Mini Project

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

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

head(wisc.df)
```

```
         diagnosis radius_mean texture_mean perimeter_mean area_mean
842302           M       17.99        10.38         122.80    1001.0
842517           M       20.57        17.77         132.90    1326.0
84300903         M       19.69        21.25         130.00    1203.0
84348301         M       11.42        20.38          77.58     386.1
84358402         M       20.29        14.34         135.10    1297.0
843786           M       12.45        15.70          82.57     477.1
         smoothness_mean compactness_mean concavity_mean concave.points_mean
842302           0.11840          0.27760         0.3001             0.14710
842517           0.08474          0.07864         0.0869             0.07017
84300903         0.10960          0.15990         0.1974             0.12790
84348301         0.14250          0.28390         0.2414             0.10520
84358402         0.10030          0.13280         0.1980             0.10430
843786           0.12780          0.17000         0.1578             0.08089
         symmetry_mean fractal_dimension_mean radius_se texture_se perimeter_se
842302          0.2419                0.07871    1.0950     0.9053        8.589
842517          0.1812                0.05667    0.5435     0.7339        3.398
84300903        0.2069                0.05999    0.7456     0.7869        4.585
84348301        0.2597                0.09744    0.4956     1.1560        3.445
84358402        0.1809                0.05883    0.7572     0.7813        5.438
843786          0.2087                0.07613    0.3345     0.8902        2.217
         area_se smoothness_se compactness_se concavity_se concave.points_se
842302    153.40      0.006399        0.04904      0.05373           0.01587
842517     74.08      0.005225        0.01308      0.01860           0.01340
```

```
84300903   94.03      0.006150        0.04006      0.03832           0.02058
84348301   27.23      0.009110        0.07458      0.05661           0.01867
84358402   94.44      0.011490        0.02461      0.05688           0.01885
843786     27.19      0.007510        0.03345      0.03672           0.01137
         symmetry_se fractal_dimension_se radius_worst texture_worst
842302       0.03003             0.006193        25.38         17.33
842517       0.01389             0.003532        24.99         23.41
84300903     0.02250             0.004571        23.57         25.53
84348301     0.05963             0.009208        14.91         26.50
84358402     0.01756             0.005115        22.54         16.67
843786       0.02165             0.005082        15.47         23.75
         perimeter_worst area_worst smoothness_worst compactness_worst
842302            184.60     2019.0           0.1622            0.6656
842517            158.80     1956.0           0.1238            0.1866
84300903          152.50     1709.0           0.1444            0.4245
84348301           98.87      567.7           0.2098            0.8663
84358402          152.20     1575.0           0.1374            0.2050
843786            103.40      741.6           0.1791            0.5249
         concavity_worst concave.points_worst symmetry_worst
842302            0.7119               0.2654         0.4601
842517            0.2416               0.1860         0.2750
84300903          0.4504               0.2430         0.3613
84348301          0.6869               0.2575         0.6638
84358402          0.4000               0.1625         0.2364
843786            0.5355               0.1741         0.3985
         fractal_dimension_worst
842302                   0.11890
842517                   0.08902
84300903                 0.08758
84348301                 0.17300
84358402                 0.07678
843786                   0.12440
```

To remove the first column and avoid including diagnosis in our analysis:

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

And to save the first diagnosis column for later:

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

Q1: How many observations are in this dataset?

```
n.observations <- nrow(wisc.data)
n.observations
```

```
[1] 569
```

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

```
n.malignant <- table(wisc.df$diagnosis)["M"]
n.malignant
```

```
  M
212
```

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

```
n._mean <- length(grep("_mean", colnames(wisc.data)))
n._mean
```

```
[1] 10
```

PCA

```
# Check column means and standard deviations for scaling
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 with scaling and look at summary

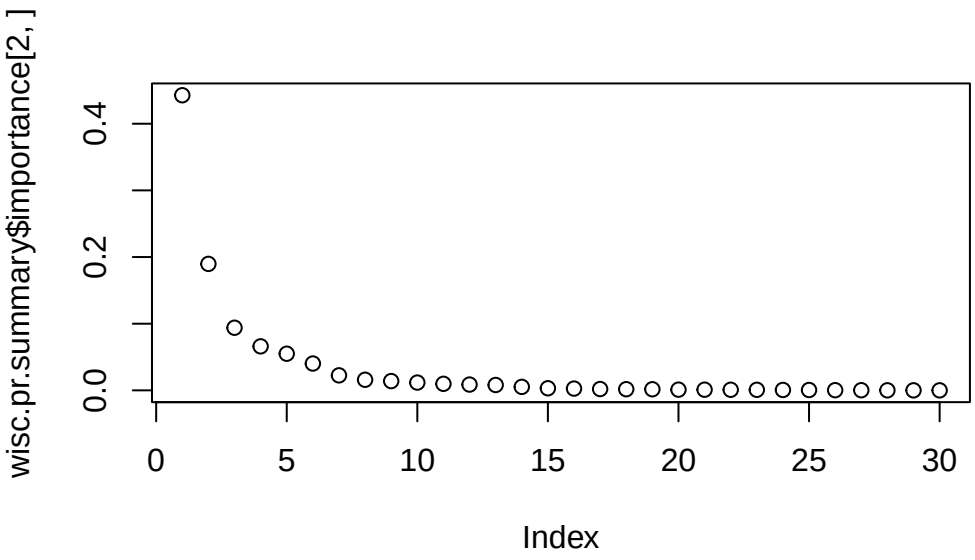
```
# Perform PCA on wisc.data by completing the following code
wisc.pr <- prcomp(wisc.data, scale = T)
summary(wisc.pr)
```

```
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
```

