Class 8: Breast Cancer Mini Project

Barry (PID: 911)

The goal of this mini-project is for you to explore a complete analysis using the unsupervised learning techniques covered in class. You'll extend what you've learned by combining PCA as a preprocessing step to clustering using data that consist of measurements of cell nuclei of human breast masses.

Our data fro today come from FNA of breast tissue. Let's read this data into R.

```
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
```

Q. How many observations/samples/patients/rows?

There are 569 individuals in this dataset.

Q What is in the `$diagnosis` column? How many of each type?

```
sum(wisc.df$diagnosis == "M")
```

```
[1] 212
```

```
sum(wisc.df$diagnosis == "B")
```

```
[1] 357
```

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

```
  B   M
357 212
```

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

```
colnames(wisc.df)
```

```
 [1] "diagnosis"               "radius_mean"
 [3] "texture_mean"            "perimeter_mean"
 [5] "area_mean"               "smoothness_mean"
 [7] "compactness_mean"        "concavity_mean"
 [9] "concave.points_mean"     "symmetry_mean"
[11] "fractal_dimension_mean"  "radius_se"
[13] "texture_se"              "perimeter_se"
[15] "area_se"                 "smoothness_se"
[17] "compactness_se"          "concavity_se"
[19] "concave.points_se"       "symmetry_se"
[21] "fractal_dimension_se"    "radius_worst"
[23] "texture_worst"           "perimeter_worst"
[25] "area_worst"              "smoothness_worst"
[27] "compactness_worst"       "concavity_worst"
[29] "concave.points_worst"    "symmetry_worst"
[31] "fractal_dimension_worst"
```

```
length( grep("_mean", colnames(wisc.df), value=TRUE) )
```

```
[1] 10
```

Q. How many variables/dimensions have we?

```
ncol(wisc.df)
```

```
[1] 31
```

Save the diagnosis for reference later

```
diagnosis <- as.factor(wisc.df$diagnosis)
```

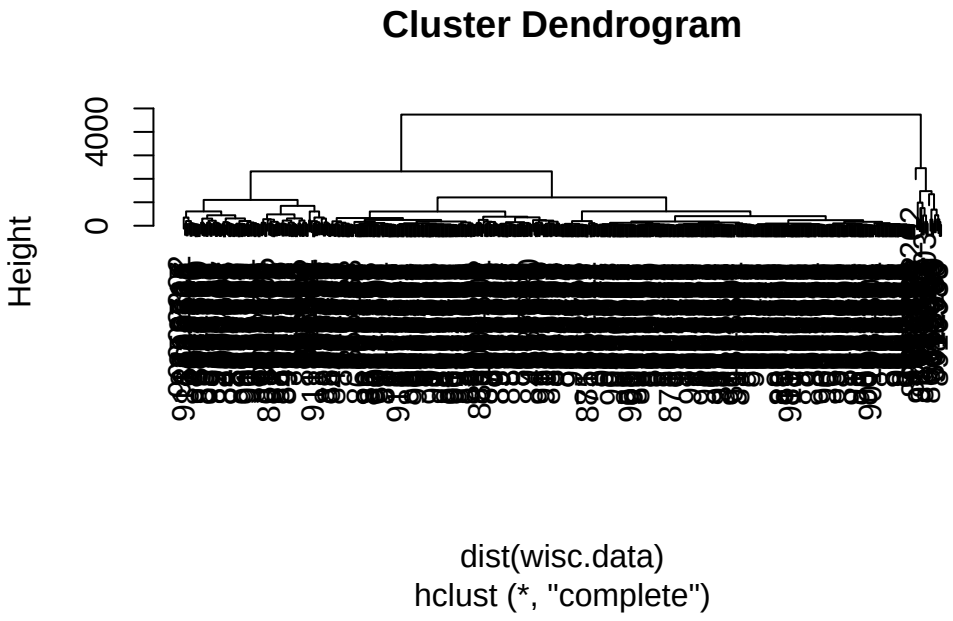
and remove or exclude this column form any of our analysis

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

Let's try clustering this data:

Hierarchical Clustering with `hclust()`

```
wisc.hc <- hclust( dist(wisc.data) )
plot(wisc.hc)
```



Principal Component Analysis

Let's try PCA on this data. Before doing any analysis like this we should check if our input data needs to be scalled first?

