Unsupervised Learning Mini-Project

```
# 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  X
842302                   0.11890 NA
842517                   0.08902 NA
84300903                 0.08758 NA
84348301                 0.17300 NA
84358402                 0.07678 NA
843786                   0.12440 NA
```

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

```
         radius_mean texture_mean perimeter_mean area_mean smoothness_mean
842302         17.99        10.38         122.80    1001.0         0.11840
842517         20.57        17.77         132.90    1326.0         0.08474
84300903       19.69        21.25         130.00    1203.0         0.10960
```

```
84348301       11.42        20.38          77.58     386.1          0.14250
84358402       20.29        14.34         135.10    1297.0          0.10030
843786         12.45        15.70          82.57     477.1          0.12780
         compactness_mean concavity_mean concave.points_mean symmetry_mean
842302            0.27760         0.3001             0.14710        0.2419
842517            0.07864         0.0869             0.07017        0.1812
84300903          0.15990         0.1974             0.12790        0.2069
84348301          0.28390         0.2414             0.10520        0.2597
84358402          0.13280         0.1980             0.10430        0.1809
843786            0.17000         0.1578             0.08089        0.2087
         fractal_dimension_mean radius_se texture_se perimeter_se area_se
842302                  0.07871    1.0950     0.9053        8.589  153.40
842517                  0.05667    0.5435     0.7339        3.398   74.08
84300903                0.05999    0.7456     0.7869        4.585   94.03
84348301                0.09744    0.4956     1.1560        3.445   27.23
84358402                0.05883    0.7572     0.7813        5.438   94.44
843786                  0.07613    0.3345     0.8902        2.217   27.19
         smoothness_se compactness_se concavity_se concave.points_se
842302        0.006399        0.04904      0.05373           0.01587
842517        0.005225        0.01308      0.01860           0.01340
84300903      0.006150        0.04006      0.03832           0.02058
84348301      0.009110        0.07458      0.05661           0.01867
84358402      0.011490        0.02461      0.05688           0.01885
843786        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  X
842302                   0.11890 NA
842517                   0.08902 NA
84300903                 0.08758 NA
84348301                 0.17300 NA
84358402                 0.07678 NA
843786                   0.12440 NA
```

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

```
[1] "M" "M" "M" "M" "M" "M"
```

```
is.vector(diagnosis) == TRUE
```

```
[1] TRUE
```

Q1. How many observations are in this dataset?

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

```
[1] 569
```

569 observations.

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

```
sum(diagnosis == "B")
```

```
[1] 357
```

357 observations.

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

```
features <- as.vector(colnames(wisc.data))
sum(grepl("_mean", features))
```

```
[1] 10
```

