class08_Mini-Project

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1. Exploratory data analysis

Preparing the data

First, download and import our data using the `read.csv()` function to read the CSV (comma-separated values) file.

Assign the result to an object called `wisc.df`.

```
# 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)
```

Examine our input data to ensure column names are set correctly.

```
# We can use the View() or head() functions here
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
```

Note: The first column, `wisc.df$diagnosis` is a pathologist provided expert diagnosis. We will not be using this for our unsupervised analysis as it is essentially the "answer" to the question which cell samples are malignant or benign.

To make sure we don't accidentally include this in our analysis, create a new data.frame that omits this first column.

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

Finally, setup a separate new vector called diagnosis that contains the data from the diagnosis column of the original dataset. We will store this as a factor (useful for plotting) and use this later to check our results.

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

Exploratory data analysis

Explore the data you created before (wisc.data and diagnosis) to answer the following questions.

Q1. How many observations are in this dataset?

```
dim(wisc.data)
```

```
## [1] 569  30
```

Answer: There are 569 observations (number of rows) in this dataset.

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

```
length(grep("M", diagnosis))
```

```
## [1] 212
```

Answer: 212 observations have a malignant diagnosis.

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

```
length(grep(pattern = "_mean", x = colnames(wisc.data)))
```

```
## [1] 10
```

Answer: 10 variables/features in the data are suffixed with `_mean`.

2. Principal Component Analysis

Performing PCA

The next step in your analysis is to perform principal component analysis (PCA) on `wisc.data`.

It is important to check if the data need to be scaled before performing PCA. Recall two common reasons for scaling data include:

- The input variables use different units of measurement.
- The input variables have significantly different variances.

Check the mean and standard deviation of the features (i.e. columns) of the `wisc.data` to determine if the data should be scaled. Use the colMeans() and apply() functions like you've done before.

```
# 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
```

Execute PCA with the prcomp() function on the `wisc.data`, scaling if appropriate, and assign the output model to `wisc.pr`.

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

Inspect a summary of the results with the summary() function.

```
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)?

Answer: 44.27% (PC1's Proportion of Variance = 0.4427) 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?

Answer: First 3 PCs (PC1-PC3) are required to describe at least 70% of the original variance. (PC2's Cumulative Proportion 0.6324 and PC3's Cumulative Proportion 0.72636)

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

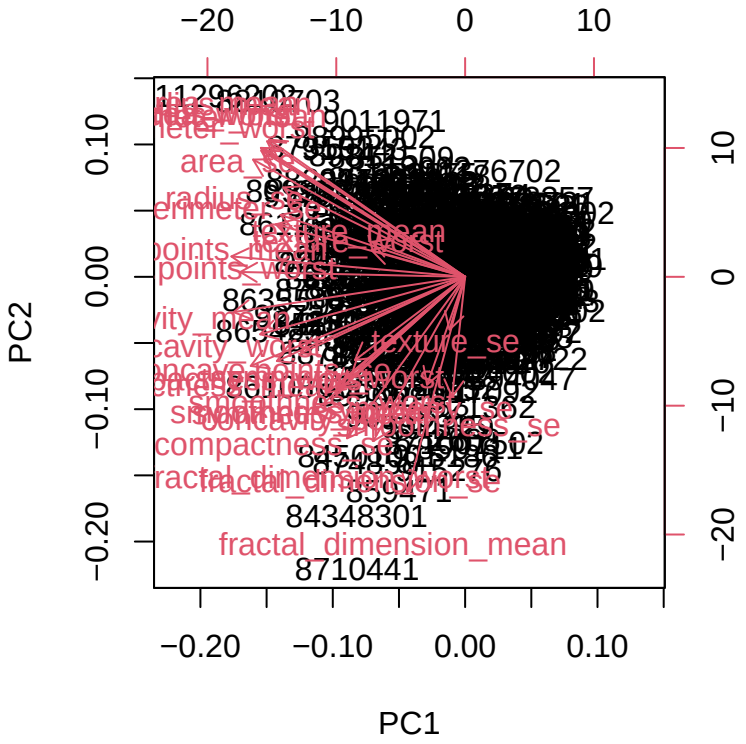
Answer: First 7 PCs (PC1-PC7) are required to describe at least 90% of the original variance. (PC6's Cumulative Proportion 0.88759 and PC7's Cumulative Proportion 0.91010)

Interpreting PCA results

Now you will use some visualizations to better understand your PCA model. A common visualization for PCA results is the so-called biplot.

Create a biplot of the `wisc.pr` using the biplot() function.

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



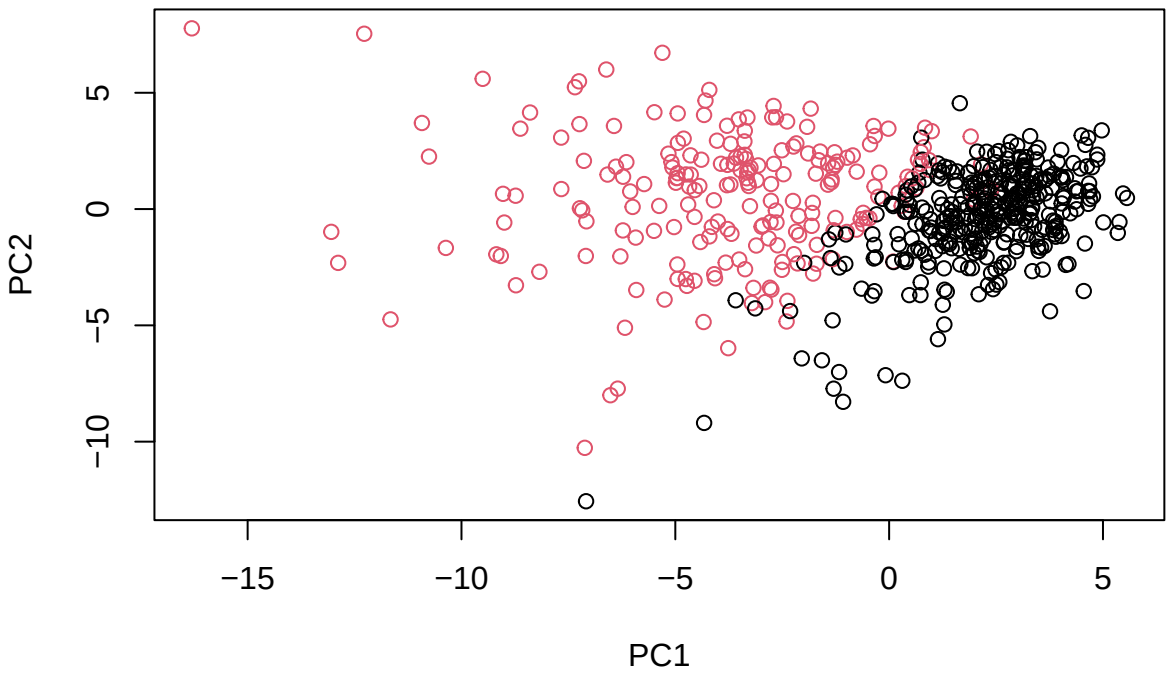
Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?

Answer: Generated biplot is hard to understand because it displays all data including non-trivial values and variable names. We can't clearly see a pattern of observations and distinguish.

This is a hot mess of a plot and we will need to generate our own plots to make sense of this PCA result.

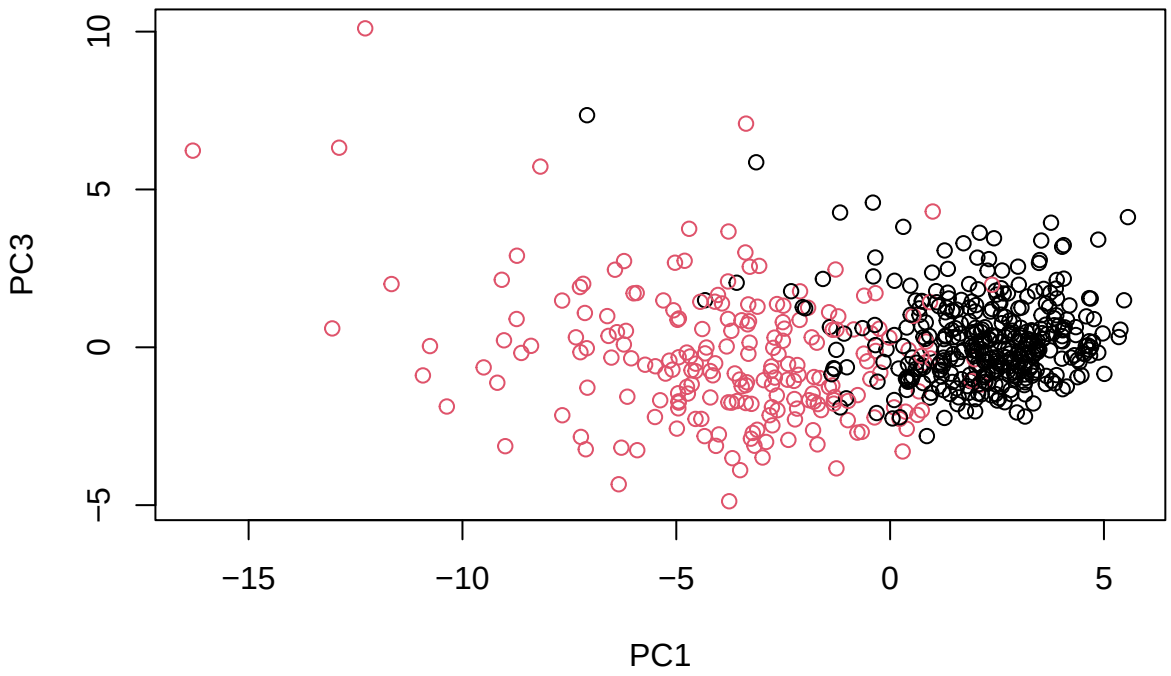
Rownames are used as the plotting character for biplots like this one which can make trends rather hard to see. So lets generate a more standard scatter plot of each observation along principal components 1 and 2 (i.e. a plot of PC1 vs PC2 available as the first two columns of `wisc.pr$x`) and color the points by the diagnosis.