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

0.4427

```
wisc.pr.summary <- summary(wisc.pr)
plot(wisc.pr.summary$importance[2,])
```



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

```
sum(wisc.pr.summary$importance[3,] < .70) + 1
```

```
[1] 3
```

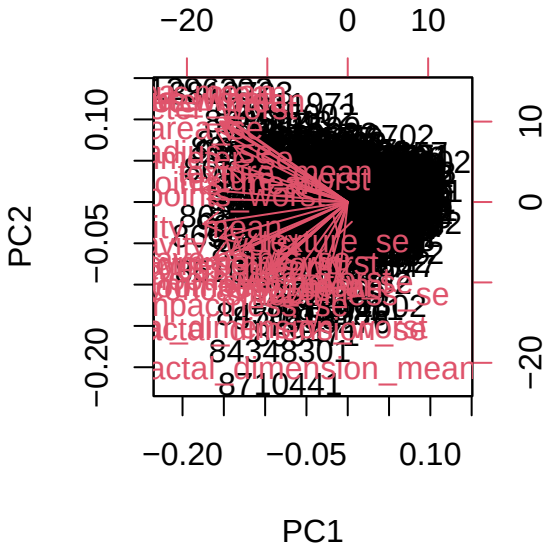
Q6. How many principal components (PCs) are required to describe at least 90% of the original variance in the data?

```
sum(wisc.pr.summary$importance[3,] < .90) + 1
```

```
[1] 7
```

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

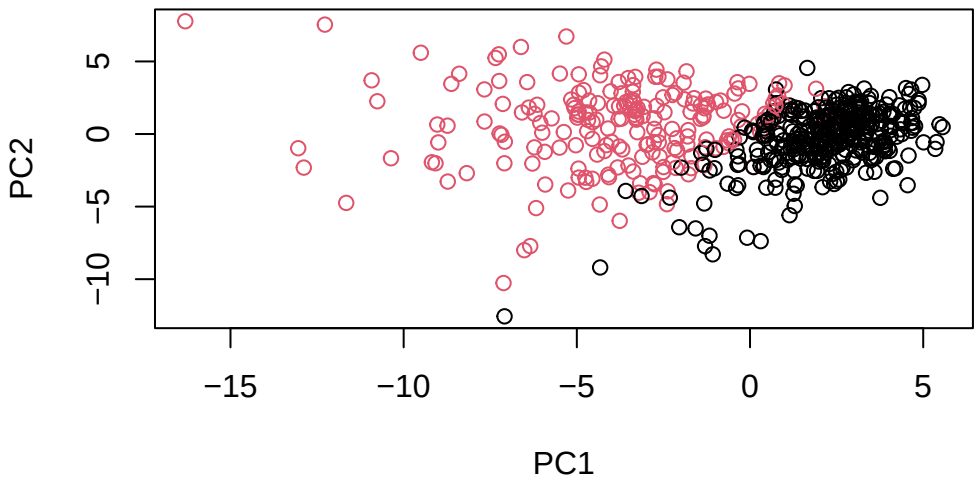
```
biplot(wisc.pr)
```



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

This plot is difficult to understand because the data points are not clearly differentiated and you can't read any of the labels. It's just a mess.

