Class 8: Breast Cancer Mini Project

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About

In today's lab we will work with fine needle aspiration (FNA) of breast mass data from the University of Wisconsin.

Data Import

```
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
```

Q1. How many patients/individuals are in this dataset?

```
nrow(wisc.df)
```

```
[1] 569
```

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

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

```
[1] 212
```

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

```
  B   M
357 212
```

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

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

```
[1] 31
```

```
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"
```

```
inds <- grep("_mean", colnames(wisc.df))
length(inds)
```

```
[1] 10
```

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

```
 [1] "radius_mean"            "texture_mean"           "perimeter_mean"
 [4] "area_mean"              "smoothness_mean"        "compactness_mean"
 [7] "concavity_mean"         "concave.points_mean"    "symmetry_mean"
[10] "fractal_dimension_mean"
```

Initial Analysis

Before analysis I want to take out the expert diagnoses column (aka the answrer) from our dataset.

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

```
[1] M M M M M M
Levels: B M
```

```
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
842302                   0.11890
842517                   0.08902
84300903                 0.08758
84348301                 0.17300
```

```
84358402                    0.07678
843786                      0.12440
```

Clustering

We can try a kmeans() clustering first

```
km <- kmeans(wisc.data, centers = 2)
table(km$cluster)
```

```
  1   2
131 438
```

```
table(diagnosis)
```

```
diagnosis
  B   M
357 212
```

Cross-table

```
table(km$cluster, diagnosis)
```

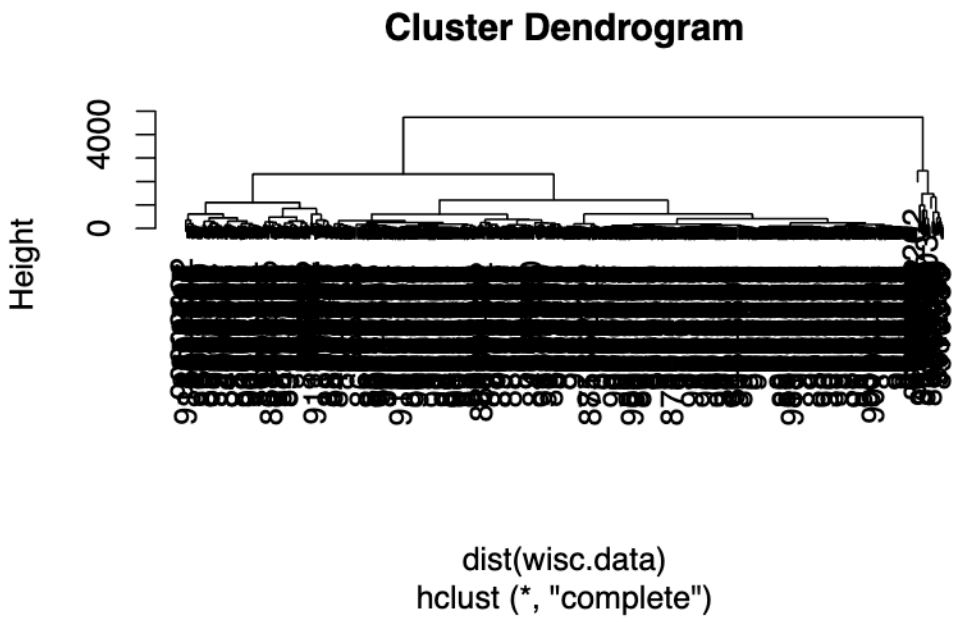
```
   diagnosis
      B   M
  1   1 130
  2 356  82
```

Let's try `hclust()` the key input required for `hclust()` is a distance matrix as produced by the `dist()` function

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

I can make a tree like figure

```
plot(hc)
```



Do we need to scale the data?

We can look at the sd of ach column (original variable)

```
round(apply(wisc.data, 2, sd))
```

```
          radius_mean           texture_mean         perimeter_mean
                    4                      4                     24
            area_mean        smoothness_mean       compactness_mean
                  352                      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
                    2                     45                      0
      compactness_se         concavity_se    concave.points_se
                    0                      0                      0
        symmetry_se   fractal_dimension_se         radius_worst
                    0                      0                      5
      texture_worst        perimeter_worst           area_worst
                    6                     34                    569
```

```
     smoothness_worst       compactness_worst         concavity_worst
                    0                       0                       0
concave.points_worst         symmetry_worst fractal_dimension_worst
                    0                       0                       0
```