```
diagnosis <- factor(wisc.df$diagnosis)
# Scatter plot observations by components 1 and 2
plot(wisc.pr$x[, 1:2], col = as.factor(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 compmonents 1 and 3
plot(wisc.pr$x[, c(1,3)], col=diagnosis, xlab="PC1", ylab="PC3")
```

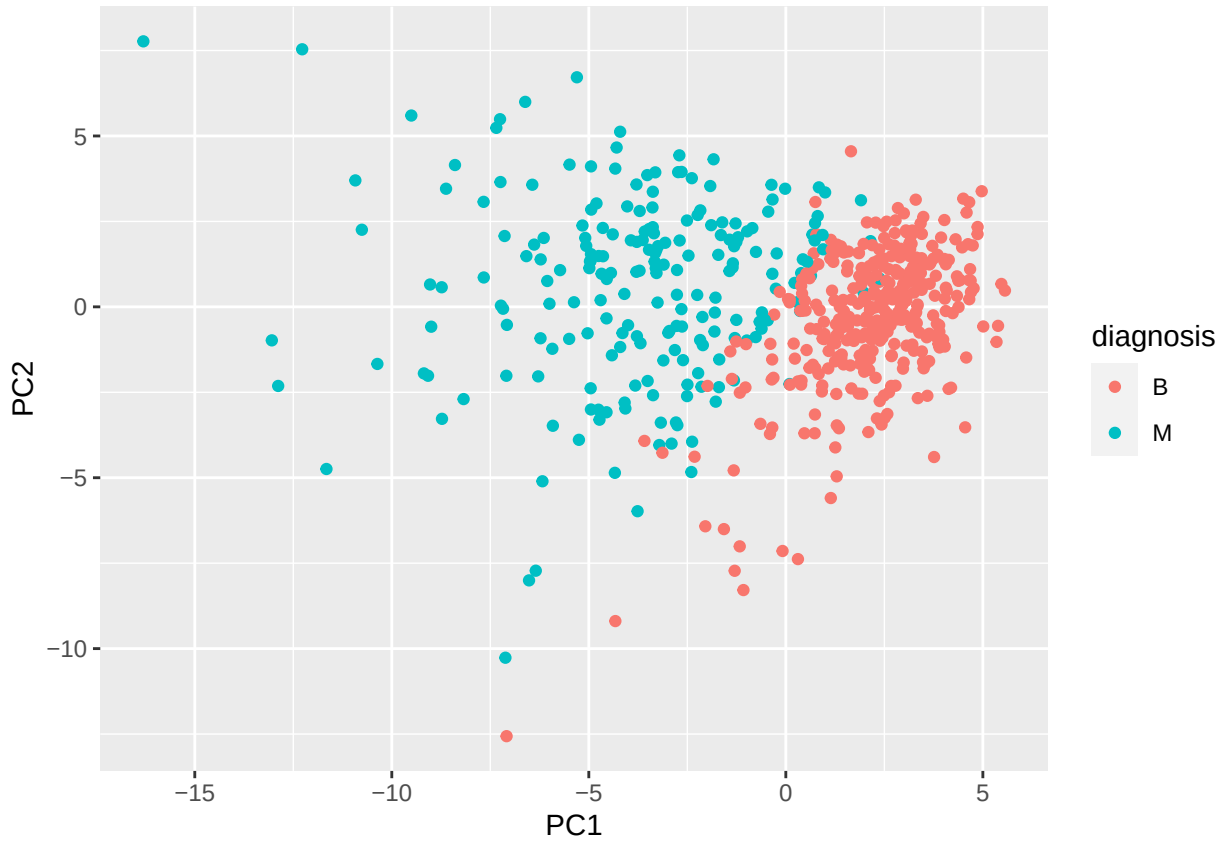


Answer:

Because principal component 2 explains more variance in the original data than principal component 3, you can see that the first plot has a cleaner cut separating the two subgroups. Overall, the plots indicate that principal component 1 is capturing a separation of malignant (red) from benign (black) samples.

Use the ggplot2 package to make a more fancy figure of these results. Remember that ggplot requires a data.frame as input and we will also need to add our diagnosis vector as a column if we want to use it for mapping to the plot color aesthetic.

```
# 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

We will produce scree plots showing the proportion of variance explained as the number of principal components increases. The data from PCA must be prepared for these plots, as there is not a built-in function in base R to create them directly from the PCA model.

