Class08

Fan Wu(PID:A15127541)

Table of contents

Data was downloaded from the class website as a CSV file.

Data Import

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

# Complete the following code to input the data and store as wisc.df
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
```

The first column `diagnosis` is the expert opinion on the sample(i.e. patient FNA).

```
head(wisc.df$diagnosis)
```

```
[1] "M" "M" "M" "M" "M" "M"
```

Remove the diagnosis from data for subsequent analysis

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

```
[1] 569  30
```

Store the diagnosis as a vector for use later when we compare our results to those from experts in the field

```
# Create diagnosis vector for later
diagnosis <- factor(wisc.df$diagnosis)
```

Q1. How many observations are in this dataset?

There are 569 observations/patients in the dataset

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

There are 212 malignant diagnosis

```
#finds out how many Benign/ Malignant there are in the sample
table(diagnosis)
```

```
diagnosis
  B   M
357 212
```

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

```
variables <- colnames(wisc.data)

grep("_mean", variables)
```

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

```
results <- grep("_mean", variables, value = T)

results
```

```
 [1] "radius_mean"            "texture_mean"           "perimeter_mean"
 [4] "area_mean"              "smoothness_mean"        "compactness_mean"
 [7] "concavity_mean"         "concave.points_mean"    "symmetry_mean"
[10] "fractal_dimension_mean"
```

```
total_use_of_mean <- length(results)
total_use_of_mean
```

```
[1] 10
```

Principal Component Analysis (PCA)

In general we want to scale and center our data prior to PCA, to ensure that each features contribute equally to the analysis

The `prcomp()` function to do PCA has a `scale = FALSE` default.

We almost always want to set `scale = True` in `prcomp()`, so that certain columns/variables with large standard deviation and mean won't impact when ccompared to others just because the units of measurement are on different scales.

```
# Check column means and standard deviations
wisc_mean <- colMeans(wisc.data)

wisc_sd <- apply(wisc.data,2,sd)

max(wisc_mean)
```

```
[1] 880.5831
```

```
min(wisc_mean)
```

```
[1] 0.003794904
```

```
max(wisc_sd)
```

```
[1] 569.357
```

```
min(wisc_sd)
```

```
[1] 0.002646071
```

```
# 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)
```

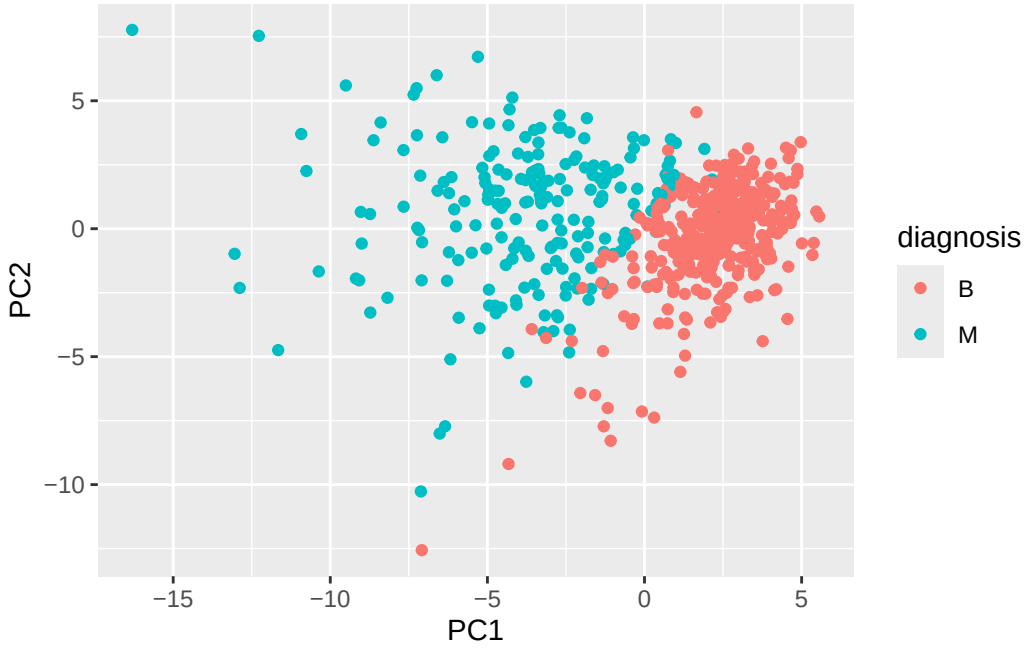
```
Importance of components:
                          PC1    PC2     PC3     PC4     PC5     PC6     PC7
Standard deviation     3.6444 2.3857 1.67867 1.40735 1.28403 1.09880 0.82172
Proportion of Variance 0.4427 0.1897 0.09393 0.06602 0.05496 0.04025 0.02251
Cumulative Proportion  0.4427 0.6324 0.72636 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
```

The main PC result figure is called a “score plot” or “PC plot” or “ordination plot”...