10 features.

```
# 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
                    X
                   NA
```

```
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
                     X
                    NA
```

```r
# Perform PCA on wisc.data by completing the following code
wisc.pr <- prcomp(wisc.data[,colnames(wisc.data) != "X"], scale=TRUE)
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

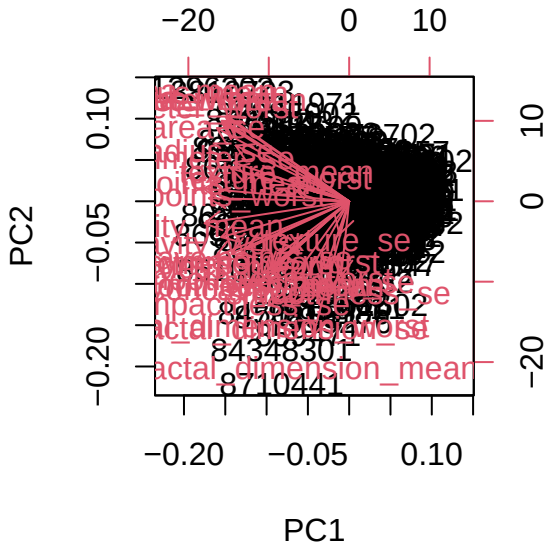
Q5. How many principal components (PCs) are required to describe at least 70% of the original variance in the data?

Three ("Cumulative Proportion" first exceeds 0.7 at PC3).

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

Three ("Cumulative Proportion" first exceeds 0.9 at PC7).

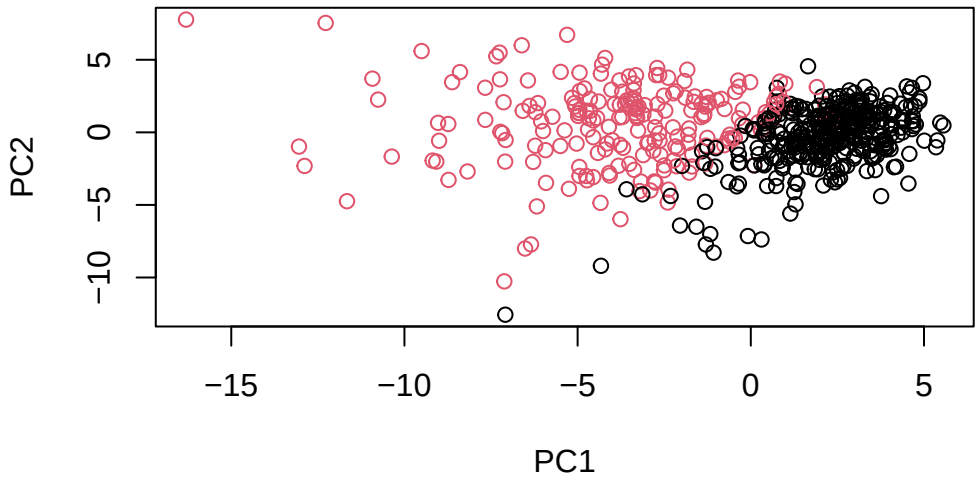
```
biplot(wisc.pr)
```



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

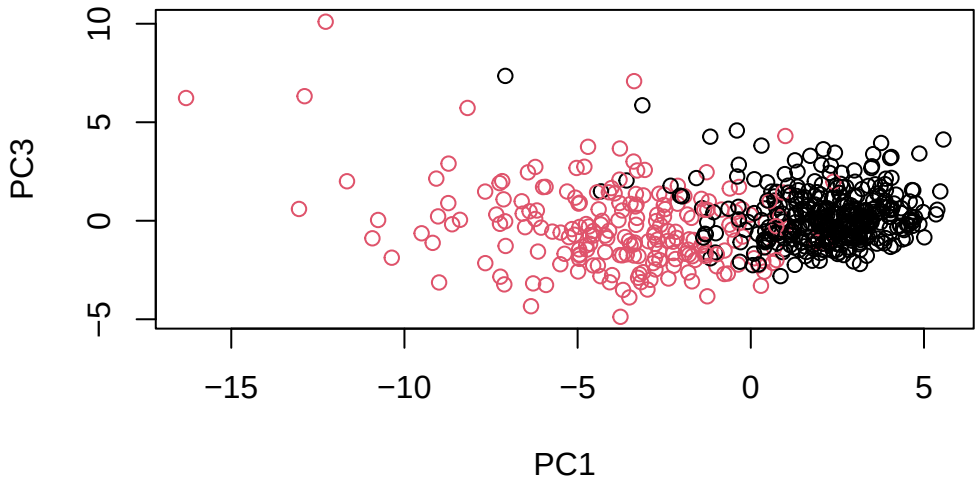
It is too crowded due to row names being plotted.

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



Q8

```
# Repeat for components 1 and 3
plot(wisc.pr$x[,"PC1"], wisc.pr$x[,"PC3"], col = as.factor(diagnosis), xlab = "PC1", ylab
```



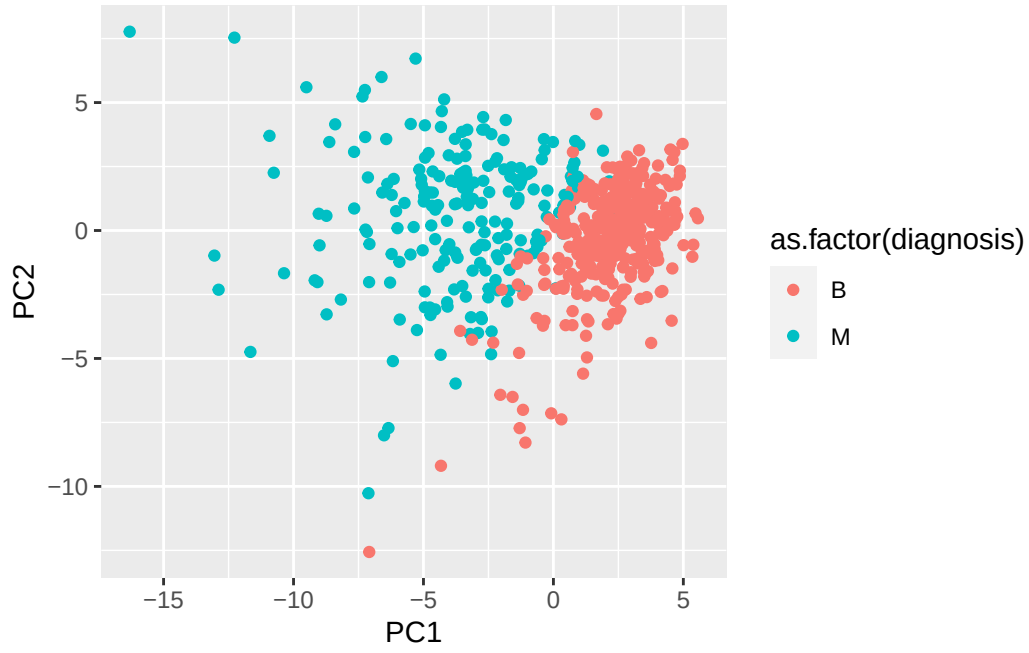
The variation along the vertical axis is less in PC3 than in PC2, because PC3 is less strong as a contributor.

