UNSUPERVISED LEARNING IN R

Introduction to the case study

Objectives

- Complete analysis using unsupervised learning
  - Reinforce what you've already learned
  - Add steps not covered before (e.g. preparing data, selecting good features for supervised learning)
  - Emphasize creativity

Example use case

- Human breast mass data:
  - Ten features measured of each cell nuclei
  - Summary information is provided for each group of cells
  - Includes diagnosis: benign (not cancerous) and malignant (cancerous)

Will not use this for modeling, as it is the target variable

Source: K. P. Bennett and O. L. Mangasarian: "Robust Linear Programming Discrimination of Two Linearly Inseparable Sets"

Overall steps

- Download data and prepare data for modeling
- Exploratory data analysis (# observations, # features, etc.)
- Perform PCA and interpret results
- Complete two types of clustering
- Understand and compare the two types
- Combine PCA and clustering

Review: PCA in R

```
> pr.iris <- prcomp(x = iris[-5], scale = FALSE, center = TRUE)
> summary(pr.iris)
Importance of components:
                          PC1     PC2    PC3     PC4
Standard deviation     2.0563 0.49262 0.2797 0.15439
Proportion of Variance 0.9246 0.05307 0.0171 0.00521
Cumulative Proportion  0.9246 0.97769 0.9948 1.00000
```

Unsupervised learning is open-ended

- Steps in this use case are only one example of what can be done
- There are other approaches to analyzing this dataset

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Let’s practice!

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PCA review and next steps

Review thus far

- Downloaded data and prepared it for modeling
- Exploratory data analysis
- Performed principal component analysis

Next steps

- Complete hierarchical clustering
- Complete k-means clustering
- Combine PCA and clustering
- Contrast results of hierarchical clustering with diagnosis
- Compare hierarchical and k-means clustering results
- PCA as a pre-processing step for clustering

Review: Hierarchical clustering in R

```
> # Calculates similarity as Euclidean distance between observations
> s <- dist(x)
> # Returns hierarchical clustering model
> hclust(s)

Call:
hclust(d = s)

Cluster method   : complete
Distance         : euclidean
Number of objects: 50
```

x is a data matrix

Review: k-means in R

```
> # k-means algorithm with 5 centers, run 20 times
> kmeans(x, centers = 5, nstart = 20)
```

- One observation per row, one feature per column
- k-means has a random component
- Run algorithm multiple times to improve odds of the best model

