Class 8: Mini Project

Elena

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#Exploring Data

Preparing Data

```
#Downloaded file from class website and imported into project folder
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
```

```
#Removing diagnosis column
wisc.data <- wisc.df[,-1]
head(wisc.data)
```

```
         radius_mean texture_mean perimeter_mean area_mean smoothness_mean
```

```
          17.99        10.38         122.80    1001.0         0.11840
          20.57        17.77         132.90    1326.0         0.08474
          19.69        21.25         130.00    1203.0         0.10960
          11.42        20.38          77.58     386.1         0.14250
          20.29        14.34         135.10    1297.0         0.10030
          12.45        15.70          82.57     477.1         0.12780
         compactness_mean concavity_mean concave.points_mean symmetry_mean
           0.27760         0.3001             0.14710        0.2419
           0.07864         0.0869             0.07017        0.1812
           0.15990         0.1974             0.12790        0.2069
           0.28390         0.2414             0.10520        0.2597
           0.13280         0.1980             0.10430        0.1809
           0.17000         0.1578             0.08089        0.2087
         fractal_dimension_mean radius_se texture_se perimeter_se area_se
                        0.07871    1.0950     0.9053        8.589  153.40
                        0.05667    0.5435     0.7339        3.398   74.08
                        0.05999    0.7456     0.7869        4.585   94.03
                        0.09744    0.4956     1.1560        3.445   27.23
                        0.05883    0.7572     0.7813        5.438   94.44
                        0.07613    0.3345     0.8902        2.217   27.19
         smoothness_se compactness_se concavity_se concave.points_se
              0.006399        0.04904      0.05373           0.01587
              0.005225        0.01308      0.01860           0.01340
              0.006150        0.04006      0.03832           0.02058
              0.009110        0.07458      0.05661           0.01867
              0.011490        0.02461      0.05688           0.01885
              0.007510        0.03345      0.03672           0.01137
         symmetry_se fractal_dimension_se radius_worst texture_worst
             0.03003             0.006193        25.38         17.33
             0.01389             0.003532        24.99         23.41
             0.02250             0.004571        23.57         25.53
             0.05963             0.009208        14.91         26.50
             0.01756             0.005115        22.54         16.67
             0.02165             0.005082        15.47         23.75
         perimeter_worst area_worst smoothness_worst compactness_worst
                  184.60     2019.0           0.1622            0.6656
                  158.80     1956.0           0.1238            0.1866
                  152.50     1709.0           0.1444            0.4245
                   98.87      567.7           0.2098            0.8663
                  152.20     1575.0           0.1374            0.2050
                  103.40      741.6           0.1791            0.5249
         concavity_worst concave.points_worst symmetry_worst
                  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
```

```
#Saving diagnosis data for later
diagnosis <- as.factor(wisc.df$diagnosis)
head(diagnosis)
```

```
[1] M M M M M M
Levels: B M
```

Q1. How many observations are in this dataset?

There are 569 observations in the dataset.

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

```
[1] 569
```

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

212 observations have a malignant diagnosis.

```
table(diagnosis)
```

```
diagnosis
  B   M
357 212
```

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

10 features in the data are suffixed with _mean.

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

```
[1] 10
```

PCA

Performing PCA

Let's try PCA on this data to see what major features might be hidden in this high dimensional data that are hard to see any other way.

Do we need to "scale" this data before PCA? We look at the mean and SD of the variables (i.e. columns)

```
#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)
```

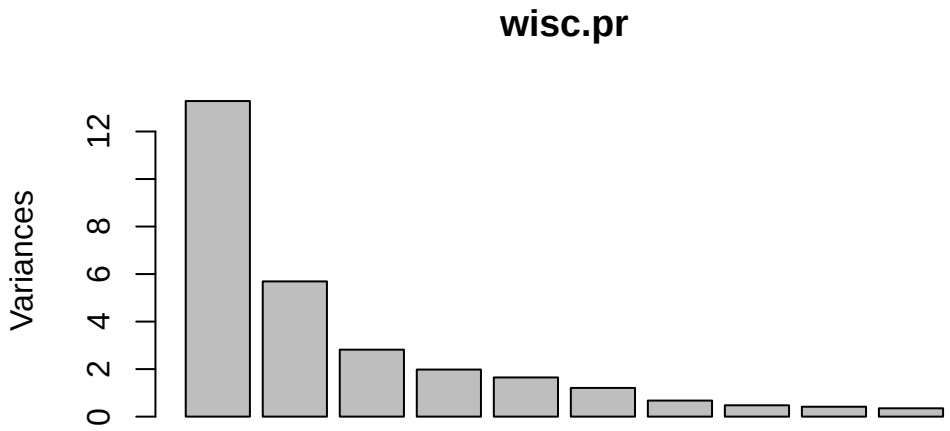
```
           radius_mean            texture_mean          perimeter_mean
          3.524049e+00            4.301036e+00            2.429898e+01
             area_mean         smoothness_mean        compactness_mean
          3.519141e+02            1.406413e-02            5.281276e-02
       concavity_mean     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
```

```
#Perform PCA on wisc.data
#Scale due to different units
wisc.pr <- prcomp(wisc.data,scale=T)
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
```

```
plot(wisc.pr)
```



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

44.27%.