```
library(ggplot2)

# wisc.pr$x

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



Q4. From your results, what proportion of the original variance is captured by the first principal components (PC1)?

44.27%

```
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
```

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

3 PCs

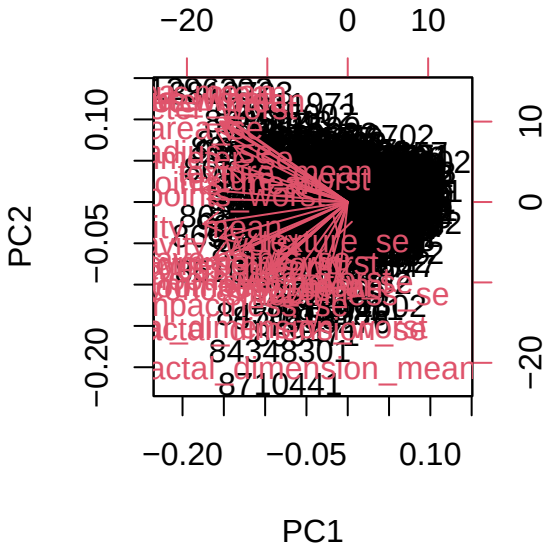
Q6. How many principal components (PCs) are required to describe at least 90% of the original variance in the data?

7 PCs

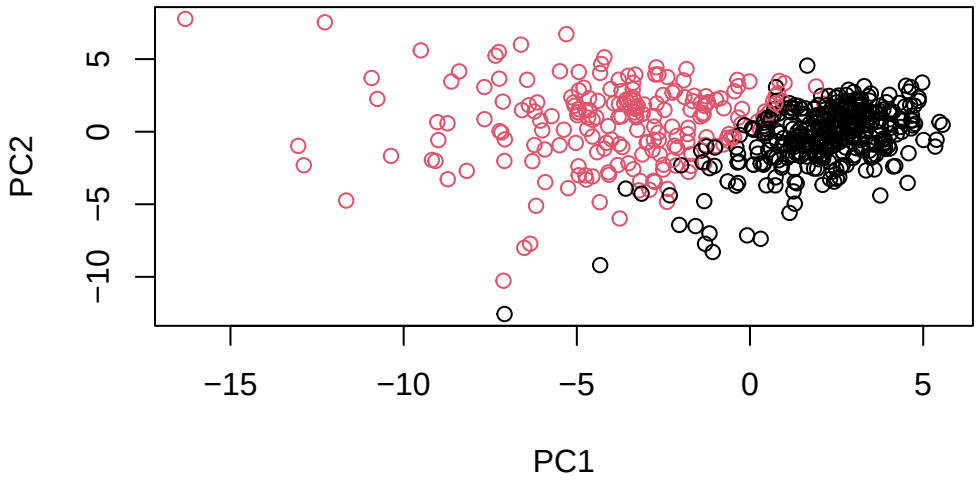
Create a biplot of the wisc.pr using the biplot() function. > Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?

Very packed; It's hard to understand, because there are so many dimensions involved.