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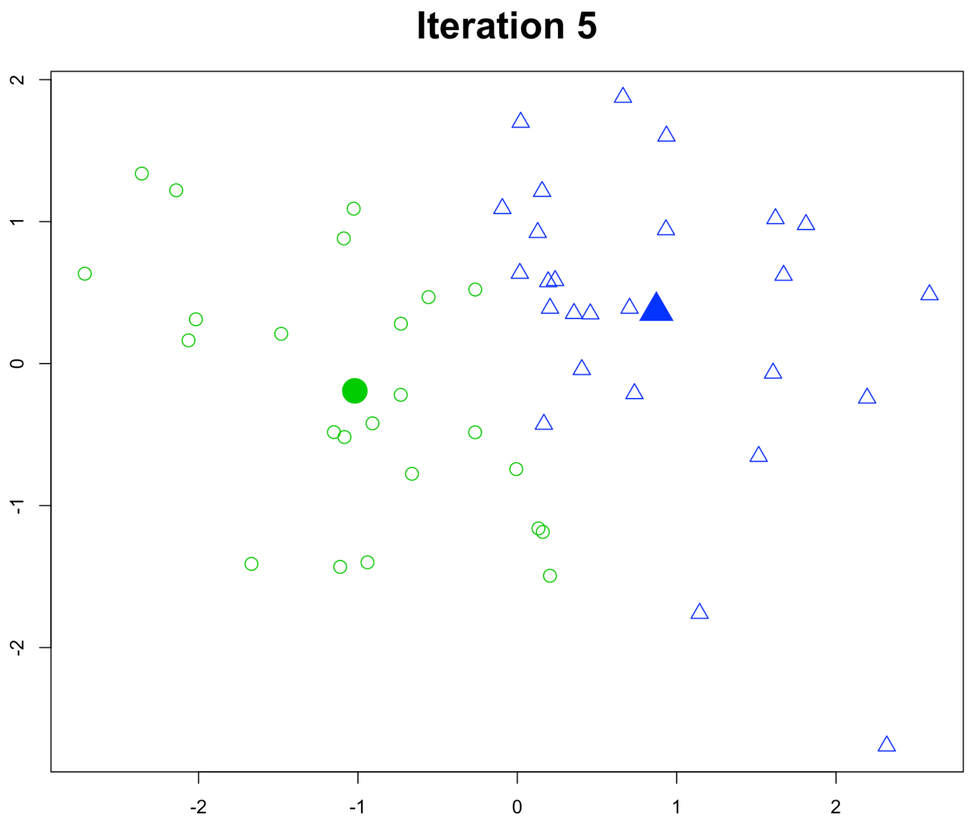
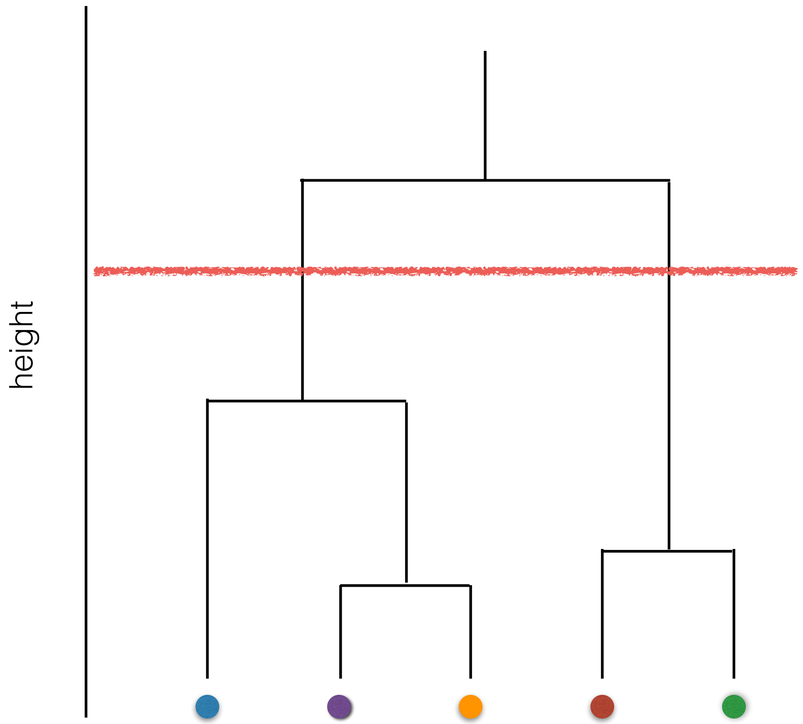
Wrap-up and review