Side-note:

```
head(mtcars)
```

```
                   mpg cyl disp  hp drat    wt  qsec vs am gear carb
Mazda RX4         21.0   6  160 110 3.90 2.620 16.46  0  1    4    4
Mazda RX4 Wag     21.0   6  160 110 3.90 2.875 17.02  0  1    4    4
Datsun 710        22.8   4  108  93 3.85 2.320 18.61  1  1    4    1
Hornet 4 Drive    21.4   6  258 110 3.08 3.215 19.44  1  0    3    1
Hornet Sportabout 18.7   8  360 175 3.15 3.440 17.02  0  0    3    2
Valiant           18.1   6  225 105 2.76 3.460 20.22  1  0    3    1
```

```
apply(mtcars, 2, mean)
```

```
      mpg        cyl       disp         hp       drat         wt       qsec
20.090625   6.187500 230.721875 146.687500   3.596563   3.217250  17.848750
       vs         am       gear       carb
 0.437500   0.406250   3.687500   2.812500
```

```
apply(mtcars, 2, sd)
```

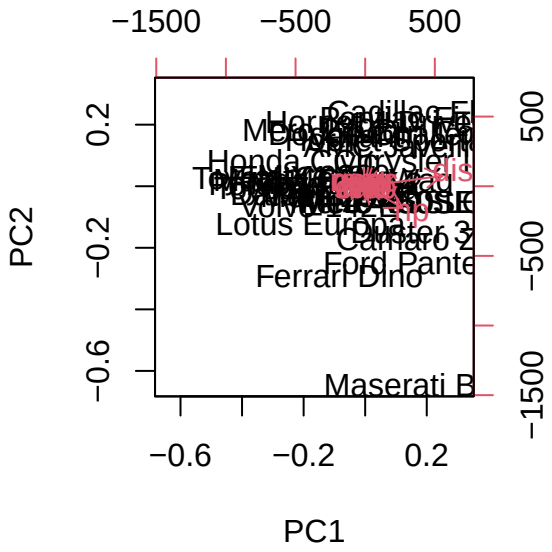
```
      mpg        cyl       disp         hp       drat         wt
6.0269481  1.7859216 123.9386938 68.5628685  0.5346787  0.9784574
     qsec         vs         am       gear       carb
1.7869432  0.5040161  0.4989909  0.7378041  1.6152000
```

Let's try a PCA on this car dataset

```
pc <- prcomp(mtcars)
summary(pc)
```

```
Importance of components:
                          PC1      PC2     PC3     PC4     PC5     PC6    PC7
Standard deviation     136.533 38.14808 3.07102 1.30665 0.90649 0.66354 0.3086
Proportion of Variance   0.927  0.07237 0.00047 0.00008 0.00004 0.00002 0.0000
Cumulative Proportion    0.927  0.99937 0.99984 0.99992 0.99996 0.99998 1.0000
                          PC8    PC9   PC10   PC11
Standard deviation     0.286 0.2507 0.2107 0.1984
Proportion of Variance 0.000 0.0000 0.0000 0.0000
Cumulative Proportion  1.000 1.0000 1.0000 1.0000
```

```r
biplot(pc)
```

