Class 08: Breast Cancer Mini Project

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Background

The goal of this mini-project is for you to explore a complete analysis using the unsupervised learning techniques covered in class. We'll extend what we learned by combining PCA as a preprocessing step to clustering using data that consist of measurements of cell nuclei of human breast masses. This expands on our RNA-Seq analysis from last day.

The data itself comes from the Wisconsin Breast Cancer Diagnostic Data Set first reported by K. P. Benne and O. L. Mangasarian: "Robust Linear Programming Discrimination of Two Linearly Inseparable Sets".

Values in this data set describe characteristics of the cell nuclei present in digitized images of a fine needle aspiration (FNA) of a breast mass.

Data import

The data is available as a CSV from the class website:

```r
# Import data
fna.data <- "WisconsinCancer.csv"
wisc.df <- read.csv(fna.data, row.names=1)
```

Make sure we do not include patient (sample) ID for the further analysis.

```r
diagnosis <- as.factor(wisc.df$diagnosis)
wisc.data <- wisc.df[, -1]
wisc.data <- subset(wisc.data, select = -X)
```

Q1. How many observations are in this dataset?

There are 569 observations in this dataset.

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

There are 212 observations.

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

There are 10 variables with _mean.

Principal Component Analysis (PCA)

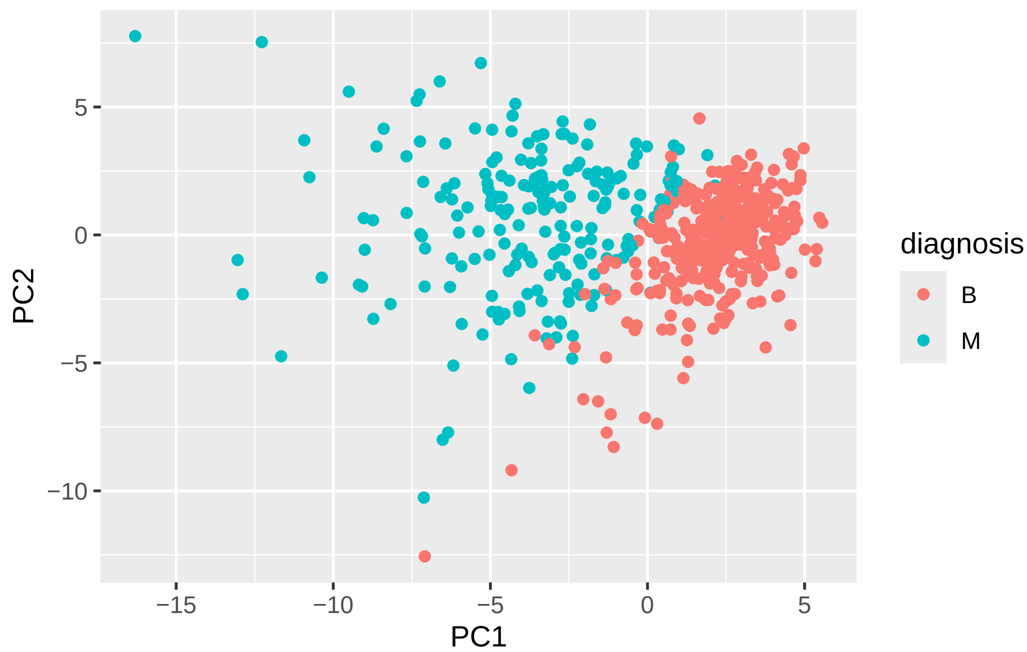
The main function in base R for PCA is called `prcomp()`. A optional argument `scale` should nearly always be switched to `scale=TRUE` for this function.

