Class 08: Machine Learning Mini Project

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Breast Cancer Project

Exploring data from the University of Wisconsin Cancer Center on breast biopsy data.

```
wisc.data <- read.csv("WisconsinCancer.csv", row.names = 1)
head(wisc.data)
```

```
         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
```

Q1. How many observations are in this dataset?

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

```
[1] 569
```

There are 569 patients in this dataset.

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

```
table(wisc.data[, 1])
```

```
  B   M
357 212
```

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

```
length(grep("_mean$", names(wisc.data)))
```

```
[1] 10
```

Save the diagnosis for later use as a reference to compare how well we do with PCA etc.

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

```
  [1] M M M M M M M M M M M M M M M M M B B B M M M M M M M M M M M M M M
 [38] B M M M M M M M M B M B B B B B M M B M M B B B B M B M M B B B B M B M M
 [75] B M B M M B B B M M B M M M B B B M B B M M B B B M M B B B B M B B M B B
[112] B B B B B B M M M B M M B B B M M B M B M M B M M B B M B B M B B B B M B
[149] B B B B B B B B M B B B B M M B M B B M M B B M M B B B B M B B M M M B M
[186] B M B B B M B B M M B M M M M B M M M B M B M B B M B M M M M B B M M B B
[223] B M B B B B B M M B B M B B M M B M B B B B M B B B B B M B M M M M M M M
[260] M M M M M M M B B B B B B M B M B B M B B M B M M B B B B B B B B B B B B
[297] B M B B M B M B B B B B B B B B B B B B B M B B B M B M B B B B M M M B B
[334] B B M B M B M B B B M B B B B B B B M M M B B B B B B B B B B M M B M M M
[371] M B M M B B B B B M B B B B B M B B B M B B M M B B B B B B B M B B B B B B
[408] B M B B B B B M B B M B B B B B B B B B B B B M B M M B M B B B B B M B B
[445] M B M B B M B M B B B B B B B B B M M B B B B B B M B B B B B B B B B B M B
[482] B B B B B B M B M B B M B B B B B B M M B M B M B B B B B M B B M B M B M M
[519] B B B M B B B B B B B B B B B M B M M B B B B B B B B B B B B B B B B B B B
[556] B B B B B B B M M M M M M B
Levels: B M
```

Now, exclude the diagnosis column from the data

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

Q. How many “dimensions”, “variables”, and “columns” are there in this dataset?

```
dim(wisc)
```

```
[1] 569  30
```

```
ncol(wisc)
```

```
[1] 30
```

Principal Component Analysis (PCA)

To perform PCA in R we can use the `prcomp()` function. It takes a numerical dataset input and optional `scale=FALSE/TRUE` argument.

Generally, `scale=TRUE` should always be set but let's make sure by checking if the mean and standard deviation are different across these 30 columns.

```
round( colMeans(wisc))
```

```
            radius_mean            texture_mean          perimeter_mean
                     14                      19                      92
              area_mean         smoothness_mean        compactness_mean
                    655                       0                       0
         concavity_mean     concave.points_mean          symmetry_mean
                      0                       0                       0
 fractal_dimension_mean              radius_se             texture_se
                      0                       0                       1
           perimeter_se                area_se          smoothness_se
                      3                      40                       0
         compactness_se           concavity_se       concave.points_se
                      0                       0                       0
           symmetry_se    fractal_dimension_se            radius_worst
                      0                       0                      16
         texture_worst         perimeter_worst              area_worst
                     26                     107                     881
     smoothness_worst       compactness_worst         concavity_worst
                      0                       0                       0
  concave.points_worst         symmetry_worst fractal_dimension_worst
                      0                       0                       0
```

```
pca <- prcomp(wisc, scale = TRUE)
summary(pca)
```

```
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)?

44.27% is captured by PC1.

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

Three principal components are required.

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

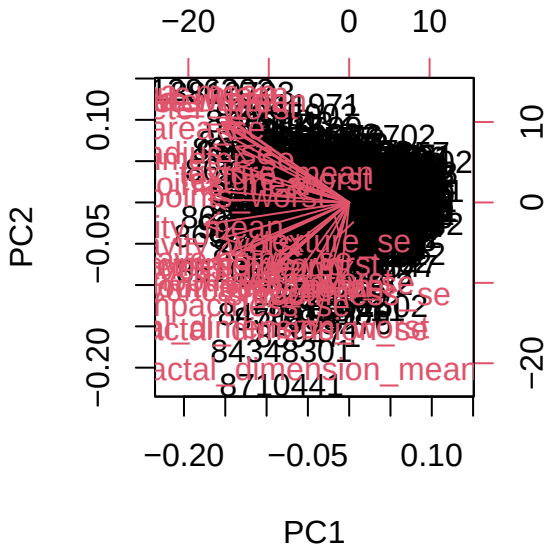
Seven principal components are required

