Class 08: Mini Project

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Outline

TOday we will apply the machine learning method we introduced last class on breast cancer biopsy from fine needle aspiration.

Preparing the data

The data is supplied on CSV format. Downloaded from class website and saved to project folder. We want the patient id (first col) to be name of rows, instead of being analyzed as data.

```
wisc.df <- read.csv("WisconsinCancer.csv", row.names=1)
```

Examine input data.

```
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 want to exclude the *diagnosis* column for the aim of PCA. Delete and make a new *wisc.data* data frame for analysis, and save diagnosis to a new vector *diagnosis*

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

Exploratory data analysis

Q1. How many observations are in this dataset?

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

```
[1] 569
```

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

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

```
[1] 212
```

```
#or
table(diagnosis)
```

```
diagnosis
  B   M
357 212
```

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

```
# We can find objects with certain pattern by `grep(pattern, x)`
length(grep("_mean", colnames(wisc.df)))
```

```
[1] 10
```

Principal Component Analysis

Performing PCA

It is important to check if the data need to be scaled before performing PCA. Two common reasons for scaling data include: - The input variables use different units of measurement. - The input variables have significantly different variances.

The upshot here is we set `scale = TRUE` argument to `prcomp()`.

```
# Check column means and standard deviations
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)? - Cumulative Proportion of PC1 = 0.4427

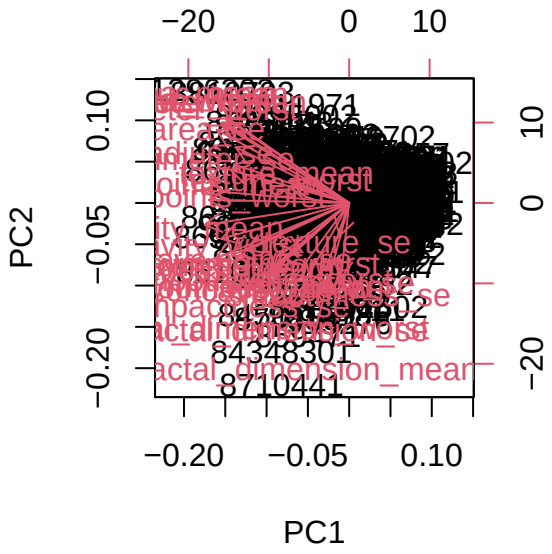
Q5. How many principal components (PCs) are required to describe at least 70% of the original variance in the data? - 3, because cumulative proportion reaches 70% at PC3.

Q6. How many principal components (PCs) are required to describe at least 90% of the original variance in the data? - 7.

Interpreting PCA results

Visualization is a useful tool to interpret PCA data. A common visualization for PCA results is the so-called biplot (function: `biplot()`)

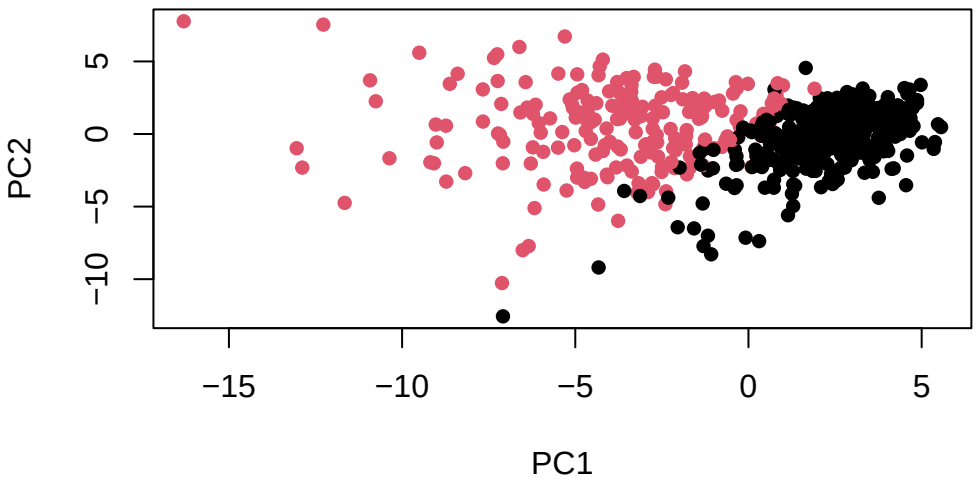
```
biplot(wisc.pr)
```



Problem: Row names are used as the plotting character for biplots like this one which can make trends rather hard to see.

