Class 08: Machine Learning Mini Project

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Exploratory Data Analysis

```r
# Save your input data file into your Project directory
fna.data <- "https://bioboot.github.io/bimm143_S20/class-material/WisconsinCancer.csv"

# Complete the following code to input the data and store as wisc.df
wisc.df <- read.csv(fna.data, row.names=1)
```

```r
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
```

```
wisc.data <- wisc.df[,-1]
```

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

Q1

How many observations are in this data set?

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

```
[1] 569
```

The amount of observations in this data set is 569

Q2

How many of these observations have a malignant diagnosis?

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

```
  B   M 
357 212 
```

The amount of observations in this data set that have a malignant diagnosis is 212

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

- The `grep()` function will be useful here

```r
length(grep("_mean", colnames(wisc.data), wisc.data))
```

```
[1] 10
```

The amount of variables in that data sset suffixed with _mean is 10

Principal Component Analysis

```r
# 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 
```

```r
apply(wisc.data,2,sd)
```

```
            radius_mean            texture_mean          perimeter_mean 
           3.524049e+00            4.301036e+00            2.429898e+01 
              area_mean         smoothness_mean        compactness_mean 
           3.519141e+02            1.406413e-02            5.281276e-02 
         concavity_mean     concave.points_mean           symmetry_mean 
           7.971981e-02            3.880284e-02            2.741428e-02 
 fractal_dimension_mean               radius_se              texture_se 
           7.060363e-03            2.773127e-01            5.516484e-01 
           perimeter_se                 area_se           smoothness_se 
           2.021855e+00            4.549101e+01            3.002518e-03 
         compactness_se            concavity_se       concave.points_se 
           1.790818e-02            3.018606e-02            6.170285e-03 
            symmetry_se    fractal_dimension_se            radius_worst 
           8.266372e-03            2.646071e-03            4.833242e+00 
          texture_worst         perimeter_worst              area_worst 
           6.146258e+00            3.360254e+01            5.693570e+02 
       smoothness_worst       compactness_worst         concavity_worst 
           2.283243e-02            1.573365e-01            2.086243e-01 
```

```
  concave.points_worst          symmetry_worst fractal_dimension_worst 
          6.573234e-02            6.186747e-02            1.806127e-02 
```

```r
# Perform PCA on wisc.data
wisc.pr <- prcomp(wisc.data, scale=TRUE)
# Perform a summary on the PC 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
```

Q4

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

The proportion of the original variance captured by PC1 is .4427.

