Class 08: Machine Learning Mini Project

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Breast Cancer Project

Today we are going to explore some data from the University of Wisconsin Cancer Center on breast biopsy data.

1. Exploratory data analysis

```
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
```

```
# Create diagnosis vector for later
diagnosis <- wisc.df$diagnosis
diagnosis
```

```
  [1] "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M"
 [19] "M" "B" "B" "B" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M"
 [37] "M" "B" "M" "M" "M" "M" "M" "M" "M" "M" "B" "M" "B" "B" "B" "B" "B" "M"
 [55] "M" "B" "M" "M" "B" "B" "B" "B" "M" "B" "M" "M" "B" "B" "B" "B" "M" "B"
 [73] "M" "M" "B" "M" "B" "M" "M" "B" "B" "B" "M" "M" "B" "M" "M" "M" "B" "B"
 [91] "B" "M" "B" "B" "M" "M" "B" "B" "B" "M" "M" "B" "B" "B" "B" "M" "B" "B"
[109] "M" "B" "B" "B" "B" "B" "B" "B" "B" "M" "M" "M" "B" "M" "M" "B" "B" "B"
[127] "M" "M" "B" "M" "B" "M" "M" "B" "M" "M" "B" "B" "M" "B" "B" "M" "B" "B"
[145] "B" "B" "M" "B" "B" "B" "B" "B" "B" "B" "B" "B" "M" "B" "B" "B" "B" "M"
[163] "M" "B" "M" "B" "B" "M" "M" "B" "B" "M" "M" "B" "B" "B" "B" "M" "B" "B"
[181] "M" "M" "M" "B" "M" "B" "M" "B" "B" "B" "M" "B" "B" "M" "M" "B" "M" "M"
[199] "M" "M" "B" "M" "M" "M" "B" "M" "B" "M" "B" "B" "M" "B" "M" "M" "M" "M"
[217] "B" "B" "M" "M" "B" "B" "B" "M" "B" "B" "B" "B" "B" "M" "M" "B" "B" "M"
[235] "B" "B" "M" "M" "B" "M" "B" "B" "B" "B" "M" "B" "B" "B" "B" "B" "M" "B"
[253] "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "B" "B" "B" "B"
[271] "B" "B" "M" "B" "M" "B" "B" "M" "B" "B" "M" "B" "M" "M" "B" "B" "B" "B"
[289] "B" "B" "B" "B" "B" "B" "B" "B" "B" "M" "B" "B" "M" "B" "M" "B" "B" "B"
[307] "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "M" "B" "B" "B" "M" "B" "M"
[325] "B" "B" "B" "B" "M" "M" "M" "B" "B" "B" "B" "M" "B" "M" "B" "M" "B" "B"
[343] "B" "M" "B" "B" "B" "B" "B" "B" "B" "M" "M" "M" "B" "B" "B" "B" "B" "B"
[361] "B" "B" "B" "B" "B" "M" "M" "B" "M" "M" "M" "B" "M" "M" "B" "B" "B" "B"
[379] "B" "M" "B" "B" "B" "B" "B" "M" "B" "B" "B" "M" "B" "B" "M" "M" "B" "B"
[397] "B" "B" "B" "B" "M" "B" "B" "B" "B" "B" "B" "B" "M" "B" "B" "B" "B" "B"
[415] "M" "B" "B" "M" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "M" "B"
[433] "M" "M" "B" "M" "B" "B" "B" "B" "B" "M" "B" "B" "M" "B" "M" "B" "B" "M"
[451] "B" "M" "B" "B" "B" "B" "B" "B" "B" "B" "M" "M" "B" "B" "B" "B" "B" "B"
[469] "M" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "M" "B" "B" "B" "B" "B" "B"
[487] "B" "M" "B" "M" "B" "B" "M" "B" "B" "B" "B" "B" "M" "M" "B" "M" "B" "M"
[505] "B" "B" "B" "B" "B" "M" "B" "B" "M" "B" "M" "B" "M" "M" "B" "B" "B" "M"
[523] "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "M" "B" "M" "M" "B" "B" "B"
[541] "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B"
[559] "B" "B" "B" "B" "M" "M" "M" "M" "M" "M" "B"
```

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

Q1. How many patient samples are in this dataset?

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

```
[1] 569
```

There are 569 patients in this dataset.