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

3.

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

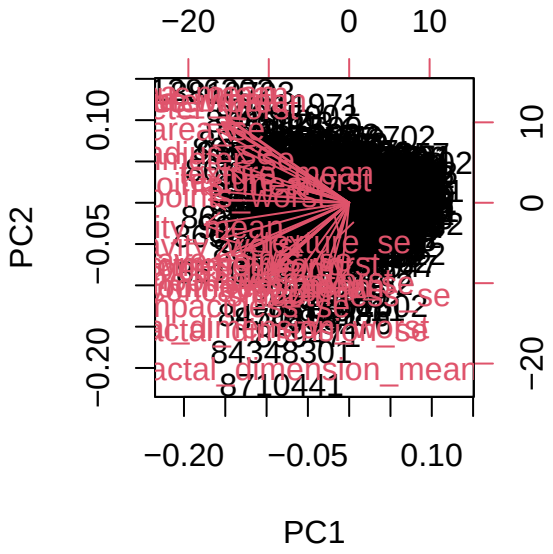
7.

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

One of our main results from methods like PCA is a so-called "score plots," "PC plots," "ordination plots," "PC1 vs PC2," etc.

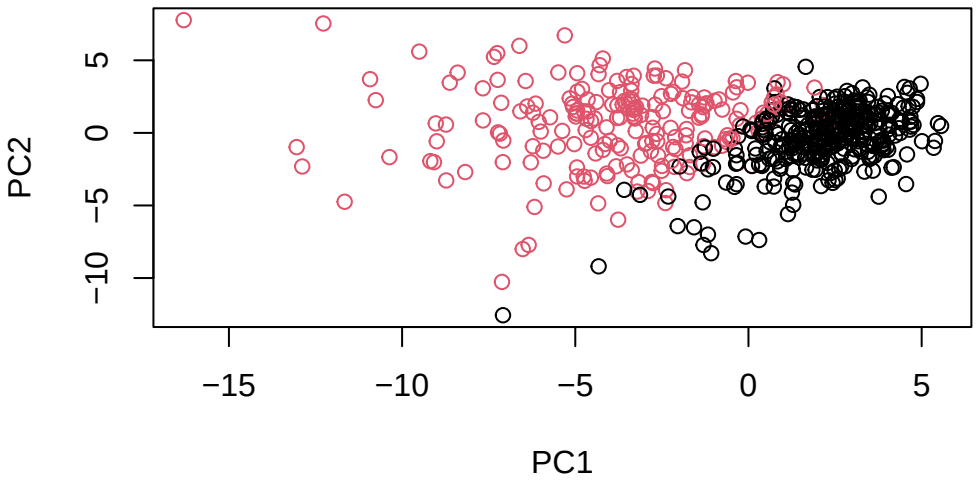
The base R `biplot()` of the PC data is difficult to understand because it has too much information and labels on it, making it difficult to read and interpret.

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



Let's make one of PC1 vs. PC2

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

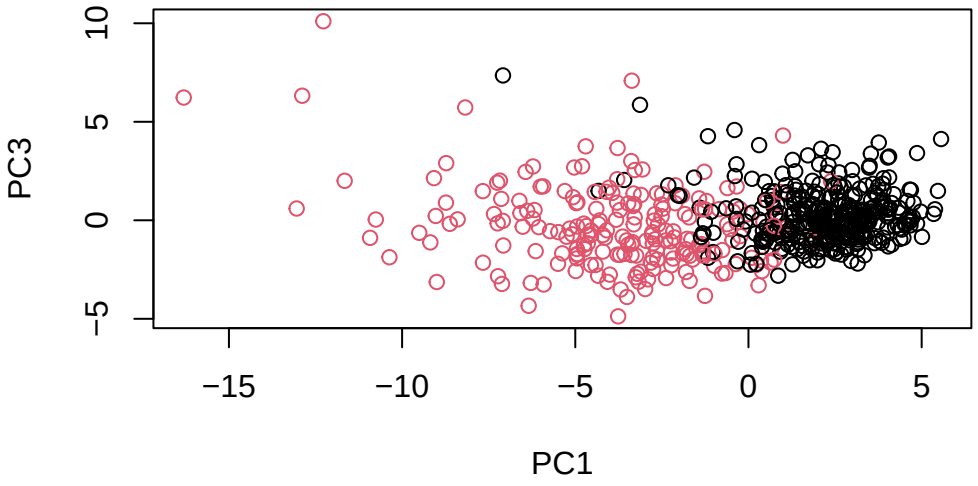


Calculating PC score: SUM(Original Read Counts * Influence); each sample is then plotted.

