Lab8: Unsupervised Learning Mini-Project

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Breast Cancer Dataset Analysis

0. Data import

```
# Save your input data file into your Project directory
fna.data <- "WisconsinCancer.csv"

# Complete the following code to input the data and store as wisc.df
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
```

```r
# The diagnosis column is not needed for the analysis
wisc.data <- wisc.df[,-1]

# Create diagnosis vector for later
```

```r
diagnosis <- as.factor(wisc.df[,1])
```

1. Exploratory Data analysis

> Q1. How many observations are in this dataset?

```r
print(paste("The number of observations is", nrow(wisc.df)))
```

```
[1] "The number of observations is 569"
```

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

```r
print(paste("The number of observations with a malignant diagnosis is",
            sum(wisc.df$diagnosis == "M")))
```

```
[1] "The number of observations with a malignant diagnosis is 212"
```

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

```r
print(paste("The number of variables with '_mean' suffix is",
            length(grep("_mean", names(wisc.df)))))
```

```
[1] "The number of variables with '_mean' suffix is 10"
```

Clustering

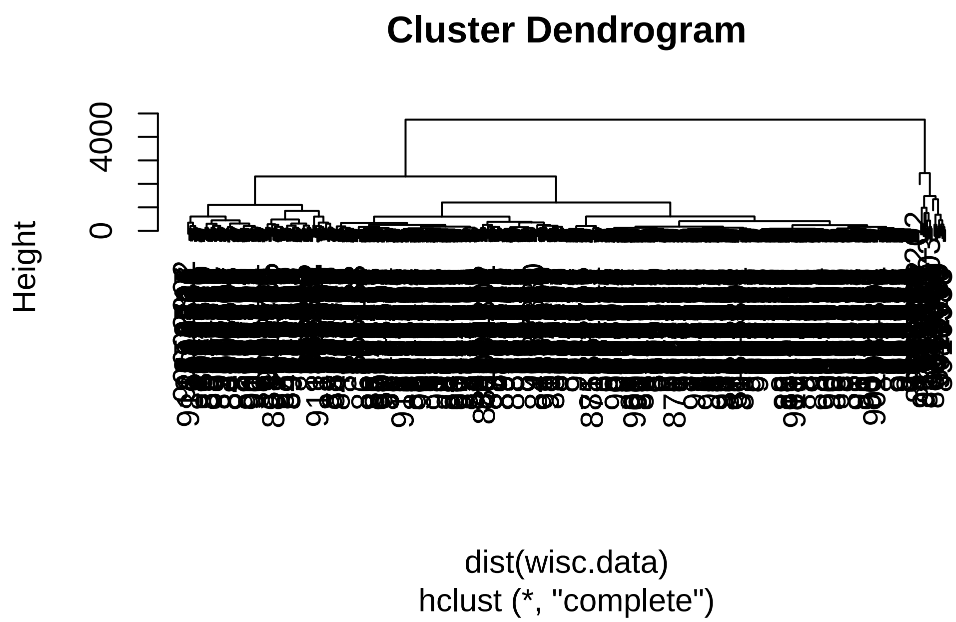
We can try k-means clustering first

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

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

Let's try hierarchical clustering

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



2. Principal Component Analysis

Check if the data needs to be scaled

```r
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 
```

```r
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 
```

The variables use different units and variance and means are thus very different. Scaling is appropriate here.

```r
wisc.pr <- prcomp(wisc.data, scale.=T)
summary(wisc.pr)
```

```
Importance of components:
                          PC1    PC2     PC3     PC4     PC5     PC6     PC7
```

