Class 08: Machine learning

```r
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
```

Q How many patient samples are in this dataset?

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

```
[1] 569
```

There're are 569 patients in this dataset

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

```

  B   M 
357 212 
```

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

```r
diagnosis <- as.factor(wisc.data$diagnosis)
# diagnosis
```

```r
ncol(wisc)
```

```
[1] 30
```

There're 30 variables in this dataset

Principle Component Analysis

```r
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
```

```r
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
```

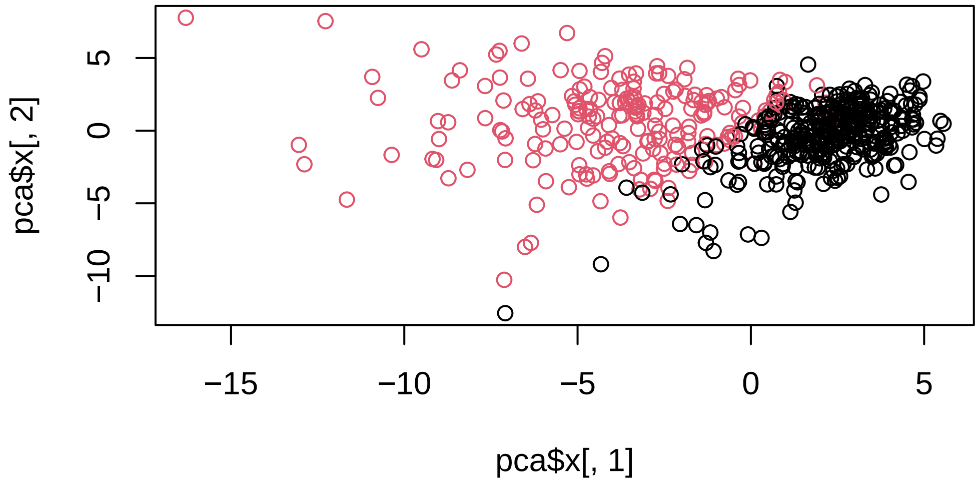
```r
attributes(pca)
```

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

$class
[1] "prcomp"
```

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

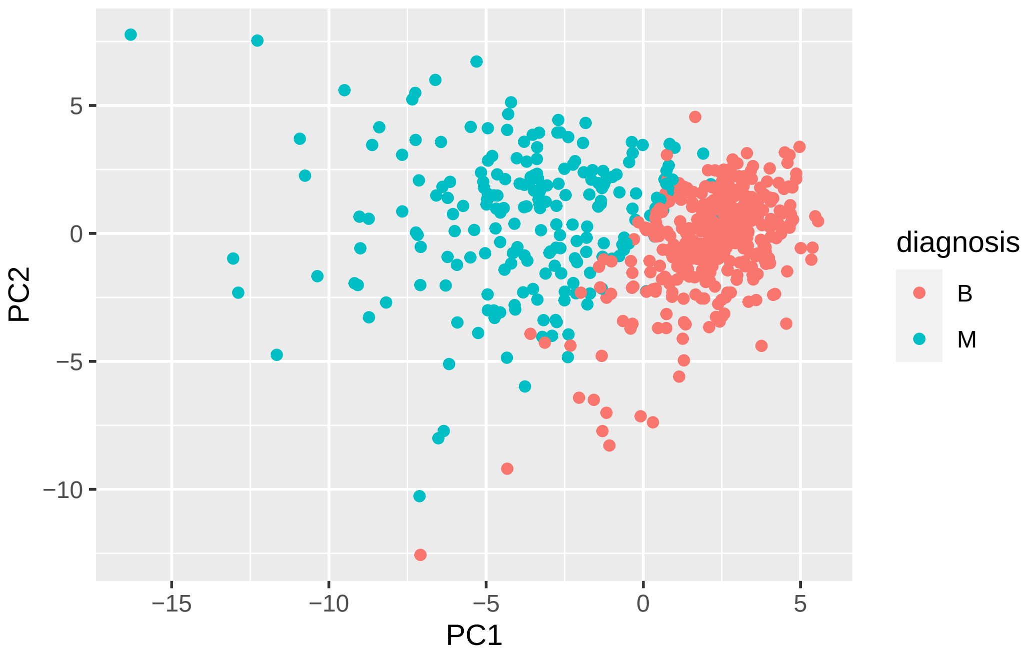
```r
plot(pca$x[,1], pca$x[,2], col=diagnosis)
```



```
library(ggplot2)

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

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



> Q How much variance is captured in the top three PCs?

They capture 72.64%

> **Q** 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`?