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

The malignant and benign patients tend to cluster together i.e. share similar characteristics. PC1 vs. PC2 gives a cleaner division between the groups than PC1 vs. PC3, because PC2 captures more variance than PC3.

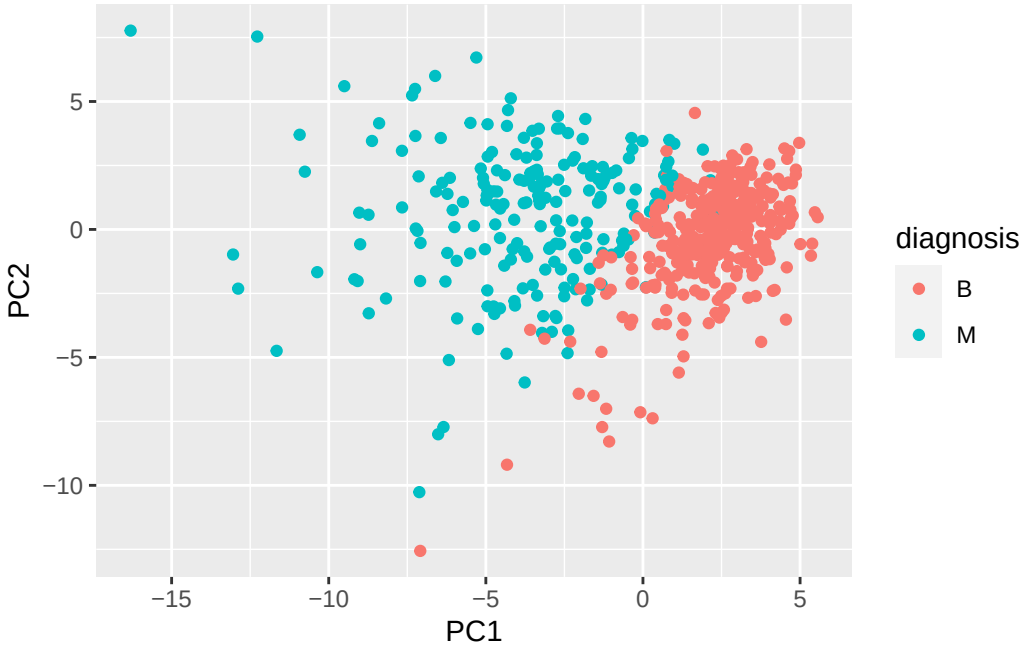
```
plot(wisc.pr$x[,1], wisc.pr$x[,3], col=diagnosis, xlab="PC1", ylab="PC3")
```




```
#Graphing with ggplot
library(ggplot2)

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

# Make a scatter plot colored by diagnosis
ggplot(df) +
  aes(PC1, PC2, col=diagnosis) +
  geom_point() +
  labs(x="PC1", y="PC2")
```