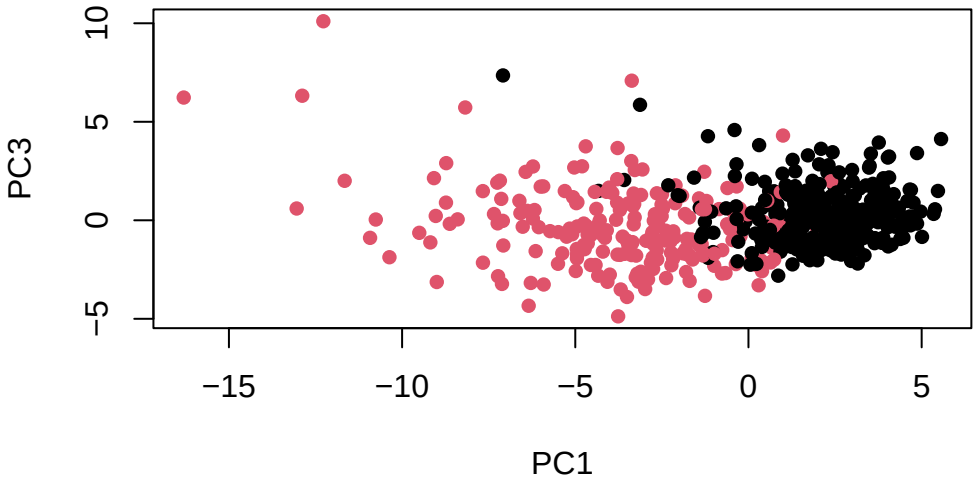
Let's make a more standard scatter plot.

```
# plot where a patient lies on new PC1 & 2 axis
plot(wisc.pr$x[,1], wisc.pr$x[,2], col = diagnosis, pch = 16, 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, pch = 16, xlab = "PC1", ylab = "PC3")
```



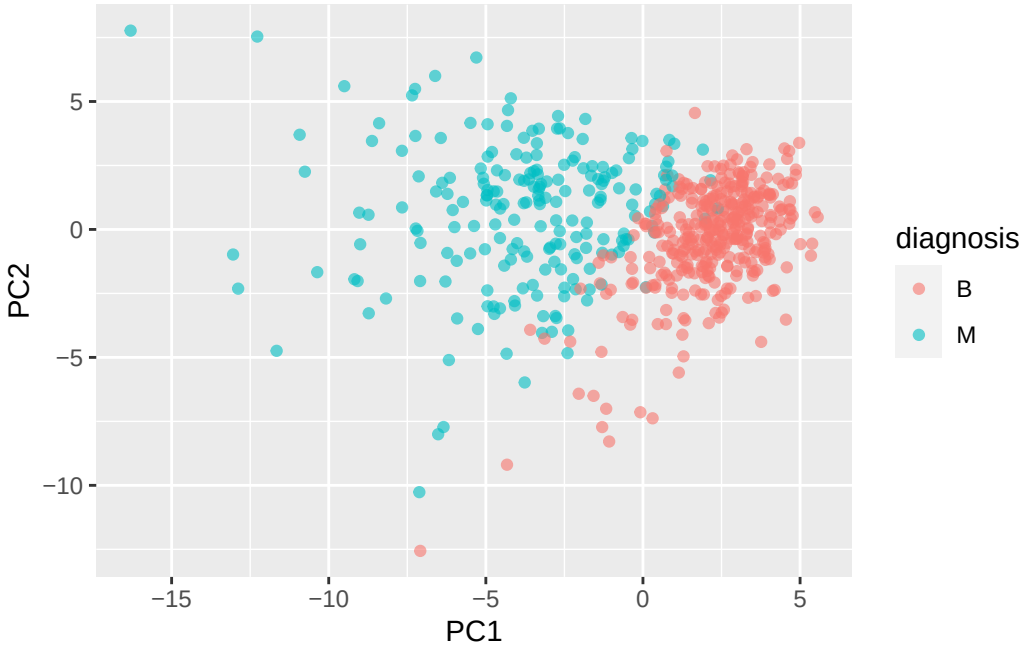
The two groups are less separated than the plot using PC1 and 2. This is because PC2 explains more difference in the data points than PC3.

