale=TRUE`.

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

```
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)?

0.4427 (about 44%)

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

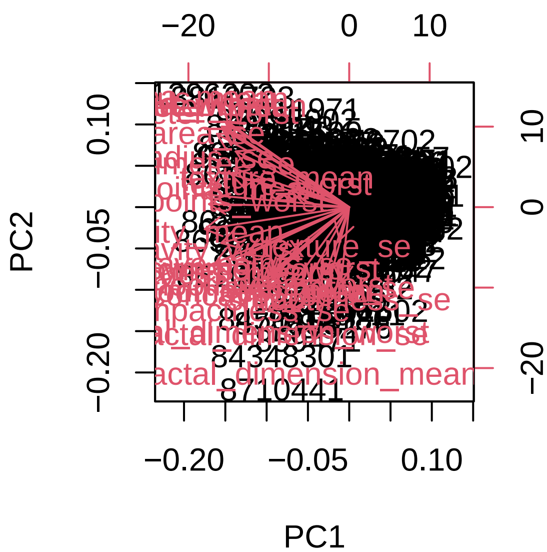
3

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

7

Interpreting PCA Results

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



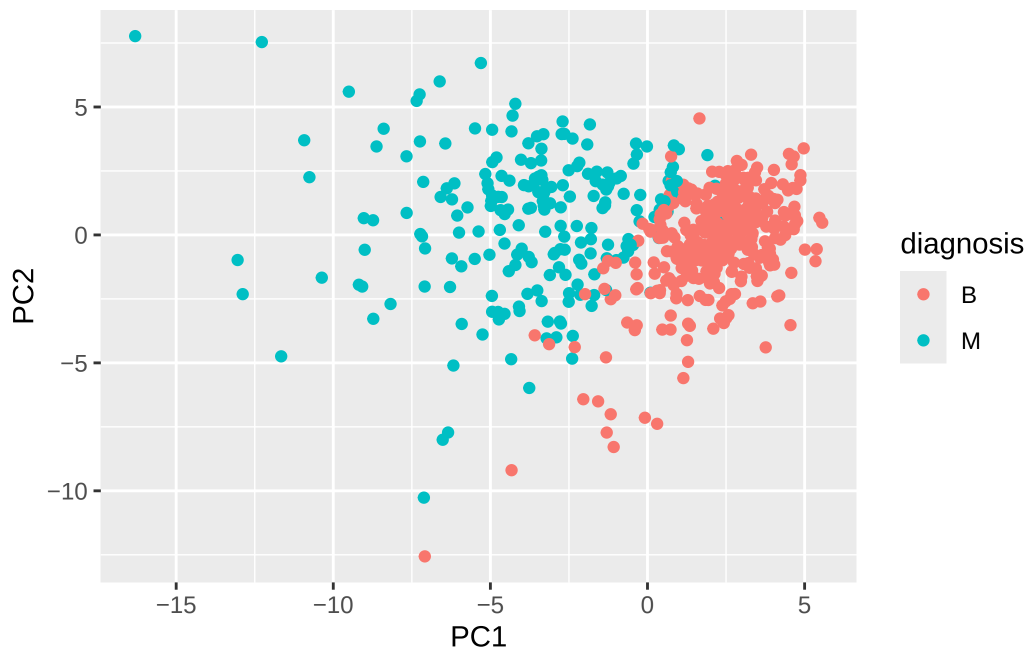
Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?

The plot is difficult to understand because of all the words overlapped onto each other.

Let's make our main result figure - the "PC plot" or "score plot", or "ordination plot"

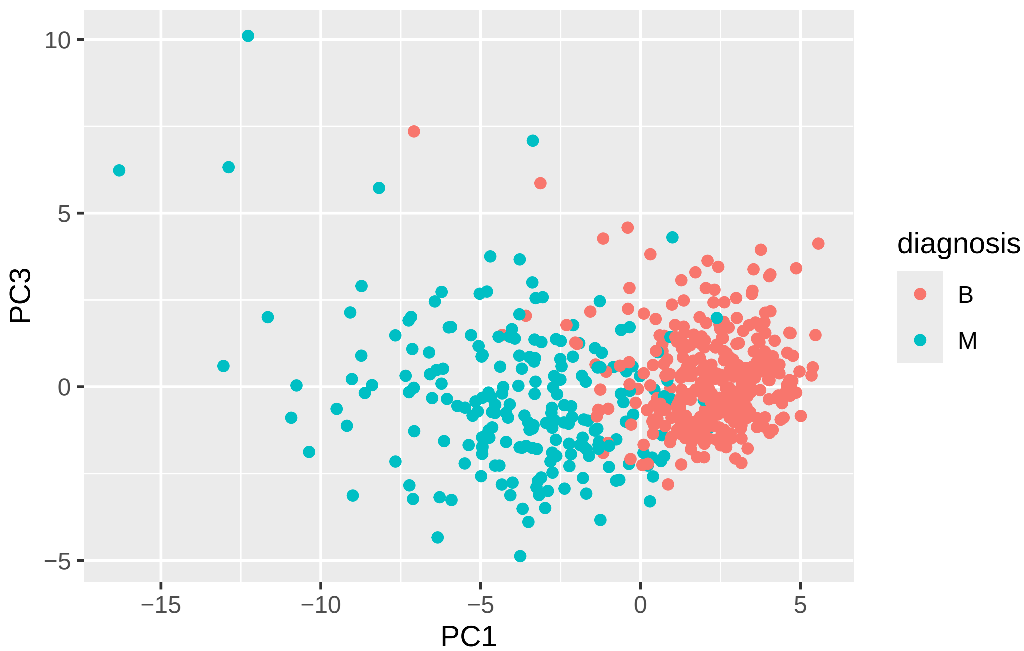
```r
library(ggplot2)

