Class 8: Mini Project

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4/28/23

1. Exploratory Data Analysis

Prepare the Data

First we need to input and read the data.

```
# Save input data file into the Project directory
wisc.df <- read.csv('WisconsinCancer.csv', 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
```

To make sure we don't accidentally include diagnosis in our analysis, lets 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]
```

Create a diagnosis vector for later

```
diagnosis <- wisc.df$diagnosis
```

Exploratory Data Analysis

Q1. How many observations are in this dataset?

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

```
[1] 569
```

There are 569 observations.

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

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

```
  B   M
357 212
```

```
diagnosis <- wisc.df$diagnosis
```

There are 212 observations that have a malignant diagnosis.

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

```
length(grep("_mean", colnames(wisc.df)))
```

```
[1] 10
```

There are 10 variables/features in the data that are suffixed with `_mean`.

2. Principal Component Analysis

Performing PCA

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

```
# 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(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
```

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

0.4427

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

```
variance <- (wisc.pr$sdev^2)
variance/(sum(variance))
```

```
 [1] 4.427203e-01 1.897118e-01 9.393163e-02 6.602135e-02 5.495768e-02
 [6] 4.024522e-02 2.250734e-02 1.588724e-02 1.389649e-02 1.168978e-02
[11] 9.797190e-03 8.705379e-03 8.045250e-03 5.233657e-03 3.137832e-03
[16] 2.662093e-03 1.979968e-03 1.753959e-03 1.649253e-03 1.038647e-03
[21] 9.990965e-04 9.146468e-04 8.113613e-04 6.018336e-04 5.160424e-04
[26] 2.725880e-04 2.300155e-04 5.297793e-05 2.496010e-05 4.434827e-06
```

Three principal components are required to describe at least 70% of the original variance in the data.

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

Seven principal components are required to describe at least 90% of the original variance in the data.

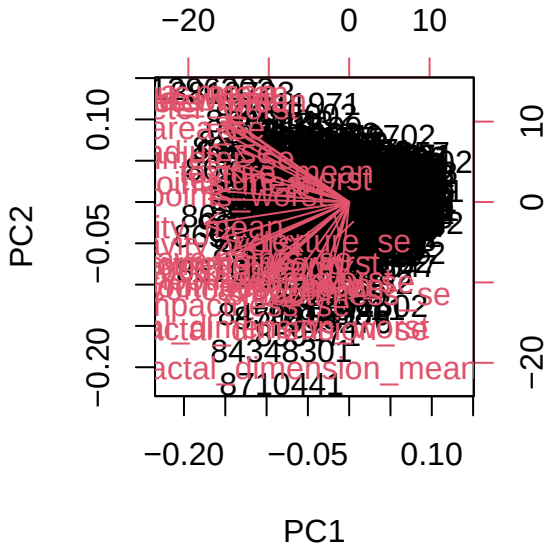
Interpreting PCA results

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

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

This plot is very messy and difficult to understand because the rownames are used as the plotting character, making it cluttered.

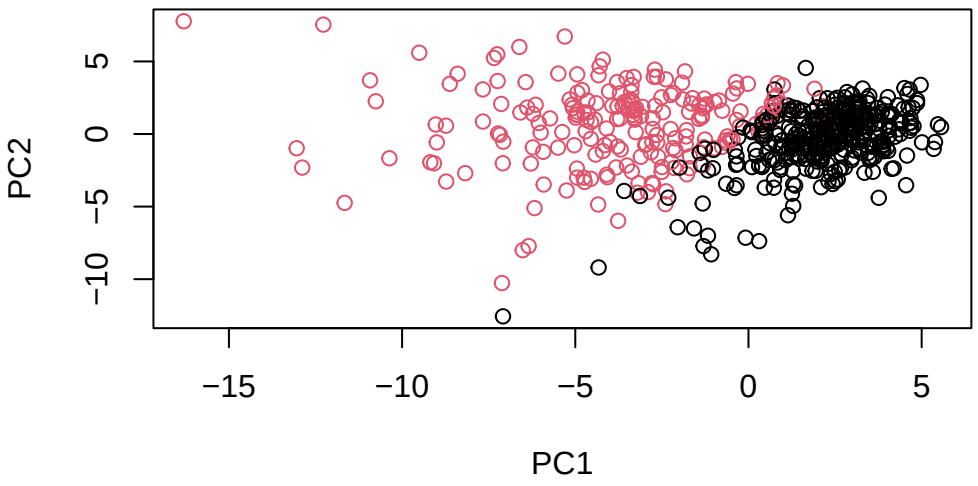
```
biplot(wisc.pr)
```



Create a cleaner plot

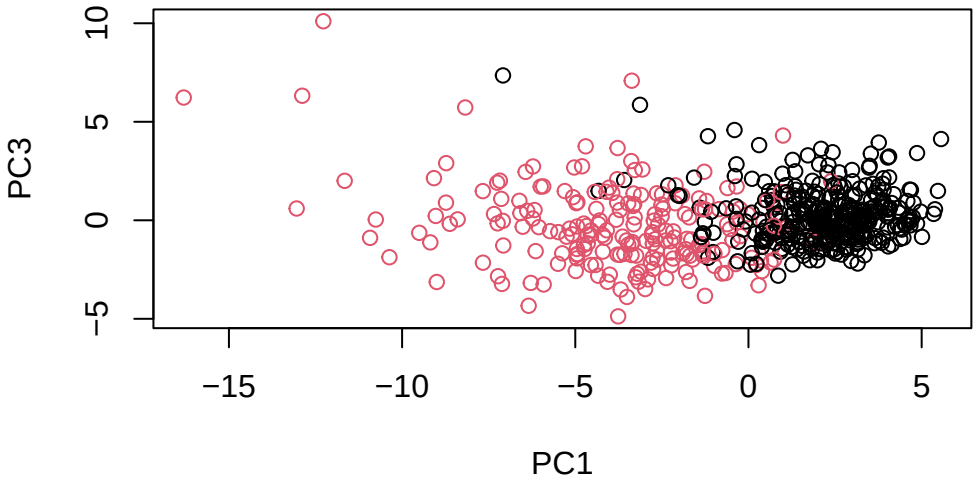
```
diagnosis <- as.factor(diagnosis)
```