```
# 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=as.factor(diagnosis)) +
  geom_point()
```

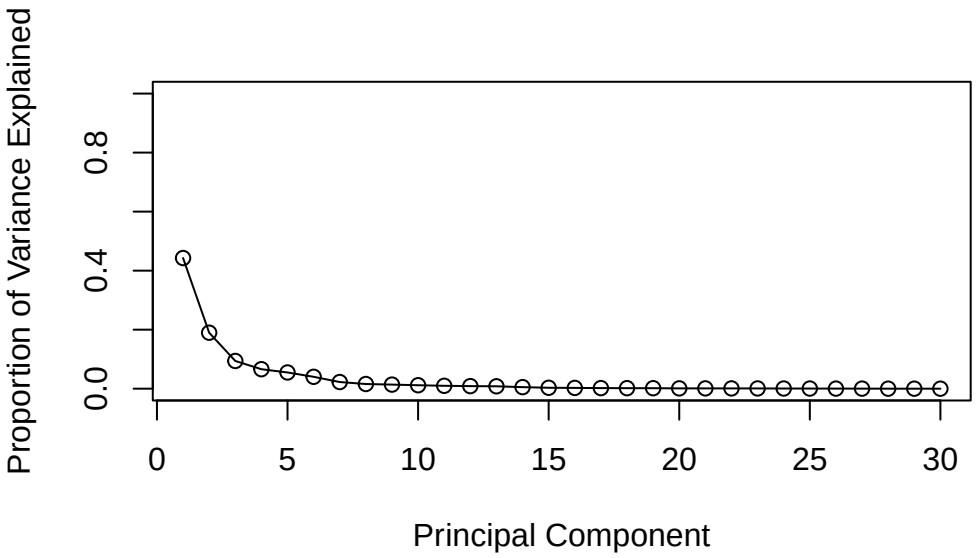



```
# Calculate variance of each component
pr.var <- wisc.pr$sdev^2
head(pr.var)
```

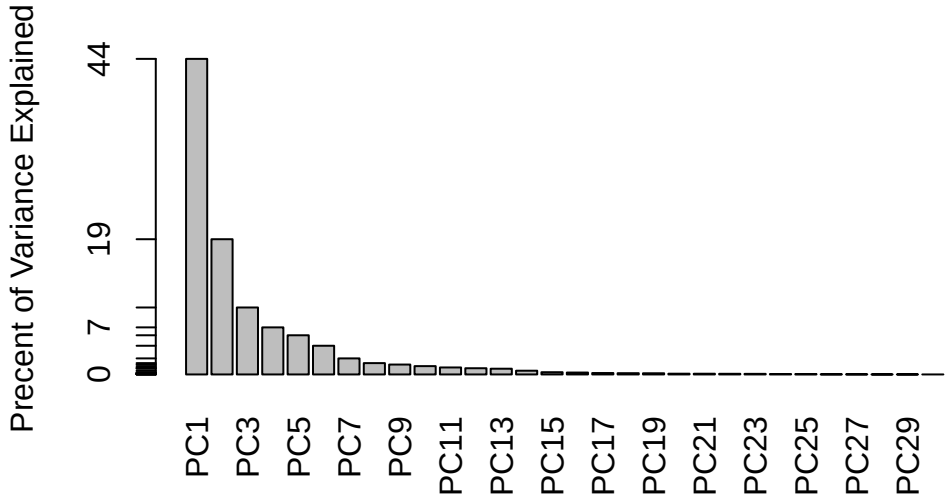
```
[1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

```
# Variance explained by each principal component: pve
pve <- wisc.pr$sdev^2 / sum(wisc.pr$sdev^2)

# Plot variance explained for each principal component
plot(pve, xlab = "Principal Component",
     ylab = "Proportion of Variance Explained",
     ylim = c(0, 1), type = "o")
```



