Class 8 Mini Project

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Preparing the data

Data is prepared in CSV format

```
# Save your input data file into your Project directory
fna.data <- "WisconsinCancer.csv"

# Input the data and store as wisc.df. `row.names=1` puts the first column into the row na
wisc.df <- read.csv(fna.data, row.names=1)
# Viewing resulting data frame to check:
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 is from a pathologist giving an expert diagnosis, which is essentially the answer to if the cells are malignant or benign, so we should omit it.

```
#Use -1 to remove first column
wisc.data <- wisc.df[,-1]
#Create diagnosis vector to check results later
diagnosis <- as.factor(wisc.df[,1])
```

Exploratory data analysis

> Q1. How many observations are in this dataset?

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

```
[1] 569
```

569 rows, so 569 observations in the dataset.

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

```
table(diagnosis)
```

```
diagnosis
  B   M
357 212
```

There are 357 benign and 212 malignant diagnoses.

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

```
#`colnames()` gives access to the column names
column_names <- colnames(wisc.data)
#`grep()` finds patterns within the names, searches for "_mean" in the column names
column_mean <- grep("_mean", column_names)
#`length()` gives the number of elements in the vector
length(column_mean)
```

```
[1] 10
```

Principal Component Analysis

First check the mean and standard deviation of the features of the data to determine if the data should be scaled.

```r
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 
```

```r
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
```

Execute PCA with `prcomp()` on the data

```
#`prcomp` creates a PCA of the data, and settting "scale" to TRUE ensures that even throug
wisc.pr <- prcomp(wisc.data, scale=TRUE)
#there are too many rows to show each individual patient, so use `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 components (PC1)?

44.27% of the original variance is captured by PC1.

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

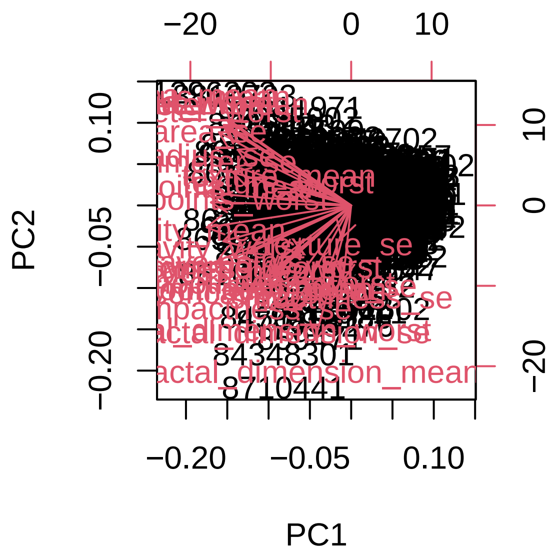
PC1-PC3. At PC3, the cumulative proportion is 72.6%.

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

PC1-PC7. At PC7, the cumulative proportion is 91%.

Interpreting PCA results

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

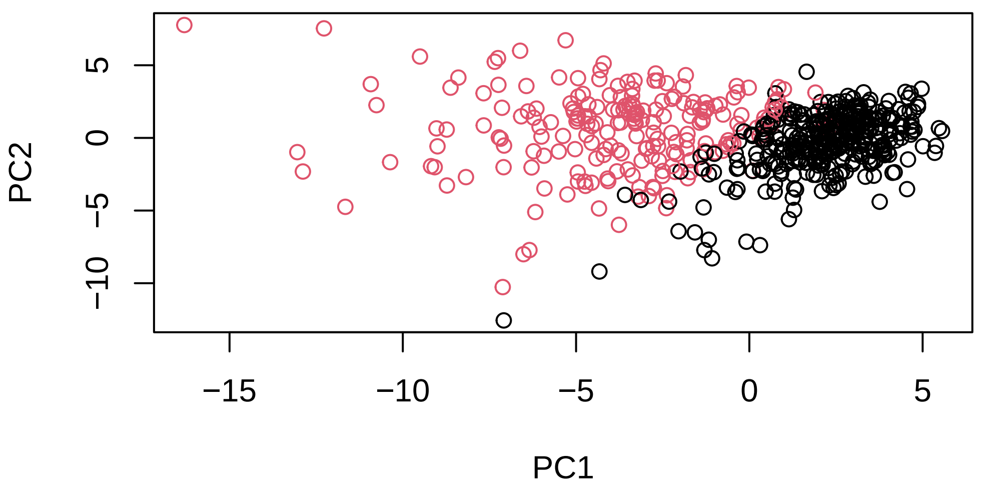


> Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?