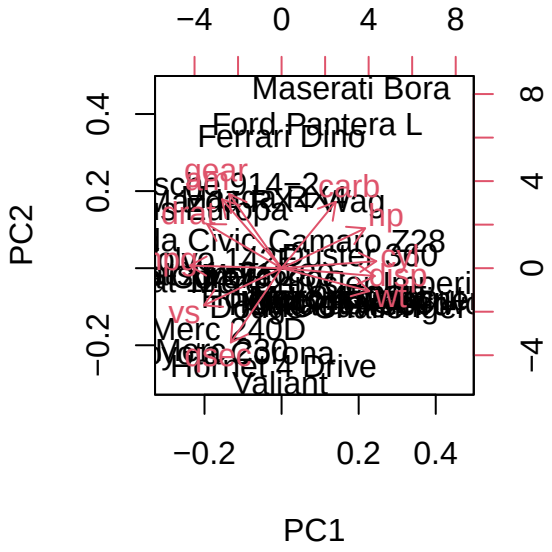



```r
pc.scale <- prcomp(mtcars, scale=TRUE)
summary(pc.scale)
```

```
Importance of components:
                          PC1    PC2     PC3     PC4     PC5     PC6    PC7
Standard deviation     2.5707 1.6280 0.79196 0.51923 0.47271 0.46000 0.3678
Proportion of Variance 0.6008 0.2409 0.05702 0.02451 0.02031 0.01924 0.0123
Cumulative Proportion  0.6008 0.8417 0.89873 0.92324 0.94356 0.96279 0.9751
```

```
                            PC8     PC9     PC10   PC11
Standard deviation     0.35057 0.2776 0.22811 0.1485
Proportion of Variance 0.01117 0.0070 0.00473 0.0020
Cumulative Proportion  0.98626 0.9933 0.99800 1.0000
```

```
biplot(pc.scale)
```



Back to our cancer data set

Do we need to scale this data set? Yes we do because the spread is very different

```
wisc.pr <- prcomp(wisc.data, scale=TRUE)
```

How well do the PCs capture the variance in the original data?

```
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
```

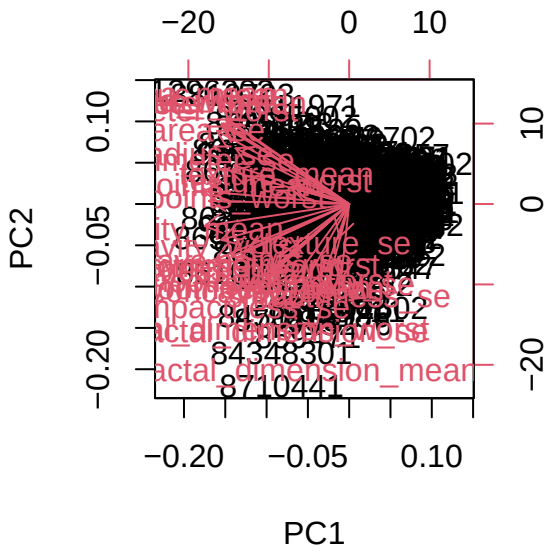
```
Proportion of Variance 0.4427 0.1897 0.09393 0.06602 0.05496 0.04025 0.02251
Cumulative Proportion  0.4427 0.6324 0.72636 0.79239 0.84734 0.88759 0.91010
                           PC8    PC9    PC10   PC11    PC12    PC13    PC14
Standard deviation     0.69037 0.6457 0.59219 0.5421 0.51104 0.49128 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
```

Our main PC score plot (a.k.a. PC plot, PC1 vs PC2, ordeiation plot).

```
attributes(wisc.pr)
```

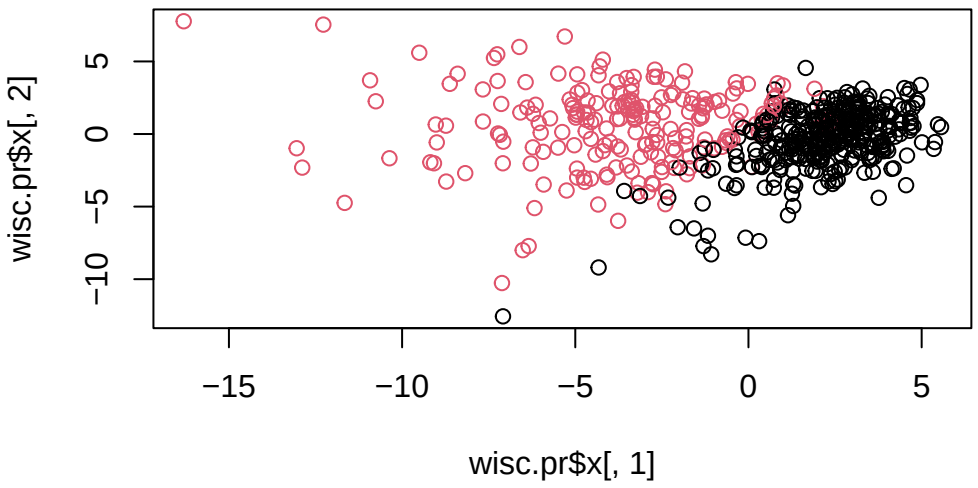
```
$names
[1] "sdev"     "rotation" "center"   "scale"    "x"

$class
[1] "prcomp"
```