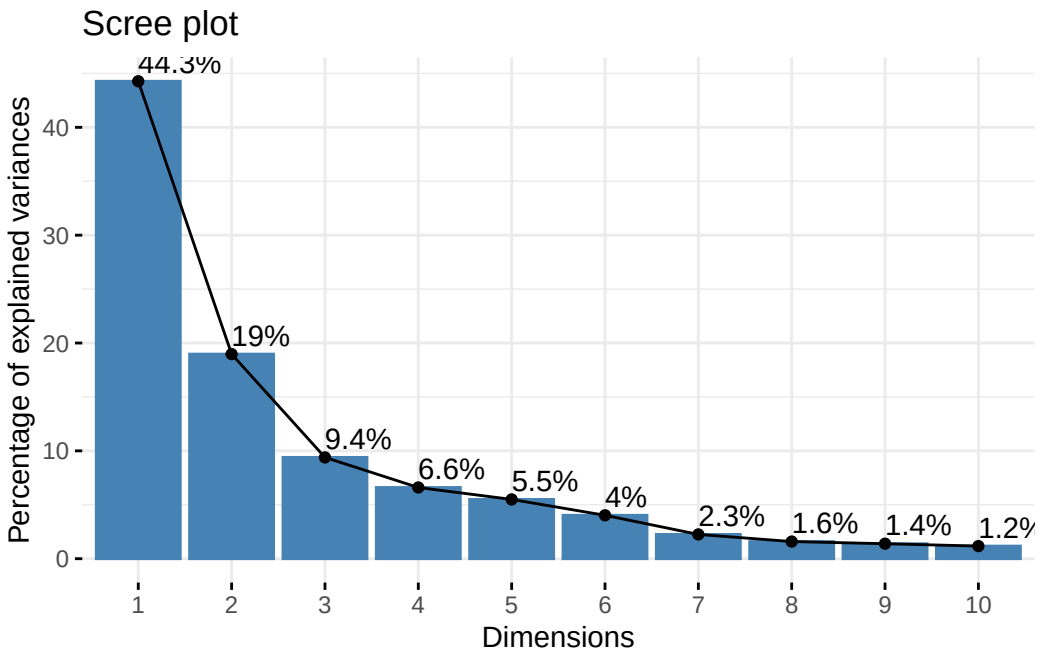

```
# Alternative scree plot of the same data, note data driven y-axis
barplot(pve, ylab = "Precent of Variance Explained",
     names.arg=paste0("PC",1:length(pve)), las=2, axes = FALSE)
axis(2, at=pve, labels=round(pve,2)*100 )
```




```
## 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 (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
```

-0.2608538.

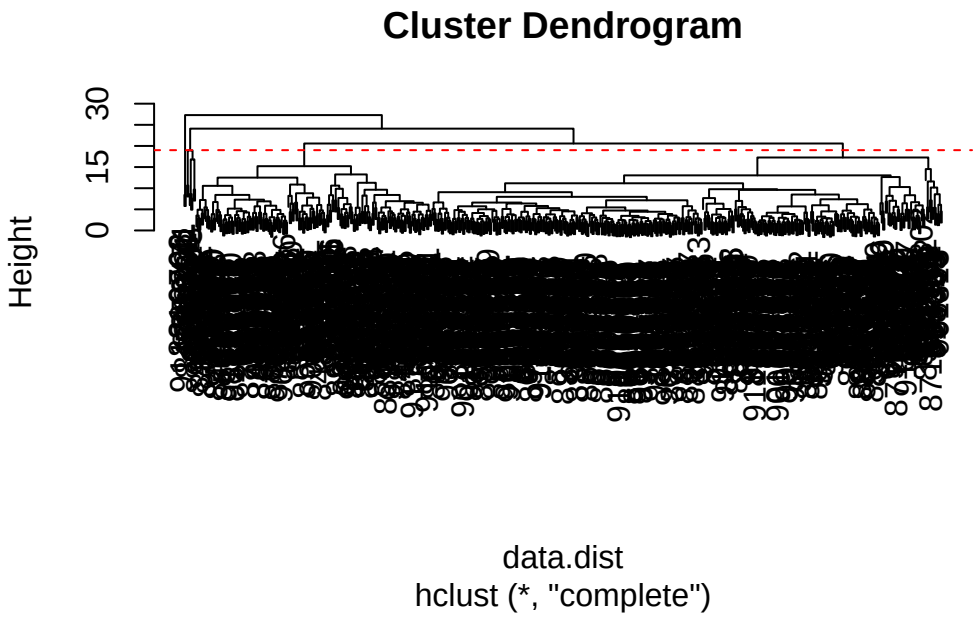
```
# Scale the wisc.data data using the "scale()" function
data.scaled <- scale(wisc.data)
```

```
data.dist <- dist(data.scaled)
```