Q2. How many cancer (M) and non-cancer (B) samples are there?

```
table(wisc.data$diagnosis)
```

```
< table of extent 0 >
```

There are 212 cancer and 357 non-cancer samples in this dataset.

```
# Now exclude the diagnosis column from the data.
wisc <- wisc.data[, -1]
```

Q3. How many "dimensions", "variable", "columns" are there in this dataset?

```
ncol(wisc)
```

```
[1] 29
```

2. Principal Component Analysis (PCA)

```
# 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
```

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

We generally always want to set `scale = TRUE` but let's make sure by checking if the mean and standard deviation values are different across there 30 columns.

```
# Perform PCA on wisc.data
pca <- prcomp(wisc.data, scale = TRUE)
```

```
# Look at summary of results
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
```

```
round(colMeans(wisc.data))
```

```
            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
```

```r
attributes(pca)
```

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

$class
[1] "prcomp"
```

Q4. How much variance is captured in the top 3 PCs?

They capture 76% of the total variance.

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

```r
# Calculate the proportion of variance explained by each PC
variance <- pca$sdev^2
prop_var <- variance / sum(variance)

# Determine the number of PCs required to explain at least 70% of the variance
cum_prop_var <- cumsum(prop_var)
num_pcs <- which.max(cum_prop_var >= 0.7)
num_pcs
```

```
[1] 3
```

3 PCs are required to describe at least 70% of the original variance in the data.

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

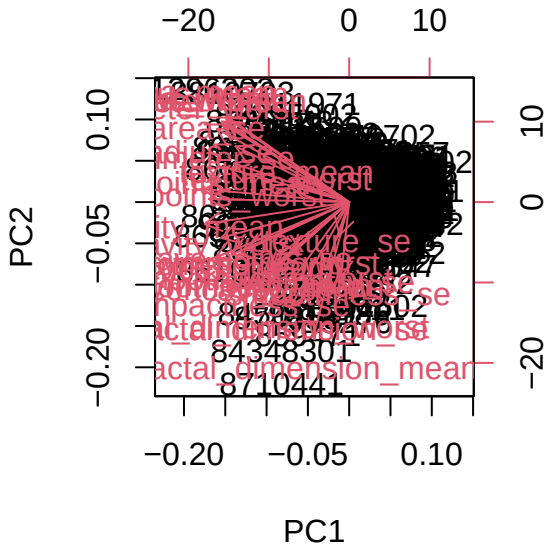
```r
# Determine the number of PCs required to explain at least 90% of the variance
cum_prop_var <- cumsum(prop_var)
num_pcs <- which.max(cum_prop_var >= 0.9)
num_pcs
```

```
[1] 7
```

7 PCs are required to describe at least 70% of the original variance in the data.

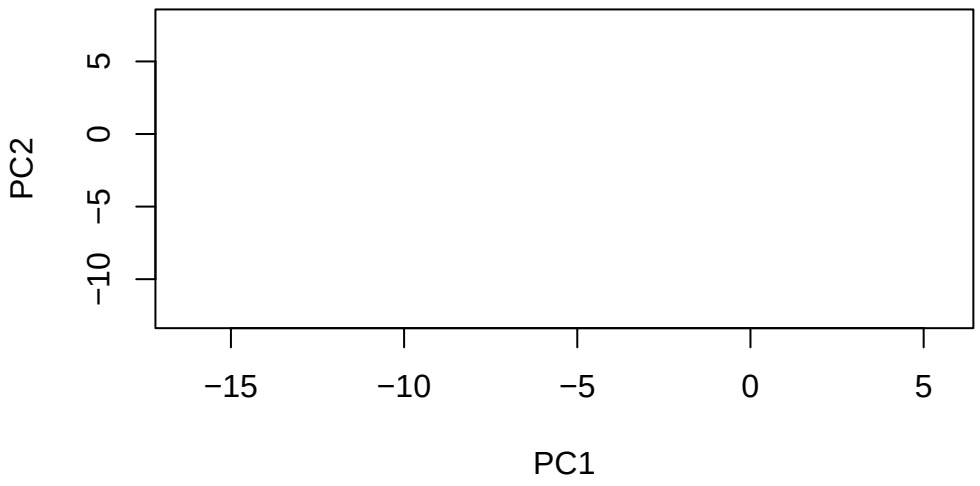
> Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?