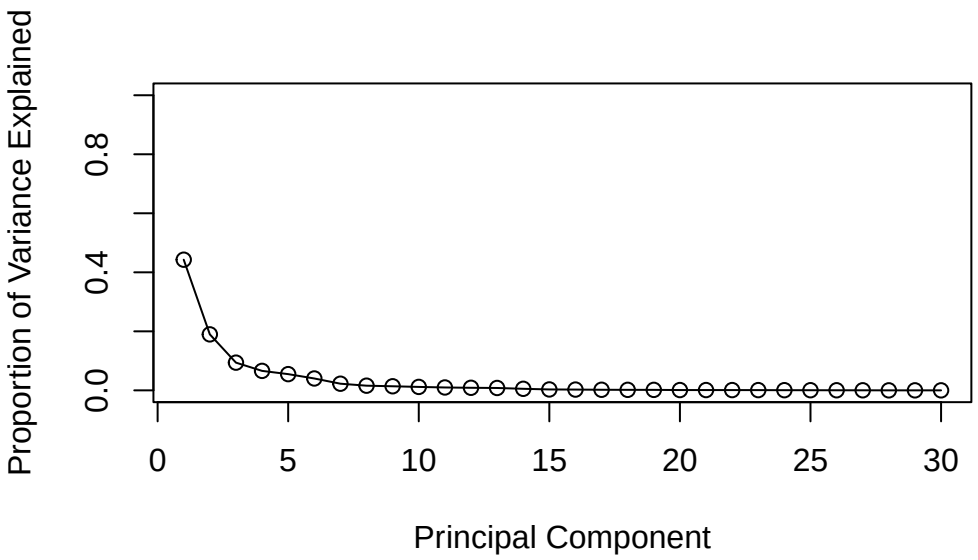
Variance

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

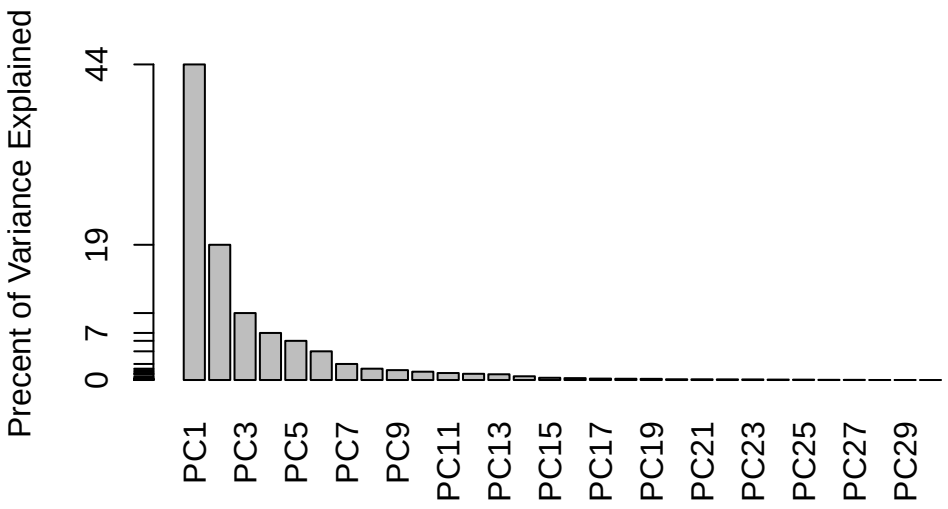
```
[1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

```
# 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 )
```



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.

-0.26085376.

```
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
```

Hierarchical Clustering

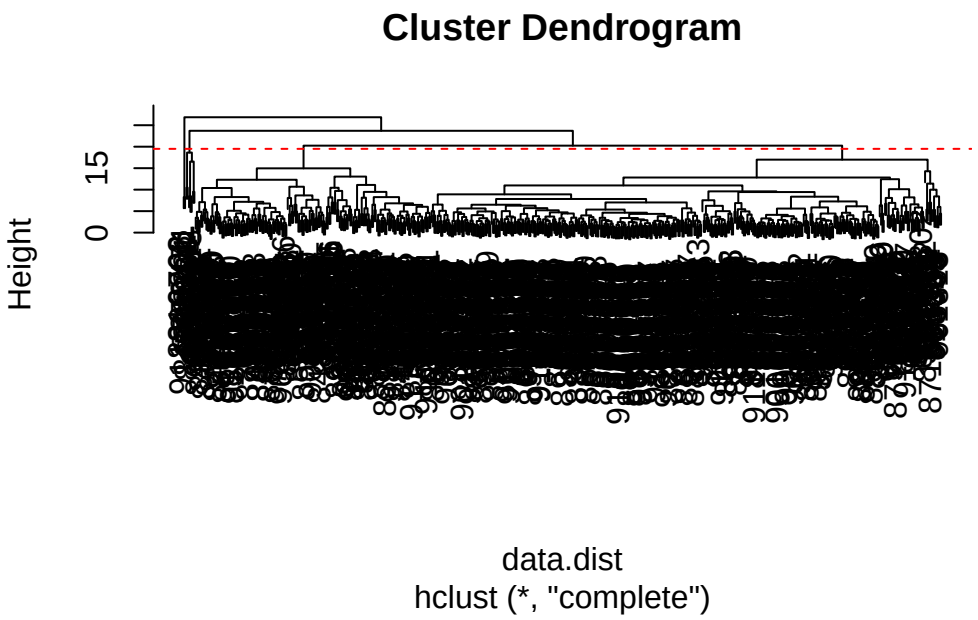
```
#Scale the wisc.data data using the "scale()" function
data.scaled <- scale(wisc.data)
```

```
#Calculate the (Euclidean) distances between all pairs of observations in the new scaled d
data.dist <- dist(data.scaled)
```

Q10. Using the plot() and abline() functions, what is the height at which the clustering model has 4 clusters?

Around 19-20.