```
plot( wisc.pr$x[, 1:2], col = diagnosis ,
     xlab = "PC1", ylab = "PC2")
```



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

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



Based on the two plots, we can tell that the distinguishing factor for the diagnosis is reliant on PC1.

Create a data.frame for ggplot

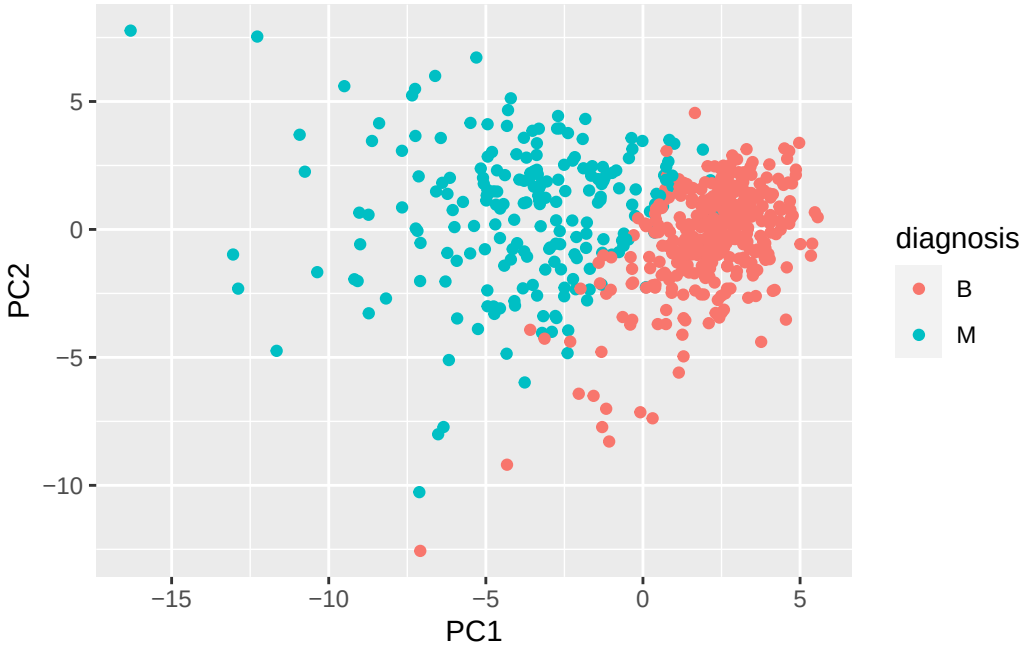
```
df <- as.data.frame(wisc.pr$x)
df$diagnosis <- diagnosis
```

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 increase.

Calculate variance of each component

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

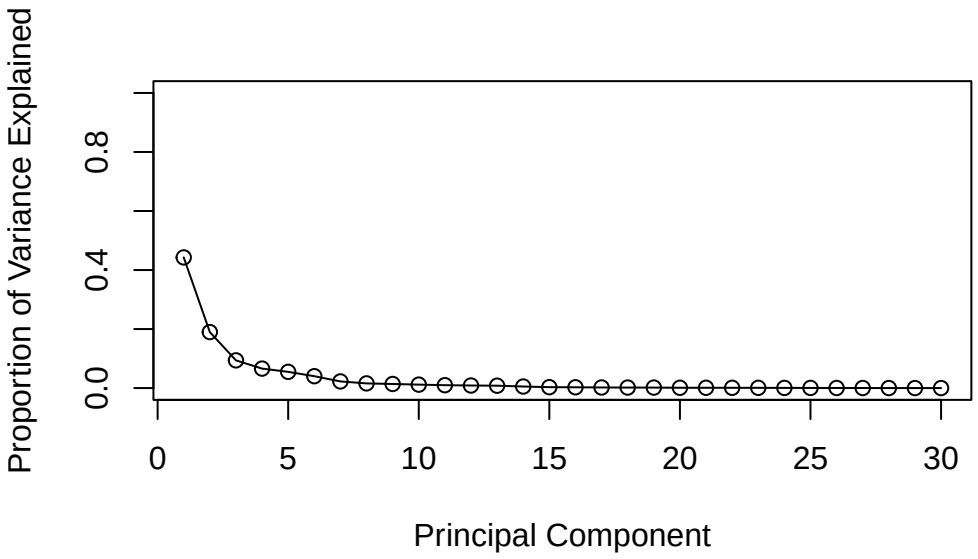
```
[1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