Yes we need to scale. We will run `prcomp` with `scale=TRUE`

```
wisc.pr <- prcomp(wisc.data, 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
```

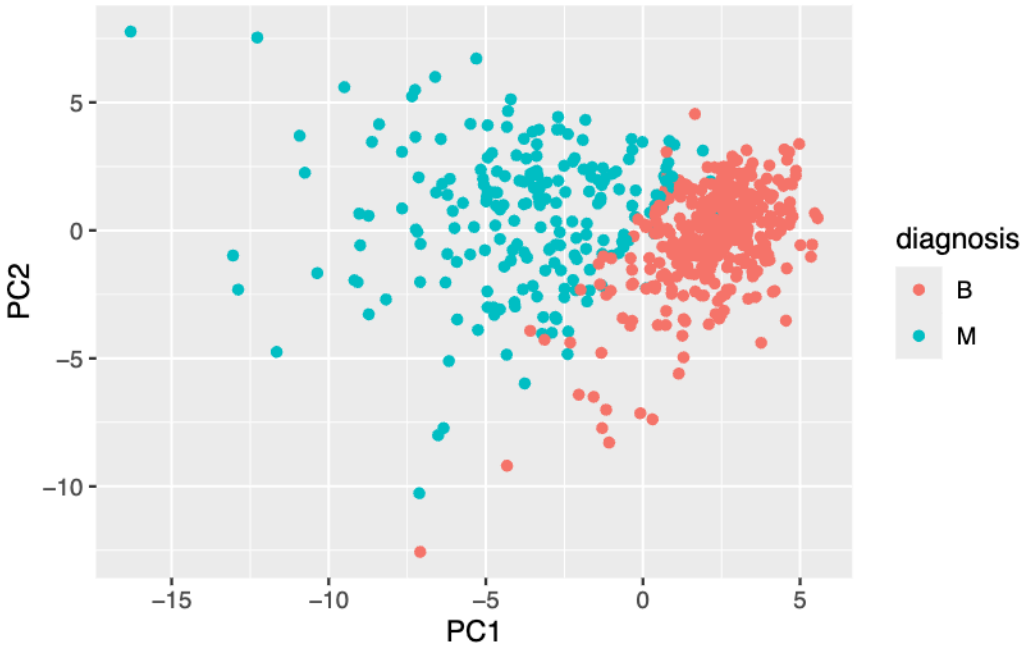
PCA

Generate our main PCA plot (score plot, PC1 vs PC2, plot..)

```
library(ggplot2)

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

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

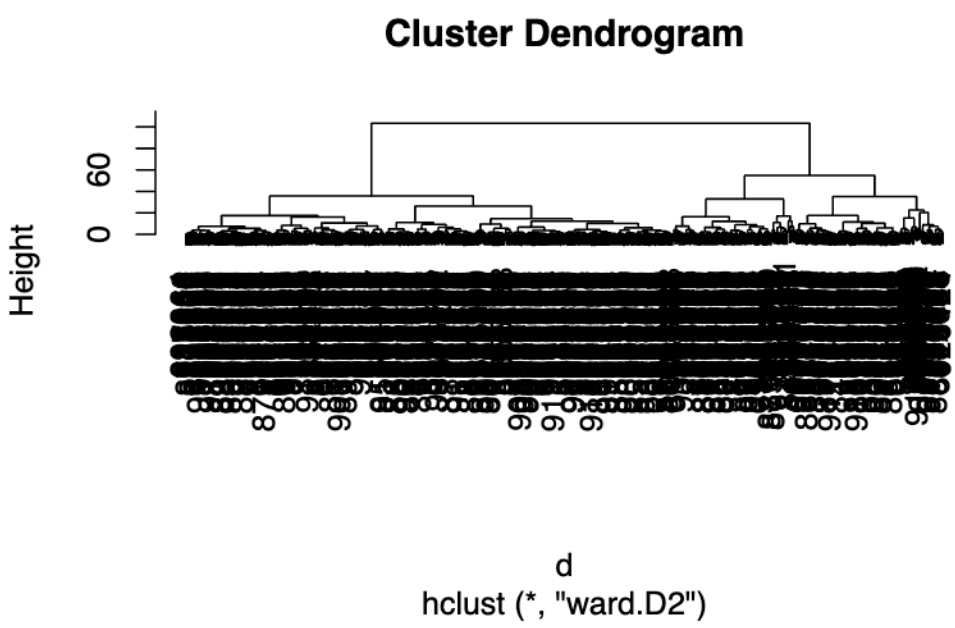


Combining Methods

Clustering on PCA results

Using the minimum number of principal components required to describe at least 90% of the variability in the data, create a hierarchical clustering model with the linkage method="ward.D2". We use Ward's criterion here because it is based on multidimensional variance like principal components analysis. Assign the results to wisc.pr.hclust.

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



To get my clustering result/membership vector I need to "cut" the tree with the `cutree()` function

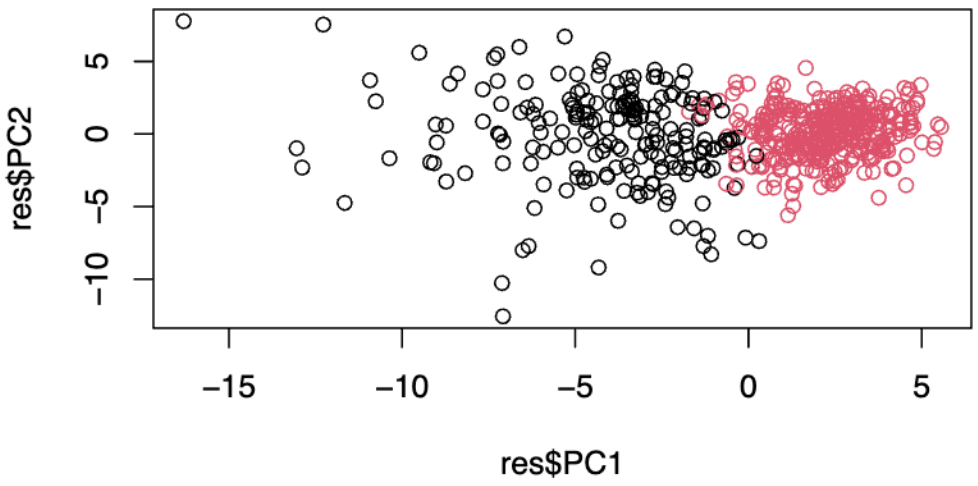
```
grps <- cutree(hc, k=2)
```

Q1. How many patients are in each cluster group?