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



These plots seem to show the benign and malignant diagnoses in separable distributions across PC1. There is slightly more overlap in subgroups in the PC1 vs PC3 plot, which makes sense because PC2 explains more variance in the data than PC3.

Variance explained

```
#calculate the variance of each component - standard deviation squared

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

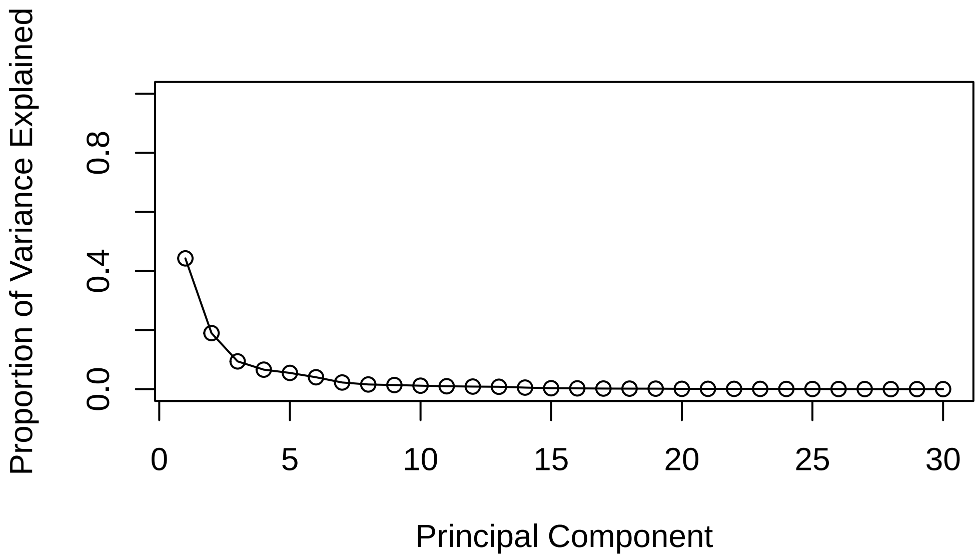
```
[1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

Calculate the variance explained by each principal component by dividing by the total variance explained of all principal components. Assign this to a variable called pve and create a plot of variance explained for each principal component.