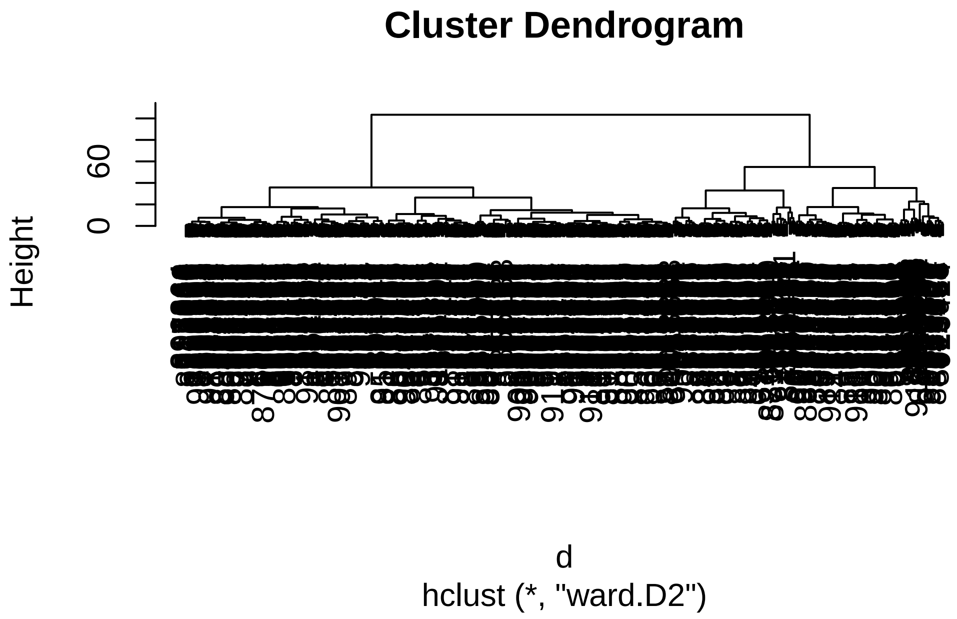
```
pca$rotation["concave.points_mean", 1]
```

```
[1] -0.2608538
```

Combine 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.

```
d <- dist(pca$x[, 1:3]) # Hclust needs a disstance matrix as input
hc <- hclust(d, method="ward.D2")
plot(hc)
```



To generate 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 
```

```
table(diagnosis)
```

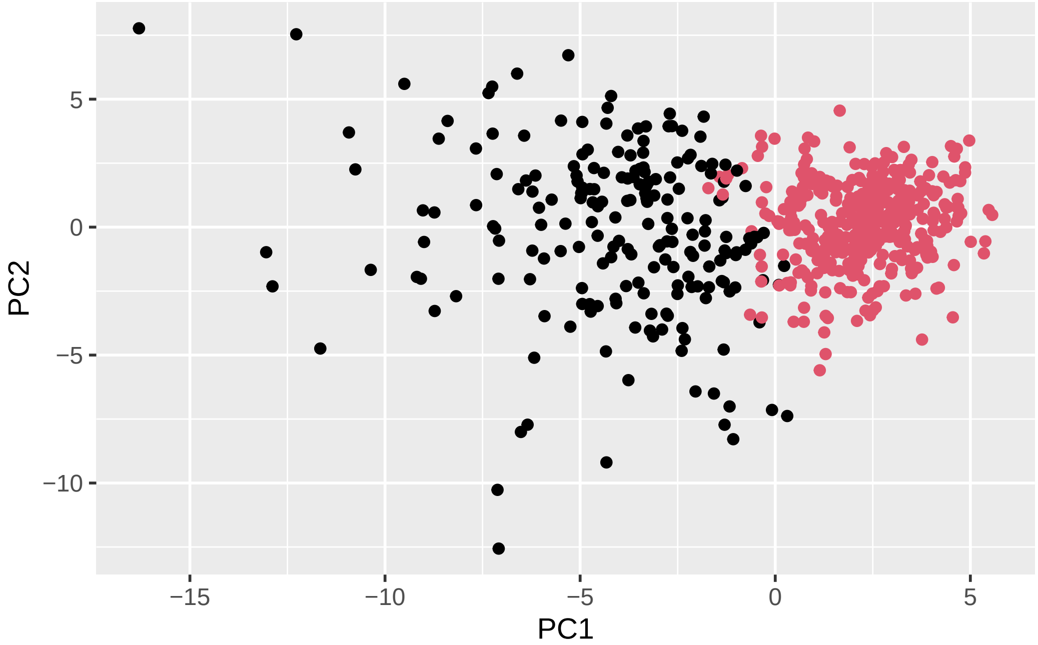
```
diagnosis
  B   M 
357 212 
```

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

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

```r
library(ggplot2)

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



> Q What is the specificity and sensitivity of our current results?

Sepc = TN/(TN + FP) = 333/(333 + 33) = 0.9098361

Sens = TP/(TP+FN) = 179/(179+24) = 0.8817734

Prediction

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

Prioritize patient 2, because it’s malignant.