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



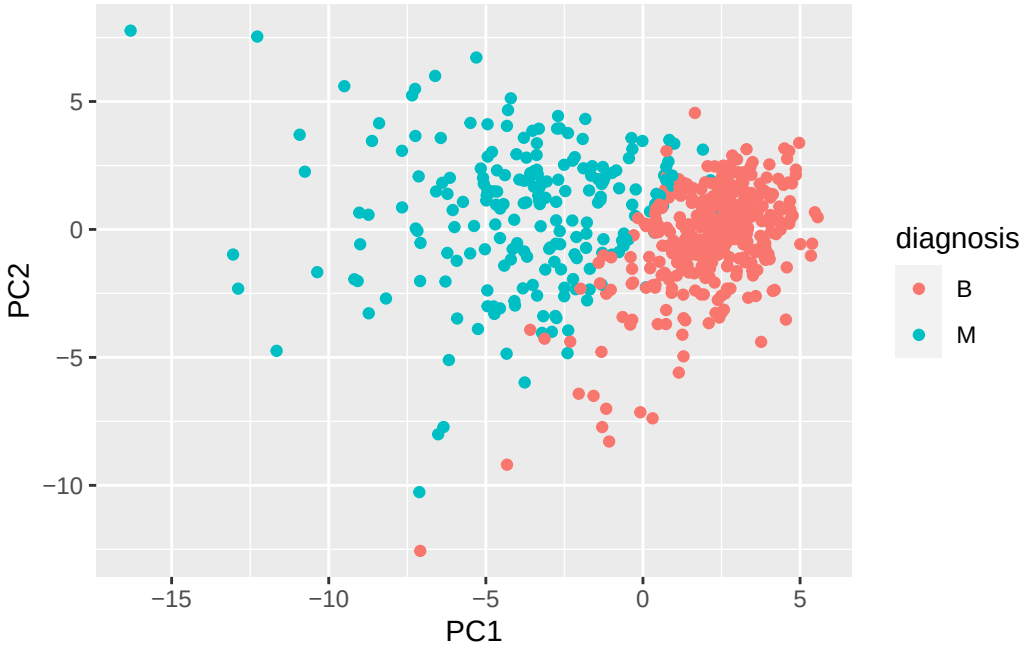
We need to build our own plot here:

```
plot(wisc.pr$x[,1], wisc.pr$x[,2], col=diagnosis)
```