Q5

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

3 PCs are required to describe at least 70% of the data

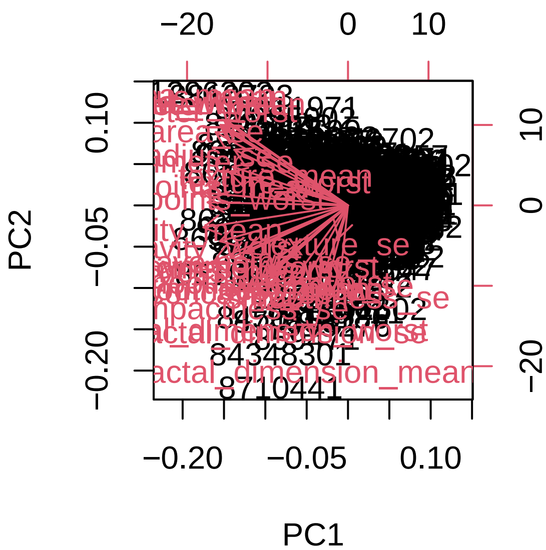
Q6

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

7 PCs are required to describe at least 90% of the data

#Plotting the PCA Data

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

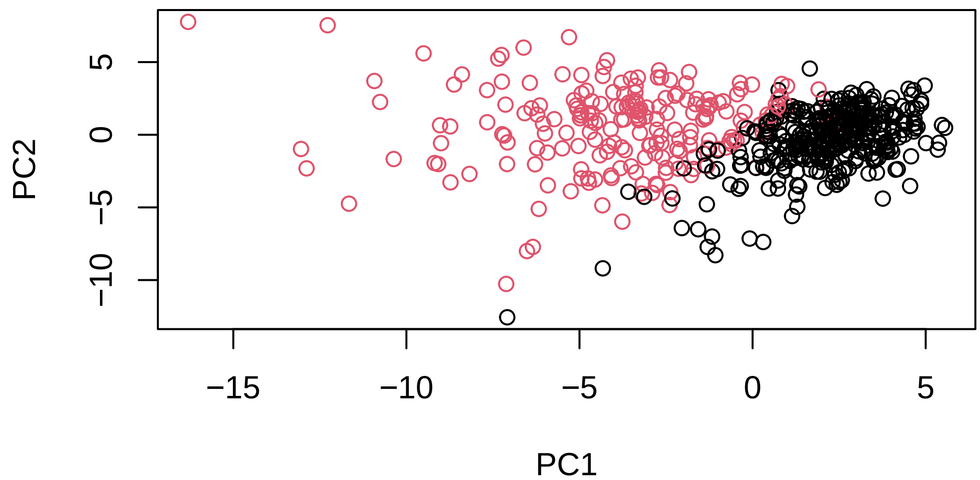


Q7

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