Case study wrap-up

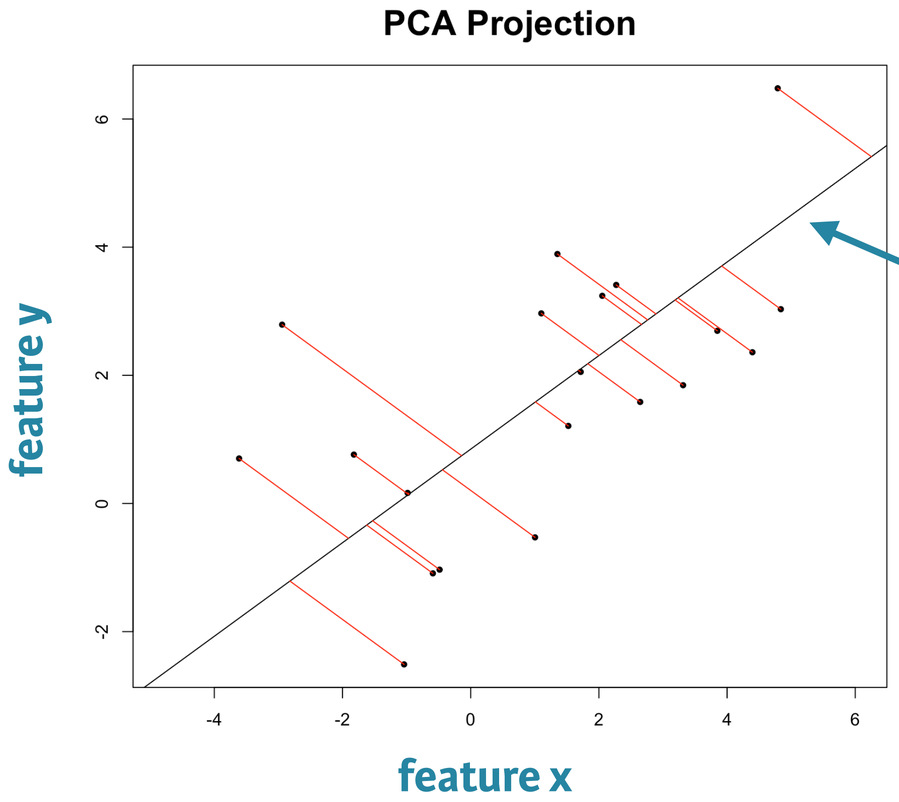
- Entire data analysis process using unsupervised learning
- Creative approach to modeling
- Prepared to tackle real world problems