```
#Create a hierarchical clustering model using complete linkage
wisc.hclust <- hclust(data.dist, method="complete")
plot(wisc.hclust)
abline(h=19.5, col="red", lty=2)
```

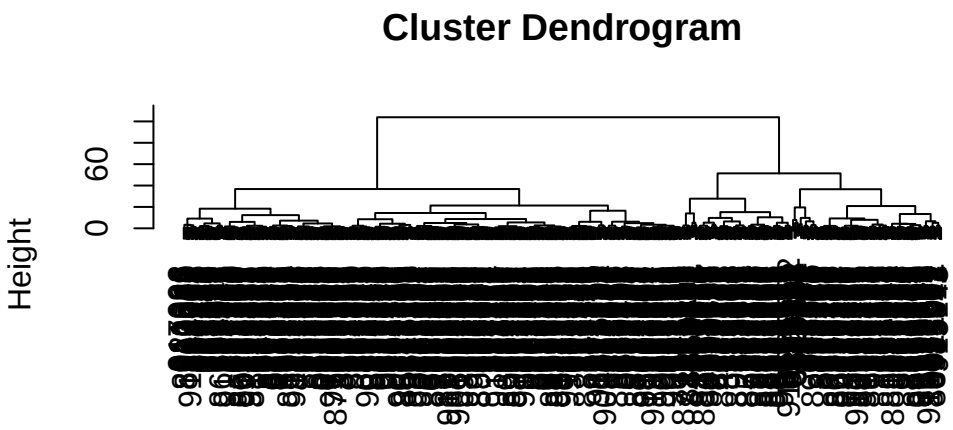


Combine methods

PCA is often used as a first step in further analysis. Here we will combine PCA and clustering.

We have our PCA results in `wisc.pr$x`.

```
wisc.pr.hclust <- hclust( dist(wisc.pr$x[,1:2]), method="ward.D2")
plot(wisc.pr.hclust)
```




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

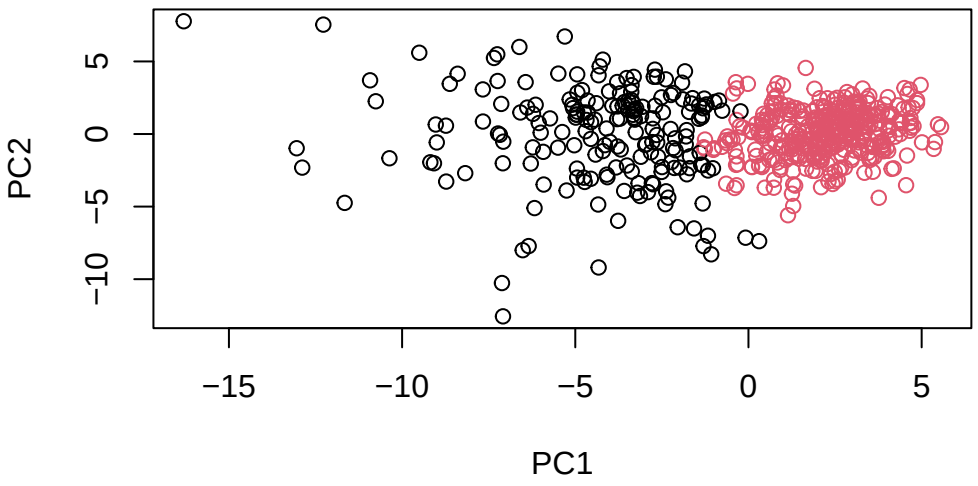
```
grps
  1   2
195 374
```

How do these "grps" i.e. clusters correspond to the expert diagnosis?

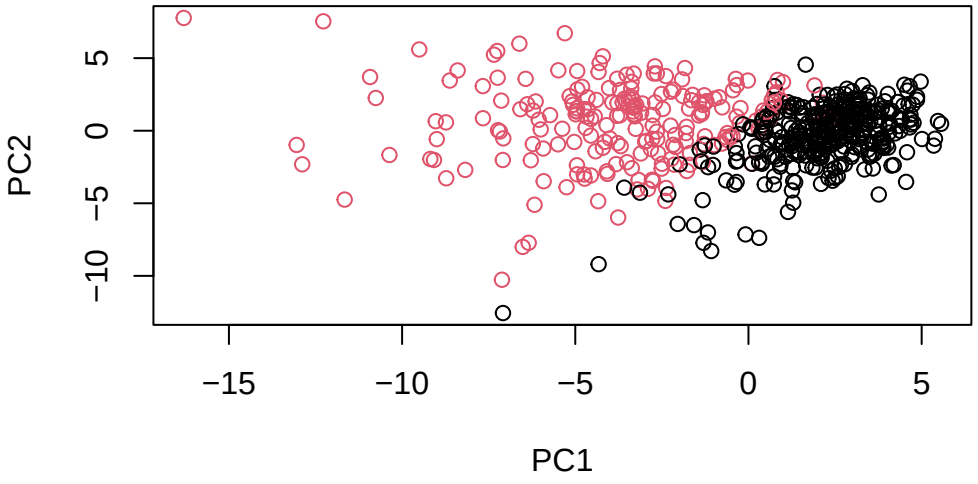
```
table(diagnosis, grps)
```