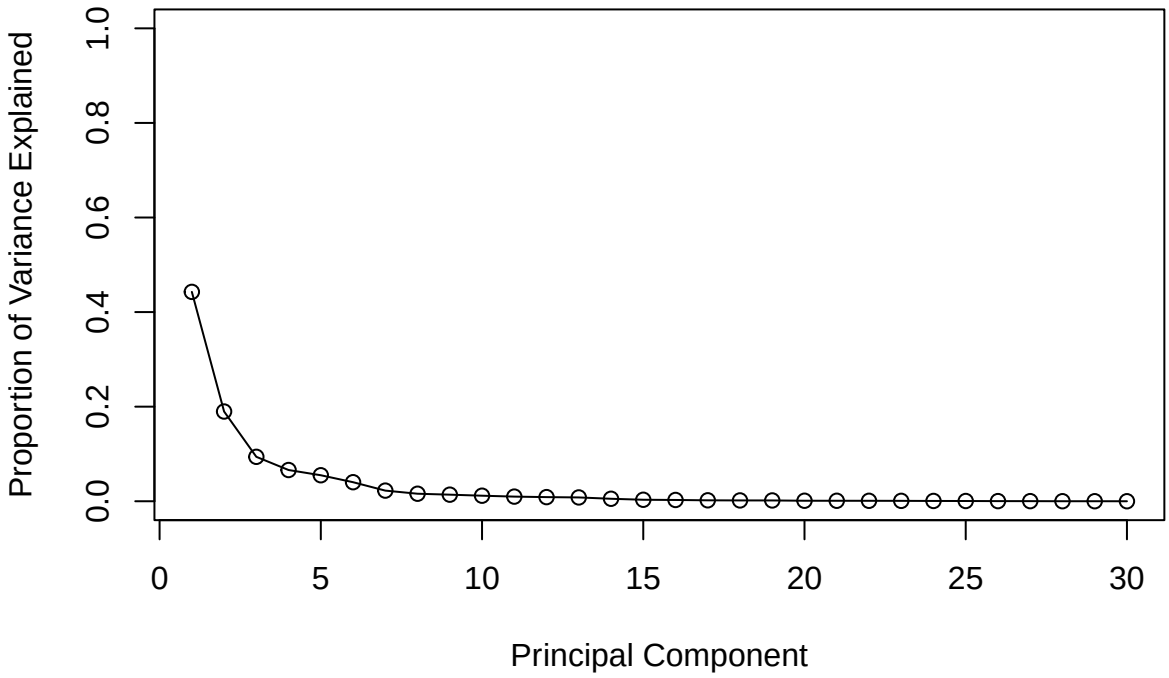
Calculate the variance of each principal component by squaring the sdev component of `wisc.pr` (i.e. `wisc.pr$sdev^2`). Save the result as an object called `pr.var`.

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

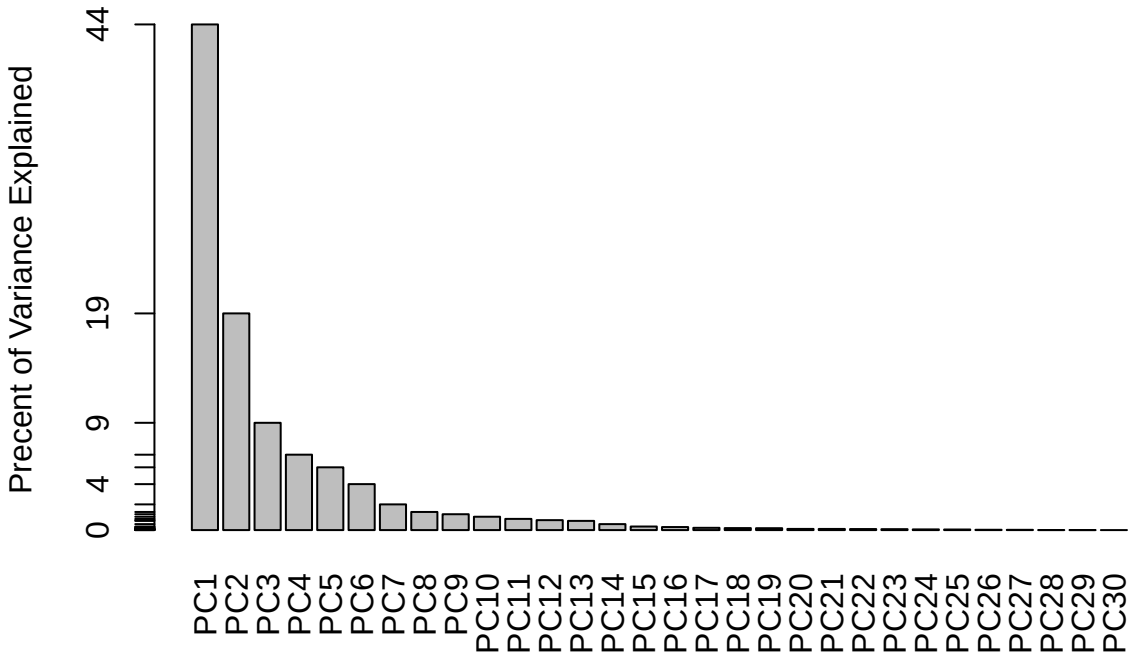
```
## [1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

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
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 =
axis(2, at=pve, labels=round(pve,2)*100 )
```



Communicating PCA results

The loadings, represented as vectors, explain the mapping from the original features to the principal components. The principal components are naturally ordered from the most variance explained to the least variance explained.

> 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["concave.points_mean",1]
```

```
## [1] -0.2608538
```

Answer: PC1's component of the loading vector for the feature concave.points_mean is -0.2608538.

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

```
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
```

Answer: First 5 PCs (PC1-PC5) are required to describe at least 80% of the original variance. (PC4's Cumulative Proportion 0.79239 and PC5's Cumulative Proportion 0.84734)

3. Hierarchical clustering

Input Data Preparation

The goal of this section is to do hierarchical clustering of the original 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`.

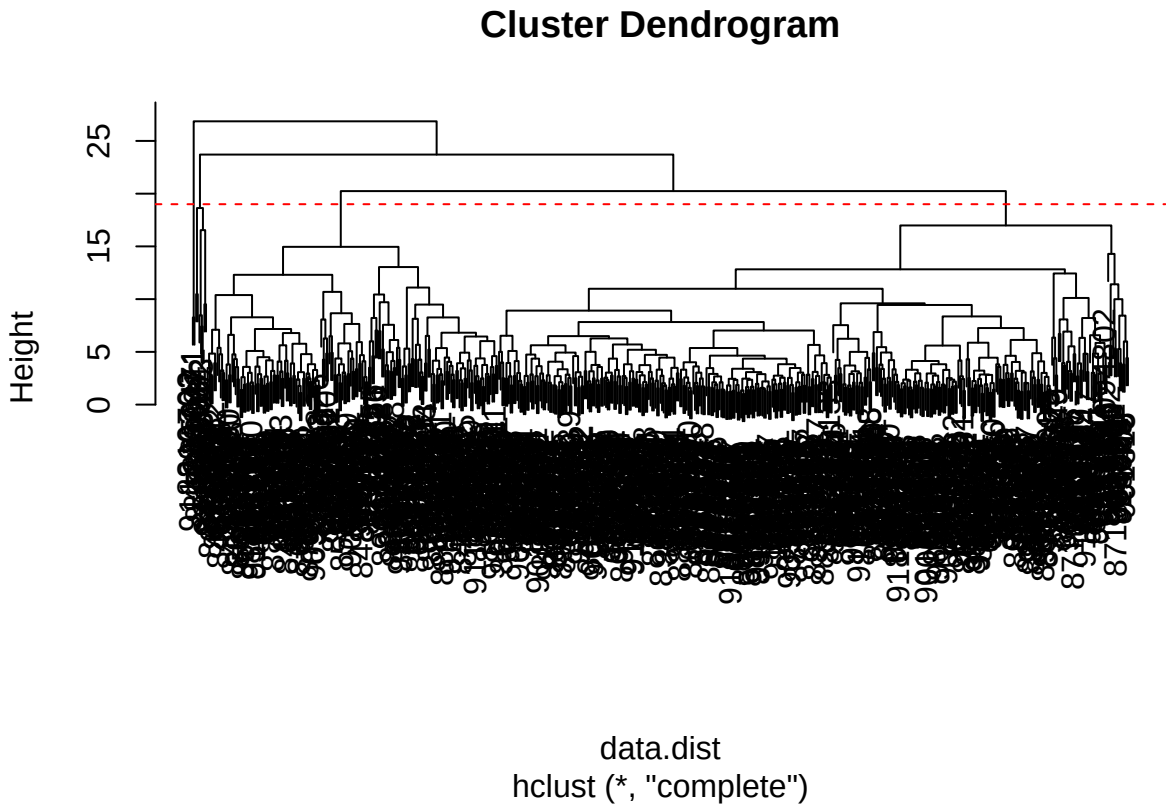
```
wisc.hclust <- hclust(data.dist, method = "complete")
```

Results of hierarchical clustering

Use the hierarchical clustering model you just created to determine a height (or distance between clusters) where a certain number of clusters exists.

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)
```