```
attributes(pca)
```

```
$names
[1] "sdev"     "rotation" "center"   "scale"    "x"

$class
[1] "prcomp"
```

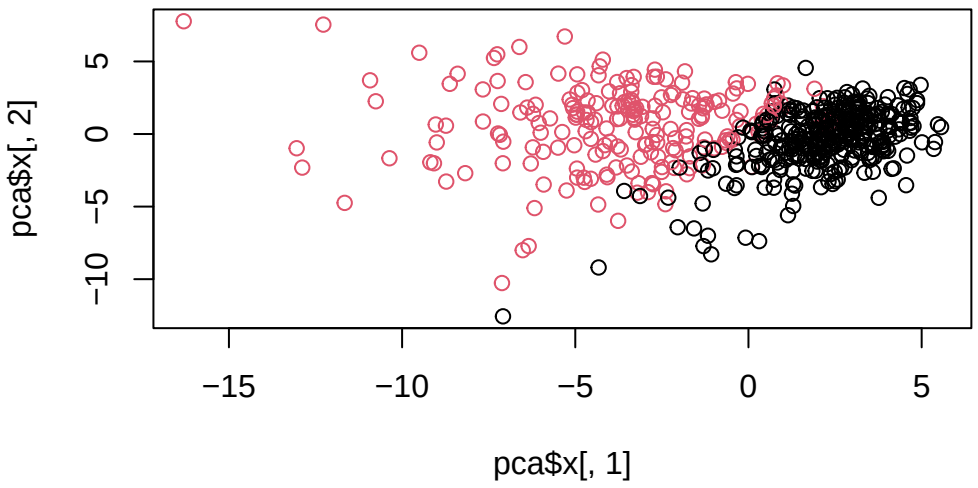
Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?

```
biplot(pca)
```

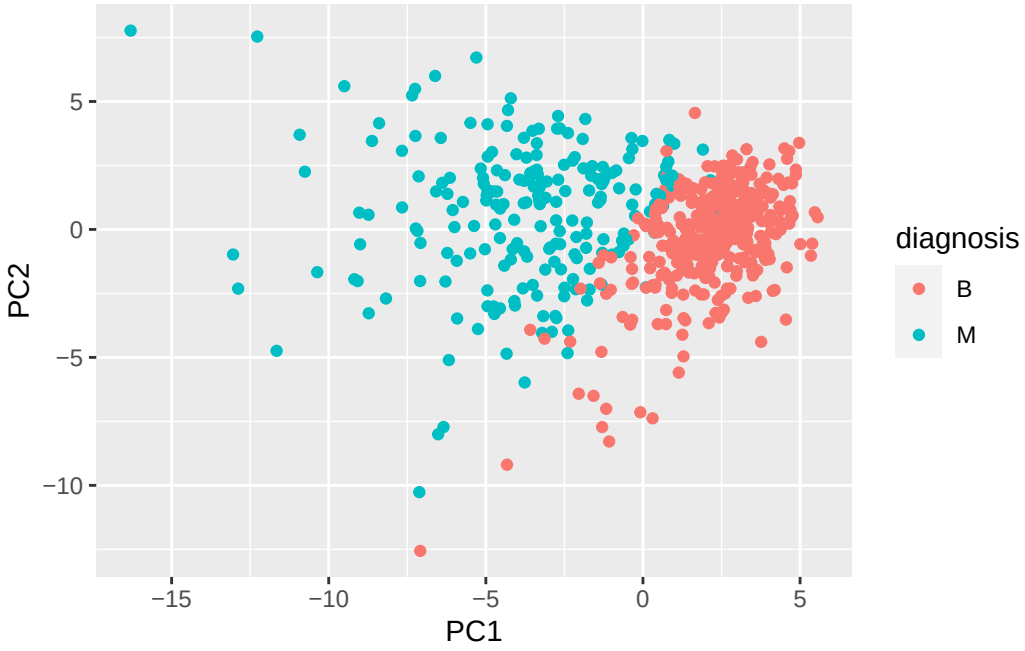


This plot stands out because it is so hard to actually read anything!