```
         grps
diagnosis   1   2
        B  18 339
        M 177  35
```

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




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



```
#install.packages("rgl")
#library(rgl)
#plot3d(wisc.pr$x[,1:3], xlab="PC 1", ylab="PC 2", zlab="PC 3", cex=1.5, size=1, type="s",
#rglwidget(width = 400, height = 400)
```

Q11. OPTIONAL: Can you find a better cluster vs diagnoses match by cutting into a different number of clusters between 2 and 10? How do you judge the quality of your result in each case?

If we cut into increasing number of clusters, we see that some clusters will have better separation of diagnoses (i.e. 0 benign and X number malignant and vice-versa). However, this will also create clusters that have very few samples or have less separation of diagnoses, which can decrease the quality of our results.

```
table(diagnosis, cutree(wisc.pr.hclust, k=2))
```

```
diagnosis   1   2
        B  18 339
        M 177  35
```

```
table(diagnosis, cutree(wisc.pr.hclust, k=3))
```

```
diagnosis   1   2   3
        B   0  18 339
        M 112  65  35
```

```
table(diagnosis, cutree(wisc.pr.hclust, k=4))
```

```
diagnosis   1   2   3   4
        B   0  18 232 107
        M 112  65  18  17
```

```
table(diagnosis, cutree(wisc.pr.hclust, k=5))
```

```
diagnosis   1   2   3   4   5
        B   0   0  18 232 107
        M  20  92  65  18  17
```

```
  table(diagnosis, cutree(wisc.pr.hclust, k=6))
```

```
diagnosis   1   2   3   4   5   6
        B   0   0   9   9 232 107
        M  20  92   3  62  18  17
```

```
  table(diagnosis, cutree(wisc.pr.hclust, k=7))
```

```
diagnosis   1   2   3   4   5   6   7
        B   0   0   9   9  70 107 162
        M  20  92   3  62  15  17   3
```

```
  table(diagnosis, cutree(wisc.pr.hclust, k=8))
```

```
diagnosis   1   2   3   4   5   6   7   8
        B   0   0   0   9   9  70 107 162
        M  20  53  39   3  62  15  17   3
```

```
  table(diagnosis, cutree(wisc.pr.hclust, k=9))
```

```
diagnosis   1   2   3   4   5   6   7   8   9
        B   0   0   0   9   9  70 107 162   0
        M  15  53  39   3  62  15  17   3   5
```

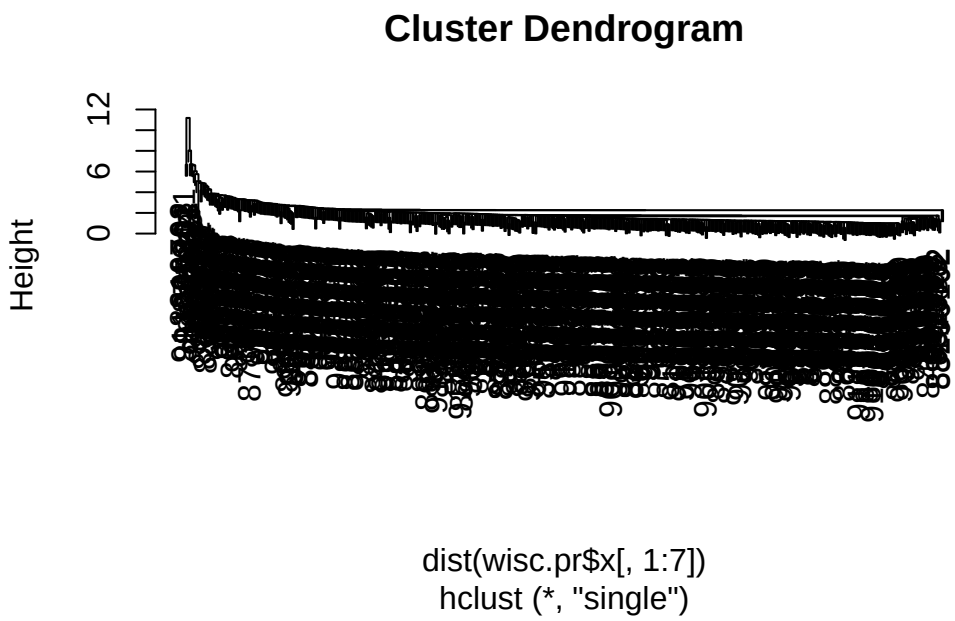
```
  table(diagnosis, cutree(wisc.pr.hclust, k=10))
```