Answer: The height is about 19 (approximation by eye).

Selecting number of clusters

Now, compare the outputs from your hierarchical clustering model to the actual diagnoses.

Use cutree() to cut the tree so that it has 4 clusters. Assign the output to the variable `wisc.hclust.clusters`.

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

Use the table() function to 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
```

Here we picked four clusters and see that cluster 1 largely corresponds to malignant cells (with diagnosis values of 1) whilst cluster 3 largely corresponds to benign cells (with diagnosis values of 0).

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

```
# Try different cluster groups (except 4 clusters)
wisc.hclust.clusters2 <- cutree(wisc.hclust, k=2)
table(wisc.hclust.clusters2, diagnosis)
```

```
##                      diagnosis
## wisc.hclust.clusters2   B   M
##                     1 357 210
##                     2   0   2
```

```
wisc.hclust.clusters3 <- cutree(wisc.hclust, k = 3)
table(wisc.hclust.clusters3, diagnosis)
```

```
##                      diagnosis
## wisc.hclust.clusters3   B   M
##                     1 355 205
##                     2   2   5
##                     3   0   2
```

```
wisc.hclust.clusters5 <- cutree(wisc.hclust, k = 5)
table(wisc.hclust.clusters5, diagnosis)
```

```
##                      diagnosis
## wisc.hclust.clusters5   B   M
##                     1  12 165
##                     2   0   5
##                     3 343  40
##                     4   2   0
##                     5   0   2
```

```
wisc.hclust.clusters6 <- cutree(wisc.hclust, k = 6)
table(wisc.hclust.clusters6, diagnosis)
```

```
##                      diagnosis
## wisc.hclust.clusters6   B   M
##                     1  12 165
##                     2   0   5
##                     3 331  39
##                     4   2   0
##                     5  12   1
##                     6   0   2
```

```
wisc.hclust.clusters7 <- cutree(wisc.hclust, k = 7)
table(wisc.hclust.clusters7, diagnosis)
```

```
##                       diagnosis
## wisc.hclust.clusters7   B   M
##                     1  12 165
##                     2   0   3
##                     3 331  39
##                     4   2   0
##                     5  12   1
##                     6   0   2
##                     7   0   2
```

```
wisc.hclust.clusters8 <- cutree(wisc.hclust, k = 8)
table(wisc.hclust.clusters8, diagnosis)
```

```
##                       diagnosis
## wisc.hclust.clusters8   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
```

```
wisc.hclust.clusters9 <- cutree(wisc.hclust, k = 9)
table(wisc.hclust.clusters9, diagnosis)
```

```
##                       diagnosis
## wisc.hclust.clusters9   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
```

```
wisc.hclust.clusters10 <- cutree(wisc.hclust, k=10)
table(wisc.hclust.clusters10, diagnosis)
```