As this is such a striking result let's see if we can use the ggplot2 package to make a more fancy figure of these results.

```
# Create a data.frame for ggplot
df <- as.data.frame(wisc.pr$x)
df$diagnosis <- diagnosis

# Load the ggplot2 package
library(ggplot2)
```

```
Warning: package 'ggplot2' was built under R version 4.3.1
```

```
# Make a scatter plot colored by diagnosis
ggplot(df) +
  aes(PC1, PC2, col=diagnosis) +
  geom_point(alpha = 0.6)
```



Variance explained

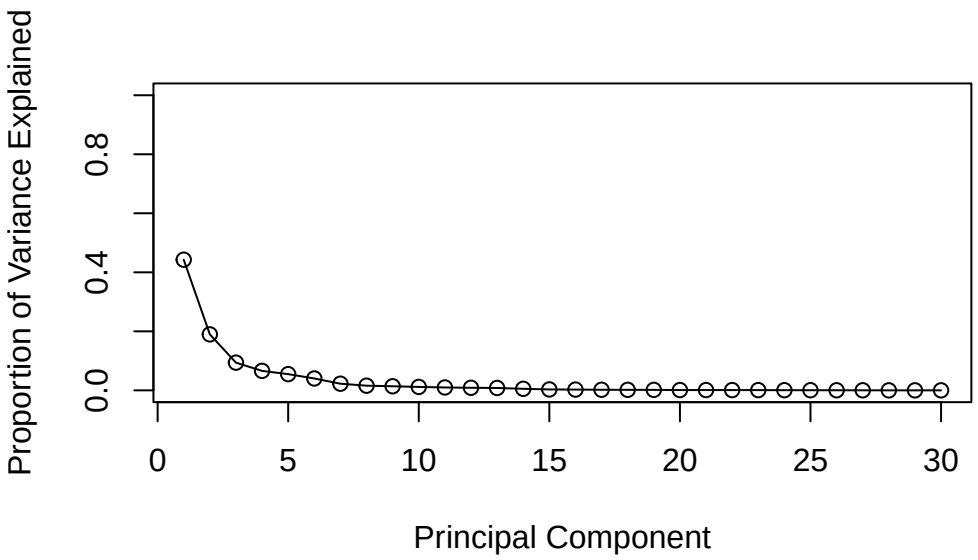
We can produce scree plots showing the proportion of variance explained as the number of principal components increases. Calculate the variance of each principal component by squaring the stdev component of data.

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

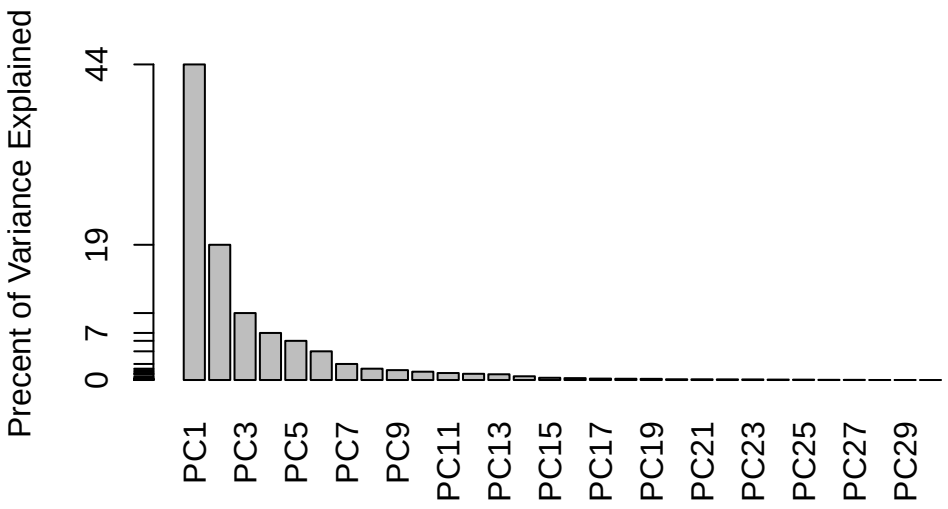
```
[1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

Then we can calculate the variance explained by each principal component by dividing by the total variance explained of all principal components.