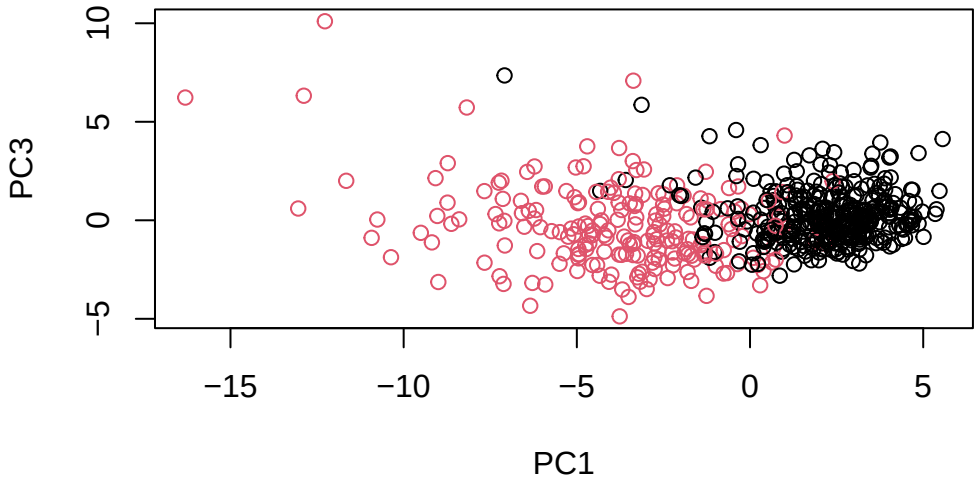
```
# Scatter plot observations by components 1 and 2
plot(wisc.pr$x, col = diagnosis,
     xlab = "PC1", ylab = "PC2")
```



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

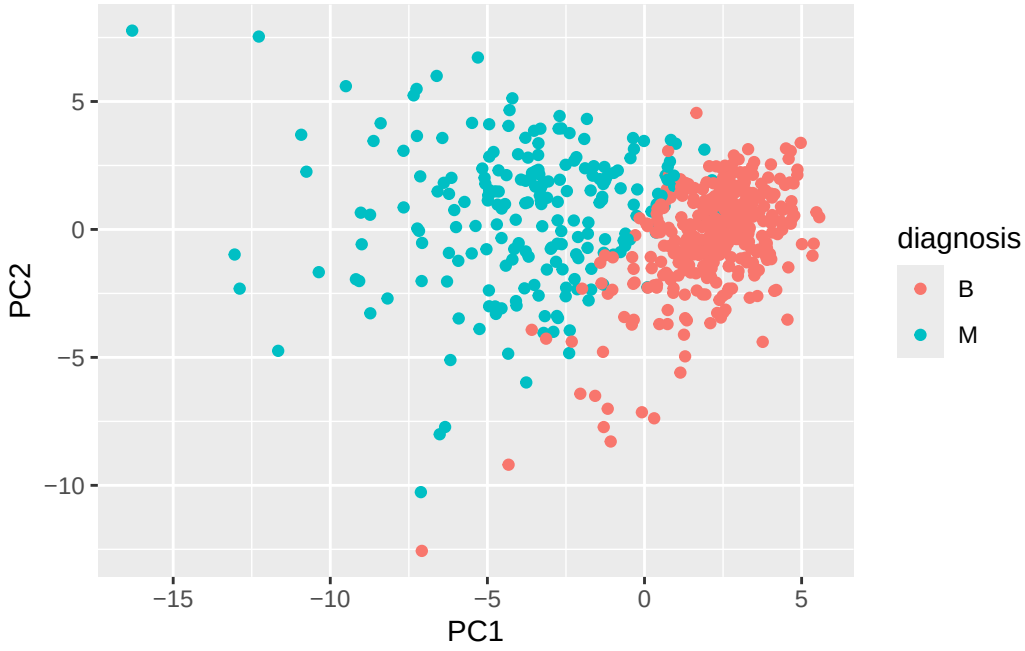
The plots are easy to interpret and differentiate between each sample. PC1 generally differentiates the malignant and benign samples, and PC2 delineates the diagnosis groups better than PC3. You can tell this because there is less overlap between the distribution of the red dots and the black dots in the PC1 vs PC2 plot compared to the PC1 vs PC3.

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



Using ggplot to make a better figure

```
# 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()
```



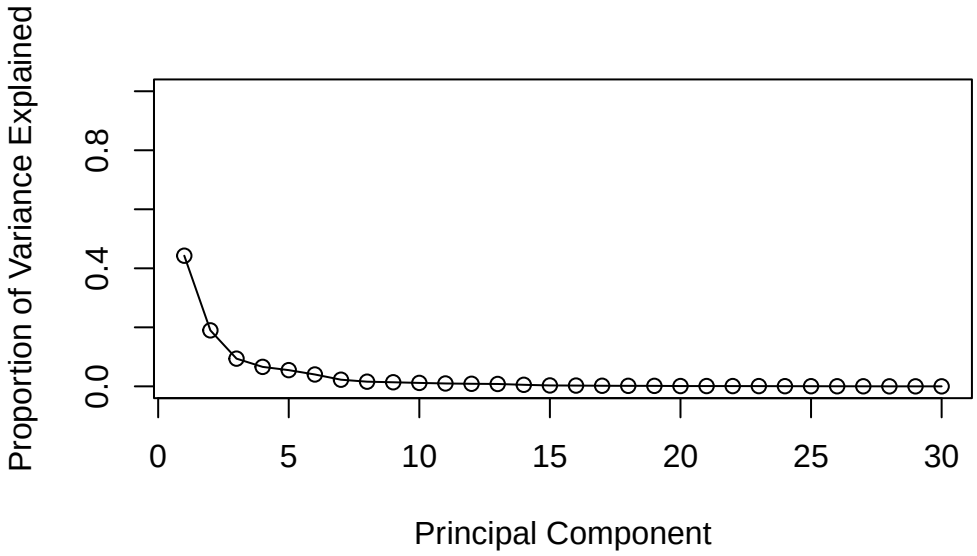
Looking at the variance

```
# 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
```