```
##                        diagnosis
## wisc.hclust.clusters10   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
```

Answer: Cutting into 4 clusters generates the optimal cluster vs diagnoses match but cutting into 5, 6, and 7 clusters generate similar outcome.

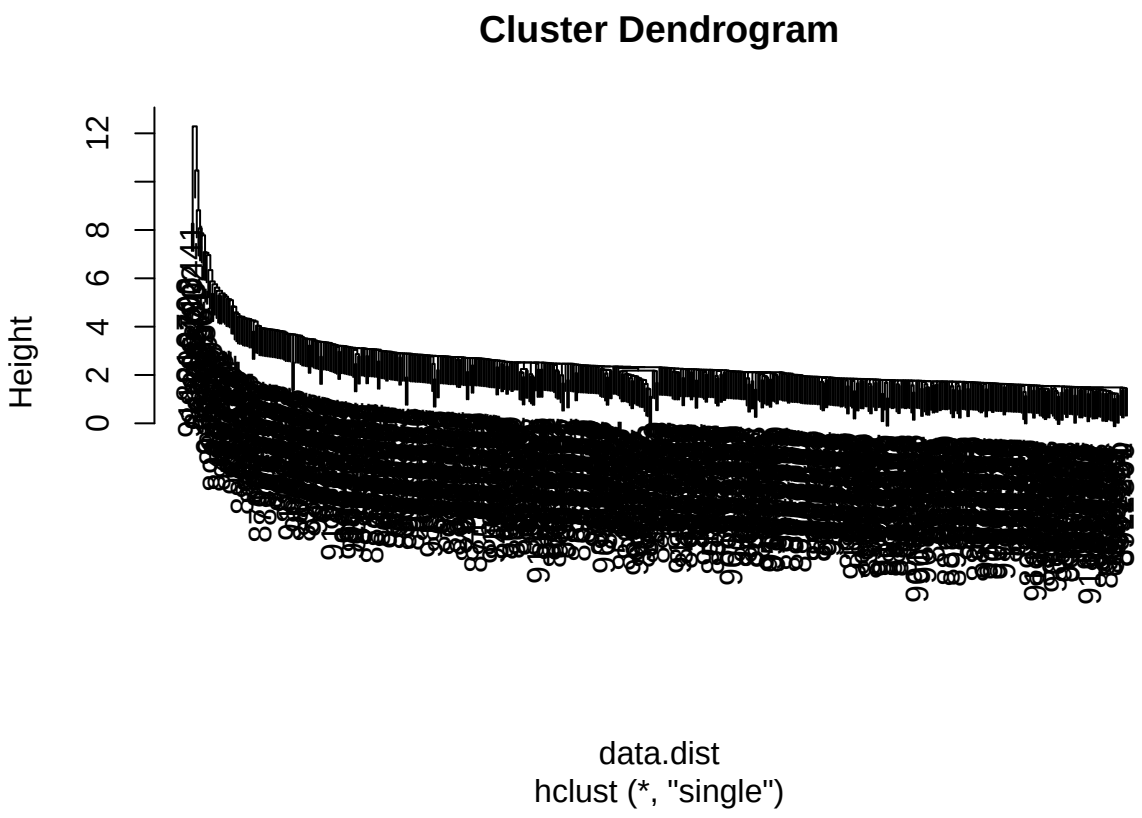
Using different methods

There are number of different "methods" we can use to combine points during the hierarchical clustering procedure. These include "single", "complete", "average" and (my favorite) "ward.D2".

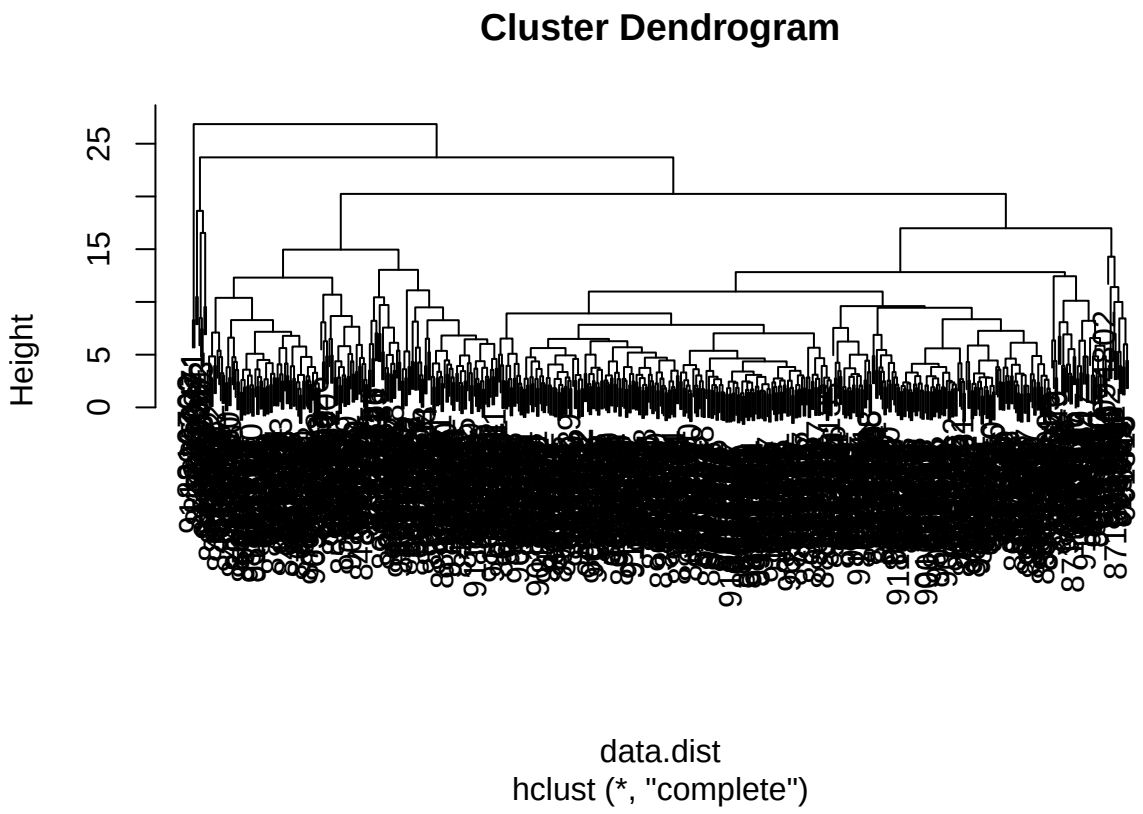
Note: The method="ward.D2"creates groups such that variance is minimized within clusters.

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

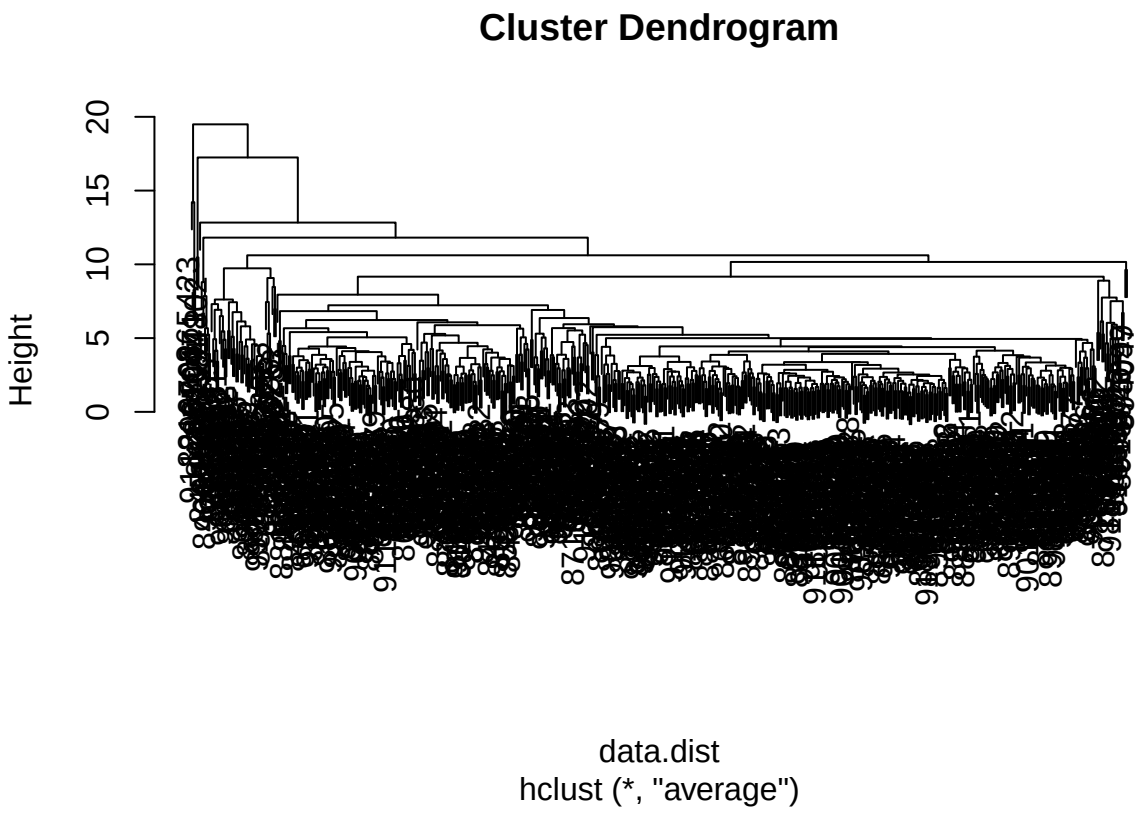
```
wisc.hclust.single <- hclust(data.dist, method="single")
wisc.hclust.complete <- hclust(data.dist, method="complete")
wisc.hclust.average <- hclust(data.dist, method="average")
wisc.hclust.ward.D2 <- hclust(data.dist, method="ward.D2")
plot(wisc.hclust.single)
```



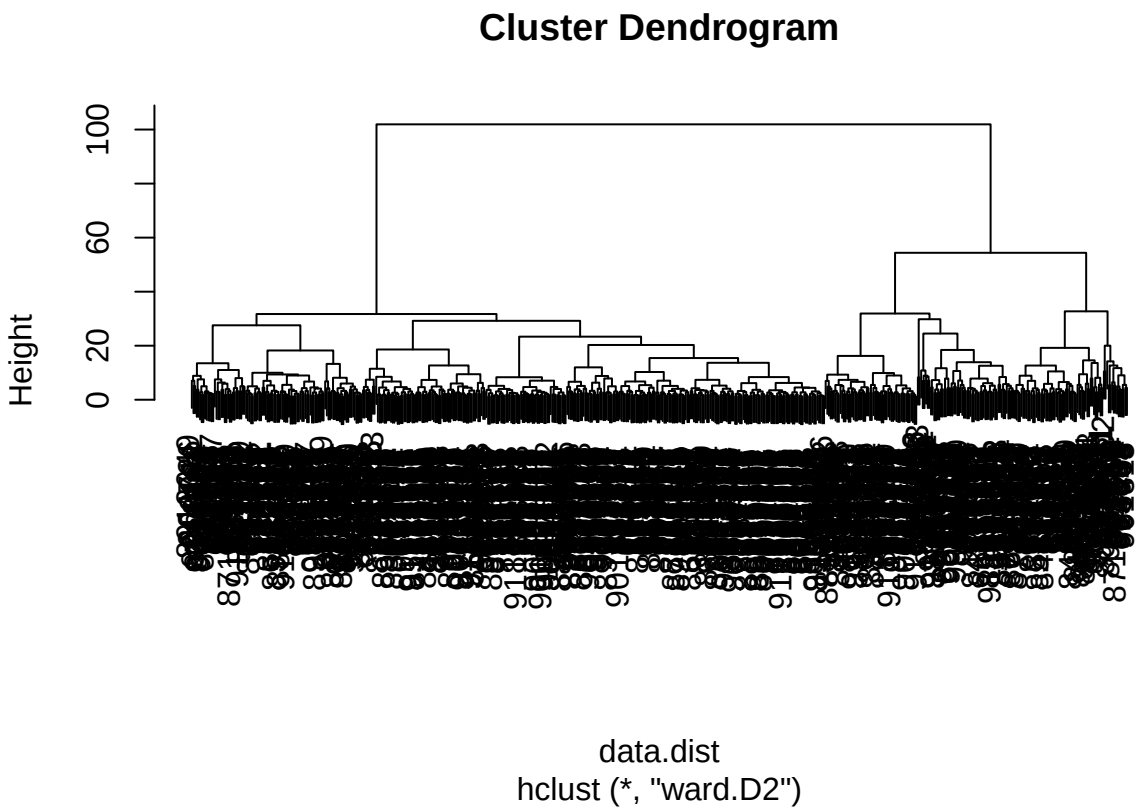
```
plot(wisc.hclust.complete)
```