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

Let's make our main result figure - the "PC plot"or "score plot", "ordienation plot" ...

```r
library(ggplot2)

ggplot(wisc.pr$x, aes(PC1, PC2, col=diagnosis)) +
  geom_point()
```

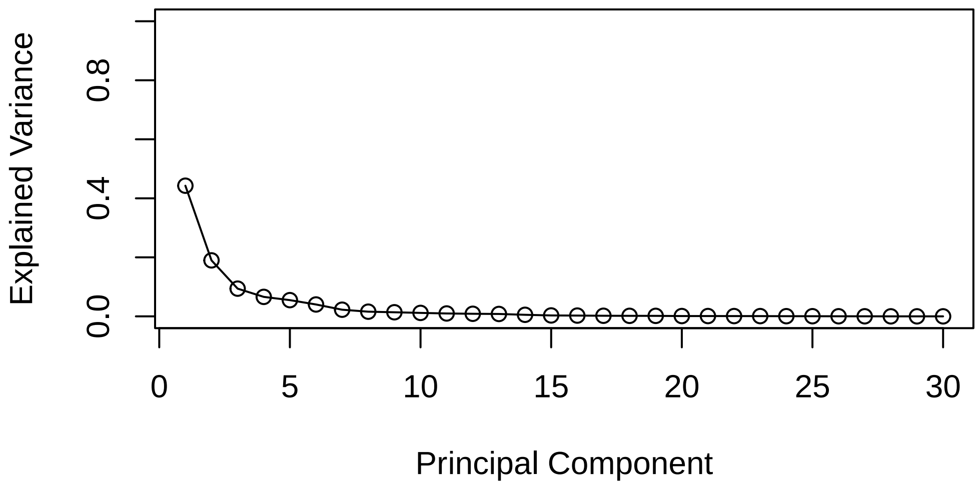


Q4. From your results, what proportion of the original variance is captured by the first principal components (PC1)?

Explained variance is 44.2720256%.

```
pve <- wisc.pr$sdev^2 / sum(wisc.pr$sdev^2)

# Plot variance explained for each principal component
plot(pve, xlab = "Principal Component",
     ylab = "Explained Variance",
     ylim = c(0, 1), type = "o")
```



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

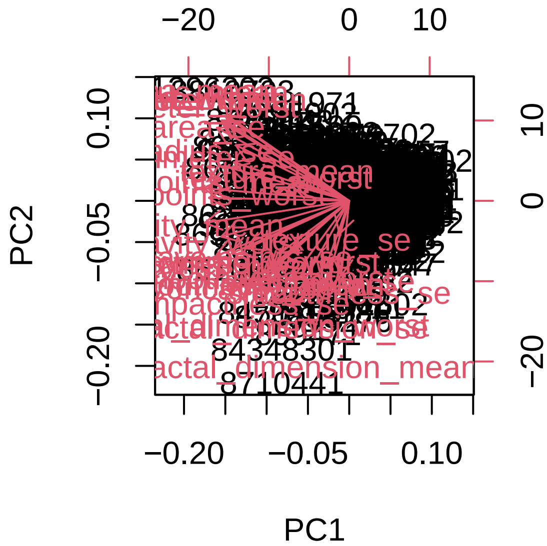
3 PCs are required to describe at least 70% of the original variance.