This plot is incredibly difficult to read as the data points are all represented by their ID numbers and are heavily overlapping and the column names are also very heavily overlapping the data making it almost impossible to read.

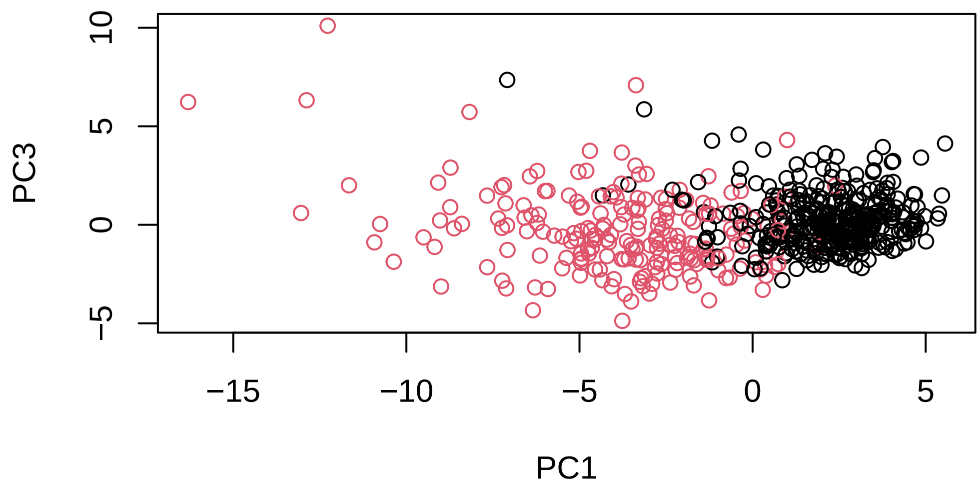
```
plot(wisc.pr$x[,c("PC1","PC2")], col = diagnosis ,
     xlab = "PC1", ylab = "PC2")
```



Q8

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

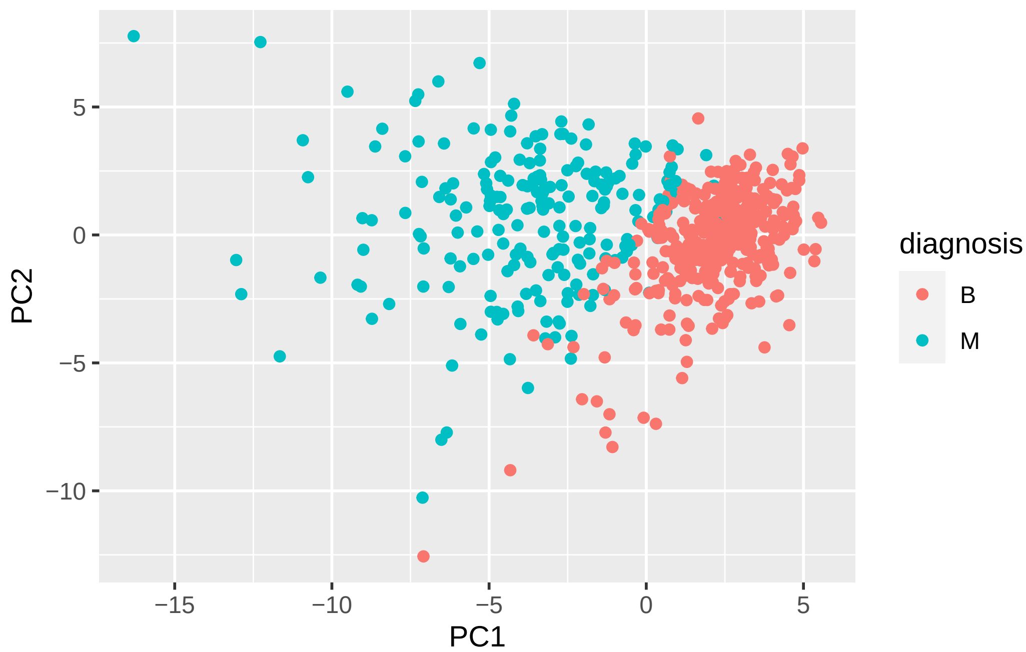
```
plot(wisc.pr$x[,c("PC1","PC3")], col = diagnosis ,
     xlab = "PC1", ylab = "PC3")
```