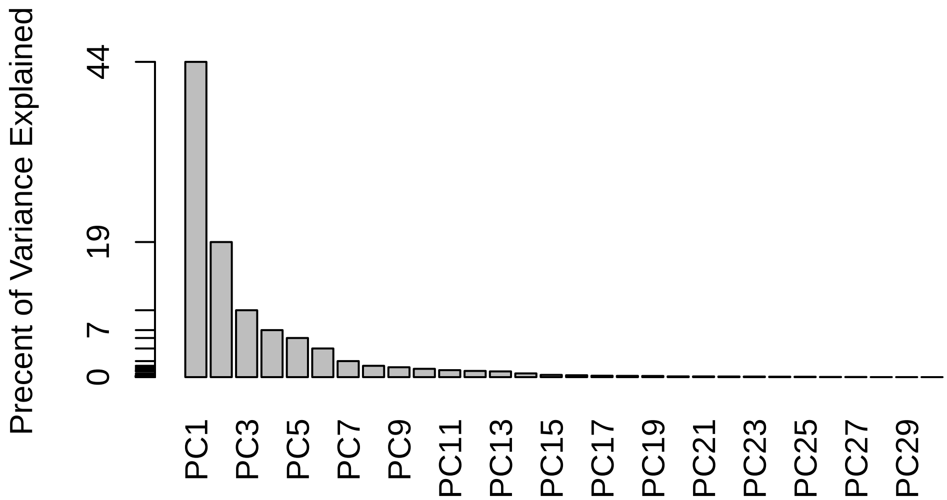
```
# Variance explained by each principal component: pve
pve <- pr.var/sum(pr.var)

# Plot variance explained for each principal component
```

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




```r
# 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 )
```



> 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.

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

```
[1] -0.2608538
```

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

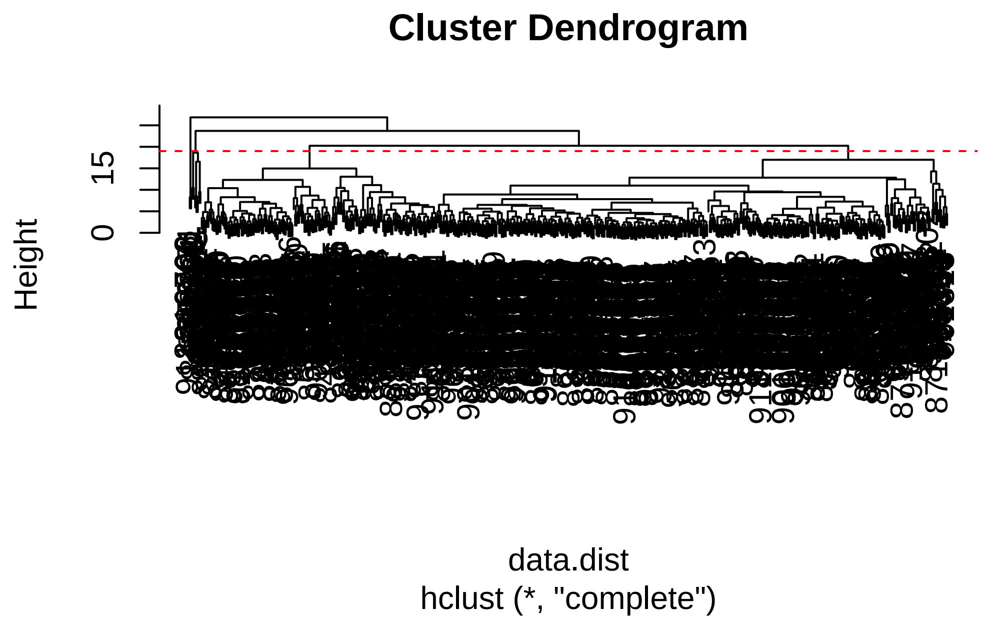
The model has 4 clusters at a height of **19**.

```
# Scale the wisc.data data using the "scale()" function
data.scaled <- scale(wisc.data)

#calculate euclidean distances
data.dist <- dist(data.scaled)

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

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



Selecting number of clusters