Calculate the variance explained by each principal component by dividing by the total variance explained of all principal components.

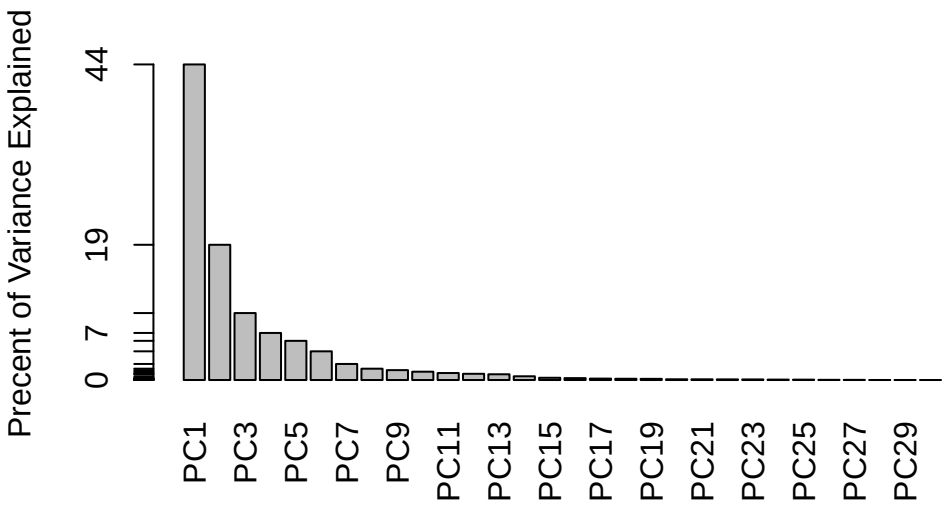
```
# Variance explained by each principal component: pve
pve <- pr.var / sum(pr.var)
```

```
# 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 )
```