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

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)
```




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

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

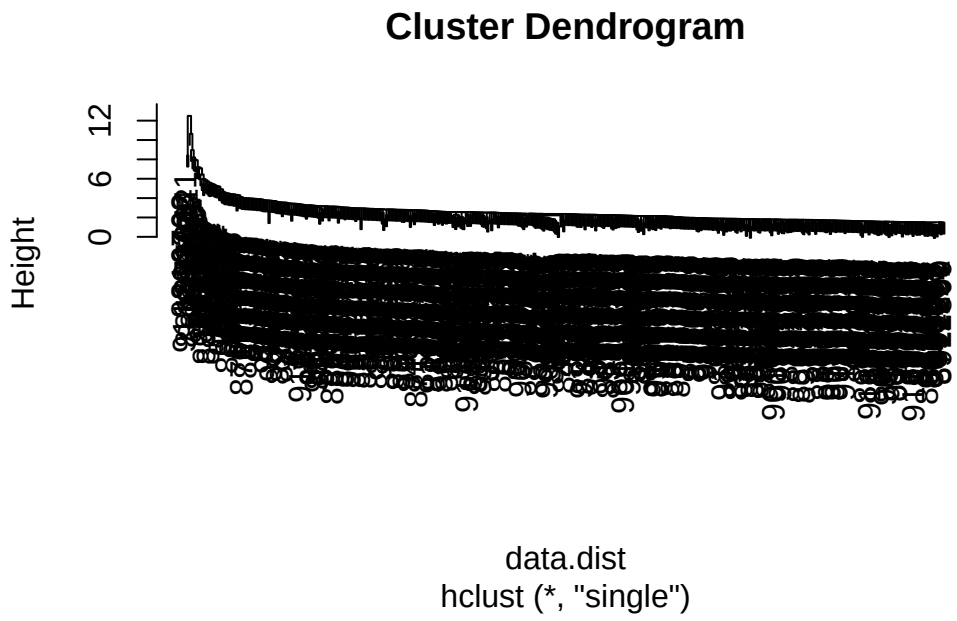
```
                    diagnosis
wisc.hclust.clusters   B   M
                   1  12 165
                   2   2   5
                   3 343  40
                   4   0   2
```

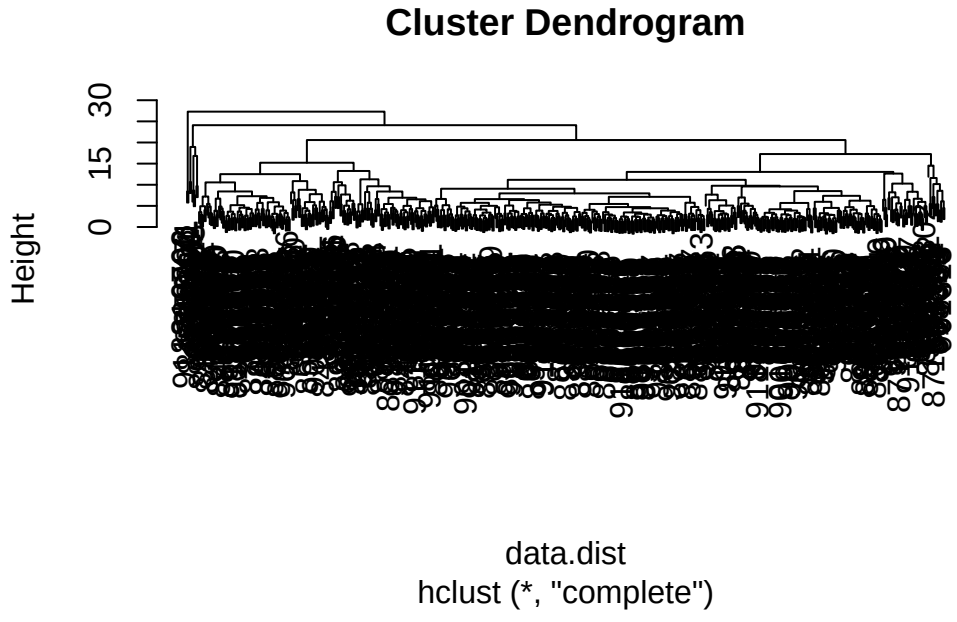