This plot is quite hard to look at, it shows all column names and patient codes, making it extremely difficult to identify points. All the points are jumbled together.

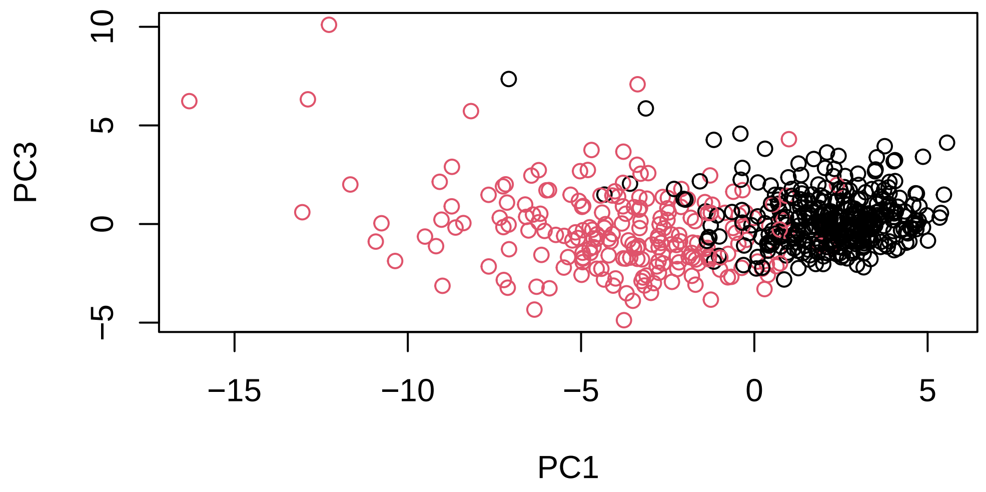
Scatter plot observations by components 1 and 2:

```r
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?

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



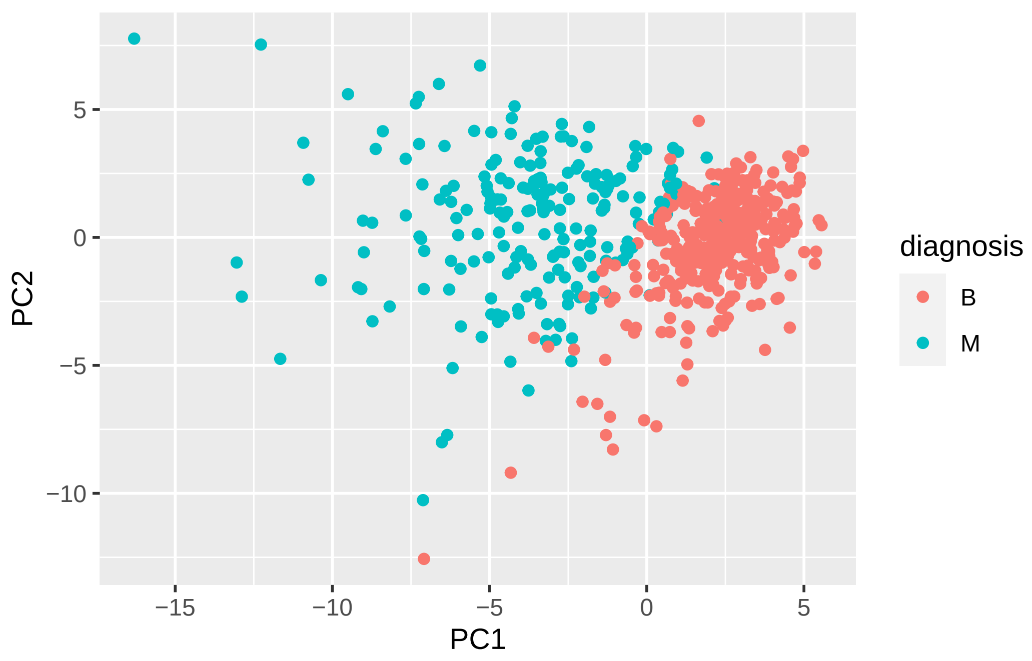
The spread of the points along the y axis is wider than the plot of PC1 vs PC2. There is also more overlap of the benign and malignant points, so the first plot has a cleaner cut separating the subgroups.

Use ggplot2 to make a fancy figure:

```r
# 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

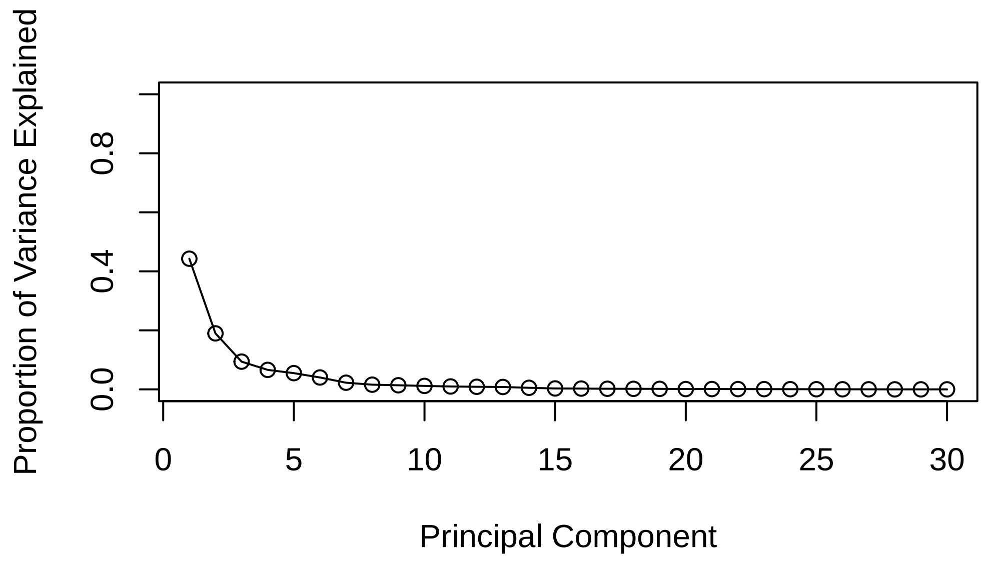
Calculating the variance of each PC by squaring the sdev component of `wisc.pr`

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

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

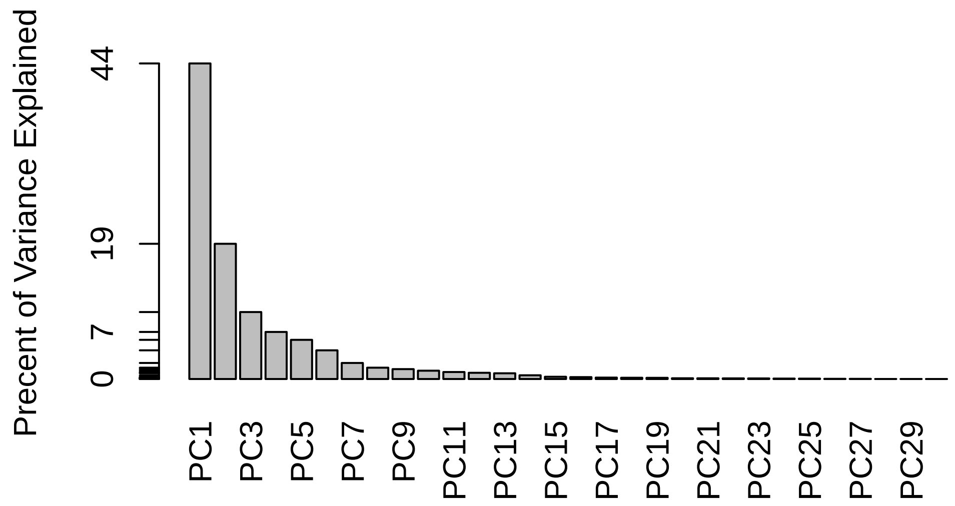
Calculating the variance explained by each PC by dividing by the total variance explained by all PCs.