```
#cut the tree so that it has 4 clusters
wisc.hclust.clusters <- cutree(wisc.hclust, k=4)

#compare the cluster membership to the actual diagnoses
table(wisc.hclust.clusters, diagnosis)
```

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

Try it with a different number of clusters:

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

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

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

> Q11. OPTIONAL: Can you find a better cluster vs diagnoses match by cutting into a different number of clusters between 2 and 10? How do you judge the quality of your result in each case?

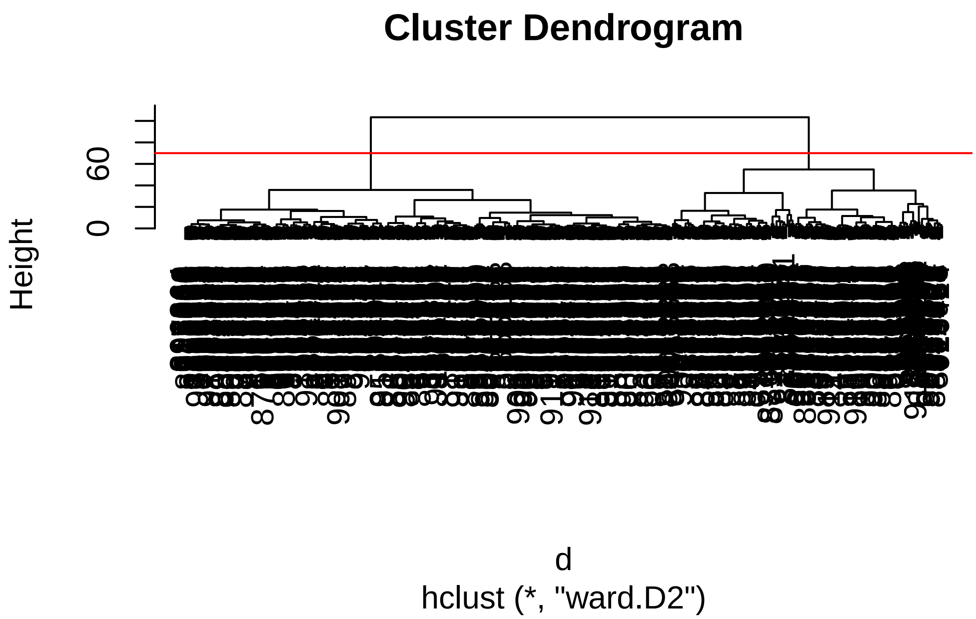
It seems like 4 clusters is the best number, decreasing from 4 leads to more mixing (less separability) between the benign and malignant subgroups within clusters, while increasing from 4 leads to extra clusters with low numbers of observations regardless of subgroup.

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

PCA gave me results that made more sense, given that with clustering it looked like two of the clusters were very close together and 2 of the 4 clusters has very little observations compared to the other 2.

Combining PCA and Clustering

```r
#only putting the first 3 PCs into the clustering
d <- dist(wisc.pr$x[,1:3])
wisc.pr.hclust <- hclust(d, method="ward.D2")
plot(wisc.pr.hclust)
abline(h=70, col="red")
```




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

```
grps
  1   2
203 366
```

> Q13. How well does the newly created model with four clusters separate out the two diagnoses?

Make a wee "cross-table"

```
#compare cluster groups to diagnosis
table(grps, diagnosis)
```

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

TP: 179 FP: 24

Sensitivity: TP/(TP+FN)

> Q14. How well do the 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.

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

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

The clustering models before PCA did worse than the one that combined methods.

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

Patient 2