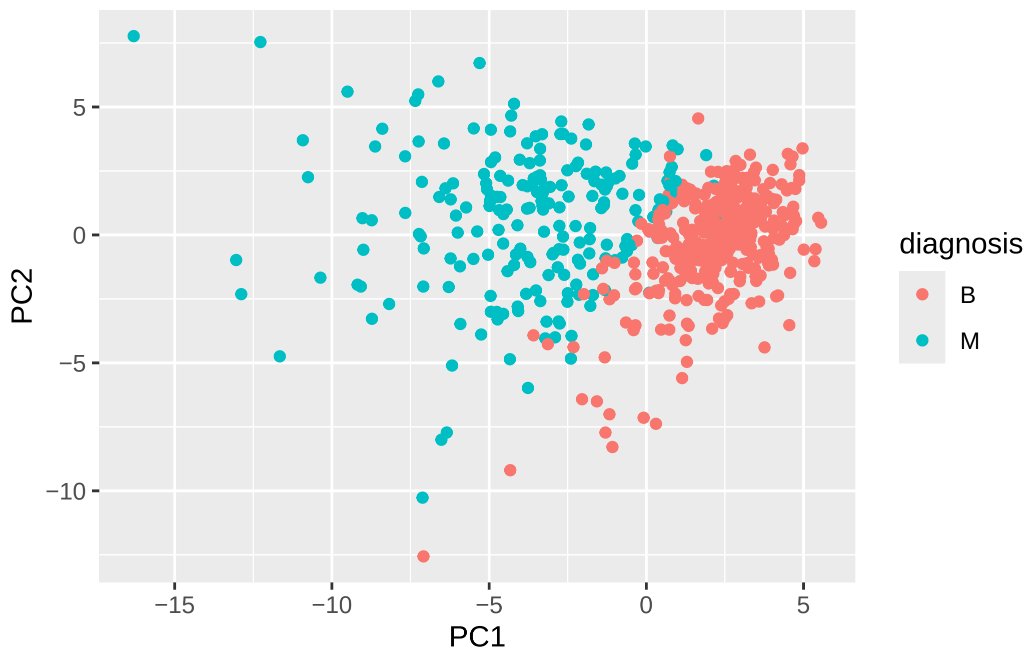
```
Standard deviation     3.6444 2.3857 1.67867 1.40735 1.28403 1.09880 0.82172
Proportion of Variance 0.4427 0.1897 0.09393 0.06602 0.05496 0.04025 0.02251
Cumulative Proportion  0.4427 0.6324 0.72636 0.79239 0.84734 0.88759 0.91010
                           PC8    PC9    PC10   PC11    PC12    PC13    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)…

```r
library(ggplot2)

# Convert pca results to dataframe
res <- as.data.frame(wisc.pr$x)

# Use ggplot
ggplot(res) + aes(x=PC1, y=PC2, col=diagnosis) + geom_point()
```



> Q4. From your results, what proportion of the original variance is captured by the first principal components (PC1)?

```
print(paste("The original variance captured by PC1 is", summary(wisc.pr)$importance[2,1]))
```

```
[1] "The original variance captured by PC1 is 0.44272"
```

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

```
PC.70 <- 1 + sum(unname(summary(wisc.pr)$importance[3,] < 0.7))
print(paste("The number of PCs required for 70% of original variance is", PC.70))
```

```
[1] "The number of PCs required for 70% of original variance is 3"
```

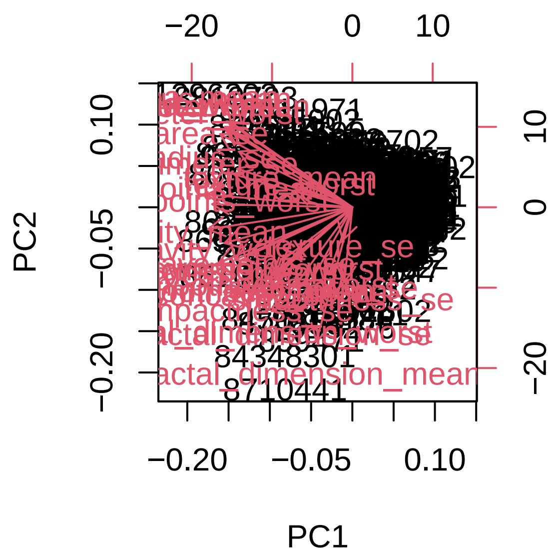
> Q6. How many principal components (PCs) are required to describe at least 90% of the original variance in the data?