Q11. OPTIONAL: Can you find a better cluster vs diagnoses match by cutting into a different number of clusters between 2 and 10? How do you judge the quality of your result in each case?

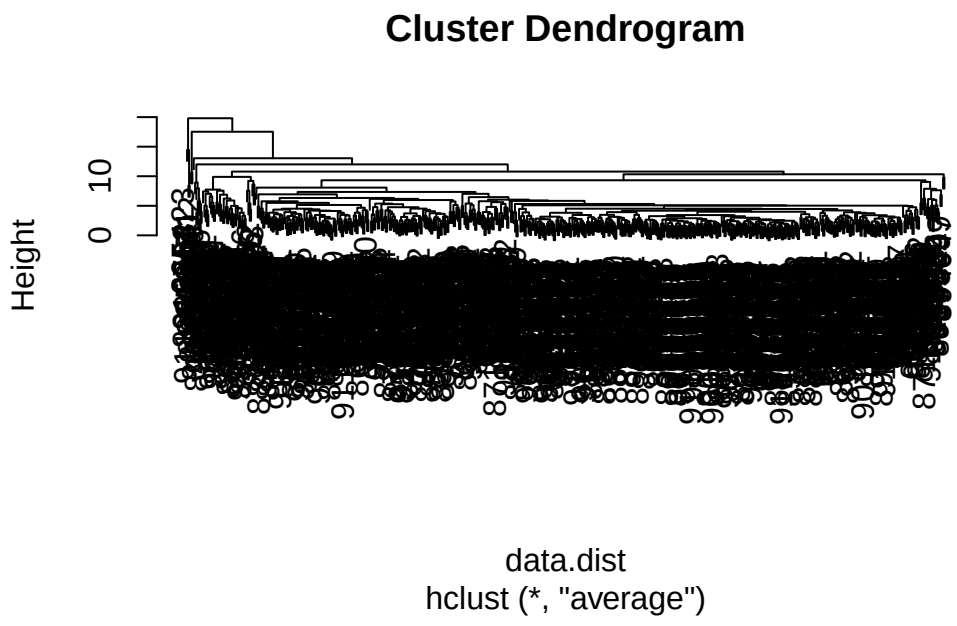
Q12. Which method gives your favorite results for the same data.dist dataset? Explain your reasoning.

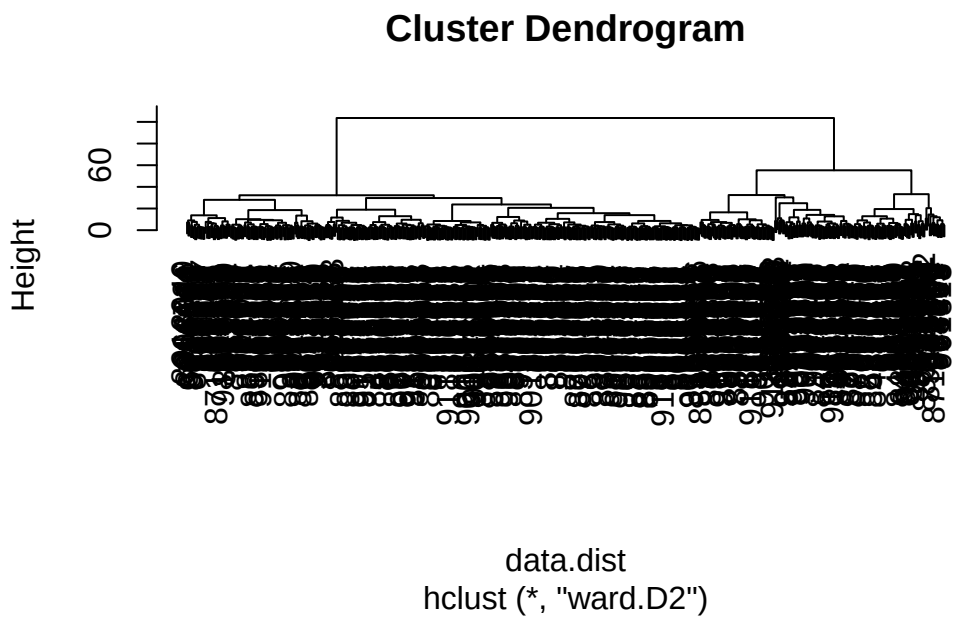
```r
methods = c("single", "complete", "average", "ward.D2")

for (i in methods){
  hclust_data <- hclust(data.dist, method=i)
  plot(hclust_data)
}
```









I prefer ward.D2, beucase it is able to categorize the data into two groups at the first clustering.