Types of clustering





Dimensionality reduction

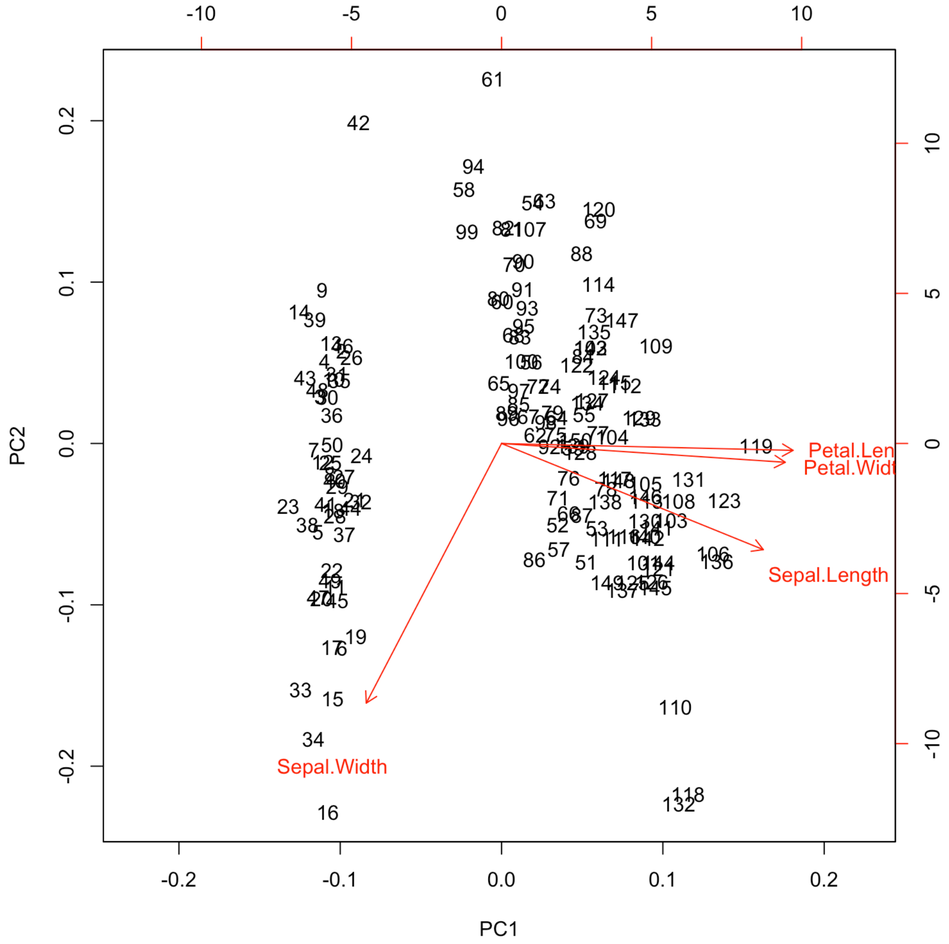


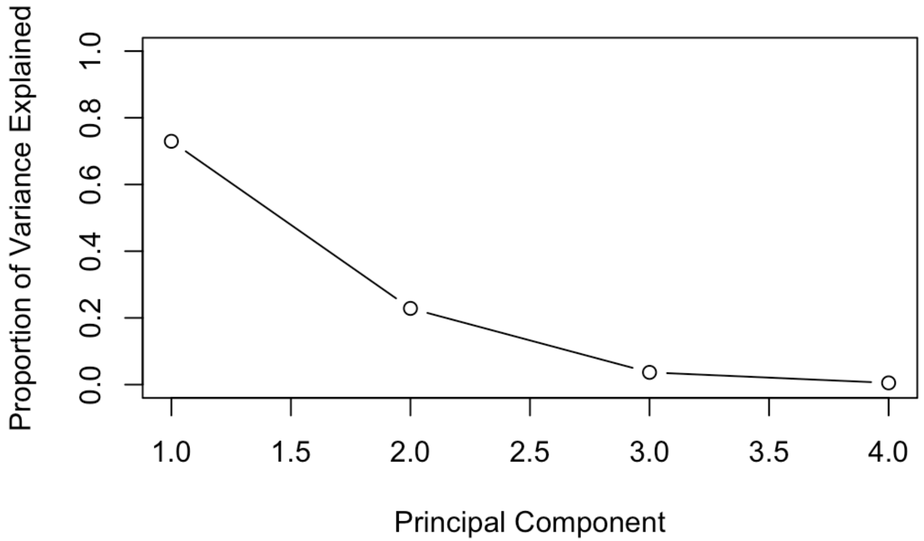
line represents new feature z,
a linear combination of x and y