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

7 PCs are required to describe at least 90% of the original variance.

Interpreting PCA results

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



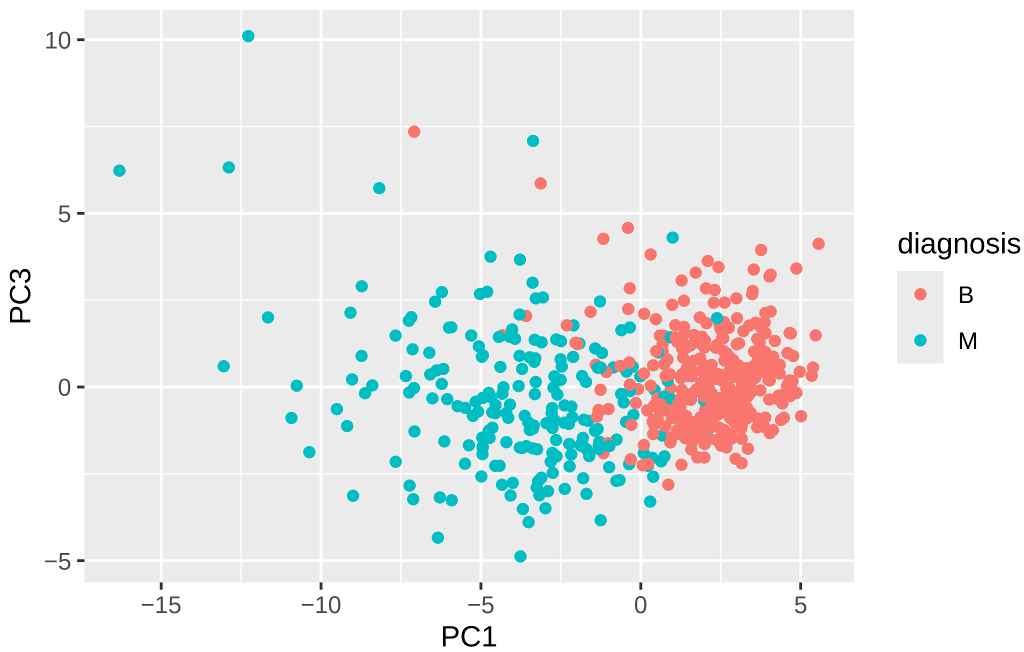
> Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?

Rownames are used to label each dots in the plot, which makes us hard to understand.

> Q8. Generate a similar plot for principal components 1 and 3. What do you notice about these plots?

```
library(ggplot2)

ggplot(wisc.pr$x, aes(PC1, PC3, col=diagnosis)) +
  geom_point() +
  labs(x="PC1", y="PC3")
```



> Q9. 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? This tells us how much this original feature contributes to the first PC.

It is -0.26. We can use `wisc.pr$rotation[, 1]['concave.points_mean']`.

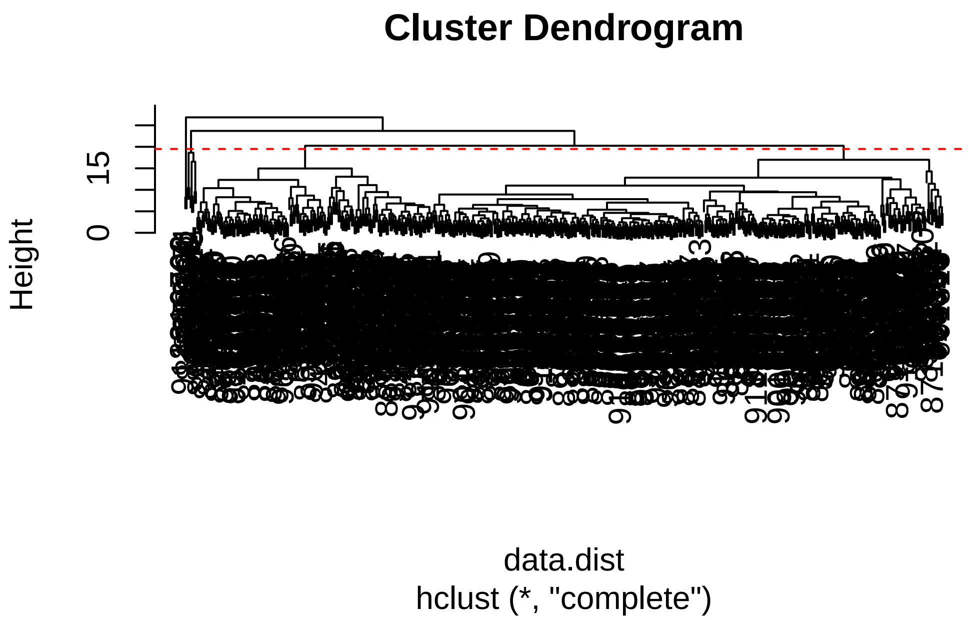
Hierarchical Clustering

```
data.scaled <- scale(wisc.data)
data.dist <- dist(data.scaled)
wisc.hclust <- hclust(data.dist, method="complete")
```

> Q10. Using the plot() and abline() functions, what is the height at which the clustering model has 4 clusters?

