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 Univesity of Wisconsin.

Data Import

```
fna.data="WisconsinCancer.csv"
wisc.df = read.csv(fna.data, 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
```

Exploratory data analysis

The first step of any data analysis, unsupervised or supervised, is to familiarize yourself with the data.Explore the data you created before (wisc.data and diagnosis) to answer the following questions:

Q1. How many observations/patients/individual samples are in this dataset?

569 Observations

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

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

```
[1] 212
```

table function super useful - it shows 357 binign and 212 malignant

```
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))
inds
```

```
 [1]  2  3  4  5  6  7  8  9 10 11
```

```
length(inds)
```

```
[1] 10
```

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

```
 [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 diagnosis column (a.k.a the answer) from our dataset.

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

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

> this will remove that first diagnosis column and print everything following the first diagnosis column

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

Clustering

We can try kmeans() clustering first.

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

```
table(km$cluster)
```

```
  1   2
131 438
```

Cross-table

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

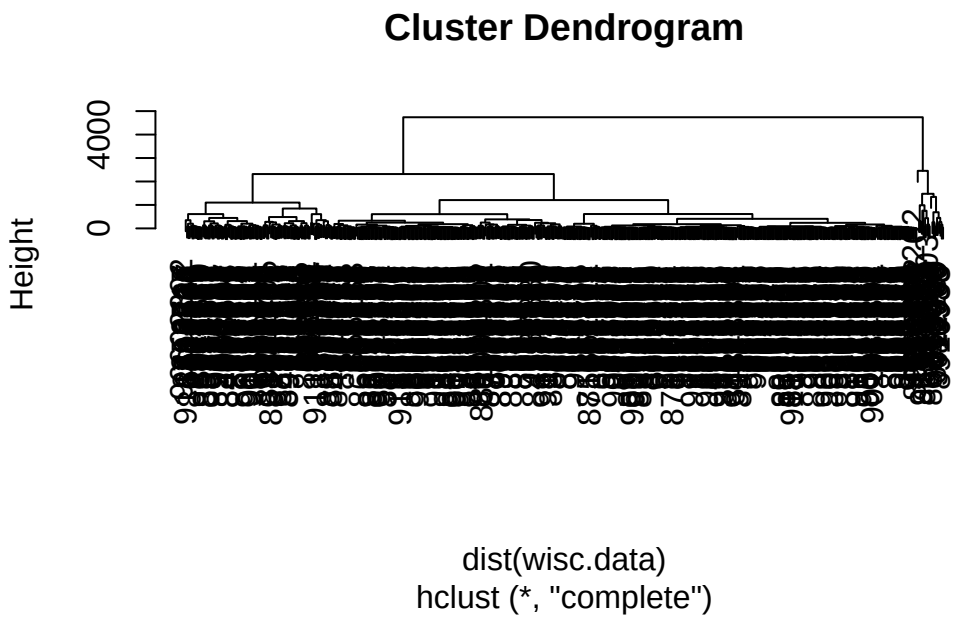
```
   diagnosis
      B   M
  1   1 130
  2 356  82
```

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 fugure

```
plot(hc)
```



PCA

Dp we need to scale the data?

We can look at the sd of each 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)
```

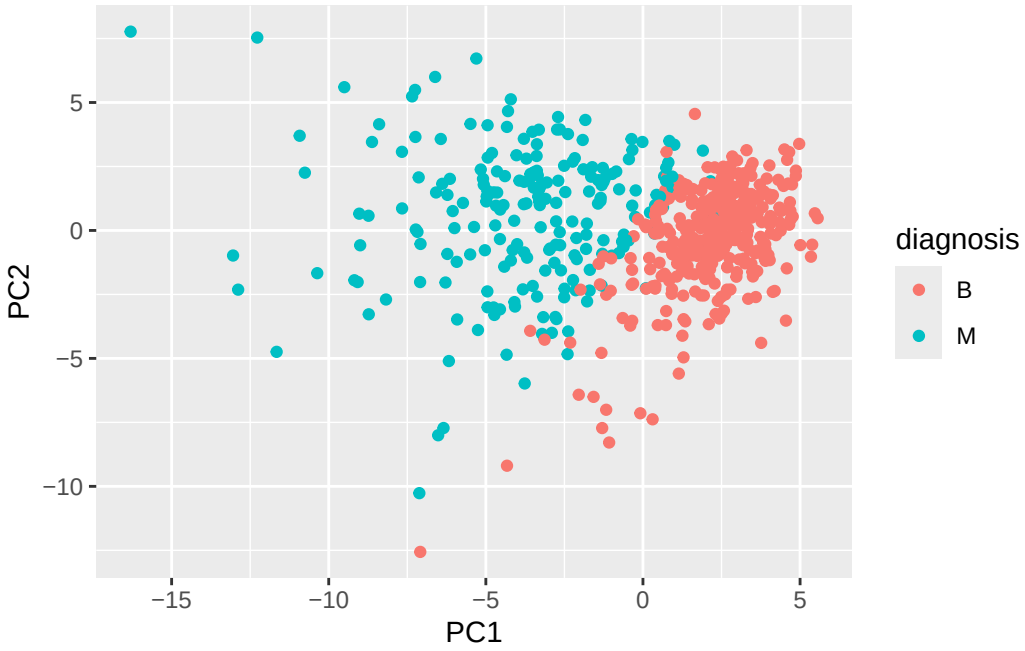
```
Importance of components:
                          PC1    PC2     PC3     PC4     PC5     PC6     PC7
Standard deviation     3.6444 2.3857 1.67867 1.40735 1.28403 1.09880 0.82172
Proportion of Variance 0.4427 0.1897 0.09393 0.06602 0.05496 0.04025 0.02251
Cumulative Proportion  0.4427 0.6324 0.72636 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
```