```
# 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")
```




```
# 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 )
```



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]
```

```
            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
```

concave.points_mean = -0.26085376

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

```
which(cumsum(pve)>0.8)[1]
```

```
[1] 5
```

Hierarchical clustering

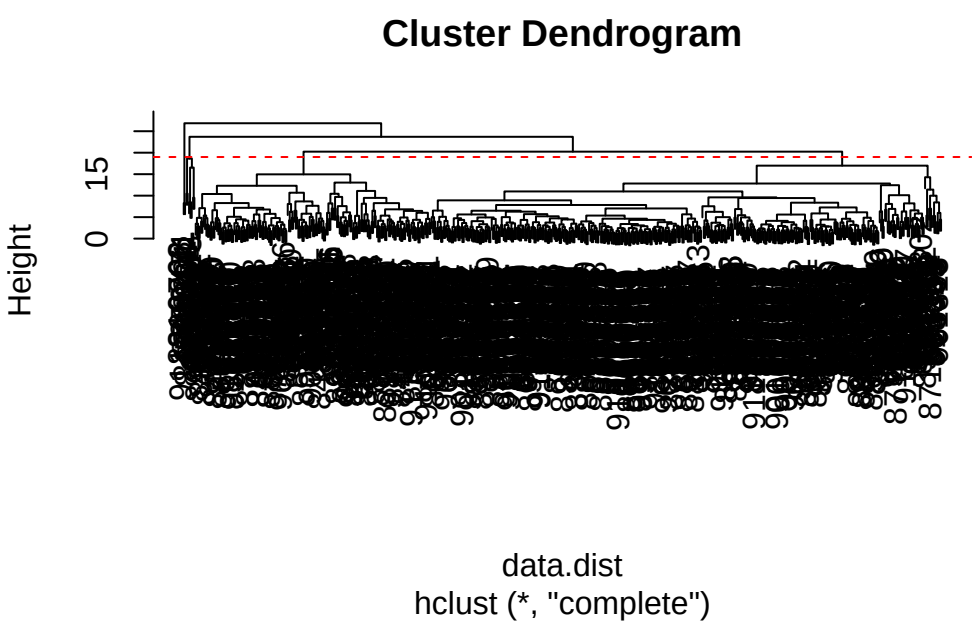
As part of the preparation for hierarchical clustering, the distance between all pairs of observations are computed.

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

# Calculate the data distance
data.dist <- dist(data.scaled)

# Create a hierarchical clustering model using complete linkage.
wisc.hclust <- hclust(data.dist, method = "complete")
```

Result of Hierarchical Clustering

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

```
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

```
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
```

Interpretation: cluster 1 corresponds to Maligant, cluster 3 corresponds to benign cells.

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

```
CDmatch <- function(x) {
  wisc.hclust.clusters.n <- cutree (wisc.hclust, k=x)
```

```
  table(wisc.hclust.clusters.n, diagnosis)
}
ncluster <- 2:10
lapply(2:10, CDmatch)
```

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

[[2]]
                     diagnosis
wisc.hclust.clusters.n   B   M
                     1 355 205
                     2   2   5
                     3   0   2

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

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

[[5]]
                     diagnosis
wisc.hclust.clusters.n   B   M
                     1  12 165
                     2   0   5
                     3 331  39
                     4   2   0
```

```
                    5  12   1
                    6   0   2

[[6]]
                     diagnosis
wisc.hclust.clusters.n   B   M
                    1  12 165
                    2   0   3
                    3 331  39
                    4   2   0
                    5  12   1
                    6   0   2
                    7   0   2