```
wisc.pr.hclust <- hclust(dist(wisc.pr$x[,1:7]), method="ward.D2")
grps <- cutree(wisc.pr.hclust, k=2)
```

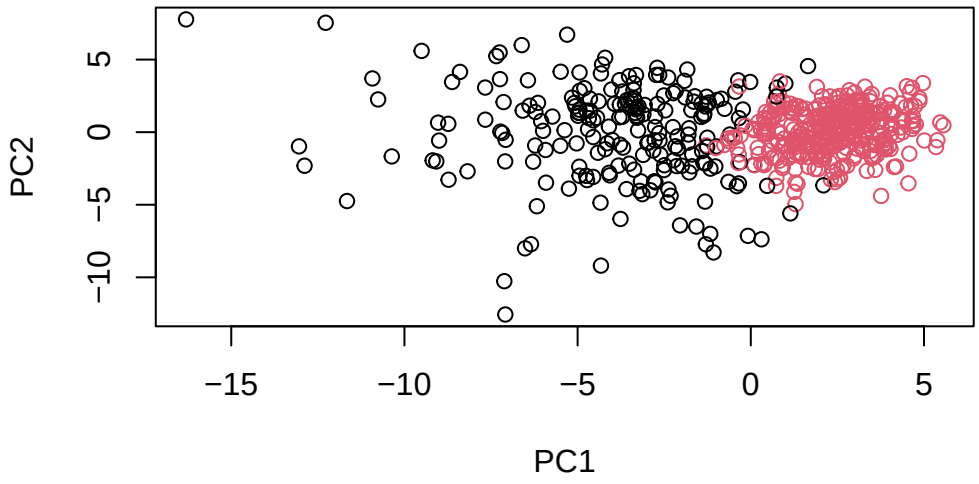
```
table(grps)
```

```
grps
  1   2
216 353
```

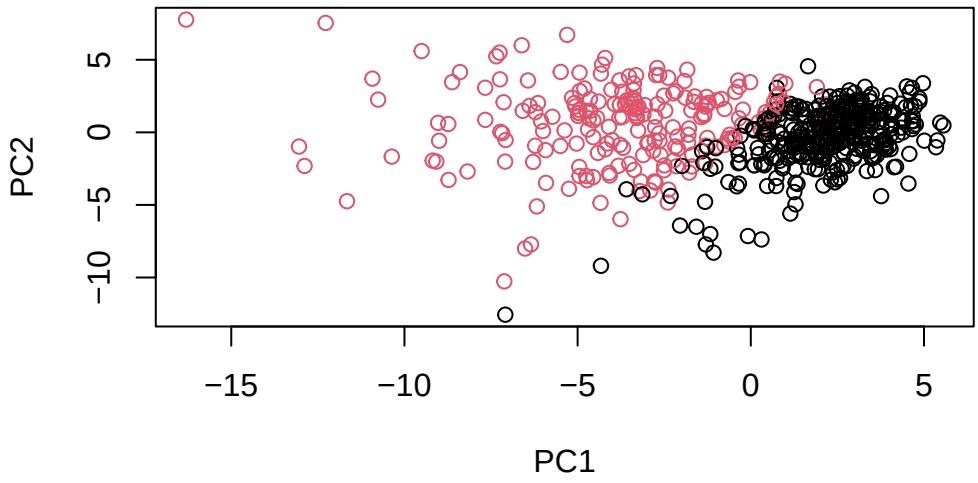
```
table(grps, diagnosis)
```

```
    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=as.factor(diagnosis))
```



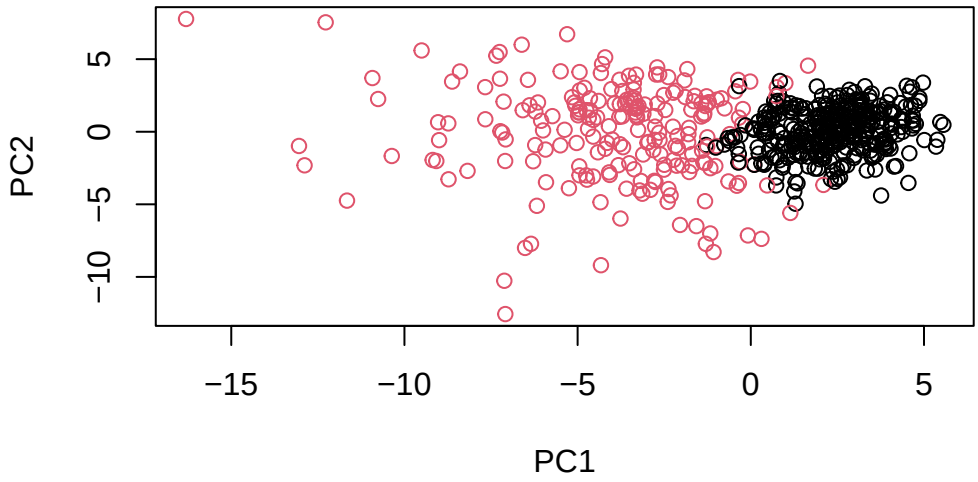