ggplot based graph

Install the package

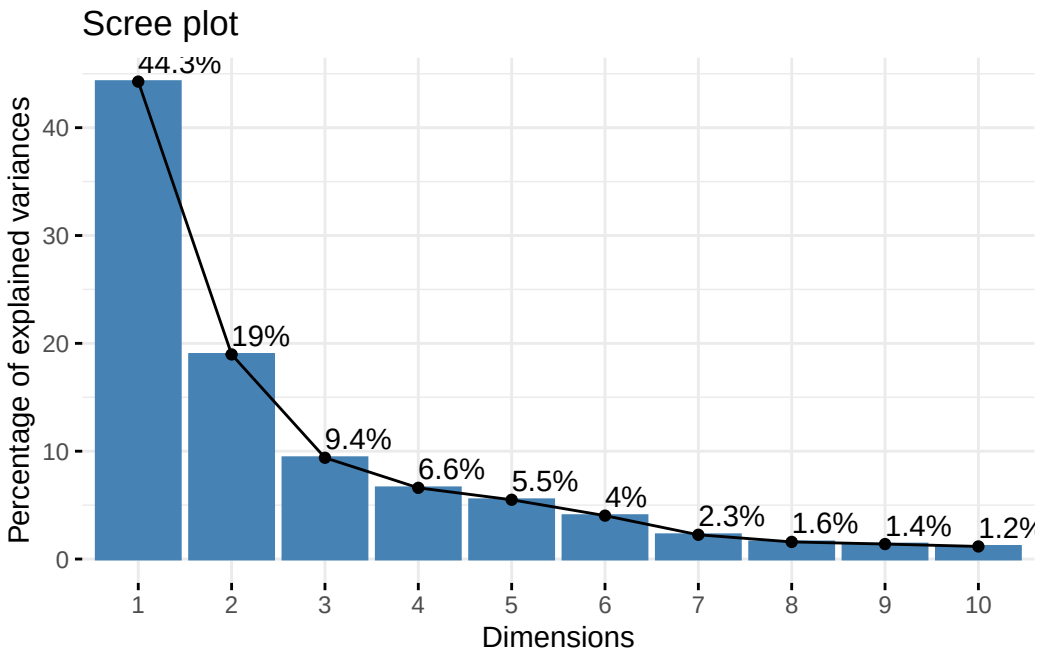
```
#install.packages("factoextra")
```

Now plot

```
library(factoextra)
```

```
Welcome! Want to learn more? See two factoextra-related books at https://goo.gl/ve3WBa
```

```
fviz_eig(wisc.pr, addlabels = TRUE)
```



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`? This tells us how much this original feature contributes to the first PC.

```
View(wisc.pr$rotation[,1])
```