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



Alternative scree plot of the same data:

```r
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 )
```



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`?

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

```
concave.points_mean
         -0.2608538
```

Component of loading vector for the feature `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?

PC1-PC5.

Hierarchical clustering

This type of clustering does not assume in advance the number of natural groups that exist in the data.

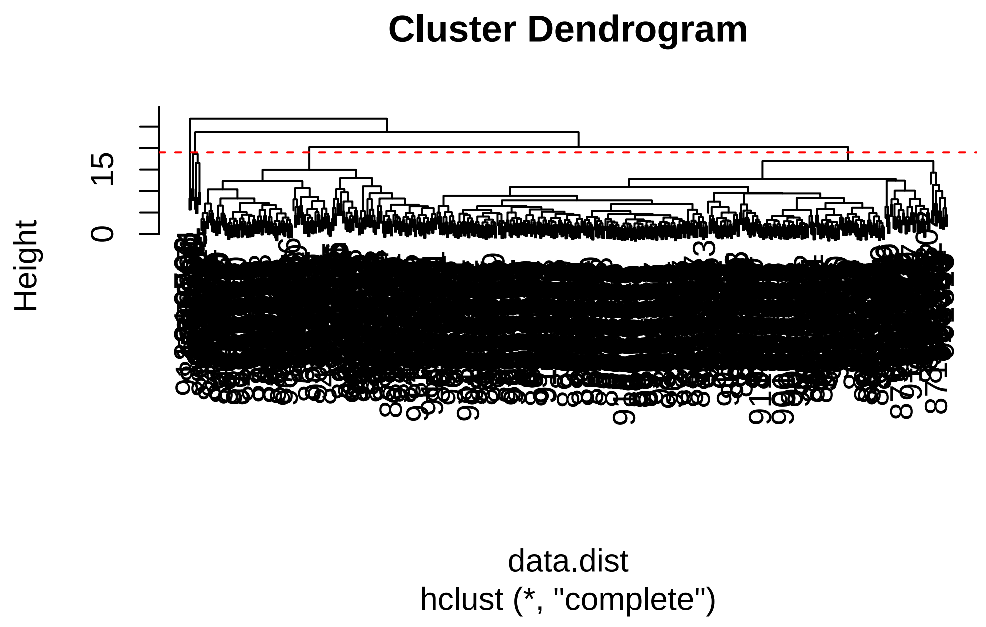
```r
#First scale the data
data.scaled <- scale(wisc.data)
#Calculate the distnaces between all pairs of observations
data.dist <- dist(data.scaled)
#Create a hierarchical clustering model using complete linkage
wisc.hclust <- hclust(data.dist, method="complete")
wisc.hclust
```

```
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)
```



Selecting number of clusters

Use `cutree()` to cut the tree so that it has 4 clusters

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

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

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

```r
wisc.hclust.clusters <- cutree(wisc.hclust, k=5)
table(wisc.hclust.clusters, diagnosis)
```