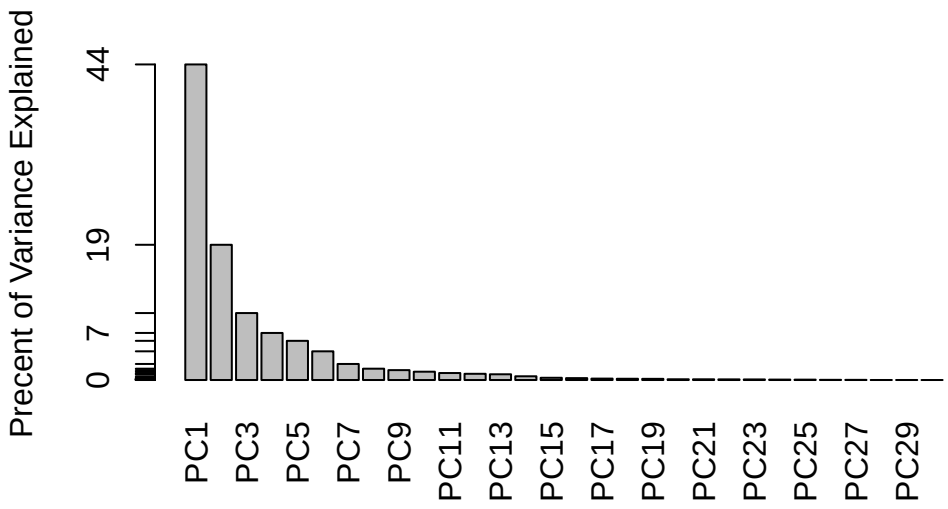
Proportion of Variance by PC

```
# 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")
```



Another alternative

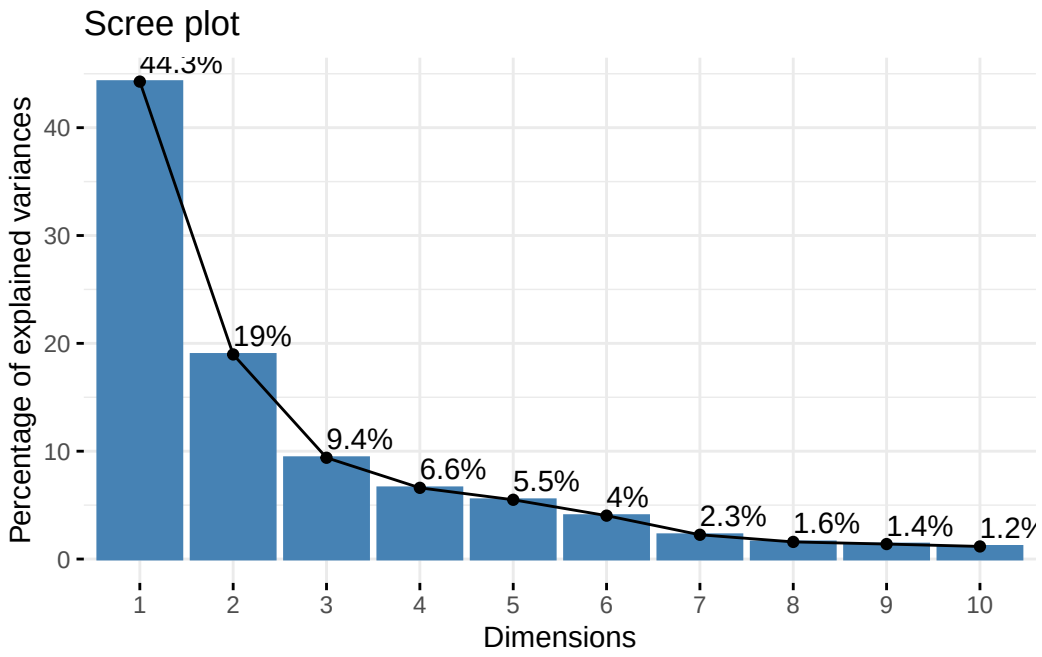
```
# Alternative scree plot of the same data, note data driven y-axis
barplot(pve, ylab = "Precent of Variance Explained",
     names.arg=paste0("PC",1:length(pve)), las=2, axes = FALSE)
axis(2, at=pve, labels=round(pve,2)*100 )
```




```
## 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 (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.