```
table(grps)
```

```
grps
  1   2
203 366
```

```
plot(res$PC1, res$PC2, col = grps)
```



Q17. Which of your analysis procedures resulted in a clustering model with the best specificity? How about sensitivity?

PCA resulted in better specificity and sensitivity.

Prediction

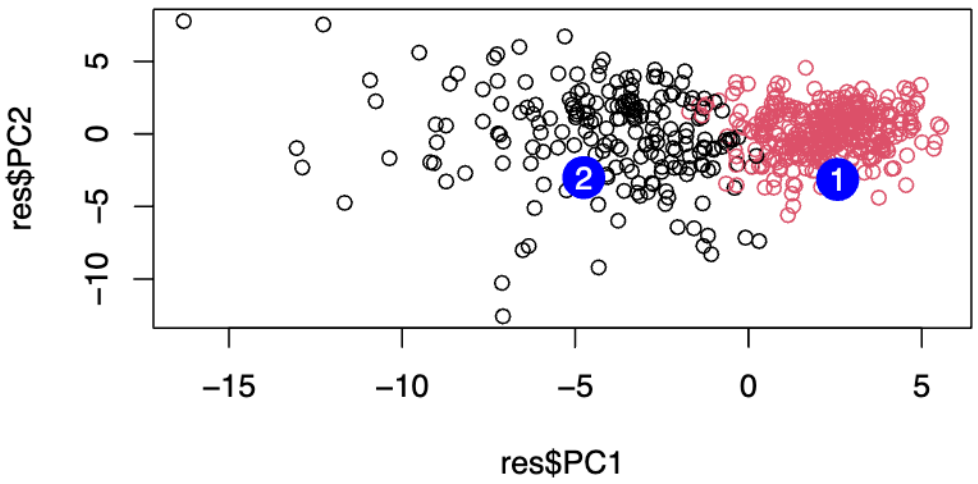
We can use our PCA result (model) to do prediction, that is take new unseen data and project it onto our new PC variables

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

```r
plot(res$PC1, res$PC2, col = grps)
points(npc[,1], npc[,2], col="blue", pch=16, cex=3)
text(npc[,1], npc[,2], labels=c(1, 2), col="white")
```



Q18. Which of these new patients should we prioritize for follow up based on your results?

Follow up with group 2

Summary

Principal Component Analysis (PCA) is a super useful method for analyzing large datasets. It works by finding new variables (PCs) that capture the most variance from the original variables in your dataset.