Make a nice ggplot version

```
pc <- as.data.frame(wisc.pr$x)

library(ggplot2)

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



Variance explained

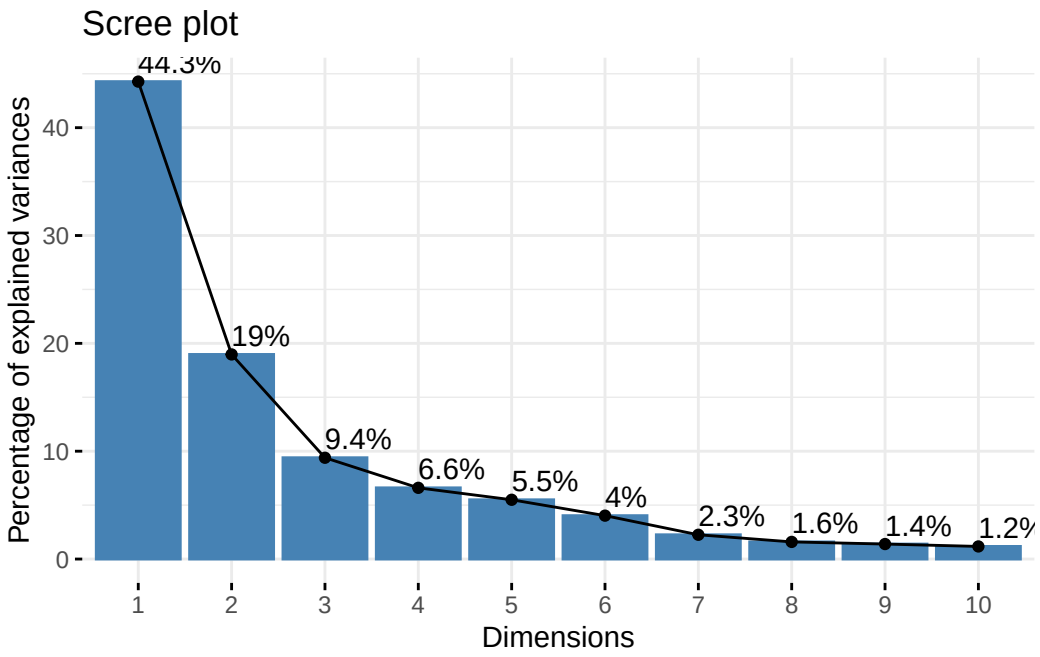
```
v <- summary(wisc.pr)
v$importance[2,]
```

```
    PC1     PC2     PC3     PC4     PC5     PC6     PC7     PC8     PC9     PC10
0.44272 0.18971 0.09393 0.06602 0.05496 0.04025 0.02251 0.01589 0.01390 0.01169
   PC11    PC12    PC13    PC14    PC15    PC16    PC17    PC18    PC19    PC20
0.00980 0.00871 0.00805 0.00523 0.00314 0.00266 0.00198 0.00175 0.00165 0.00104
   PC21    PC22    PC23    PC24    PC25    PC26    PC27    PC28    PC29    PC30
0.00100 0.00091 0.00081 0.00060 0.00052 0.00027 0.00023 0.00005 0.00002 0.00000
```

```
library(factoextra)
```

```
Welcome! Want to learn more? See two factoextra-related books at https://goo.gl/ve3WBa
```

```
fviz_eig(wisc.pr, addlabels = TRUE)
```

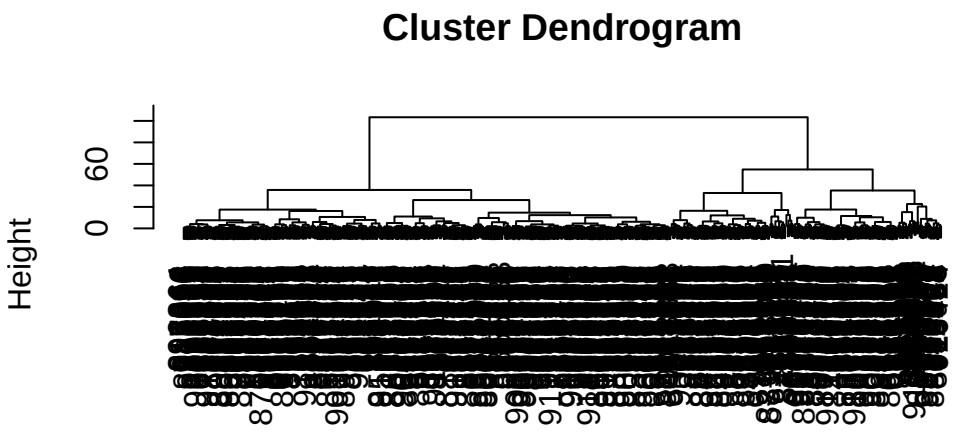


4. Combining methods

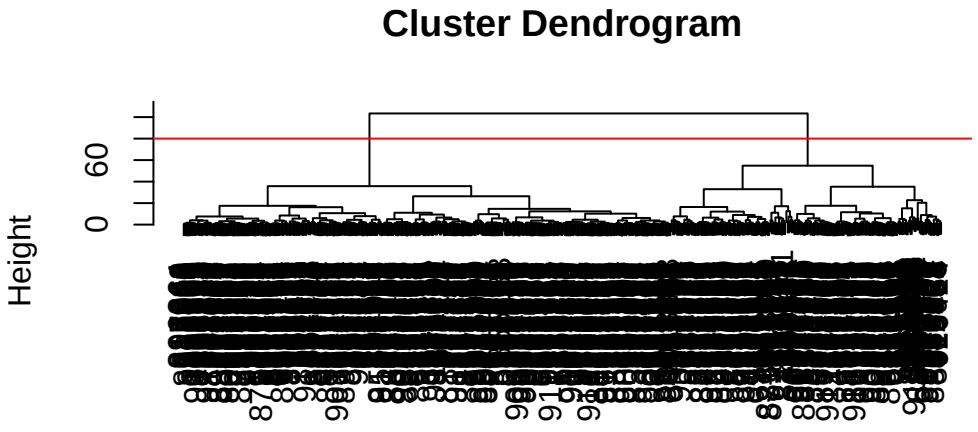
Here we will use the results of PCA as the input to a clustering analysis.

We start with using 3 PCs