[[7]]
                     diagnosis
wisc.hclust.clusters.n   B   M
                    1  12  86
                    2   0  79
                    3   0   3
                    4 331  39
                    5   2   0
                    6  12   1
                    7   0   2
                    8   0   2

[[8]]
                     diagnosis
wisc.hclust.clusters.n   B   M
                    1  12  86
                    2   0  79
                    3   0   3
                    4 331  39
                    5   2   0
                    6  12   0
                    7   0   2
                    8   0   2
                    9   0   1

[[9]]
                     diagnosis
wisc.hclust.clusters.n   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

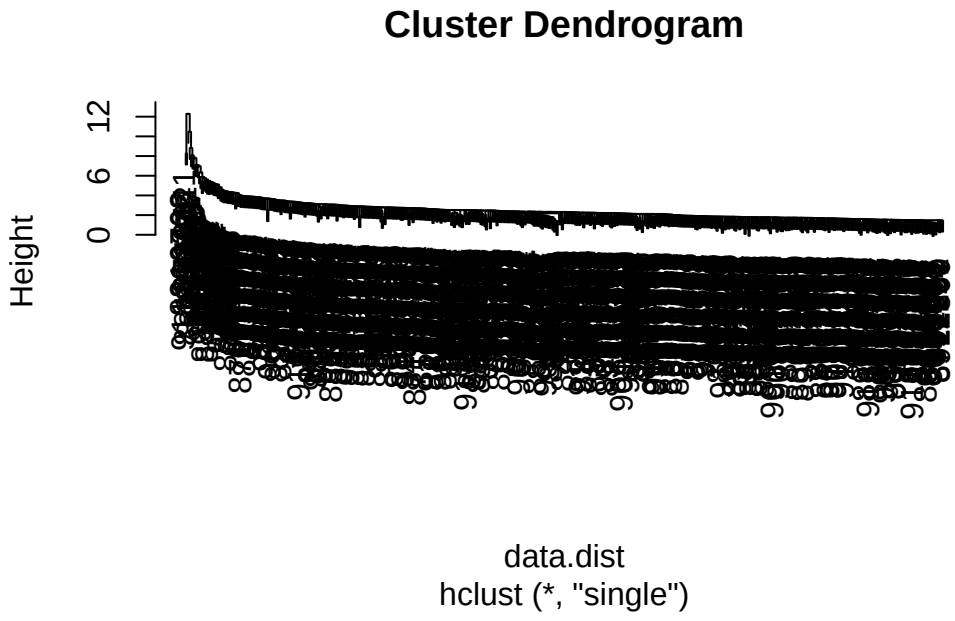
No. 4 cluster is the best solution. Lower cluster number cannot separate the malignant from benign, while higher cluster number doesn't help to improve resolution.

Using different methods

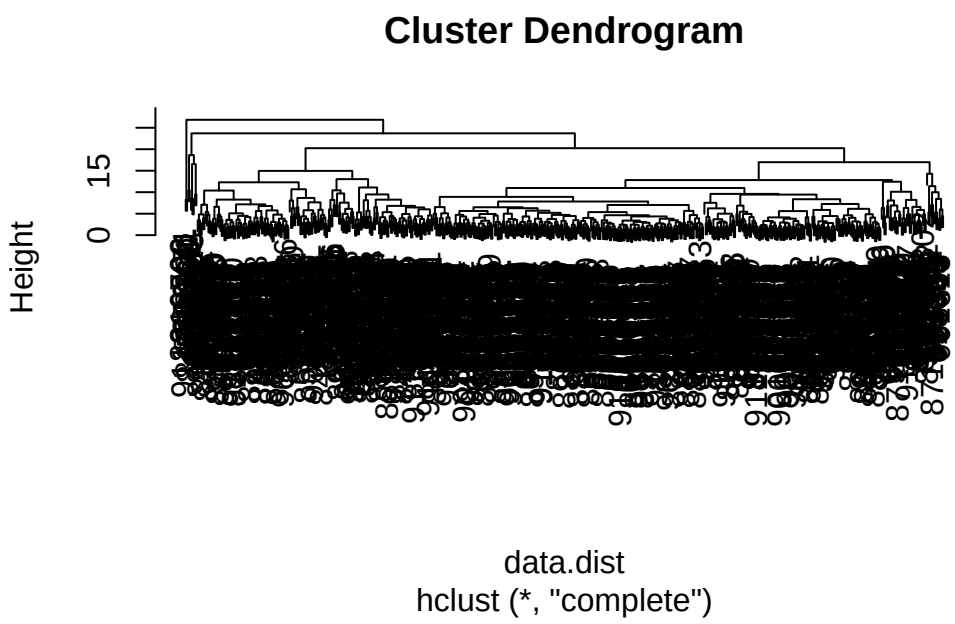
we can use to combine points during the hierarchical clustering procedure. These include "single", "complete", "average" and "ward.D2"