```
plot(pca$x[,1], pca$x[,2], col = diagnosis)
```

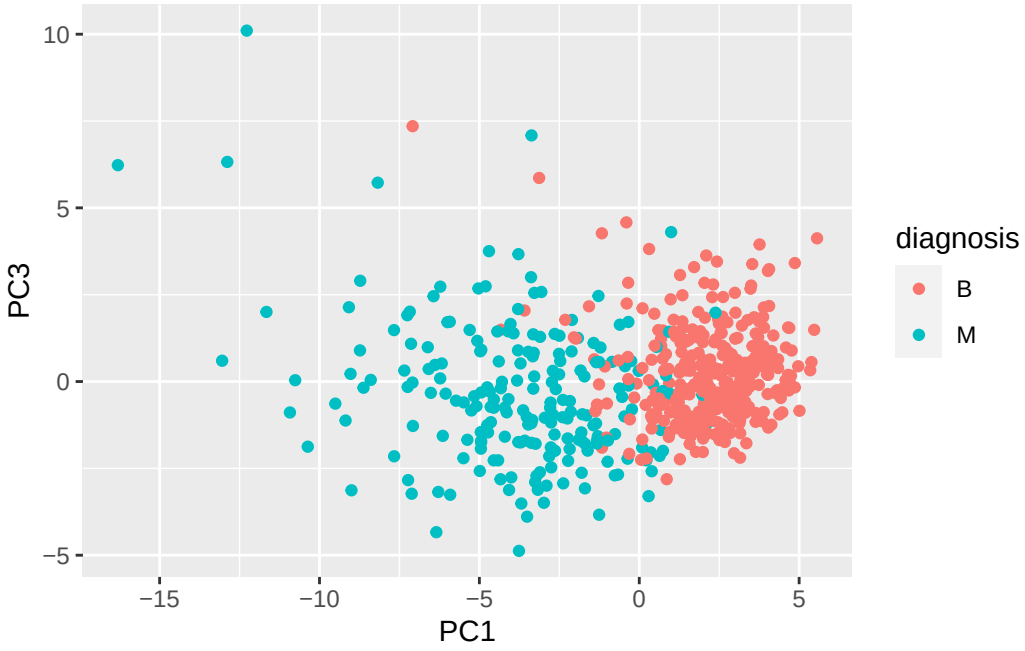



```
library(ggplot2)

x <- as.data.frame(pca$x)

ggplot(x) +
  aes(PC1, PC2, col = diagnosis) +
  geom_point()
```



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

```
y <- as.data.frame(pca$x)

ggplot(y) +
  aes(PC1, PC3, col = diagnosis) +
  geom_point()
```



I notice that these two subgroups are a little harder to tell apart because component 3 explains less variance in the original data than component 2.

> 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?

```
pca$rotation["concave.points_mean", 1]
```

```
[1] -0.2608538
```

> Q10. What is the minimum number of principal components required to explain 80% of the variance of the data?

5 principal components

Hierachical Clustering

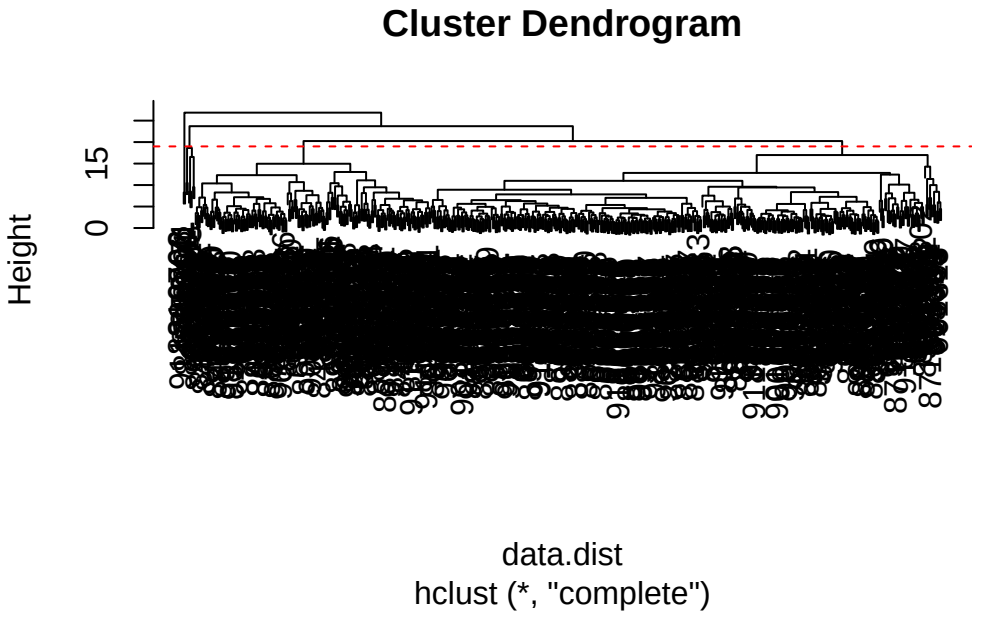
```
# Scale the wisc data using the "scale()" function
data.scaled <- scale(wisc)
```