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

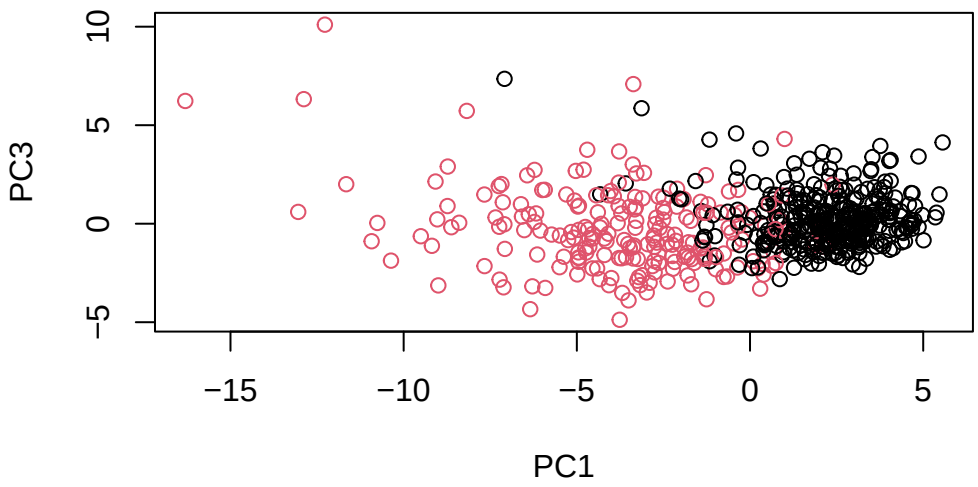



```
# Scatter plot observations by components 1 and 2
plot( wisc.pr$x , col = diagnosis ,
     xlab = "PC1", ylab = "PC2")
```



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

```
# Repeat for components 1 and 3
plot(wisc.pr$x[,c(1,3)], col = diagnosis,
     xlab = "PC1", ylab = "PC3")
```



Variance Explained

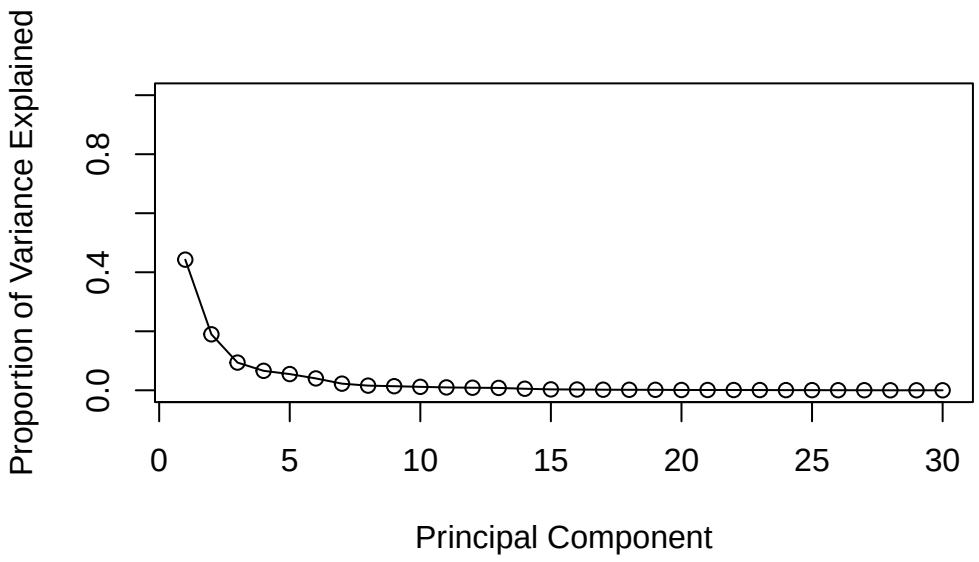
```
# Calculate variance of each component
pr.var <- wisc.pr$sdev^2
head(pr.var)
```

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

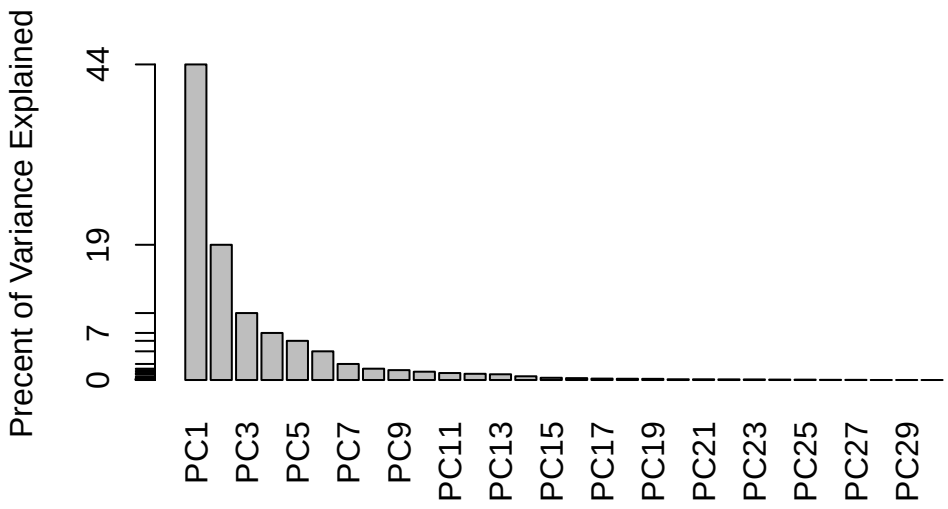
```
tot_variance = sum(pr.var)
# Variance explained by each principal component: pve
pve <- pr.var / tot_variance

# 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 )
```