```
wisc.pr$rotation["concave.points_mean", 1]
```

```
[1] -0.2608538
```

3. Hierarchical clustering

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

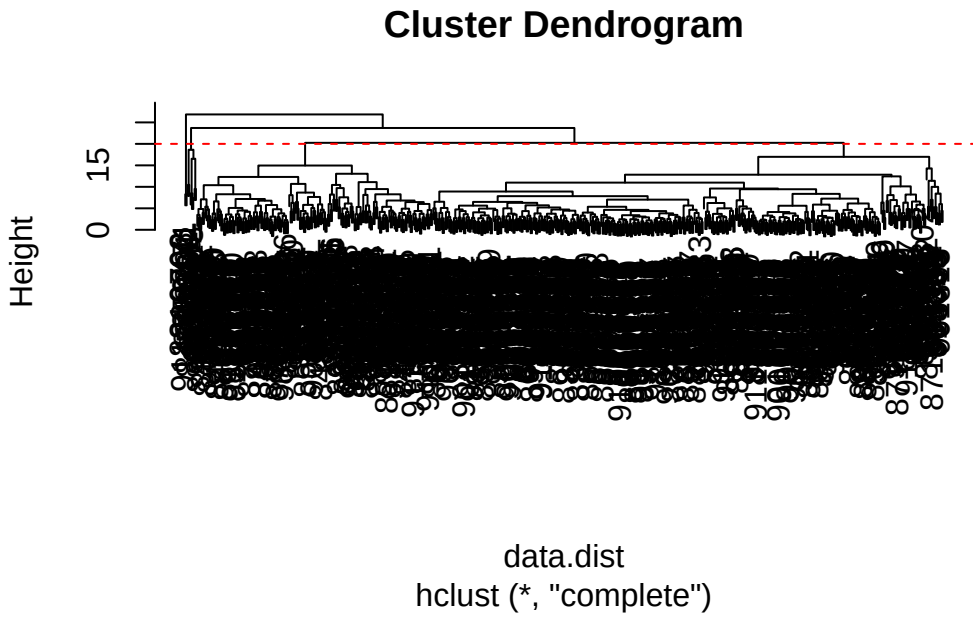
```
# Scale the wisc.data data using the "scale()" function
data.scaled <- scale(wisc.data)

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

#Create a hierarchical clustering model using complete linkage. Manually specify the method a
wisc.hclust <- hclust(data.dist, method = "complete")
```

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

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

Approximately 20. 20.24330 is closer.

```
plot(wisc.hclust)
abline(h=20, col="red", lty=2)
```



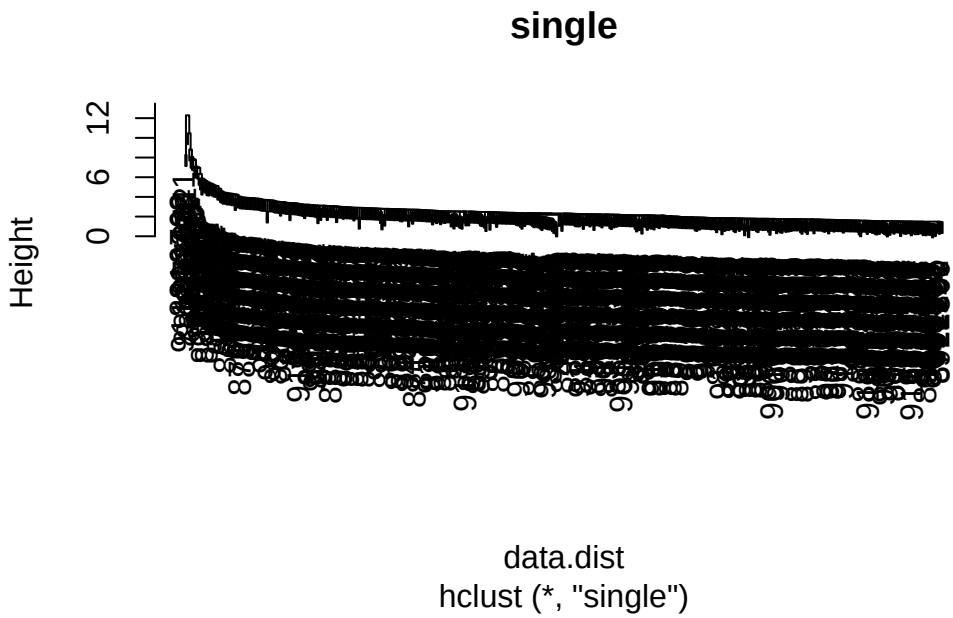
Selecting number of clusters.