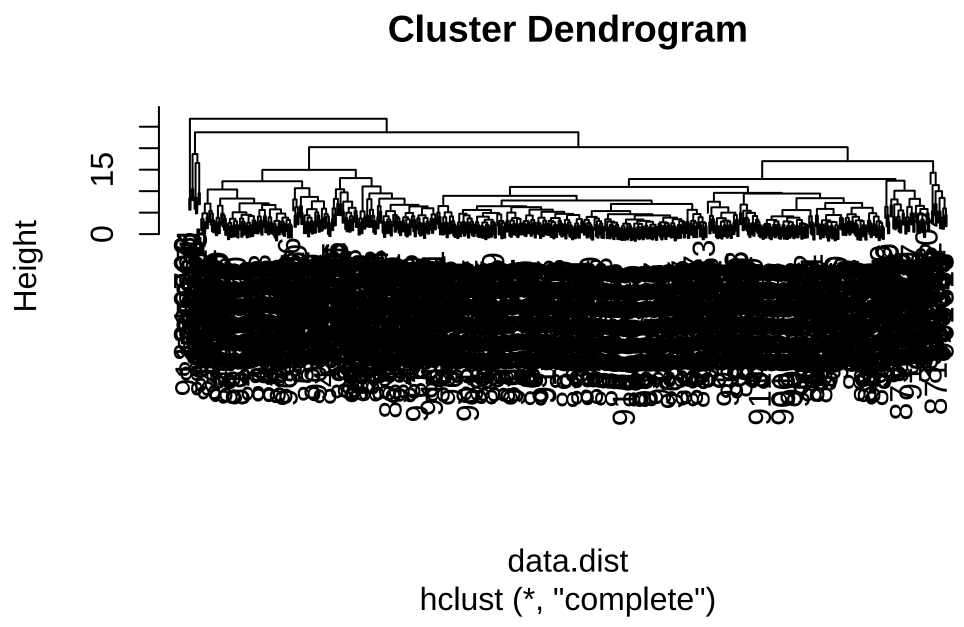
```
                    diagnosis
wisc.hclust.clusters   B   M
                   1  12 165
                   2   0   5
                   3 343  40
                   4   2   0
                   5   0   2
```

4 clusters seems to be the best, any increase in the number of clusters only increases the messiness without increasing the number of individuals within each cluster. Decreasing clusters only categorizes both B and M within the same cluster.