```
wisc.pr.hclust <- hclust( dist( wisc.pr$x[,1:3] ), method="ward.D2")
plot(wisc.pr.hclust)
```




```
plot(wisc.pr.hclust)
abline(h=80, col="red")
```



```r
grps <- cutree(wisc.pr.hclust, h=80)
table(grps)
```

```
grps
  1   2
203 366
```

```r
table(diagnosis)
```

```
diagnosis
  B   M
357 212
```

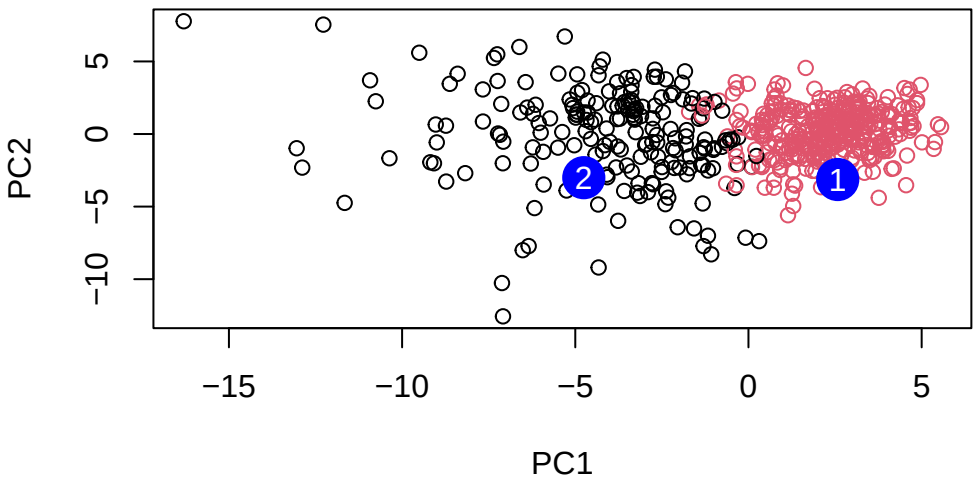
```r
table(grps, diagnosis)
```

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

Prediction

```r
url <- "https://tinyurl.com/new-samples-CSV"
new <- read.csv(url)
npc <- predict(wisc.pr, newdata=new)
```

```r
plot(wisc.pr$x[,1:2], col=grps)
points(npc[,1], npc[,2], col="blue", pch=16, cex=3)
text(npc[,1], npc[,2], c(1,2), col="white")
```


PC2
5
0
−5
−10
−15
−10
−5
0
5
PC1
2
1