```
PC.90 <- 1 + sum(unname(summary(wisc.pr)$importance[3,] < 0.9))
print(paste("The number of PCs required for 90% of original variance is", PC.90))
```

```
[1] "The number of PCs required for 90% of original variance is 7"
```

Now we can plot the PCA using `biplot()`

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



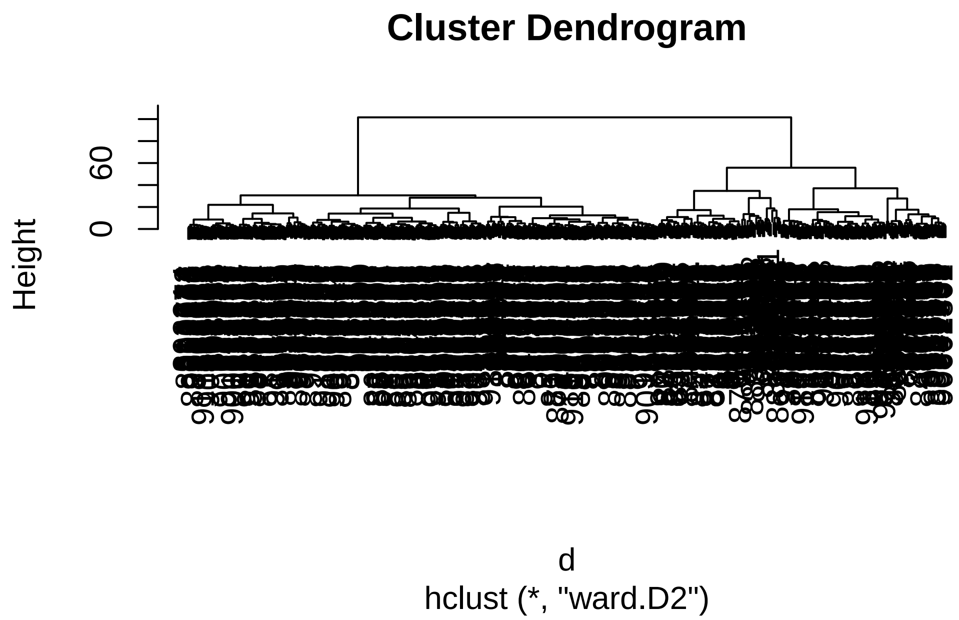
> Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?

This plot is very hard to read due to overcrowding. Too many data points (patients) and several original variables that make it difficult to observe trends. Nothing really stands out on this plot.

5. Combining Methods

Clustering on PCA results

```r
d <- dist(wisc.pr$x[,1:7])
hc <- hclust(d, method="ward.D2")
plot(hc)
```



Use `cutree()` to get membership vector

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

print(paste("There are", table(grps)[1], "patients in Group 1 and", table(grps)[2], "patie
```

```
[1] "There are 216 patients in Group 1 and 353 patients in Group 2"
```

7. Prediction

Use PCA result to do predictions, use unseen data and project it onto our new PC variables.

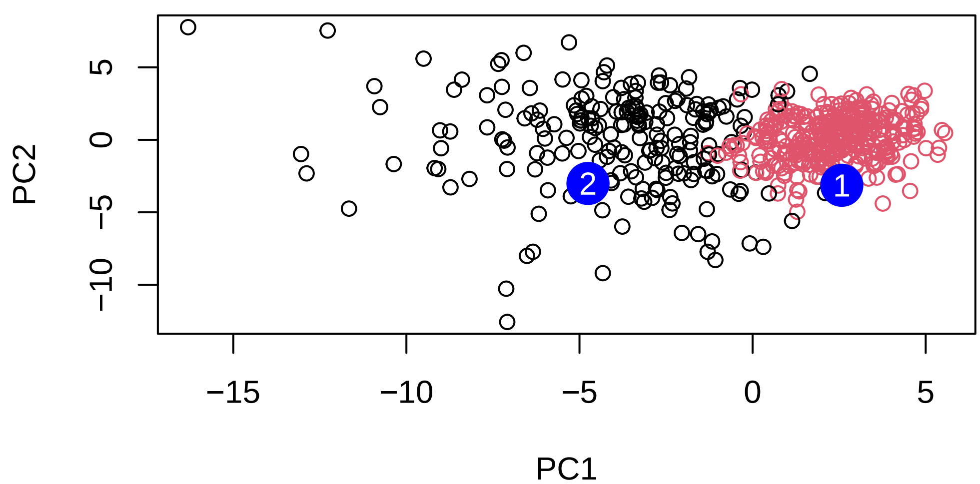
```
url <- "https://tinyurl.com/new-samples-CSV"
new <- read.csv(url)
npc <- predict(wisc.pr, newdata=new)
npc
```

```
           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
```

Now plot these two patients on a map against original data.

```
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")
```



Summary

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.