The plots look similar, but the spread for PC3 is much smaller in comparison to the previous plot.

Plotting with ggplot2

```
# 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()
```

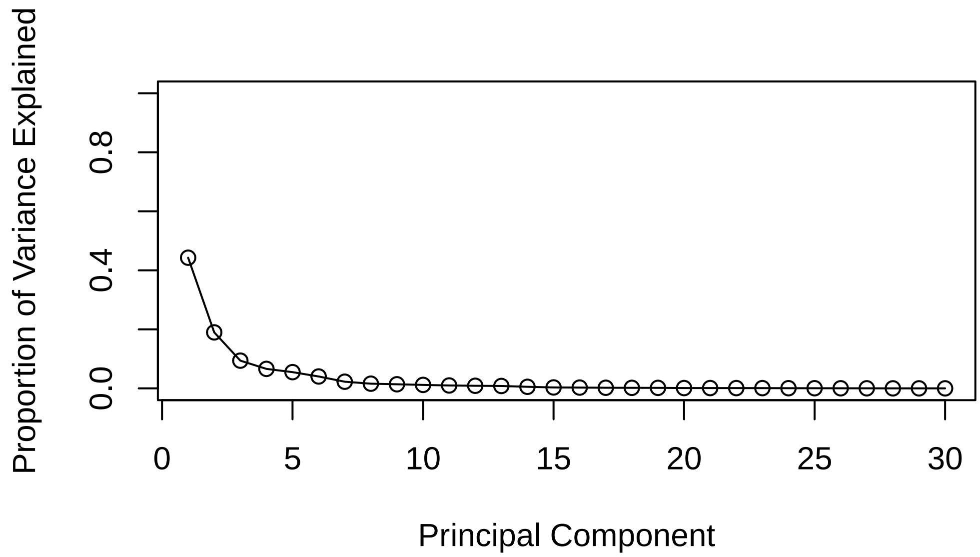


Variance Explained

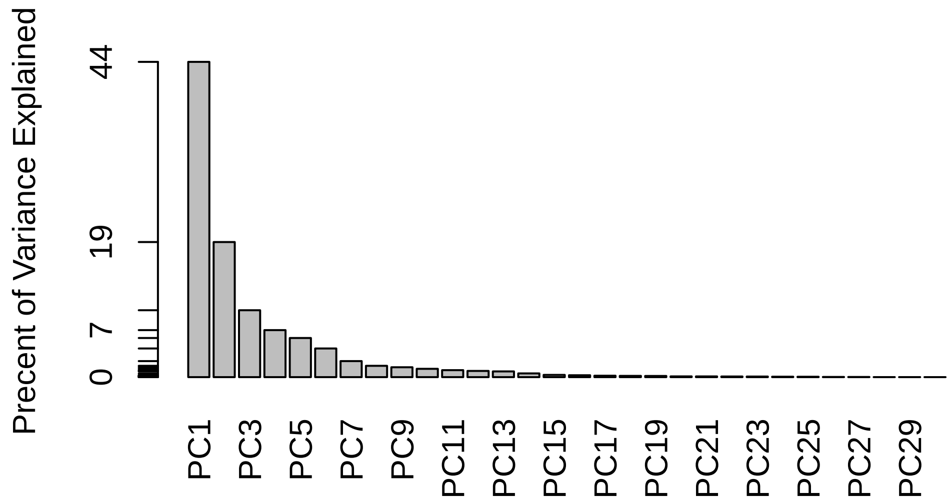
```
pr.var <- wisc.pr$sdev^2
head(pr.var)
```