```r
# Calculating Euclidean distances between all pairs of observations
data.dist <- dist(data.scaled)
```

```r
# Creating hierarchical clustering using complete linkage
wisc.hclust <- hclust(data.dist, method = "complete")
```

Q11. 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)
```




```r
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. Can you find a better cluster vs diagnoses match by cutting into a different number of clusters between 2 and 10?

```
wisc.hclust.clusters <- cutree(wisc.hclust, k = 3)
table(wisc.hclust.clusters, diagnosis)
```

```
                   diagnosis
wisc.hclust.clusters   B   M
                   1 355 205
                   2   2   5
                   3   0   2
```

Q13. Which method gives your favorite results for the same data.dist dataset? Explain your reasoning

I like ward.D2 a bit because it minimizes variance within clusters while working from the bottom up when creating the tree.

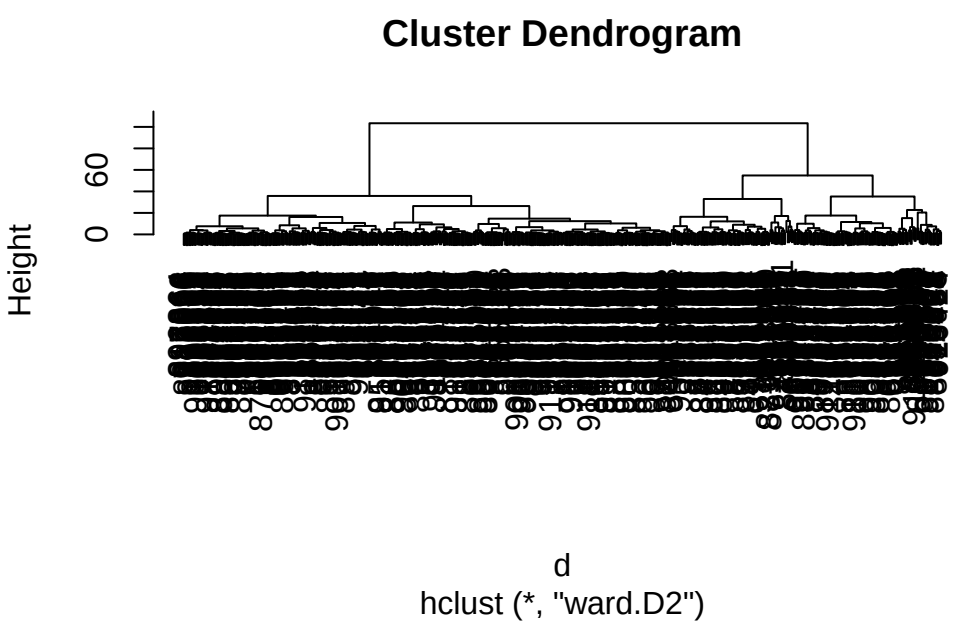
```
attributes(pca)
```

```
$names
[1] "sdev"     "rotation" "center"   "scale"    "x"

$class
[1] "prcomp"
```

Combining PCA results with clustering

We can use our new PCA variables (i.e. the scores along the PCs contained in `pca$x`) as input for other methods such as clustering.

```
# Hclust needs a distance matrix as input
d <- dist(pca$x[,1:3])

hc <- hclust(d, method = "ward.D2")
plot(hc)
```



To get our cluster membership vector we can use the `cutree()` function and specify a height (`h`) or number of groups (`k`).