```
plot(wisc.hclust.average)
```




```
plot(wisc.hclust.ward.D2)
```



Answer: `ward.D2` gives the most symmetrical and visually appealing dendrogram with 4 main clusters (optimal clustering). Branching clusters are evenly distributed and have clear groups.

4. OPTIONAL: K-means clustering

Create a k-means model on wisc.data, assigning the result to wisc.km. Be sure to create 2 clusters, corresponding to the actual number of diagnosis. Also, remember to scale the data (with the scale() function and repeat the algorithm 20 times (by setting setting the value of the nstart argument appropriately).

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

```
##    diagnosis
##       B   M
##   1 343  37
##   2  14 175
```

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

```
##                    diagnosis
## wisc.hclust.clusters   B   M
##                    1  12 165
```

```
##                    2   2   5
##                    3 343  40
##                    4   0   2
```

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

Use the table() function to compare the cluster membership of the k-means model (wisc.km$cluster) to your hierarchical clustering model from above (wisc.hclust.clusters).

```
table(wisc.hclust.clusters,wisc.km$cluster)
```

```
##
## wisc.hclust.clusters   1   2
##                    1  17 160
##                    2   0   7
##                    3 363  20
##                    4   0   2
```

Answer: Clusters 1,2 and 4 from the hclust model are equivalent to cluster 2 from the k-means model and and cluster 3 is equivalent to cluster 1. Compared to the hclust model, k-means separates the two diagnoses better as it has a higher sensitivity with fewer number of clustering.

5. Combining methods

Clustering on PCA results

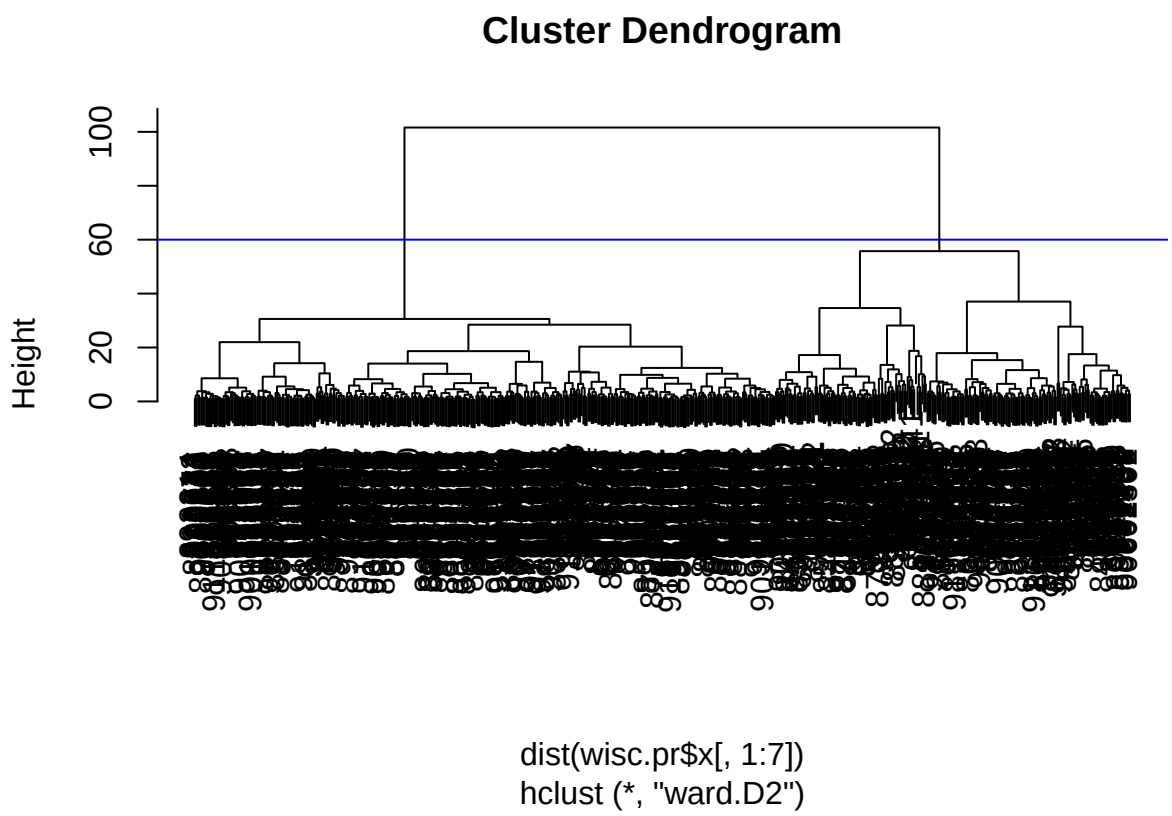
Results of the PCA analysis using `wisc.pr$x`

```
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
```

Use the first 7 principle components