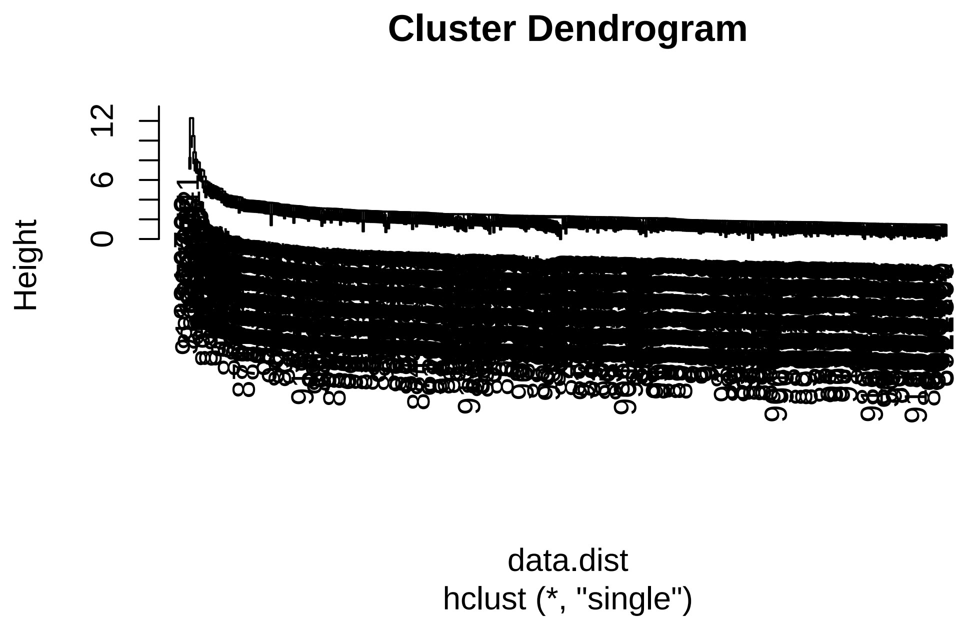
Using different methods

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

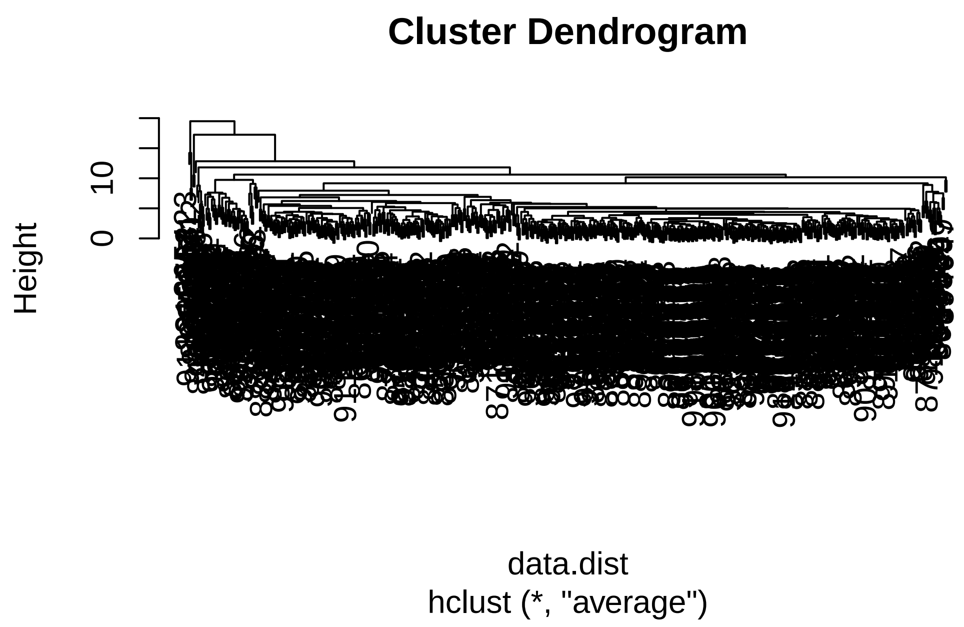
```r
wisc.hclust <- hclust(data.dist, method="complete")
plot(wisc.hclust)
```



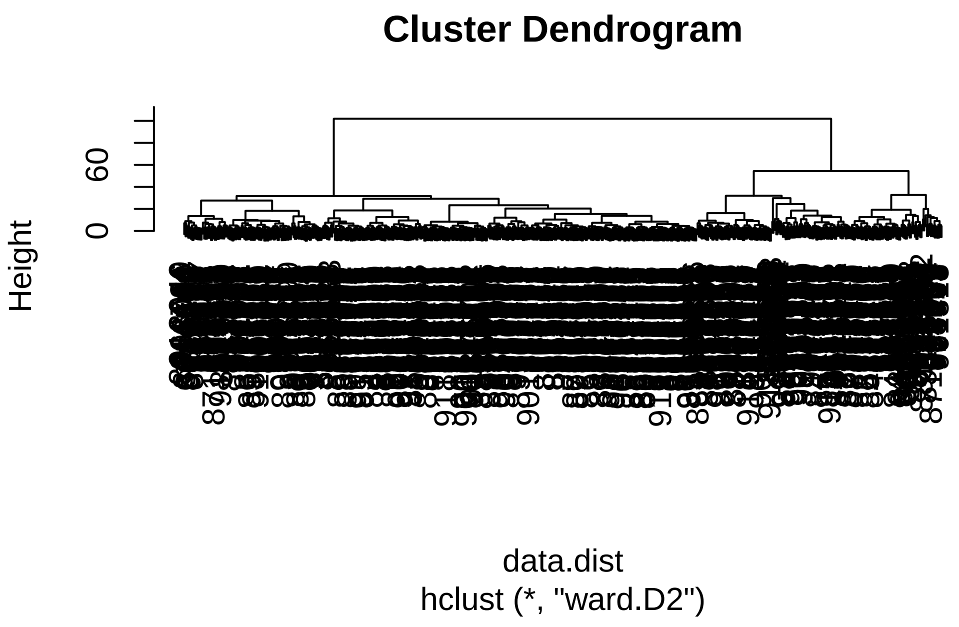
```r
wisc.hclust.single <- hclust(data.dist, method="single")
plot(wisc.hclust.single)
```



```
wisc.hclust.average <- hclust(data.dist, method="average")
plot(wisc.hclust.average)
```