Model selection

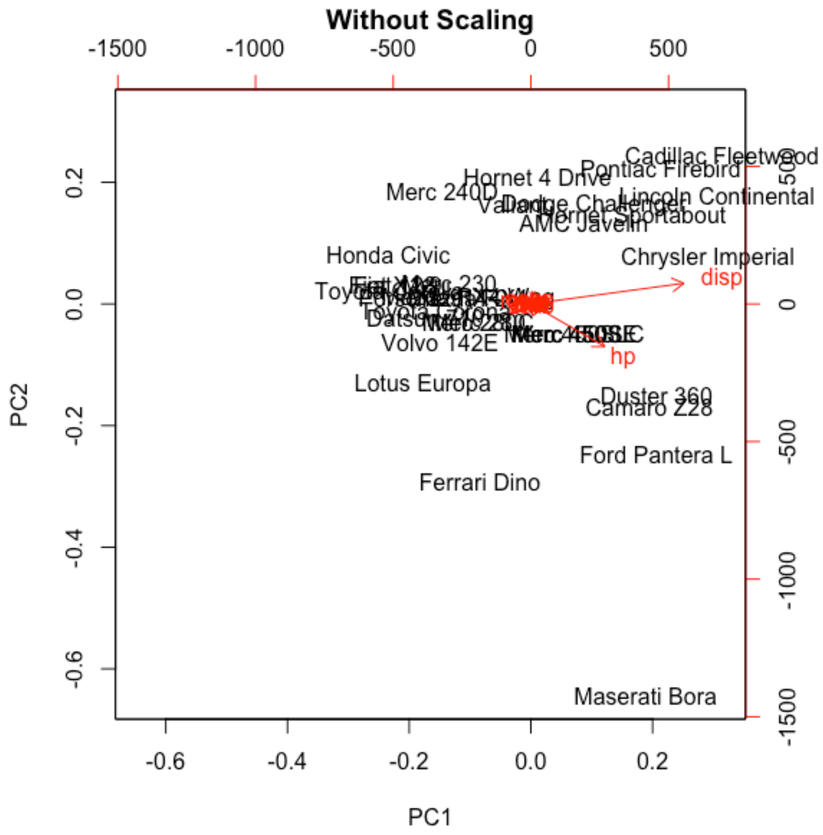
```
# Initialize total within sum of squares error: wss
> wss <- 0
>
# Look over 1 to 15 possible clusters
> for (i in 1:15) {
    # Fit the model: km.out
    km.out <- kmeans(pokemon, centers = i, nstart = 20, iter.max = 50)
    # Save the within cluster sum of squares
    wss[i] <- km.out$tot.withinss
  }
>
# Produce a scree plot
> plot(1:15, wss, type = "b",
       xlab = "Number of Clusters",
       ylab = "Within groups sum of squares")
```