```
wisc.pr.hclust<-hclust(dist(wisc.pr$x[,1:7]), method="ward.D2")
plot(wisc.pr.hclust)
abline(h=60,col="blue")
```



Above cluster dendrogram has two main branches, indicating two main clusters. Let's examine this - maybe these are malignant and benign.

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

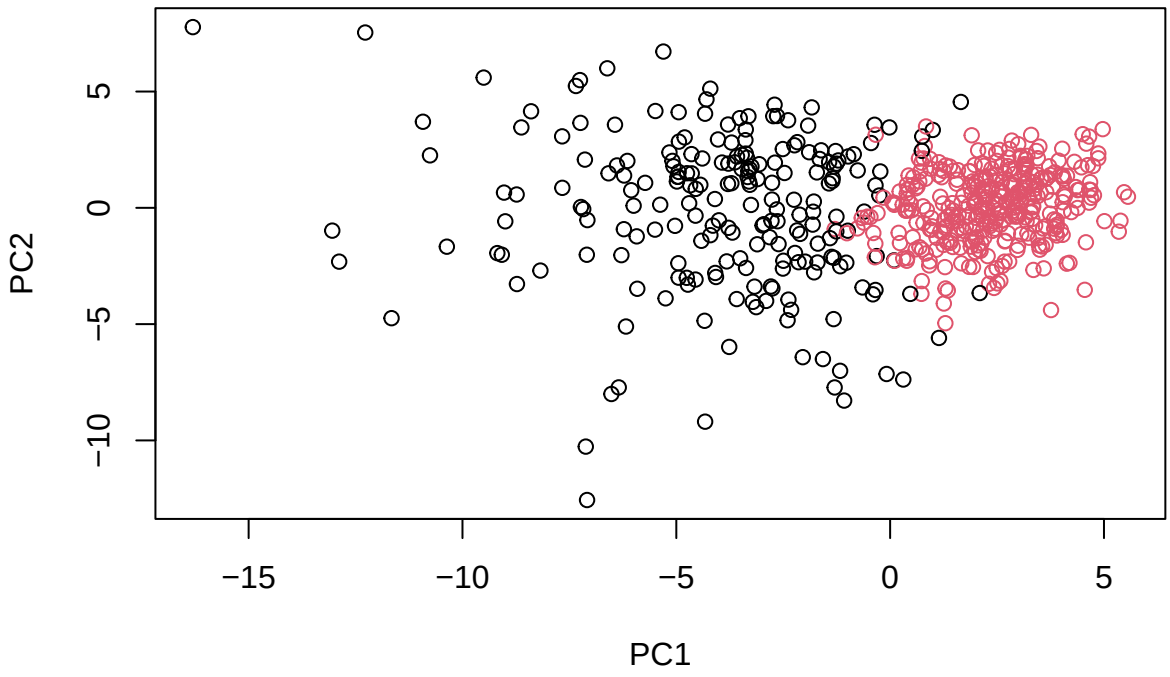
```
## grps
##   1   2
## 216 353
```

Cross table comparison of diagnosis and cluster groups

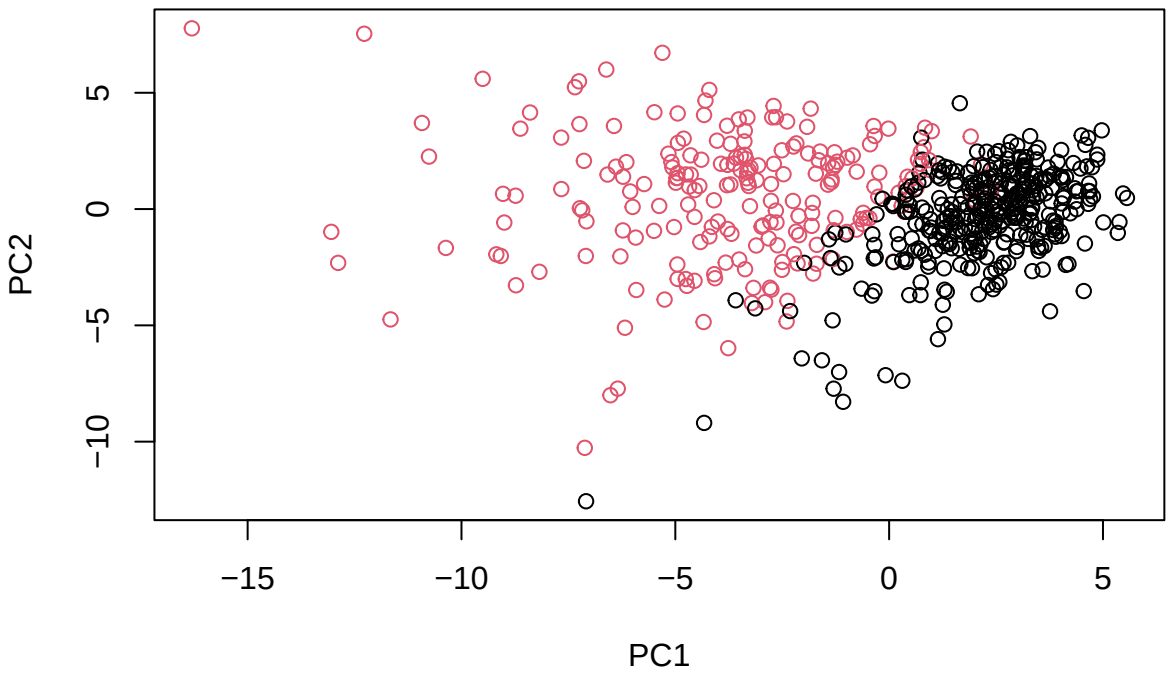
```
table(grps, diagnosis)
```

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

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




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



Note: the color swap here as the hclust cluster 1 is mostly "M" and cluster 2 is mostly "B" as we saw from the results of calling table(grps, diagnosis). To match things up we can turn our groups into a factor and reorder the levels so cluster 2 comes first and thus gets the first color (black) and cluster 1 gets the second color (red).

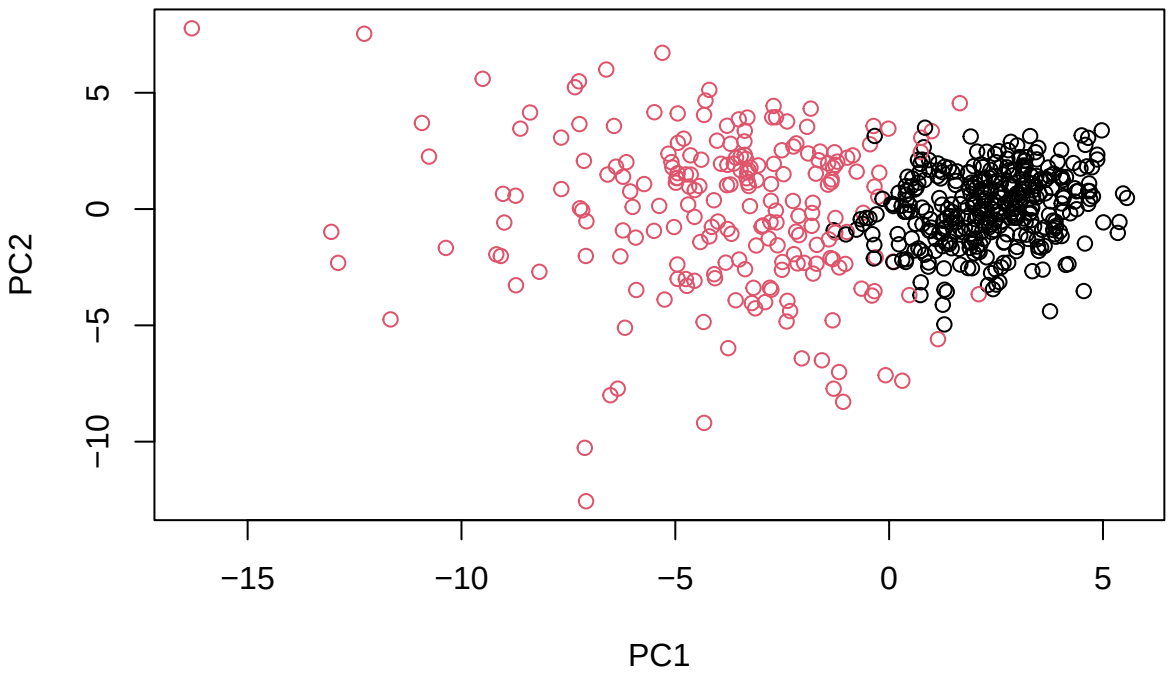
```
g <- as.factor(grps)
levels(g)
```