Communicate 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?

```
PC1_loading <- wisc.pr$rotation[,1]
PC1_loading["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?

5Pcs

```
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
```

Hierarchial Clustering

The goal of this section is to do hierarchical clustering of the original data. Recall from class that this type of clustering does not assume in advance the number of natural groups that exist in the data.

As part of the preparation for hierarchical clustering, the distance between all pairs of observations are computed. Furthermore, there are different ways to link clusters together, with single, complete, and average being the most common linkage methods.

First scale the `wisc.data` data and assign the result to `data.scaled`.

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

Calculate the (Euclidean) distances between all pairs of observations in the new scaled dataset and assign the result to `data.dist`.

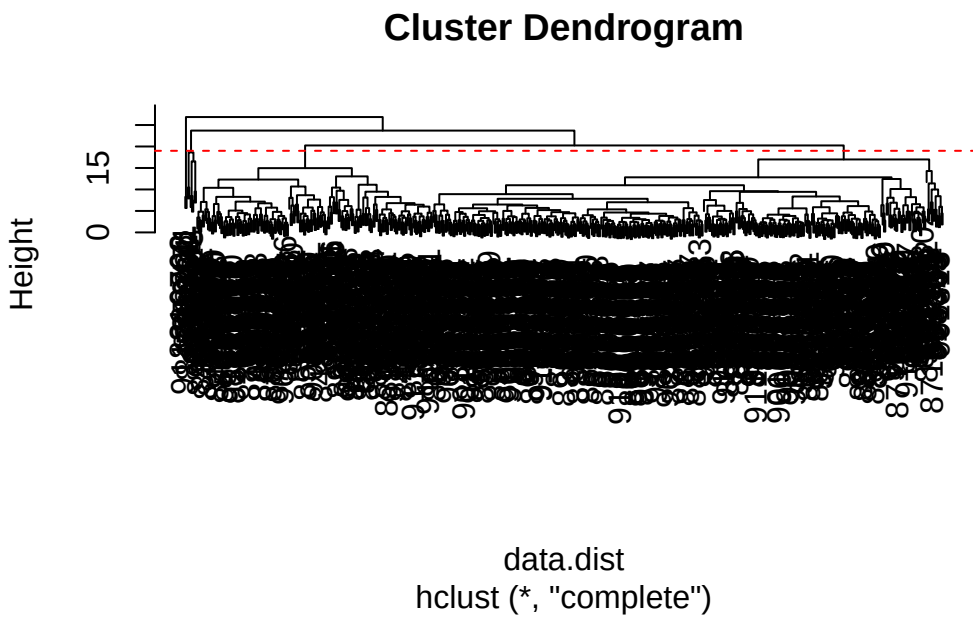
```
data.dist <- dist(data.scaled)
```

Create a hierarchical clustering model using complete linkage. Manually specify the method argument to `hclust()` and assign the results to `wisc.hclust`.

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

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

In this section, you will compare the outputs from your hierarchical clustering model to the actual diagnoses. Normally when performing unsupervised learning like this, a target variable (i.e. known answer or labels) isn't available. We do have it with this dataset, however, so it can be used to check the performance of the clustering model.

When performing supervised learning - that is, when you're trying to predict some target variable of interest and that target variable is available in the original data - using clustering to create new features may or may not improve the performance of the final model.

This exercise will help you determine if, in this case, hierarchical clustering provides a promising new feature.

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
```

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

maybe 6

Combining methods (PCA & Clustering)