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

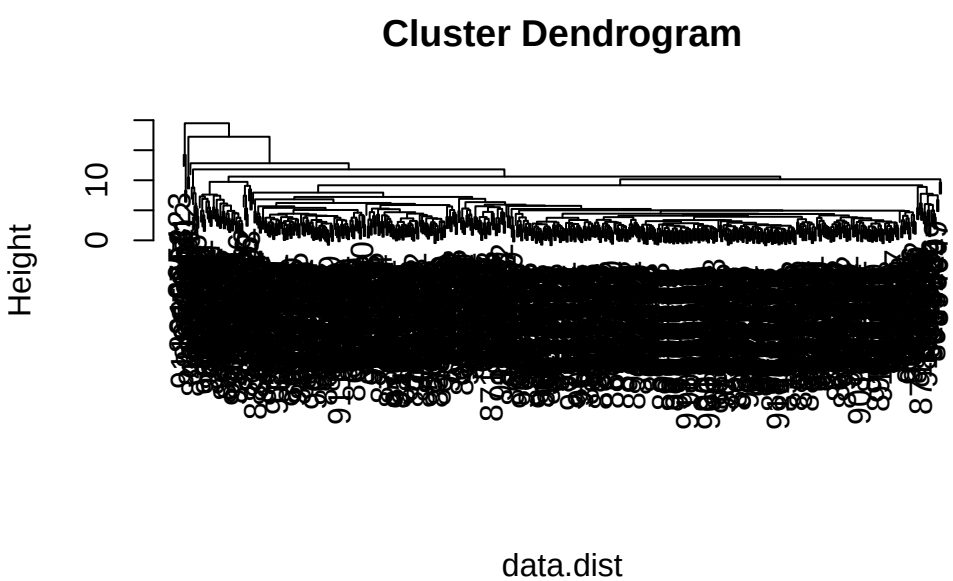
```
plot(hclust(data.dist, method = "single"))
```



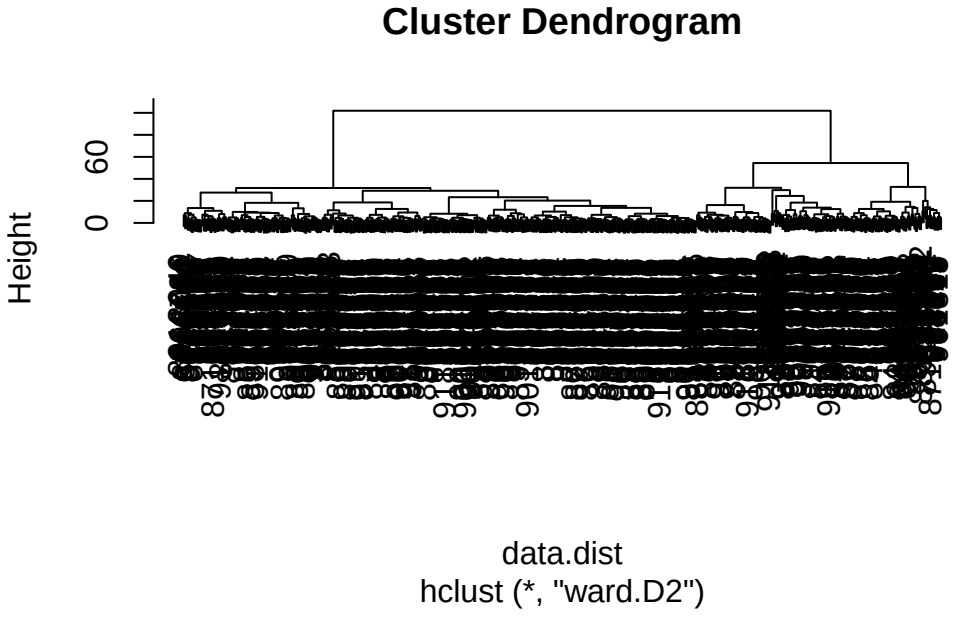
```r
plot(hclust(data.dist, method = "complete"))
```




```r
plot(hclust(data.dist, method = "average"))
```