```
#using cutree() to make 4 clusters
wisc.hclust.clusters <- cutree(wisc.hclust, k=4)

#using the table() function to compare the cluster membership to the actual diagnoses.
table(wisc.hclust.clusters, diagnosis)
```

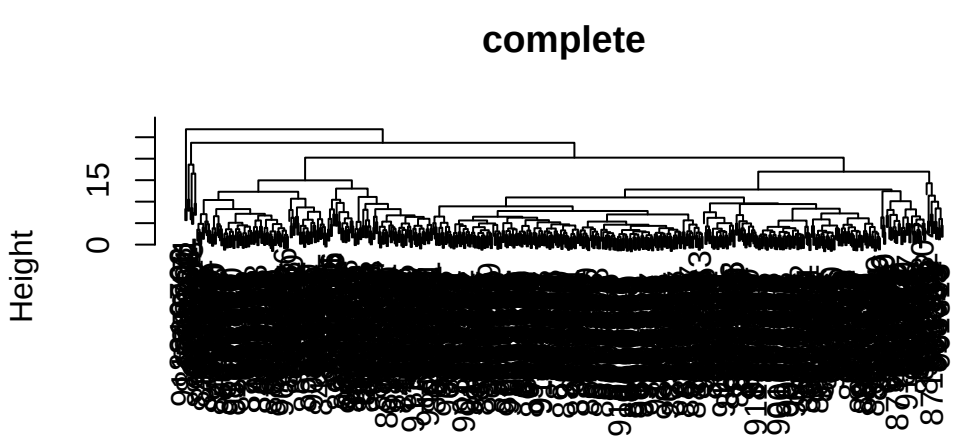
```
                    diagnosis
wisc.hclust.clusters   B   M
                   1  12 165
                   2   2   5
                   3 343  40
                   4   0   2
```

As we discussed in our last class videos 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".

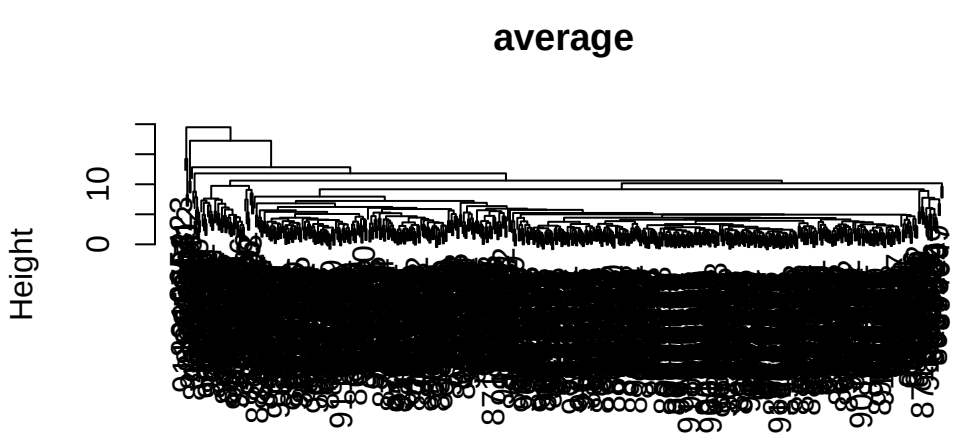
```
methods <- c("single", "complete", "average", "ward.D2")


for (method in methods) {
  hclust_result <- hclust(data.dist, method = method)
  clusters <- cutree(hclust_result, k = 2)
  plot(hclust_result, main = method)

  cat("\nClustering Method:", method, "\n")
  print(table(clusters, diagnosis))
}
```



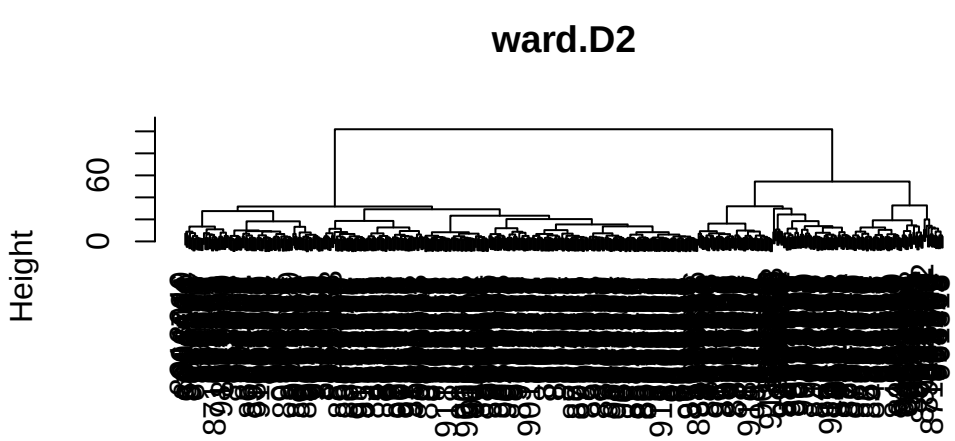

```
Clustering Method: single
        diagnosis
clusters   B   M
       1 357 210
       2   0   2
```




```
Clustering Method: complete
        diagnosis
clusters   B   M
       1 357 210
       2   0   2
```