-0.2608538

3. Hierarchical clustering

Scale the wisc.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)
```

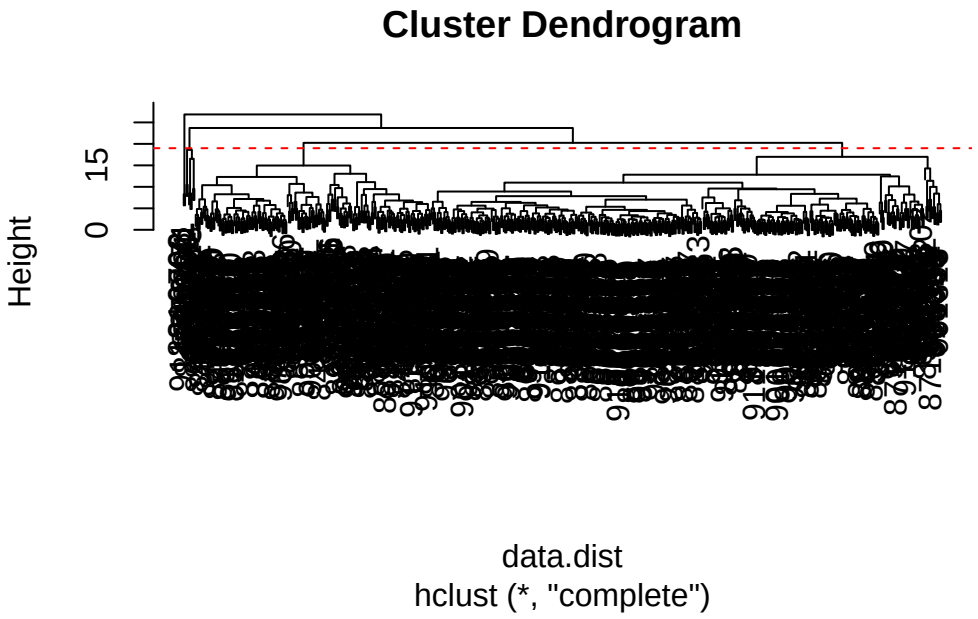
Create a hierarchical clustering model using complete linkage.

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

Results of hierarchical clustering

Q10. 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)
```



The height at which the clustering model has 4 clusters is 19.

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

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

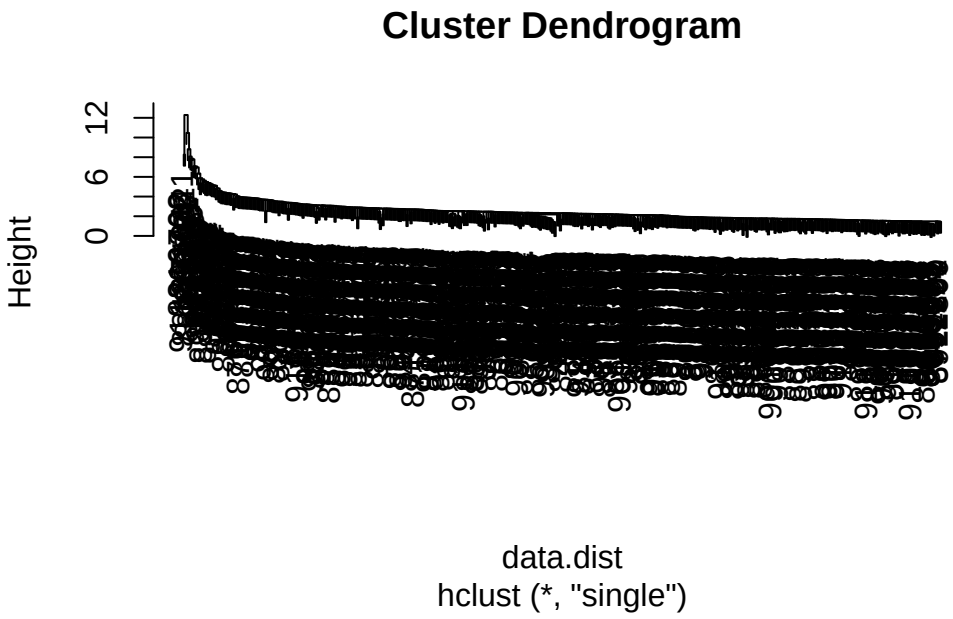
```
  2   2   5
  3 343  40
  4   0   2
```