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

```
# 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")
```



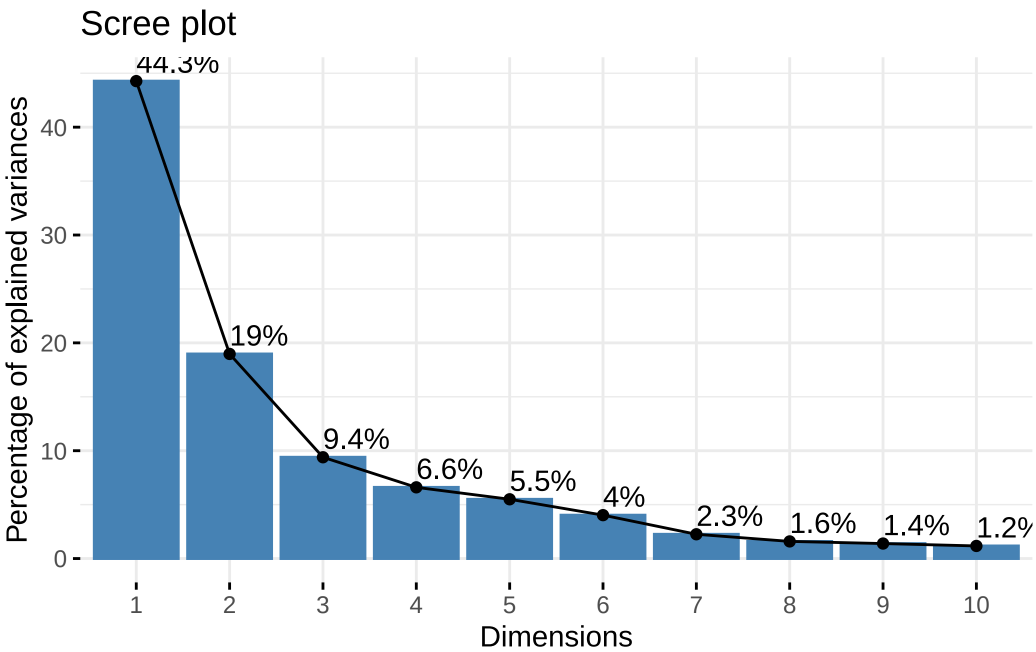

```
# Alternative scree plot of the same data, note data driven y-axis
barplot(pve, ylab = "Precent of Variance Explained",
     names.arg=paste0("PC",1:length(pve)), las=2, axes = FALSE)
axis(2, at=pve, labels=round(pve,2)*100 )
```




```
## ggplot based graph
#install.packages("factoextra")
library(factoextra)
```

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

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



Q9

For the first principal component, what is the component of the loading vector? This tells us how much this original feature contributes to the first PC.

```
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
```

The concave_points_mean is -.26085376

Hierarchical Clustering

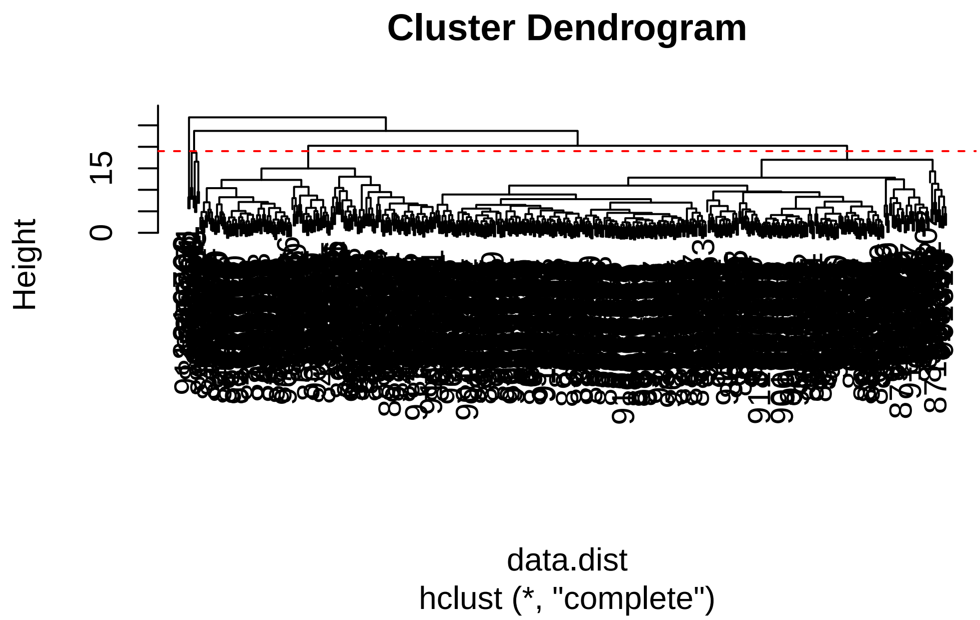
```r
# Scale the wisc.data data using the "scale()" function
data.scaled <- scale(wisc.data)

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