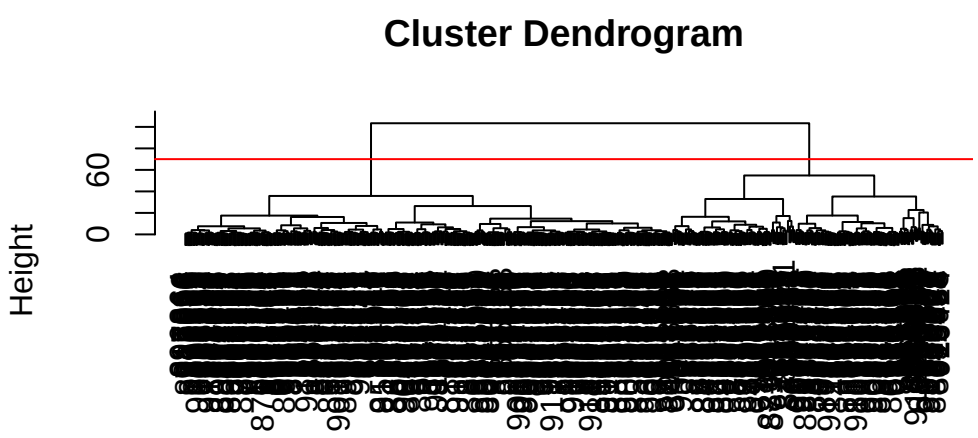
- Most important

Clustering the orginial data was not very productive. The PCA results look promising. Here we combine these methods by clustering from our PCA results. In other words, "clustering in PC space"..

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

View the tree..

```
plot(wisc.pr.hclust)
abline(h=70, col = "red")
```



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

```
## Use the distance along the first 7 PCs for clustering i.e. wisc.pr$x[, 1:7]
wisc.pr.hclust <- hclust(dist(wisc.pr$x[, 1:7]), method="ward.D2")
```

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

```
# Compare to actual diagnoses
table(wisc.pr.hclust.clusters, diagnosis)
```

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

To get our clustering membership vector (i.e. our main clustering result) we "cut the tree at a desired height or to yield a desired number of"k" groups.

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

```
grps
  1   2
216 353
```

How does this clustering grps compare to the expert diagnosis

```
# Compare to actual diagnoses
table(grps, diagnosis)
```

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

Sensitivity : TP/ (TP +FN) Specificity: TN / (TN + FP)

> 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.

K-means clustering is skipped as an optional section

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

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

7 Prediction

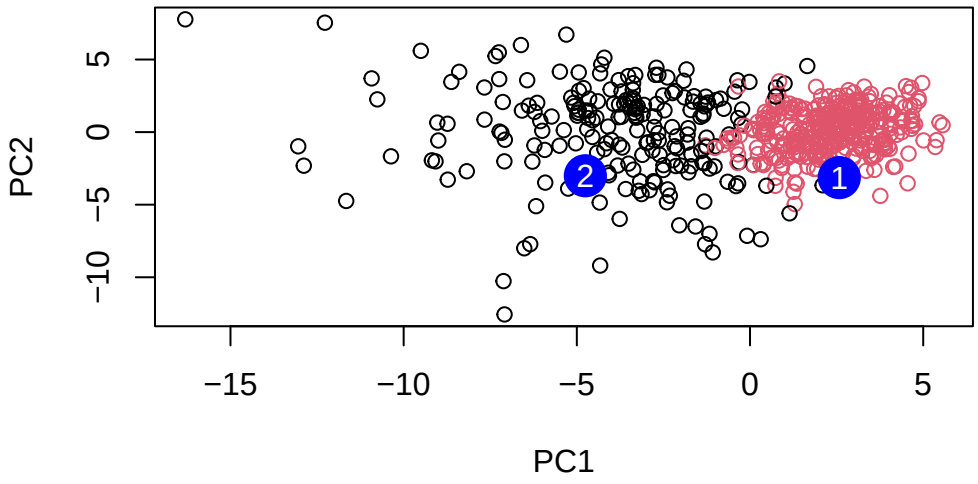
We can use our PCA model for prediction with new input patient samples

```
#url <- "new_samples.csv"
url <- "https://tinyurl.com/new-samples-CSV"
new <- read.csv(url)
npc <- predict(wisc.pr, newdata=new)
head(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
g <- as.factor(grps)

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



Q18. Which of these new patients should we prioritize for follow up based on your

results?

Group 1

```
#g <- as.factor(grps)

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

table(grps, diagnosis)
```

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