Using different methods

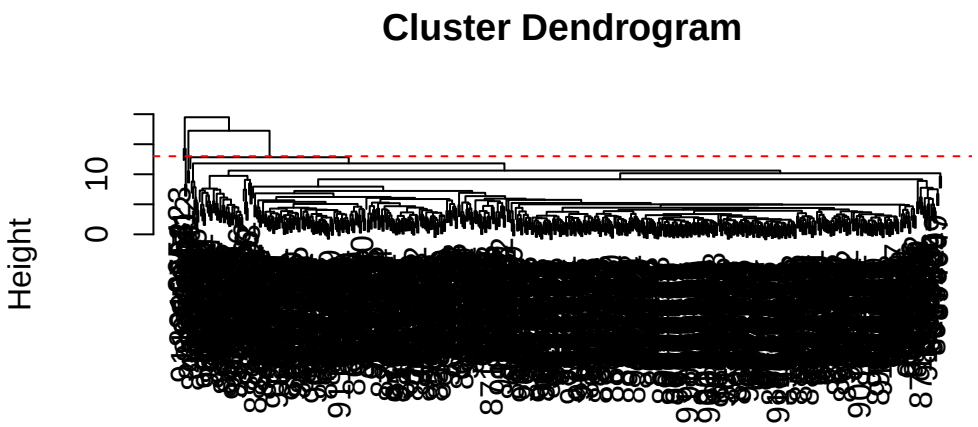
Q12. Which method gives your favorite results for the same `data.dist` dataset? Explain your reasoning.

Ward.D2 is the method that gives my favorite results for the dataset because it is a lot easier to see the clusters and it minimizes the variance within the clusters.

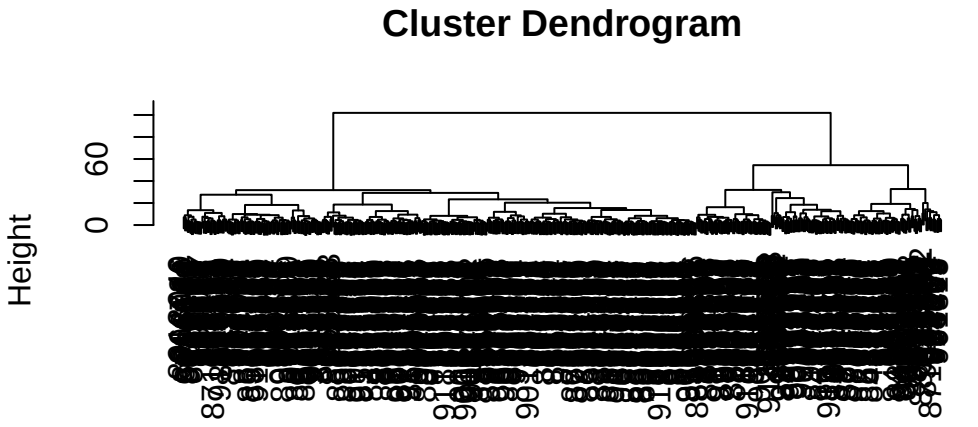
```
wisc.hclust.single <- hclust(data.dist, method = "single")
plot(wisc.hclust.single)
```




```
wisc.hclust.avg <- hclust(data.dist, method = "average")
plot(wisc.hclust.avg)
abline(h=13, col="red", lty=2)
```