```
biplot(pca)
```

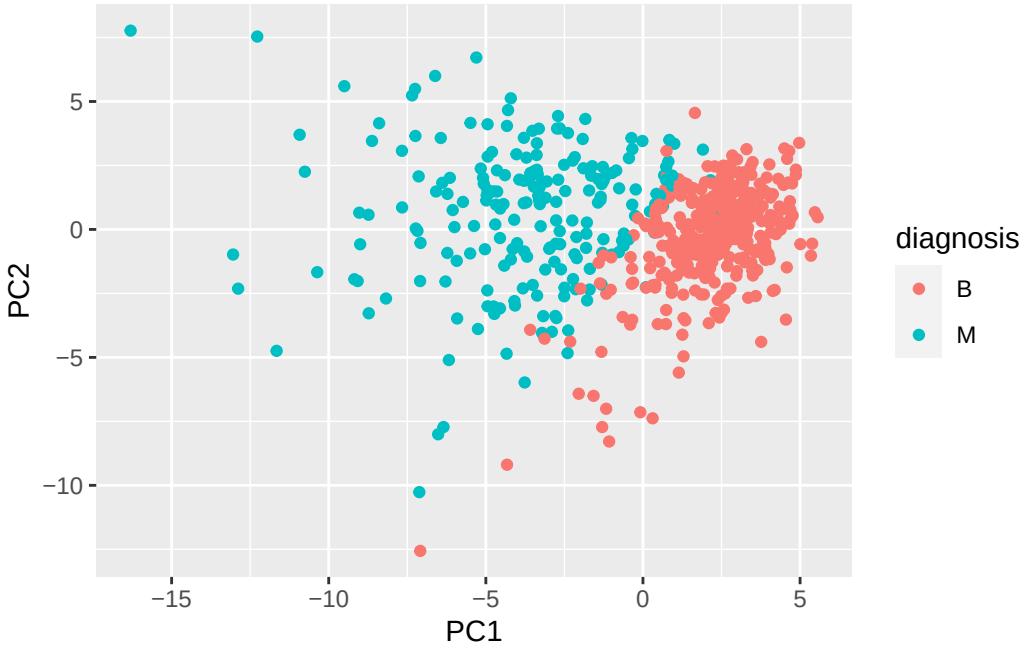


This plot is difficult to understand because there is too much information that is clustered to comprehend.

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

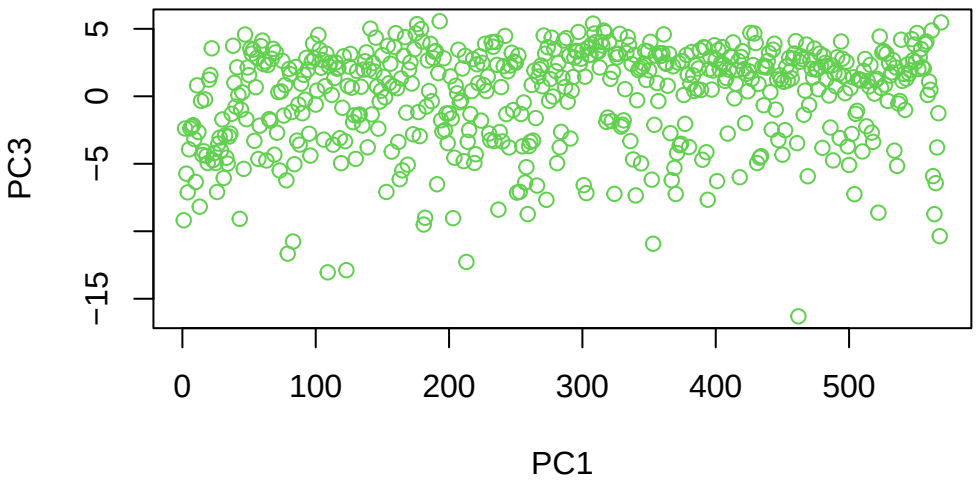



```r
# Create a data.frame for ggplot
df <- as.data.frame(pca$x)
df$diagnosis <- diagnosis