```
Clustering Method: average
         diagnosis
clusters   B   M
       1 357 209
       2   0   3
```




```
Clustering Method: ward.D2
        diagnosis
clusters   B   M
       1  20 164
       2 337  48
```

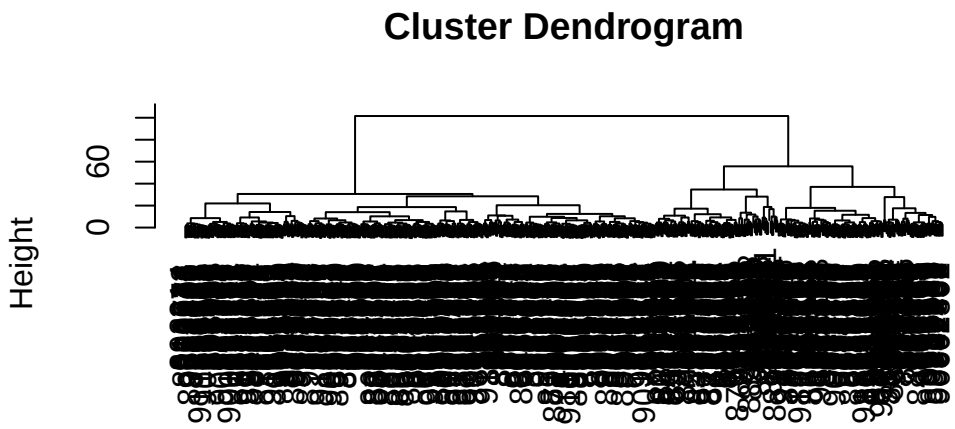
Q12. Which method gives your favorite results for the same data.dist dataset? Explain your reasoning.

The ward.D2 method gives my favorite result because it produces the best delineation between the groups while the other methods are less effective. The complete method provides groups, although they are not as differentiated. Having these groups that are well defined is important for modeling and predicting benign vs malignant tumors, so the ward.D2 method is my favorite to use for this case.

4. Combining methods

Using the minimum number of principal components required to describe at least 90% of the variability in the data, create a hierarchical clustering model with the linkage method="ward.D2". We use Ward's criterion here because it is based on multidimensional variance like principal components analysis. Assign the results to wisc.pr.hclust.

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



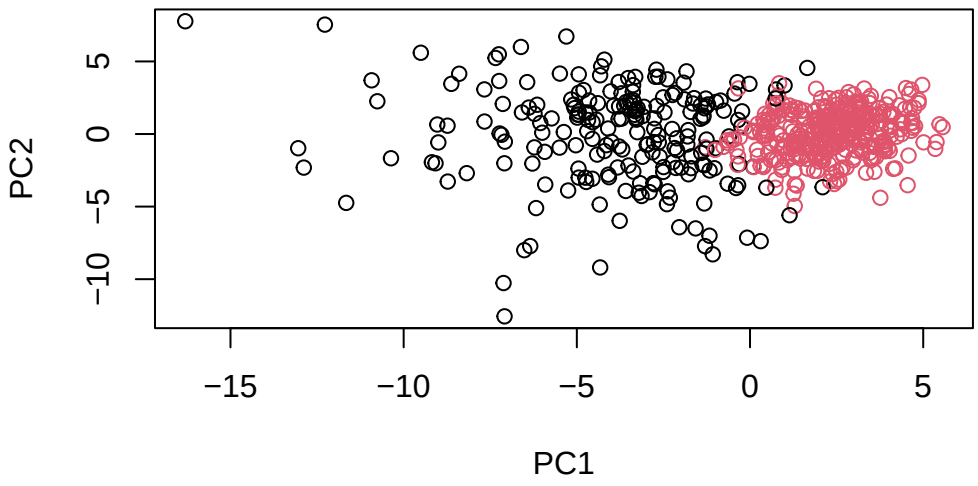

```
grps <- cutree(wisc.pr.hclust, k=2)
table(grps)
```

```
grps
  1   2
216 353
```

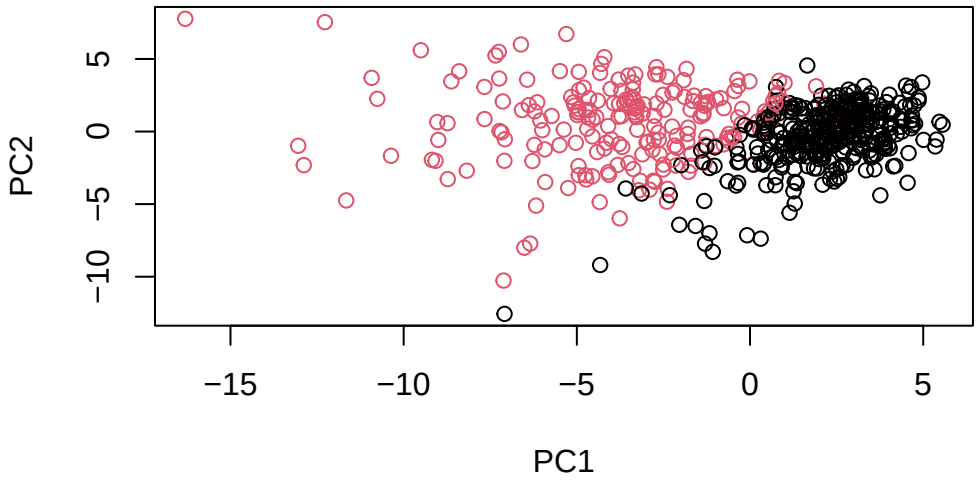
```
table(grps, diagnosis)
```