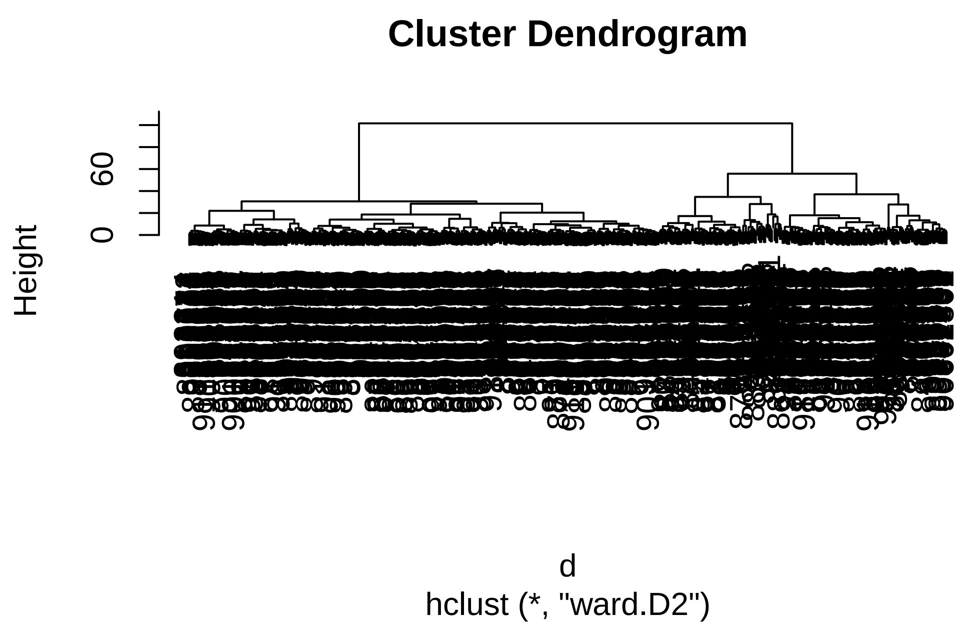
```
wisc.hclust.ward.D2 <- hclust(data.dist, method="ward.D2")
plot(wisc.hclust.ward.D2)
```



The "ward.D2" method gave the best result, it centers the height bars and makes it easy to see that our data can be sectioned into two clusters by the proportions of the height bars.

Combining methods

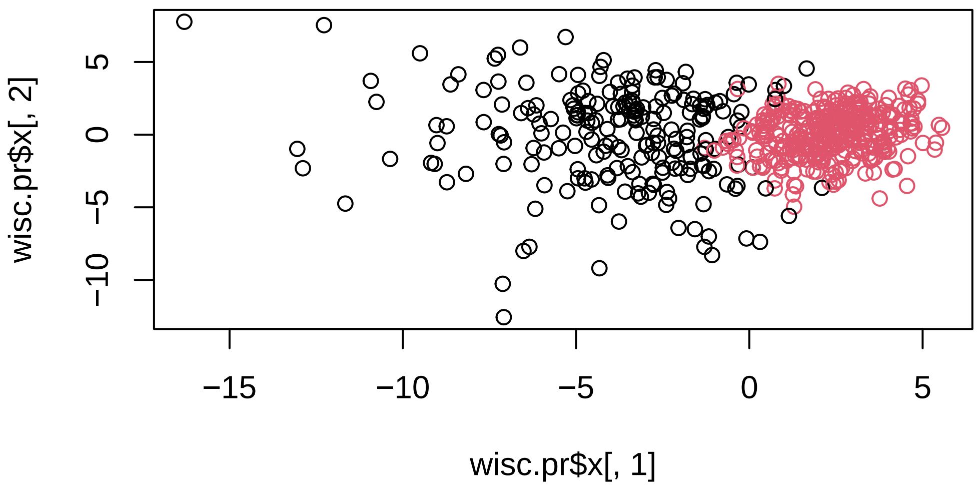
```
d <- dist(wisc.pr$x[,1:7])
wisc.pr.hclust <- hclust(d, method="ward.D2")
plot(wisc.pr.hclust)
```



Generate 2 cluster groups from this hclust object

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

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



```r
table(grps)
```

```
grps
  1   2 
216 353 
```

```r
table(diagnosis)
```

```
diagnosis
  B   M 
357 212 
```

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

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

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

The newly created model separates out the two diagnoses pretty well. Cluster 1 is mostly diagnosed as malignant. Cluster 2 is mostly diagnosed as benign. This can quantify the amount of likely false positives by looking at the individuals within each cluster that do not fall in the majority.