# Load the ggplot2 package
library(ggplot2)

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



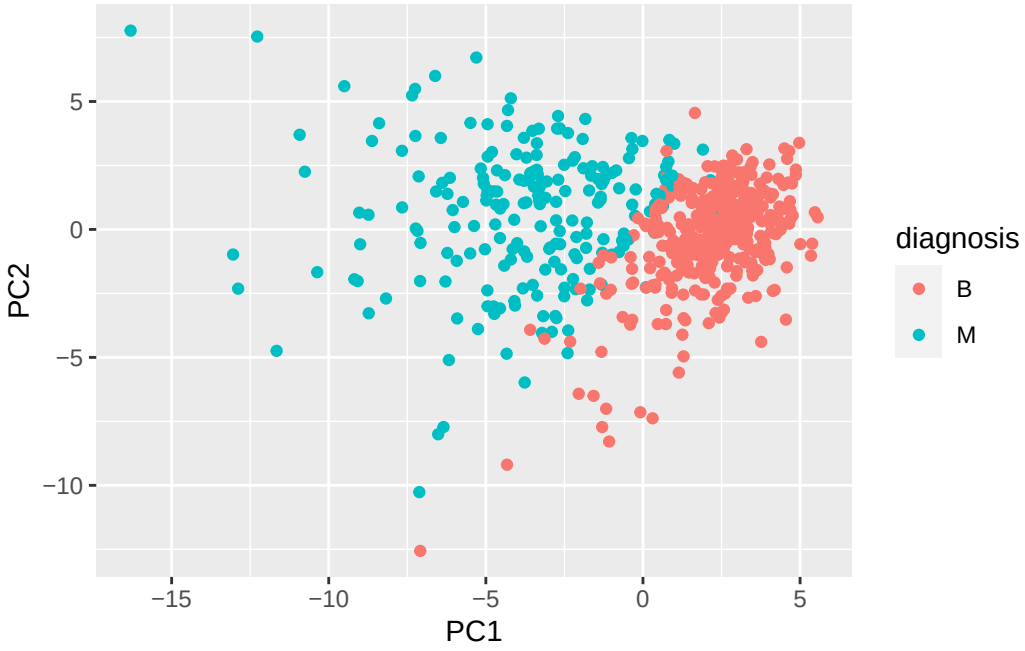
Q8. Generate a similar plot for principal components 1 and 3. What do you notice about these plots?

```
plot(pca$x[, 1], col = 3,
     xlab = "PC1", ylab = "PC3")
```



The plots indicate that PC 1 is capturing a separation of malignant (red) from benign (black) samples.

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

# Load the ggplot2 package
library(ggplot2)

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



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.

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

```
[1] -0.2608538
```

It contributes -0.26.

```
attributes(pca)
```

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

$class
[1] "prcomp"
```

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

```r
# Determine the number of PCs required to explain at least 90% of the variance
cum_prop_var <- cumsum(prop_var)
num_pcs <- which.max(cum_prop_var >= 0.8)
num_pcs
```

```
[1] 5
```

5 PCs are required to describe at least 70% of the original variance in the data.

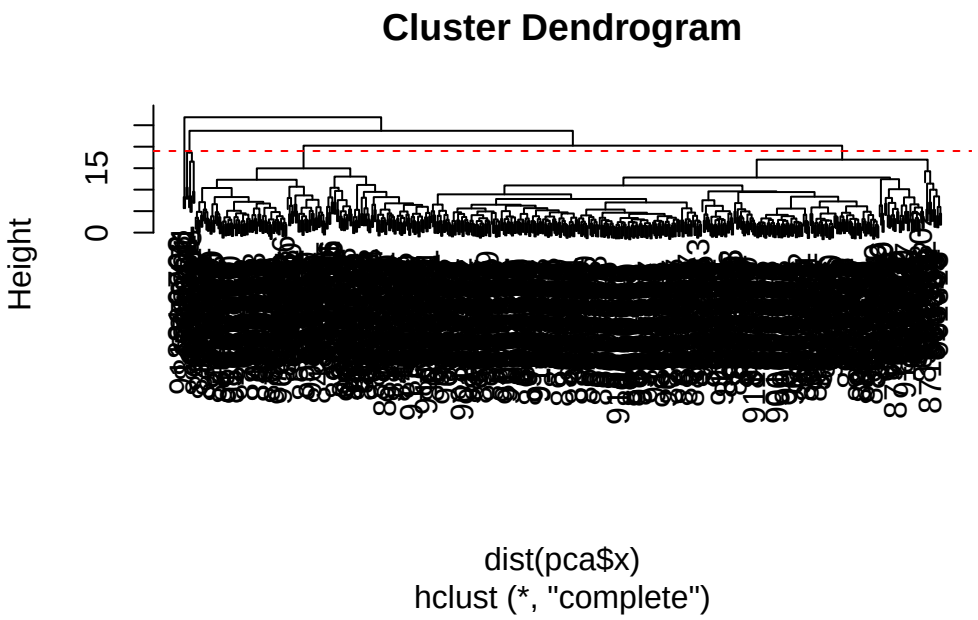
To get our cluster membership vector we can use the `cutree()` function and specify a height (`h = ___`) or number of groups (`k`).

```r
hc <- hclust(dist(pca$x), method = "complete")
grps <- cutree(hc, h = 80)
table(grps)
```

```
grps
  1
569
```

> Q11. Using the plot() and abline() functions, what is the height at which the clustering model has 4 clusters?

```r
# Plot the dendrogram
plot(hc)

# Add a horizontal line to indicate 4 clusters
abline(h = 19, col = "red", lty = 2)
```



The clustering model has 4 clusters at h = 19.