```
g <- as.factor(grps)
levels(g)
```

```
[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)
```



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

```
## 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)
```

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
```

It is able to separate the data into two groups (B and M) with as few as two rounds of clustering, which is a near-minimal number of clustering.

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
```

```
wisc.hclust.clusters_k2 <- cutree(wisc.hclust, k=2)
table(wisc.hclust.clusters_k2, diagnosis)
```

```
                      diagnosis
wisc.hclust.clusters_k2   B   M
                      1 357 210
                      2   0   2
```

The model to which PCA analysis is applied is able to separate the data into two groups (B and M) with as few as two rounds of clustering, while the previous model takes four rounds of clustering. This suggests that the PCA-incorporated model is better at separating the two groups.

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

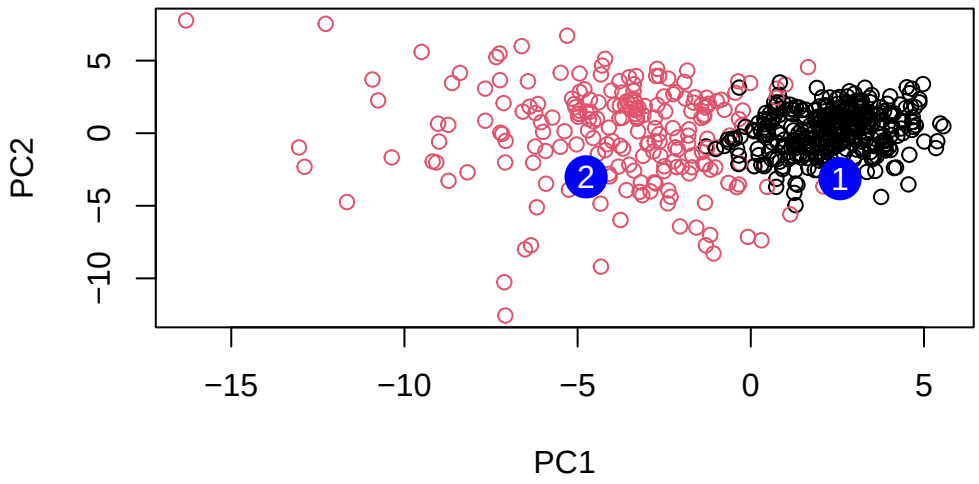
```
#url <- "new_samples.csv"
url <- "https://tinyurl.com/new-samples-CSV"
new <- read.csv(url)
new
```

```
  radius_mean texture_mean perimeter_mean area_mean smoothness_mean
1       8.598        20.98          54.66     221.8          0.1243
2      14.250        22.15          96.42     645.7          0.1049
  compactness_mean concavity_mean concave.points_mean symmetry_mean
1          0.08963         0.0300            0.009259        0.1828
2          0.20080         0.2135            0.086530        0.1949
  fractal_dimension_mean radius_se texture_se perimeter_se area_se
1                0.06757    0.3582      2.067        2.493   18.39
2                0.07292    0.7036      1.268        5.373   60.78
  smoothness_se compactness_se concavity_se concave.points_se symmetry_se
1      0.011930        0.03162      0.03000          0.009259     0.03357
2      0.009407        0.07056      0.06899          0.018480     0.01700
  fractal_dimension_se radius_worst texture_worst perimeter_worst area_worst
1             0.003048        9.565         27.04           62.06      273.9
2             0.006113       17.670         29.51          119.10      959.5
  smoothness_worst compactness_worst concavity_worst concave.points_worst
1           0.1639            0.1698         0.09001               0.02778
2           0.1640            0.6247         0.69220               0.17850
  symmetry_worst fractal_dimension_worst
1         0.2972                 0.07712
2         0.2844                 0.11320
```

```
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?

1. Compared to 2, 1 is more closely located in the intersection of the black and red groups. So there is higher chance of patient 1 being categorized into incorrect groups (pseudo result).