```
    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)
```



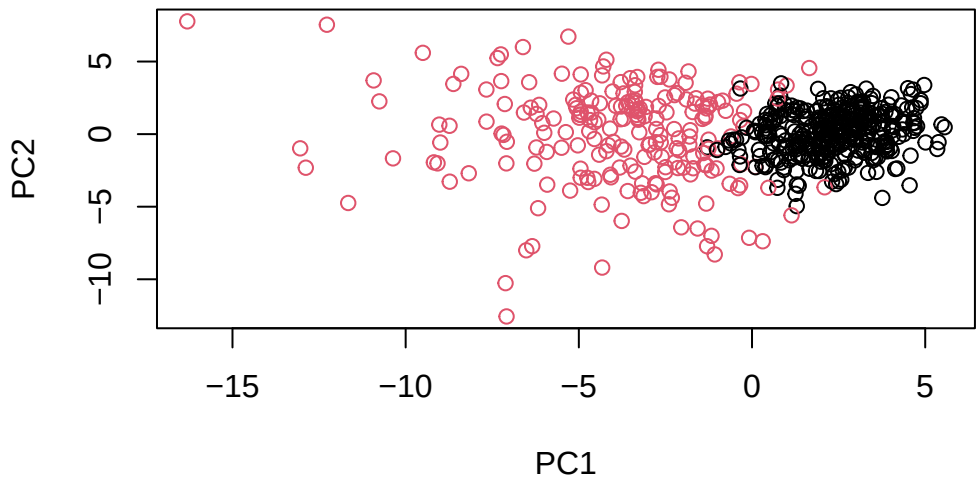
```
g <- as.factor(grps)
levels(g)
```

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

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

```
#FalsePositives
28/188 *100
```

```
[1] 14.89362
```

```
#FalseNegatives
24/329 *100
```

```
[1] 7.294833
```

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

The model separates most of the diagnoses, but not all are correctly assigned. The "false positive" rate of a B in the M cluster is 14% and the "false negative" rate of an M in the B cluster is 7%. Both seem very high and not ideal.

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
```

```
#FalsePositives
12/165 *100
```

```
[1] 7.272727
```

```
#FalseNegatives
40/343 *100
```

```
[1] 11.66181
```

The clustering in the previoius sections had a lower rate of benign samples in the predominantly malignant sample cluster but a higher rate of malignant samples in the predominantly benign sample cluster. Although overall the clustering may be better, the rate of false negatives (which is arguably a worse outcome) is much higher.

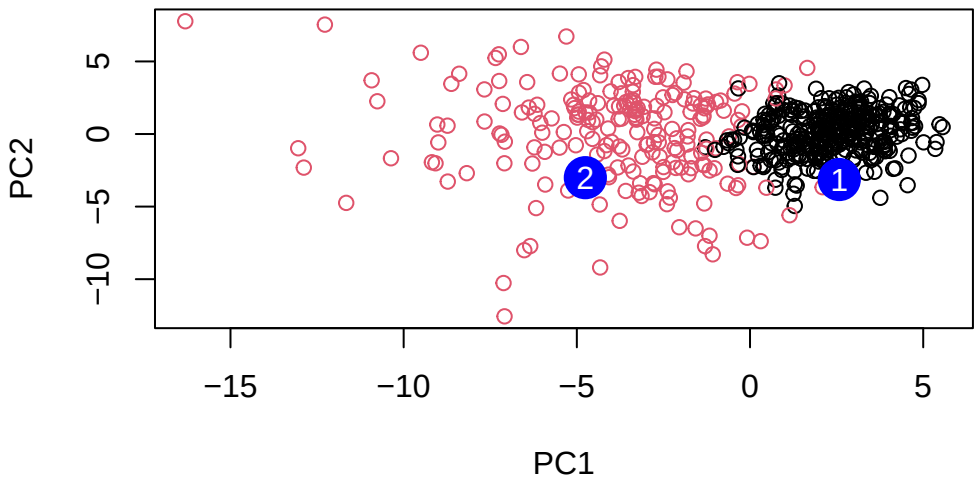
6. Prediction

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?

Sample 2 should be prioritized.