The height is 19.5.

```
plot(wisc.hclust)
abline(h = 19.5, col="red", lty=2)
```

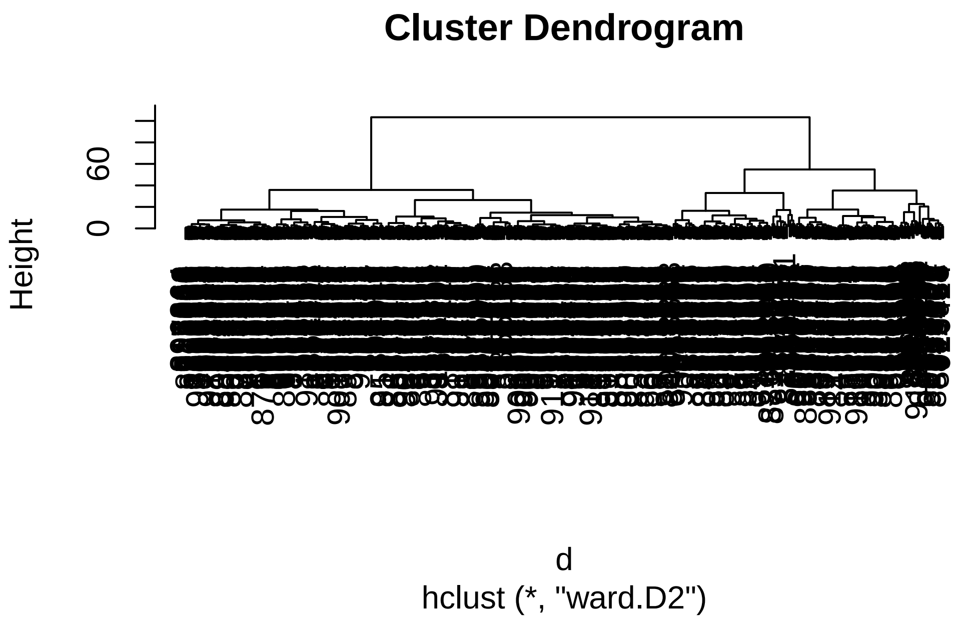



```r
grps1 <- cutree(wisc.hclust, k = 4)
table(grps1, diagnosis)
```

```
     diagnosis
grps1   B   M
    1  12 165
    2   2   5
    3 343  40
    4   0   2
```

Combining PCA + Hierarchical Clustering

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




```r
grps2 <- cutree(wisc.pr.hclust, k = 2)
```

Make a wee “cross-table”

```r
table(grps2, diagnosis)
```

```
     diagnosis
grps2   B   M
    1  24 179
    2 333  33
```

TP: 179 FP: 24

Sensitivity: TP / (TP+FN)

> Q14. How well do the hierarchical clustering models you created in previous sections (i.e. before PCA) do in terms of separating the diagnoses? Again, use the table() function to compare the output of each model (wisc.km$cluster and wisc.hclust.clusters) with the vector containing the actual diagnoses.

PCA shows the better classification performance since it makes data to be normalized, scaled, and the variables to be uncorrelated with each other.

```r
print("Previous (raw data) version")
```

```
[1] "Previous (raw data) version"
```

```r
table(grps1, diagnosis)
```

```
     diagnosis
grps1   B   M
    1  12 165
    2   2   5
    3 343  40
    4   0   2
```

```r
print("Current (pca data) version")
```

```
[1] "Current (pca data) version"
```

```r
table(grps2, diagnosis)
```

```
     diagnosis
grps2   B   M
    1  24 179
    2 333  33
```