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()
```



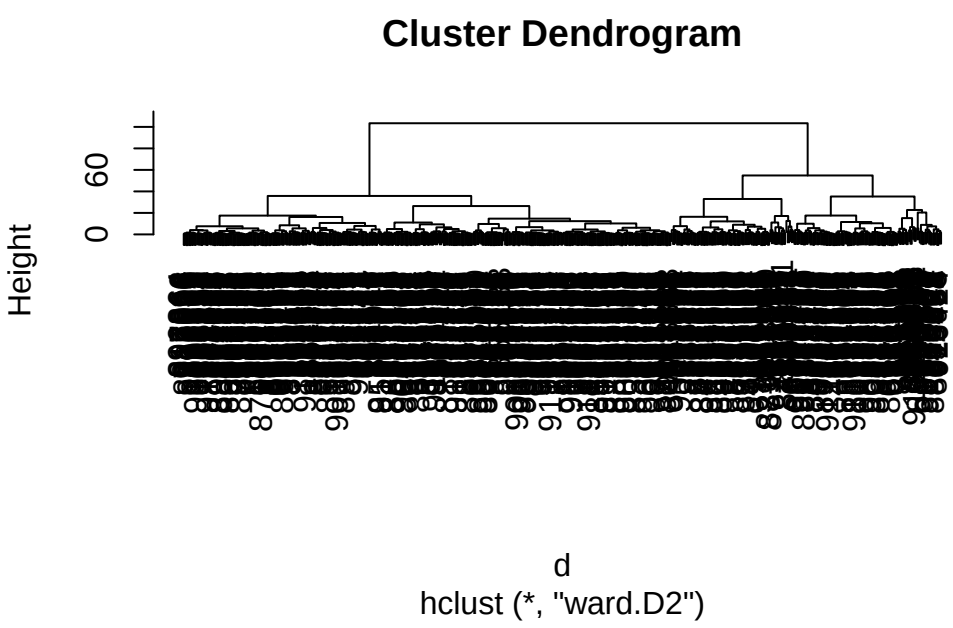
The PCA plot show a separation of Malignant (turquoise) from Benign (red) samples.

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 results/membership vector I need to "cut" the tree with the `cutree()` function.

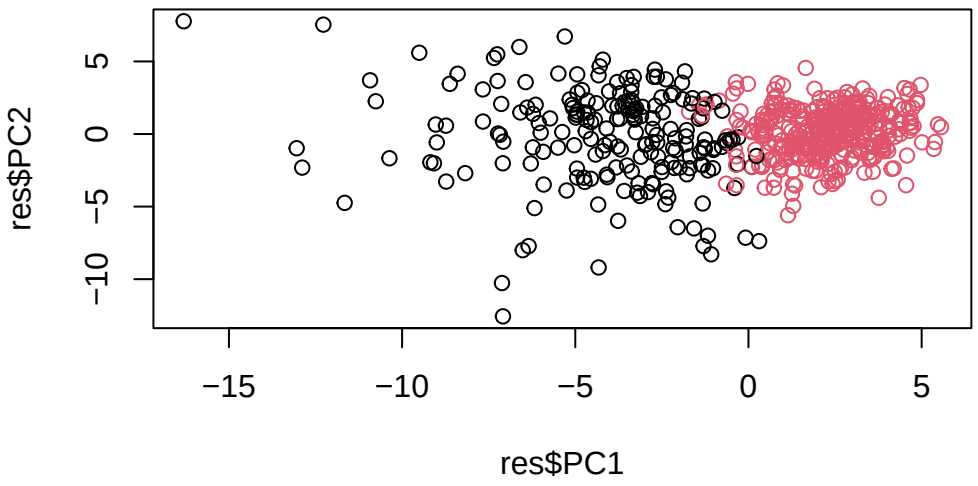
```
grps <- cutree(hc, k=2)
```

Q. How many patients are in each culster?

```
table(grps)
```

```
grps
  1   2
203 366
```

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



Prediction

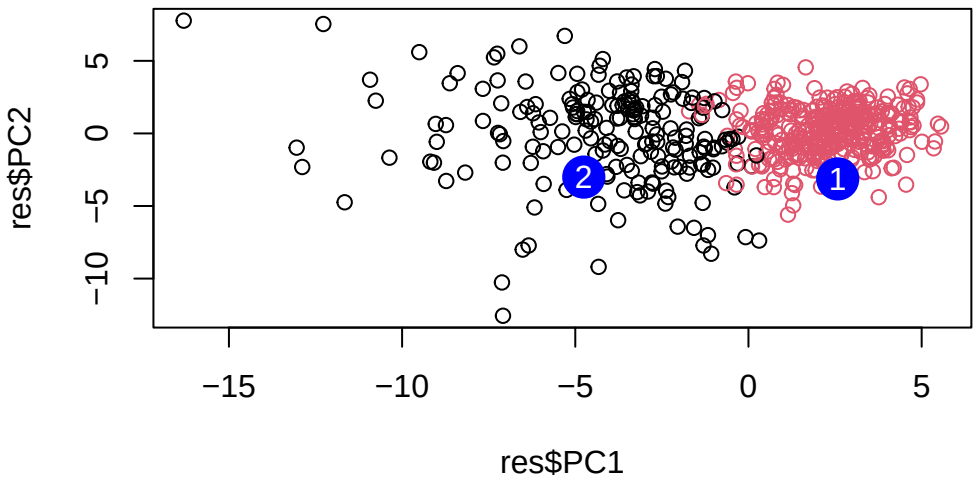
We can use our PCA result (model) to do predictions, that is take new unseen data and project it onto our new PC variables.

```
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")
```



Summary

Principle 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 original variables in your dataset.