```
Call:
hclust(d = data.dist)

Cluster method   : complete
Distance         : euclidean
Number of objects: 569
```

Q10

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

```r
plot(wisc.hclust)
abline(h=19, col="red", lty=2)
```



Selecting Numbers of Clusters

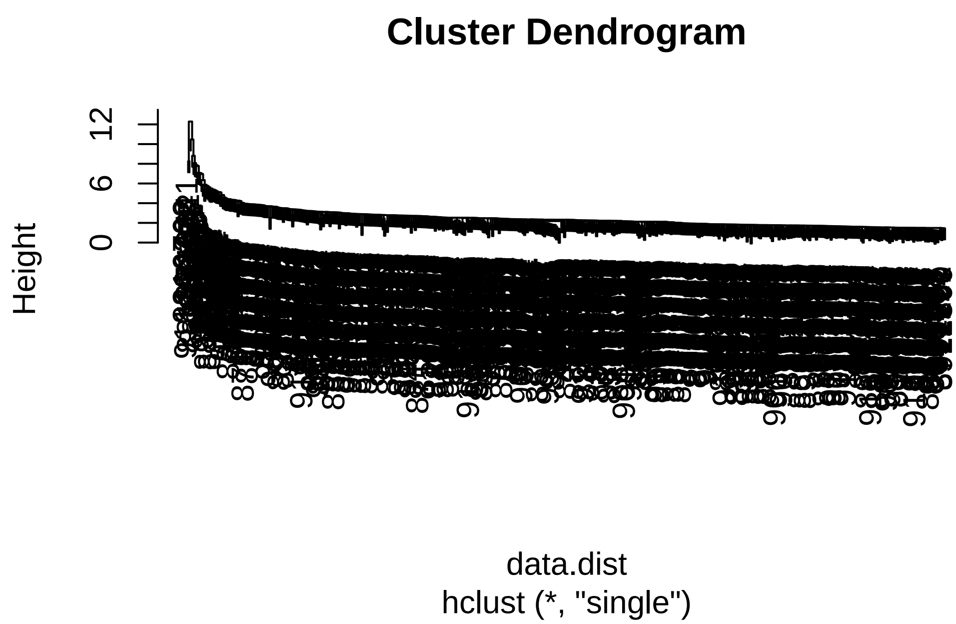
```
wisc.hclust.clusters <- cutree(wisc.hclust, k=4)
table(wisc.hclust.clusters, diagnosis)
```

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

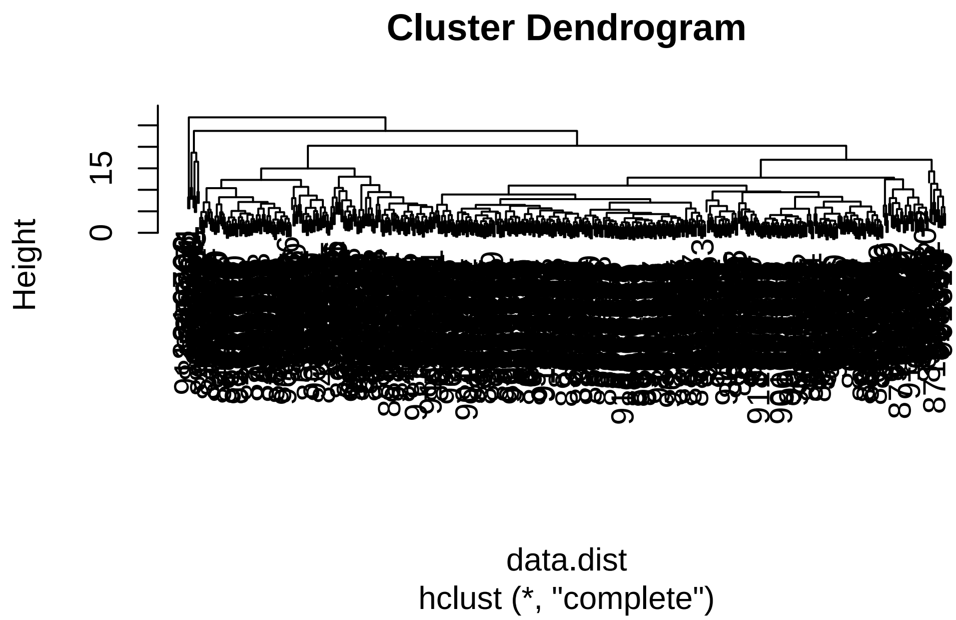
Q12

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

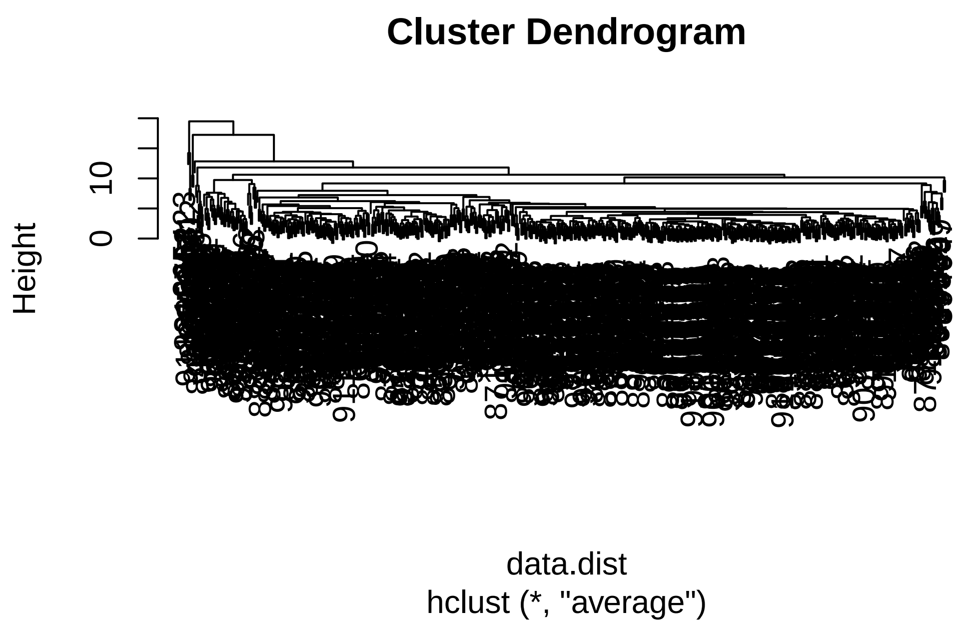
```r
wisc.hclust.s <- hclust(data.dist, method="single")
wisc.hclust.c <- hclust(data.dist, method="complete")
wisc.hclust.a <- hclust(data.dist, method="average")
wisc.hclust.w <- hclust(data.dist, method="ward.D2")