```
diagnosis   1   2   3   4   5   6   7   8   9  10
        B   0   0   0   9   9  70  77 162  30   0
        M  15  53  39   3  62  15  17   3   0   5
```

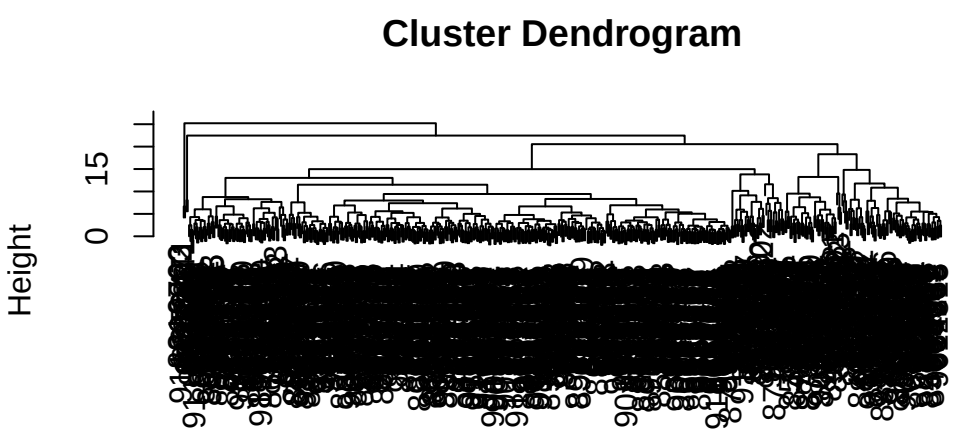
Q12. Which method gives your favorite results for the same data.dist dataset? Explain your reasoning.

The "ward.D2" method. With the other methods, the clusters are very unevenly distributed e.g., one patient sample seems to be clustered by itself, away from the other samples. The "ward.D2" method minimizes variance within clusters.

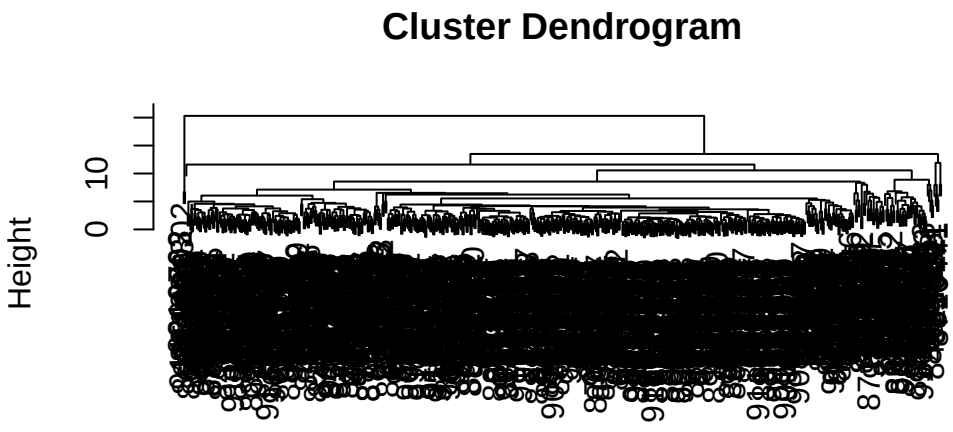
```
wisc.pr.hclust <- hclust( dist(wisc.pr$x[,1:7]), method="single")
plot(wisc.pr.hclust)
```



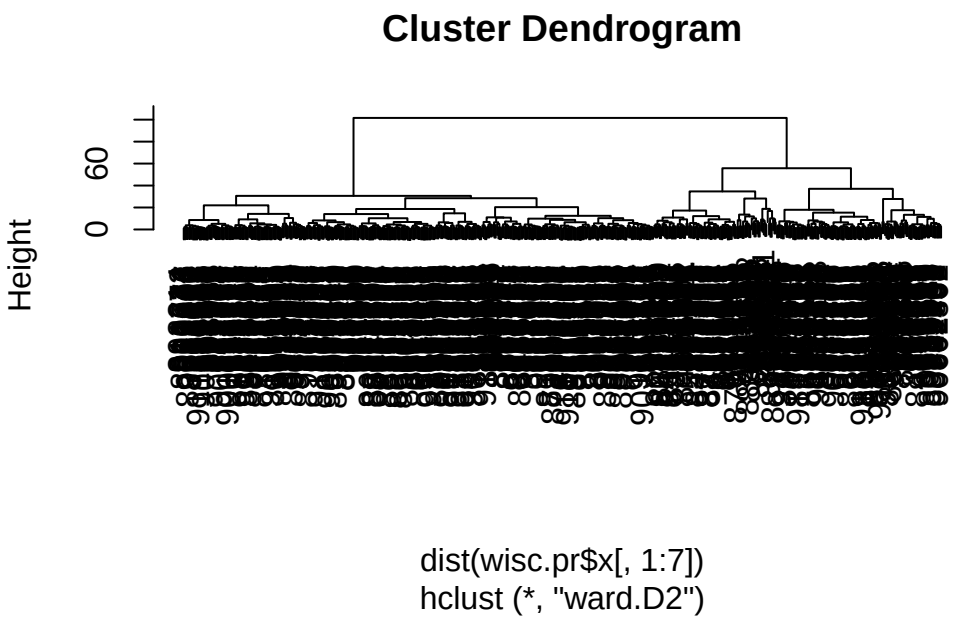