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

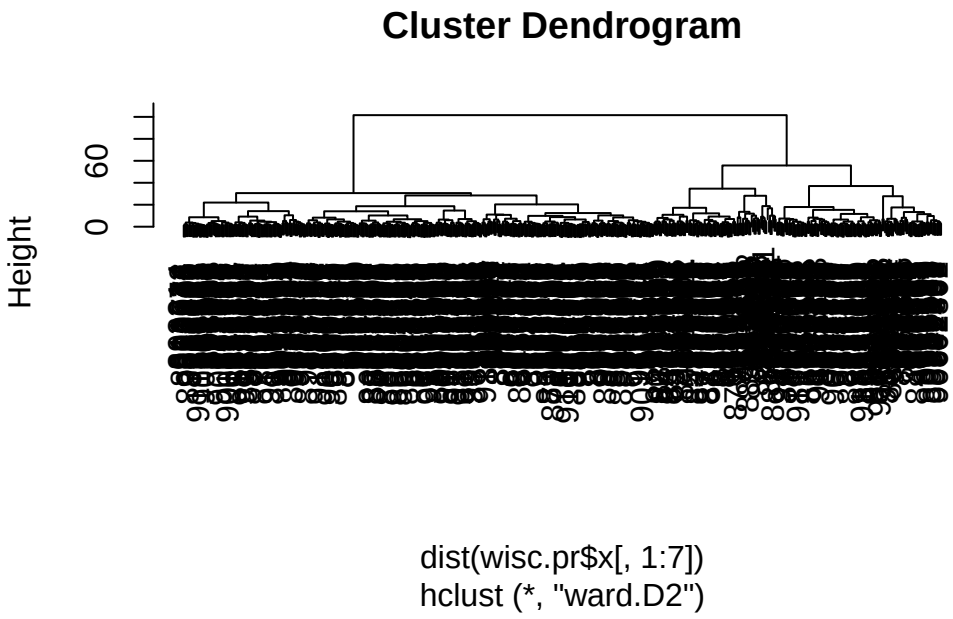


4. Combining methods

Clustering on PCA results

Let's see if PCA improves or degrades the performance of hierarchical clustering.

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




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

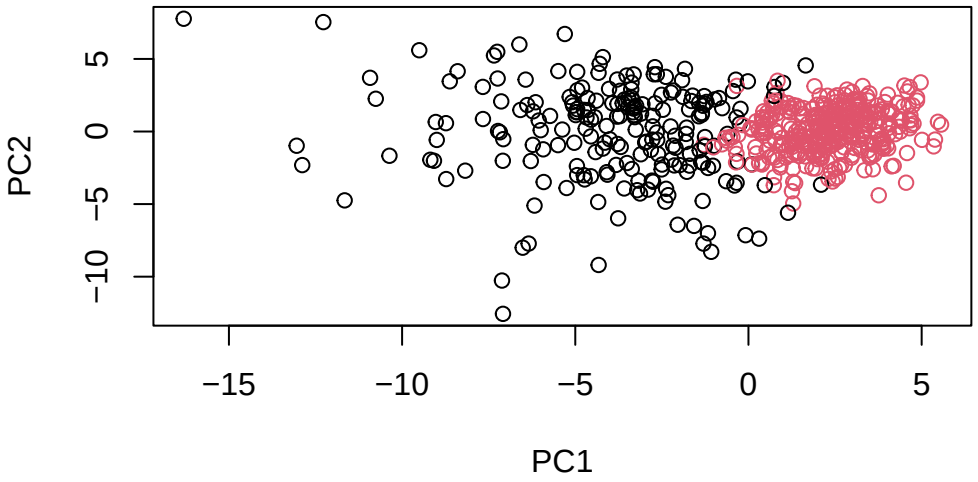
```
grps
  1   2
216 353
```

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

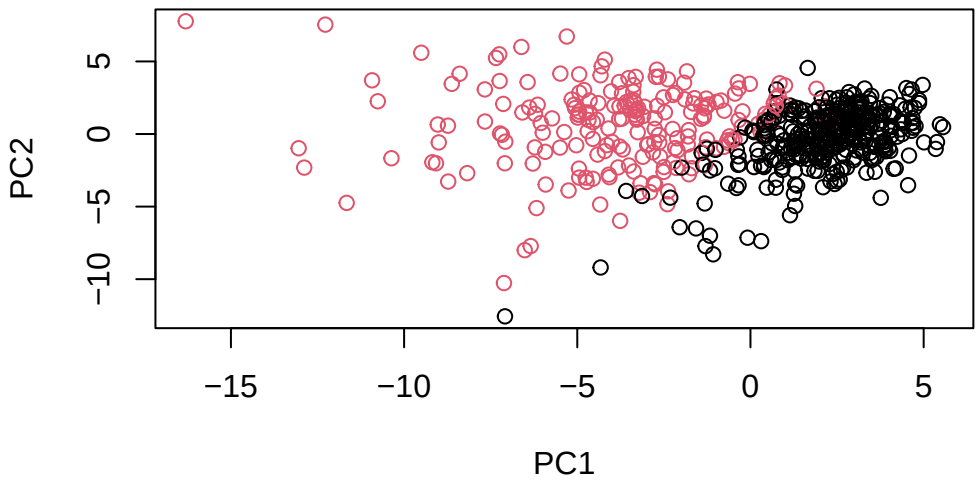
```
    diagnosis
```

```
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)
```