```
grps <- cutree(hc, h = 80)
table(grps)
```

```
grps
  1   2
203 366
```

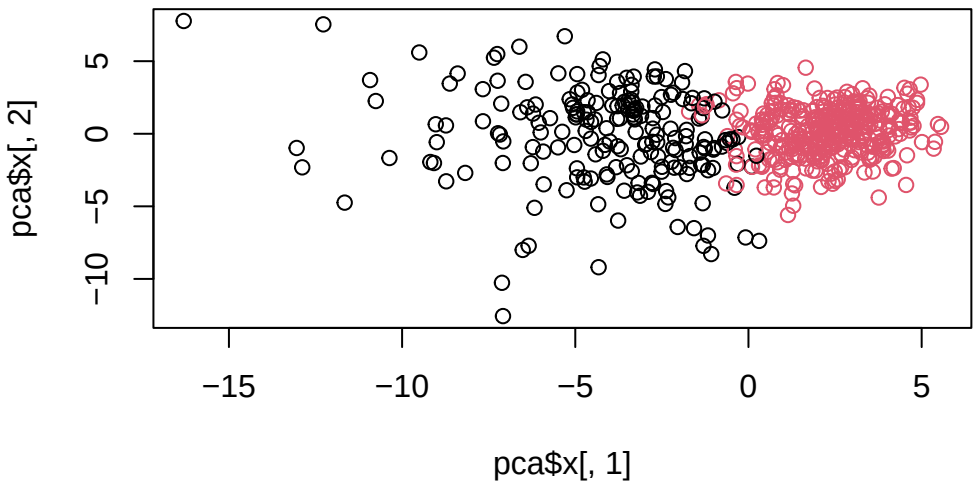
I want to find out how many diagnosis "M" and "B" are in each group.

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

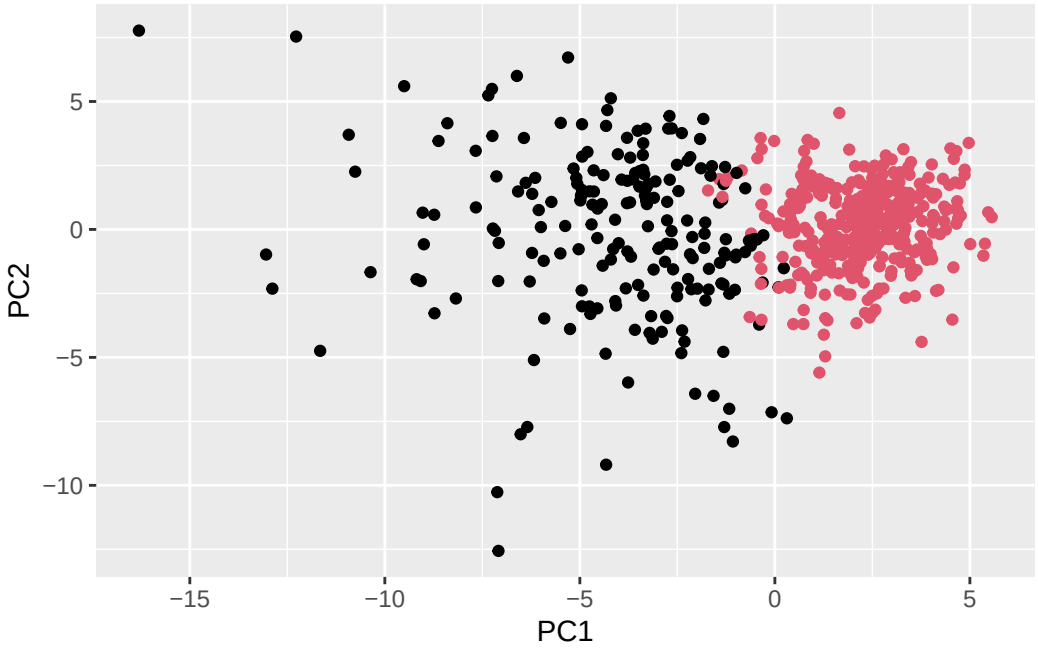
```
         grps
diagnosis   1   2
        B  24 333
        M 179  33
```

We can also plot our results using our clustering vector `grps`

```r
plot(pca$x[,1], pca$x[,2], col = grps)
```




```r
ggplot(x) +
  aes(PC1, PC2) +
  geom_point(col = grps)
```



Q15. What is the specificity and sensitivity of our current results?

```
# Specificity: True negative / (True negative + False negative)
333 / (333 + 33)
```

```
[1] 0.9098361
```

```
# Sensitivity: True positive / (True positive + False negative)
179 / (179 + 33)
```

```
[1] 0.8443396
```