```
wisc.pr.hclust <- hclust( dist(wisc.pr$x[,1:7]), method="complete")
plot(wisc.pr.hclust)
```




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



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



Q13. How well does the newly created model with four clusters separate out the two diagnoses?

With k=2, the clusters separated the diagnoses fairly well, because most patients within one cluster fell under either the benign or malignant diagnosis. However, with k=4, only 1 and 3 had good separation; 2 and 4 lacked samples and did not have good separation.

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

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

```
#Selecting number 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
```

Q14. How well do the hierarchical clustering models you created in previous sections (i.e. before PCA) do in terms of separating the diagnoses?

Separation of diagnoses seem to be similar, where one consists of mainly malignant samples and the other consists of mainly benign samples.

```
#Clustering using k-means
km <- kmeans (wisc.data, centers=2)
table(km$cluster, diagnosis)
```

```
  diagnosis
     B   M
  1   1 130
  2 356  82
```

```
#Hierarchical clustering method
wisc.pr.hclust <- hclust(dist(wisc.pr$x[,1:2]), method="ward.D2")
wisc.pr.hclust.clusters <- cutree(wisc.pr.hclust, k=2)
table(wisc.pr.hclust.clusters, diagnosis)
```

```
                     diagnosis
wisc.pr.hclust.clusters   B   M
                      1  18 177
                      2 339  35
```

Q15. OPTIONAL: Which of your analysis procedures resulted in a clustering model with the best specificity? How about sensitivity?

Best sensitivity: hierarchical clustering.

Best specificity: k-means.

```
#Sensitivity = # Samples in predominant malignant cluster / total known malignant samples
#k-means
131/(130+82)
```

```
[1] 0.6179245
```

```
#Hierarchical for first 2 PCs
(18+177)/(177+35)
```

```
[1] 0.9198113
```

```
#Specificity = # benign samples in predominantly benign cluster / total benign
#k-means
356/(1+356)
```

```
[1] 0.9971989
```

```
#Hierarchical for first 2 PCs
339/(18+339)
```

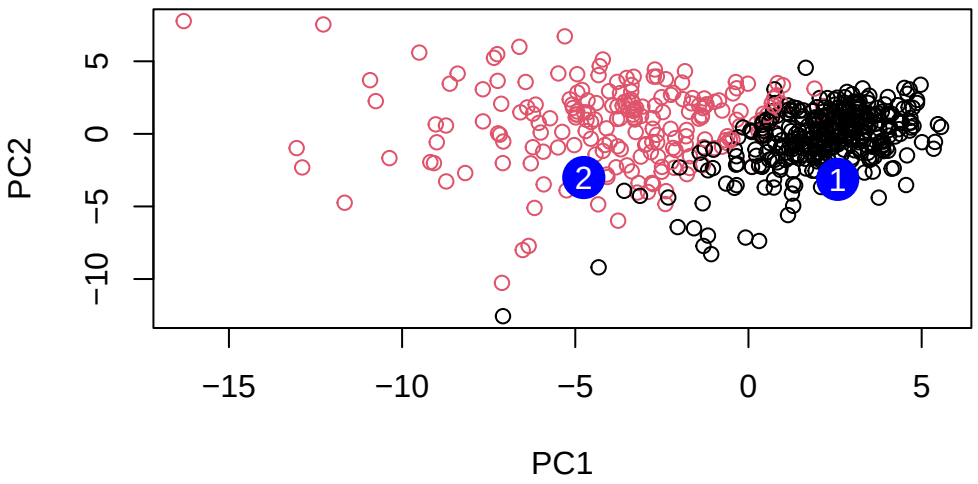
```
[1] 0.9495798
```

Prediction

```
new <- read.csv("https://tinyurl.com/new-samples-CSV")
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
```

```r
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")
```



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

Patients that had different diagnoses between the datasets (e.g., benign to malignant, or malignant to benign).