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

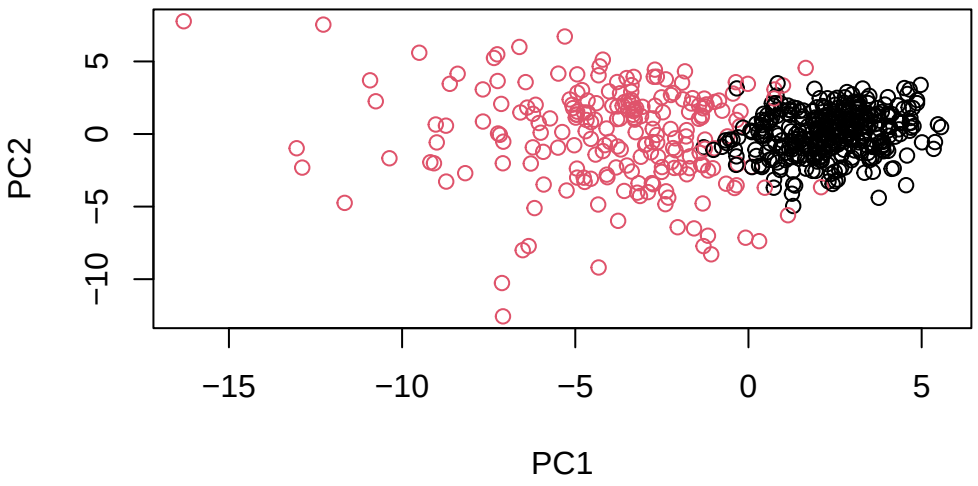
```
[1] "1" "2"
```

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

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

Plot using our re-ordered factor:

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



Cut this hierarchical clustering model into 2 clusters and assign the results to `wisc.pr.hclust.clusters`.

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

Q13. How well does the newly created model with four 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
```

The newly created model with four clusters separates out the two diagnoses pretty well.

Q14. How well do the hierarchical clustering models you created in previous sections (i.e. before PCA) do in terms of separating the diagnoses? Again, use the `table()` function to compare the output of each model (`wisc.km$cluster` and `wisc.hclust.clusters`) with the vector containing the actual diagnoses.

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

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

The hierarchical clustering models I created in previous sections do not do as well of a job separating the diagnoses as the new model does, but it still distinguishes the diagnoses.

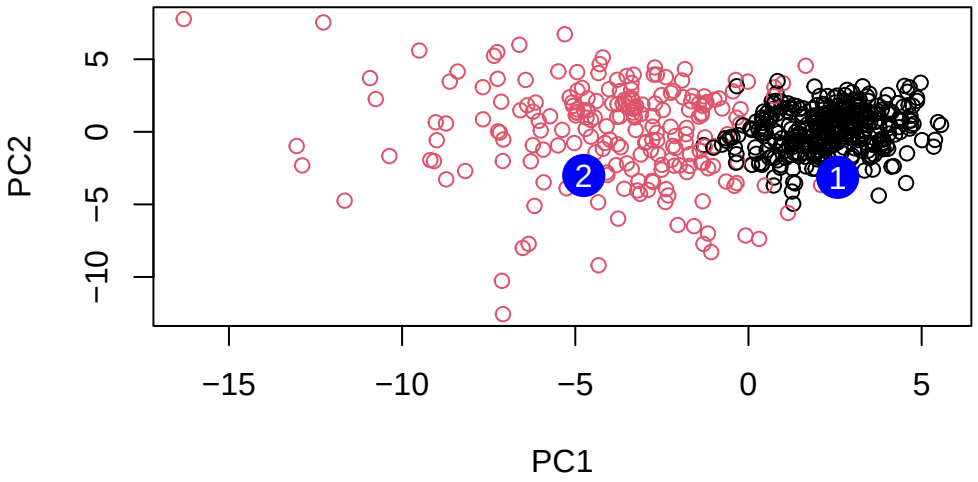
6. Prediction

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(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")
```



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

Based on my results, we should prioritize patient 2.