```
wisc.hclust.clusters <- cutree(hc, 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(hc, 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 results using the "ward.D2" method because it produces clusters of similar size and shape which are easier to visualize and understand.

Combine PCA results with clustering

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

How to find out how many diagnosis "M" and "B" there are in each group?

```
table(diagnosis)
```

```
diagnosis
  B   M
357 212
```

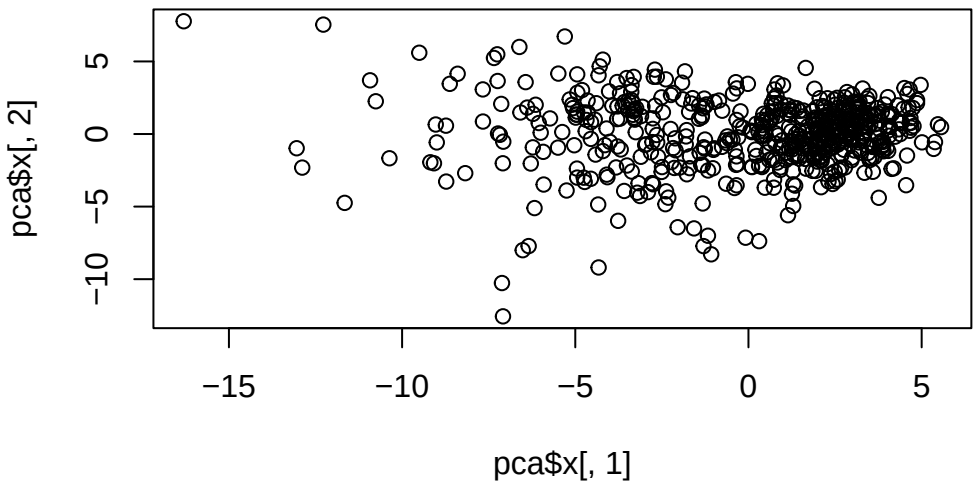
```
table(diagnosis, grps)
```

```
         grps
diagnosis   1
        B 357
        M 212
```

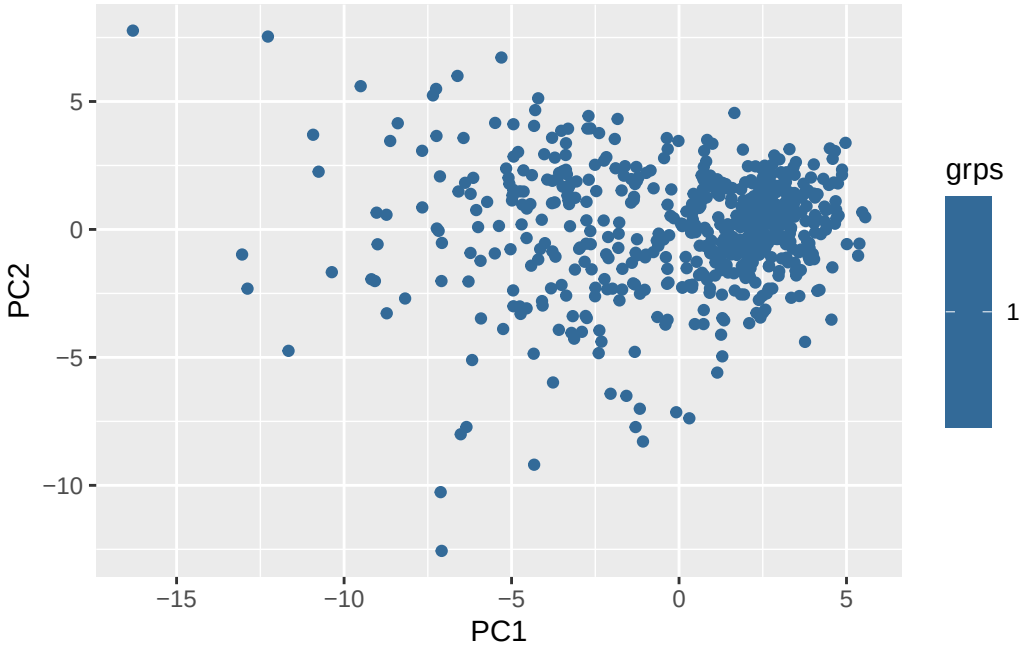
```
# G1 is labeled as M
# G2 is labeled as B
```

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

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




```
library(ggplot2)

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

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



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

Sensitivity = TP/(TP+FN) = 333/(333+33) = 0.91 Specificity = TN/(TN+FN) = 179/(24+179) = 0.88