plot(wisc.hclust.s)
```



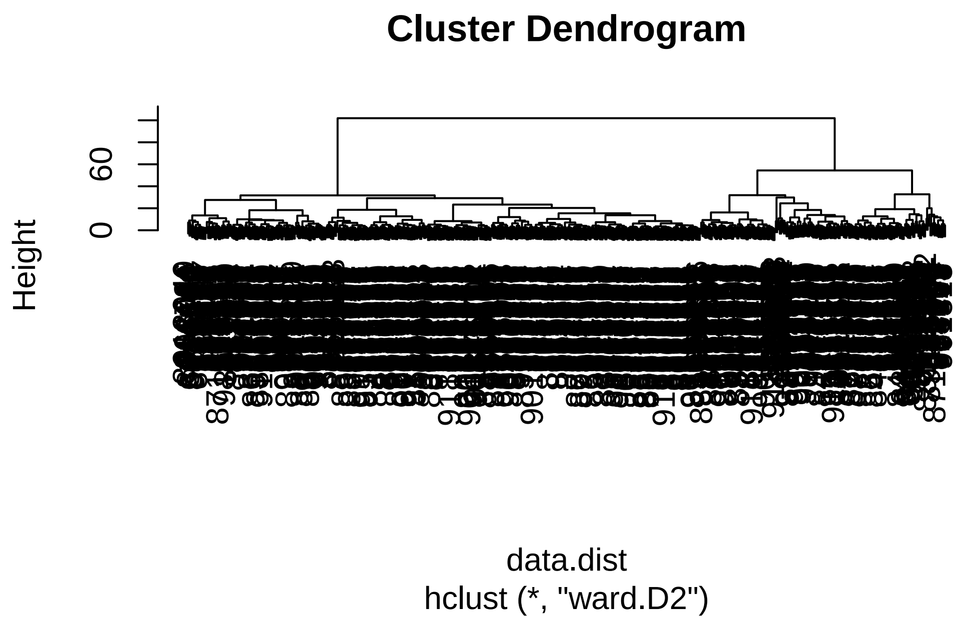

```r
plot(wisc.hclust.c)
```




```
plot(wisc.hclust.a)
```



```r
plot(wisc.hclust.w)
```



I like the `ward.D2` method because it minimizes the variance within clusters, so it appeared to cluster the data best into 2 clusters, which appeared to match out Malignant and Benign data best.

Combining Methods

```r
# Use the minimum number of principal components required to describe at least 90% of the
wisc.pr.hclust <- hclust(dist(wisc.pr$x[,1:7]), method = "ward.D2")
```

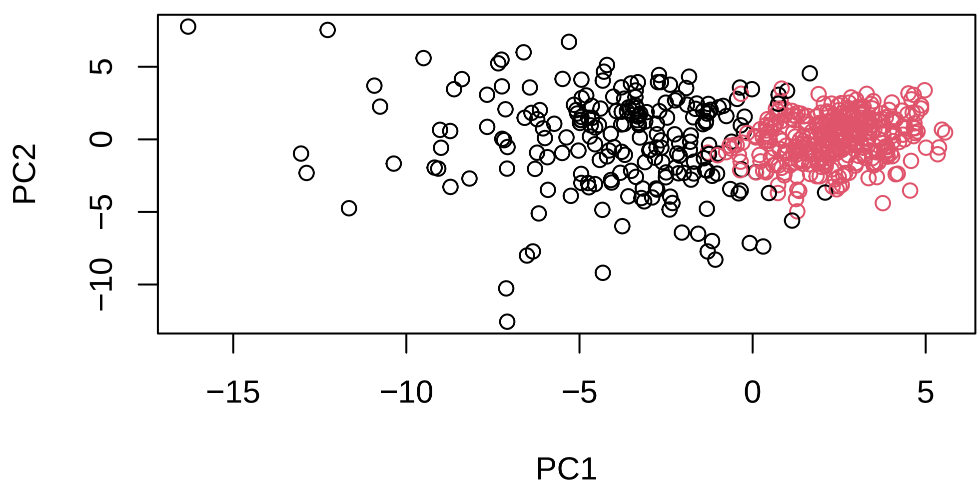
```r
grps <- cutree(wisc.pr.hclust, k=2)
table(grps)
```