```
## [1] "1" "2"
```

```
g <- relevel(g,2)
levels(g)
```

```
## [1] "2" "1"
```

```
# Plot using our re-ordered factor
plot(wisc.pr$x[,1:2], col=g)
```




```
## 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")
```

```
#Cut this hierarchical clustering model into 2 clusters
wisc.pr.hclust.clusters <- cutree(wisc.pr.hclust, k=2)
```

Q15. How well does the newly created model with 2 clusters separate out the two diagnoses?

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

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

Answer: The newly created model is better since there is a clear distinction of positive and negative results for both benign and malignant categories in each cluster. Cluster 1 primarily contains malignant diagnoses whereas Cluster 2 primarily contains benign diagnoses.

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

```
##    diagnosis
##       B   M
##   1 343  37
##   2  14 175
```

```
# hierarchical clustering model
table(wisc.hclust.clusters, diagnosis)
```

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

Answer: Both k-means and hierarchical clustering models separate the diagnoses well. In the k-means model, cluster 1 contains mostly benign cells and cluster 2 contains mostly malignant cells. in the hierarchical clustering model, cluster 3 contains mostly benign cells and clusters 1,2, and 4 contain mostly malignant cells. However, clusters 2 and 4 have such a small number of results and are can be neglected. Compared to hclust results, k-means seems to separate the two diagnoses better with higher sensitivity but same specificity.

6. Sensitivity/Specificity

Sensitivity refers to a test's ability to correctly detect ill patients who do have the condition. In our example here the sensitivity is the total number of samples in the cluster identified as predominantly malignant (cancerous) divided by the total number of known malignant samples. In other words: TP/(TP+FN).

Specificity relates to a test's ability to correctly reject healthy patients without a condition. In our example specificity is the proportion of benign (not cancerous) samples in the cluster identified as predominantly benign that are known to be benign. In other words: TN/(TN+FN).

> Q17. Which of your analysis procedures resulted in a clustering model with the best specificity? How about sensitivity?

```
# 2 branch clustering for 7 PCs
table(grps, diagnosis)
```

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

```
# k-means clustering model
table(wisc.km$cluster, diagnosis)
```

```
##    diagnosis
##       B   M
##   1 343  37
##   2  14 175
```

```
# hierarchical clustering model
table(wisc.hclust.clusters, diagnosis)
```

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

```
#sensitivity
seven_PCS_clustering_sensitivity <- 188/(188+24)
kmeans_clustering_sensitivity <- 175/(175+37)
hierarchical_clustering_sensitivity <- 172/(165+5+2+40)

#specificity
seven_PCS_clustering_specificity <- 329/(329+28)
kmeans_clustering_specificity <- 343/(343+14)
hierarchical_clustering_specificity <- 343/(343+12+2)
```

```
seven_PCS_clustering_sensitivity
```

```
## [1] 0.8867925
```

```
kmeans_clustering_sensitivity
```

```
## [1] 0.8254717
```

```
hierarchical_clustering_sensitivity
```

```
## [1] 0.8113208
```

```
seven_PCS_clustering_specificity
```

```
## [1] 0.9215686
```

```
kmeans_clustering_specificity
```

```
## [1] 0.9607843
```

```
hierarchical_clustering_specificity
```

```
## [1] 0.9607843
```

Answer: The sensitivity is 88.7% for 2-cluster clustering for first 7 PCs, 82.5% for k-means clustering, and 81.1% for hierarchical clustering. Hence, the model generated using 2-cluster clustering for first 7 PCs gives the best sensitivity. The sensitivity is 92.2% for 2-cluster clustering for first 7 PCs and 96.1% for both k-means clustering and hierarchical clustering. Hence, the model generated using either k-means clustering and hierarchical clustering gives the best specificity.

7. Prediction

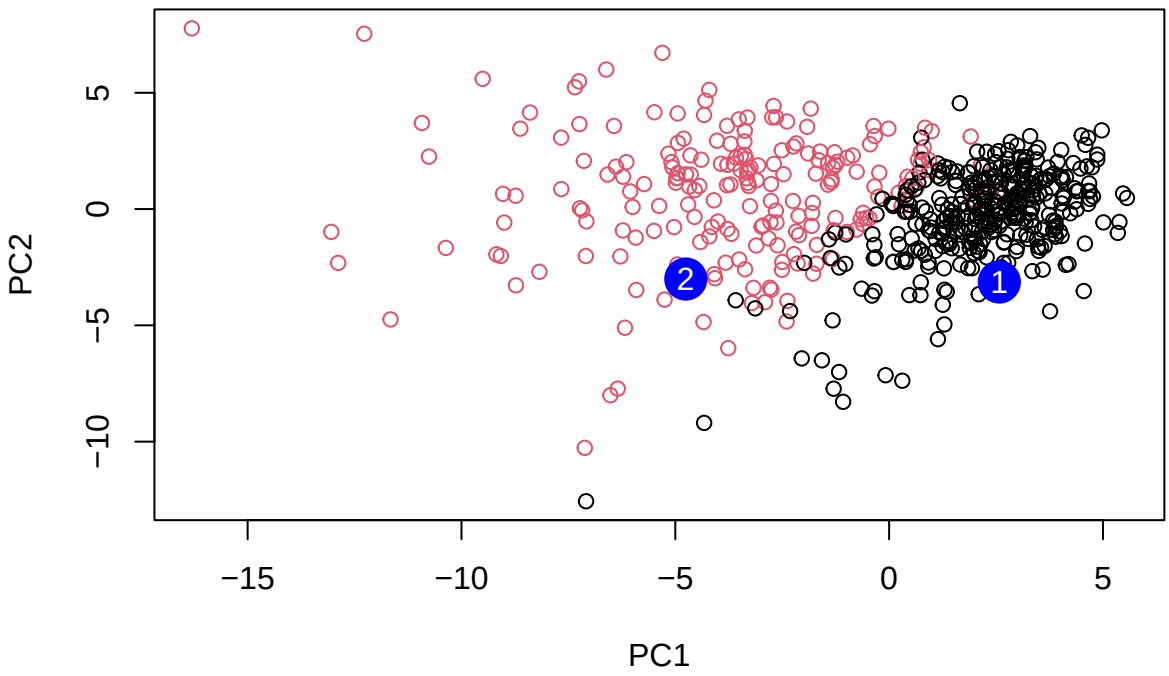
We will use the predict() function that will take our PCA model from before and new cancer cell data and project that data onto our PCA space.

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

Plot onto the PCA model

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

Answer: We should follow up on patient 2 that has cells identified as predominantly malignant.