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



"ward.D2" gives the best result as it clearly separates the population into two clusters, which is exactly what we want.

Side-note: The method="ward.D2"creates groups such that variance is minimized within clusters. This has the effect of looking for spherical clusters with the process starting with all points in individual clusters (bottom up) and then repeatedly merging a pair of clusters such that when merged there is a minimum increase in total within-cluster variance This process continues until a single group including all points (the top of the tree) is defined.

OPTIONAL: K-means clustering

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

```
  diagnosis
     B   M
1   20 134
2 337  78
```

```
wisc.hclust.wD <- hclust(data.dist, method = "ward.D2")
wisc.hclust.clusters.wD <- cutree (wisc.hclust, k=2)
table(wisc.hclust.clusters.wD, diagnosis)
```

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

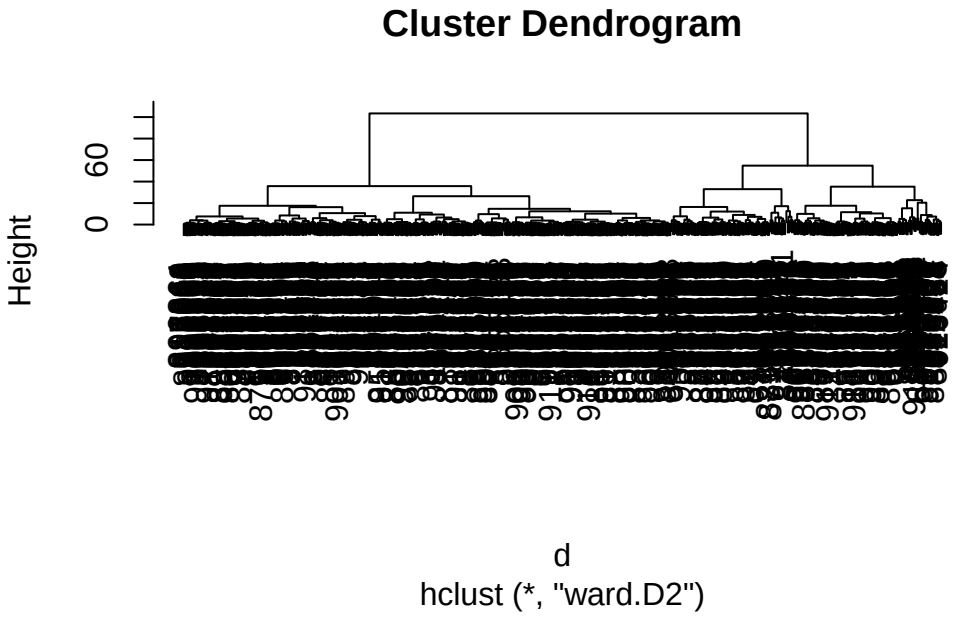
Q14. How well does k-means separate the two diagnoses? How does it compare to your hclust results?

The hclust result using "ward.D2" method produced better results in that the malignant cell is better separated from benign cells in each clusters.