```
grps
  1   2
216 353
```

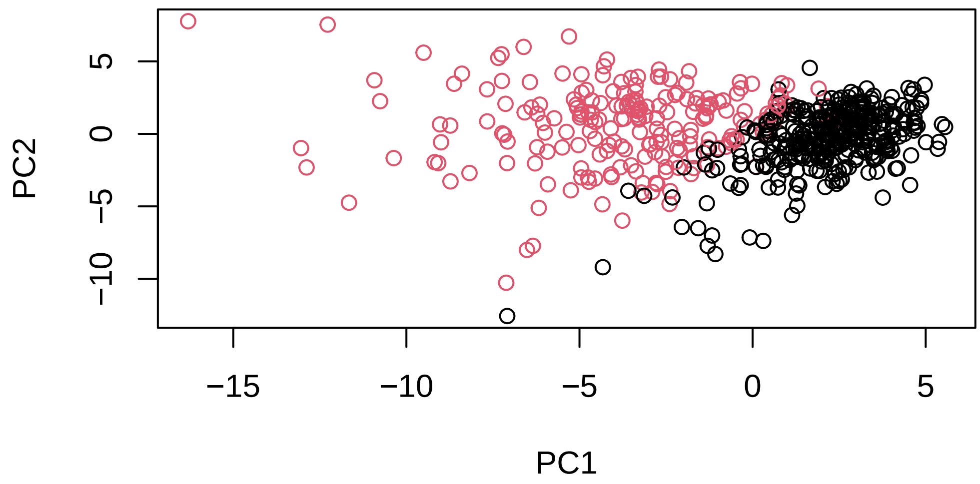
```r
table(grps, diagnosis)
```

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

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




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



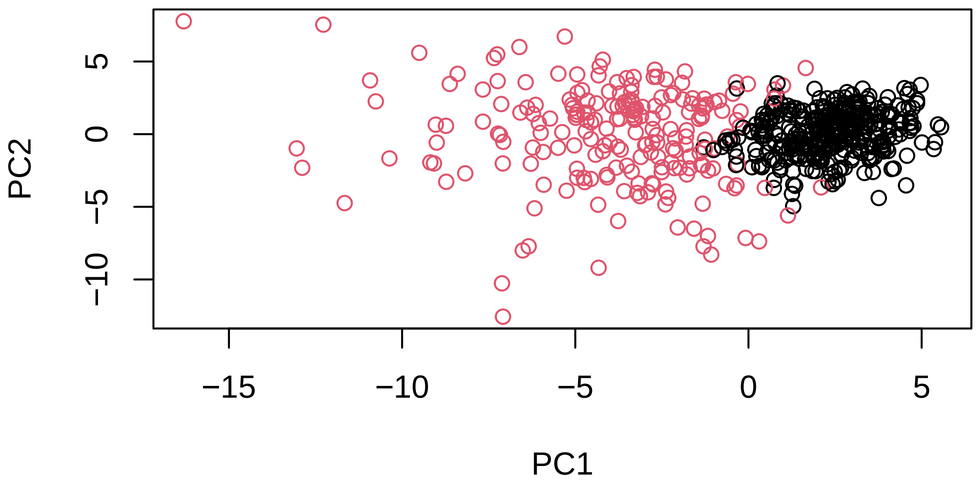

```
g <- as.factor(grps)
levels(g)
```

```
[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)
```




```
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?

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

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

The model does not seem to cluster these as well as I expected, as they are mostly correct but there are quite a few that are not clustered into the correct groupings as we expected it.

Q14

How well do the hierarchical clustering models you created in previous sections (i.e. before PCA) do in terms of separating the diagnoses?

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

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

It seems to cluster relatively well, but it has its issues and has false positives and negatives on for both diagnoses, so it is not perfect.

Prediction

Q16

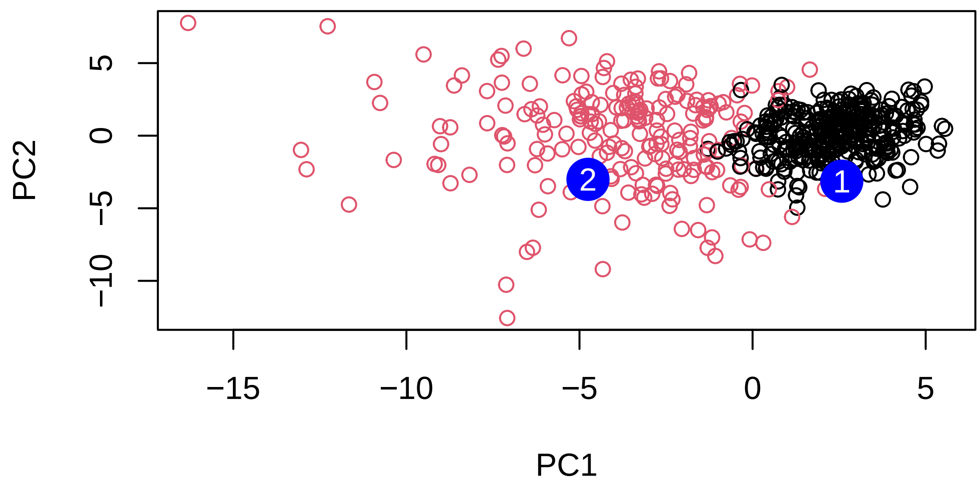
Which of these new patients should we prioritize for follow up based on your results?

```
#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")
```



Patient 2 should be prioritized because their data falls largely within the malignant cluster, so it is more likely that their tumor may be malignant.