Combining Methods

This approach will take out origional data but our PCA results and work with them.

```
# take the first 3 PCs, calculate distance matrix
d <- dist(wisc.pr$x[,1:3])
wisc.pr.hclust <- hclust(d, method = "ward.D2")
plot(wisc.pr.hclust)
```



Generate 2 cluster groups

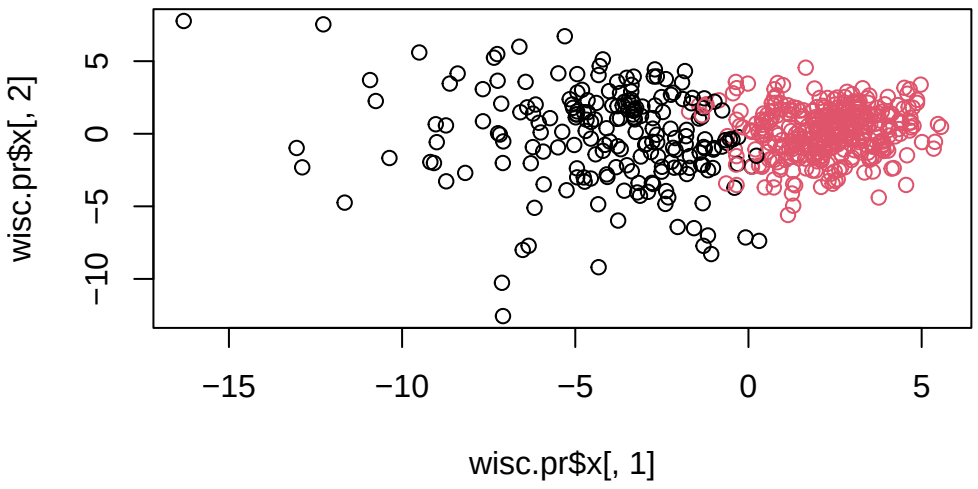
```
grps <- cutree(wisc.pr.hclust, k=2)
table(grps)
```

```
grps
  1   2
203 366
```

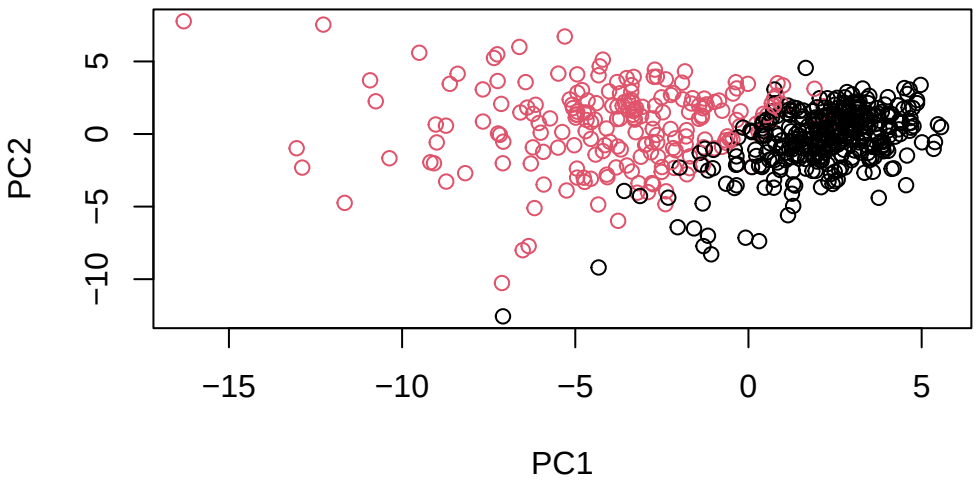
```
table(grps, diagnosis)
```

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

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




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



Q15. How well does the newly created model with four clusters separate out the two diagnoses? Compare our result with expert diagnosis

```
table(grps)
```

```
grps
  1   2
203 366
```

```
table(diagnosis)
```

```
diagnosis
  B   M
357 212
```

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

```
    diagnosis
grps   B   M
```

```
  1  24 179
  2 333  33
```

Interpretation: 24 – false positive; 33 – false negative; 179 – true negative; 333 – true positive. Given that the true values are significantly more than the negative values, the new model separates the diagnoses quite well.

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.

```
table(wisc.km$cluster, diagnosis)
```

```
  diagnosis
     B   M
1   20 134
2  337  78
```

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

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

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

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