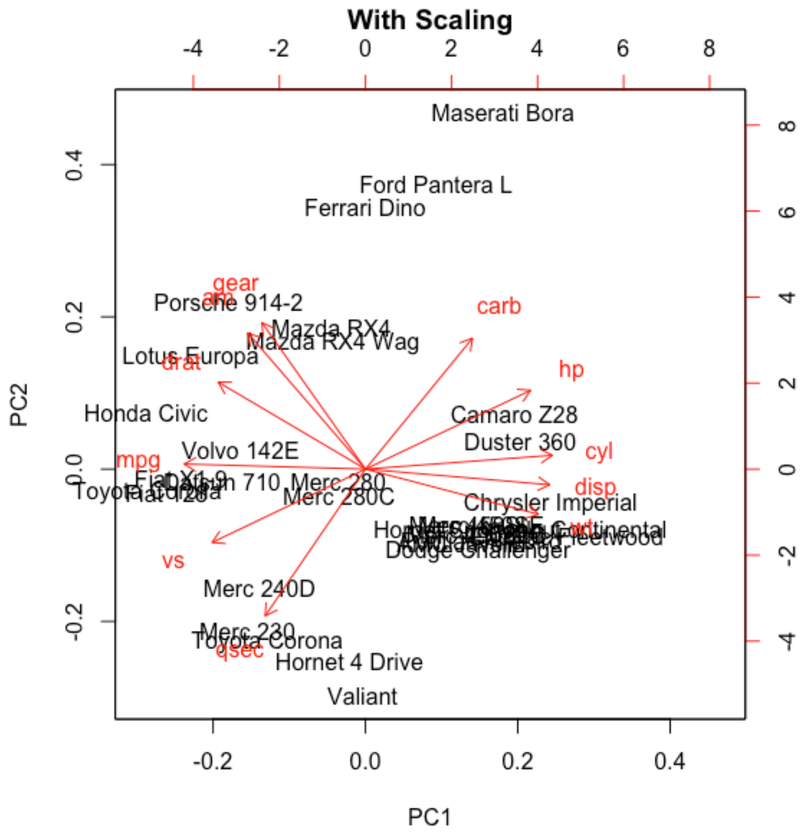
Interpreting PCA results





Importance of scaling data





Course review

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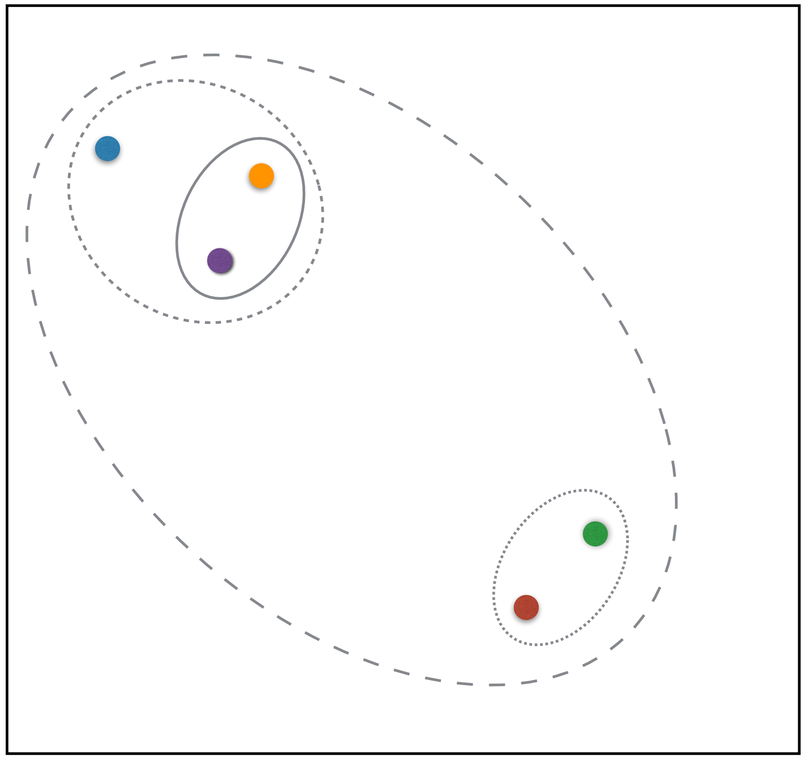
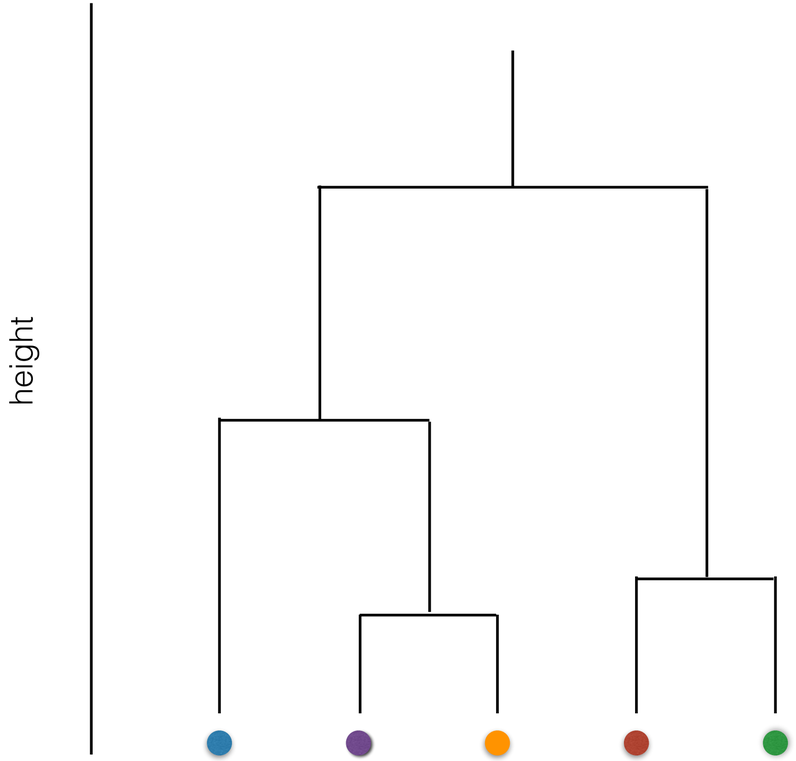
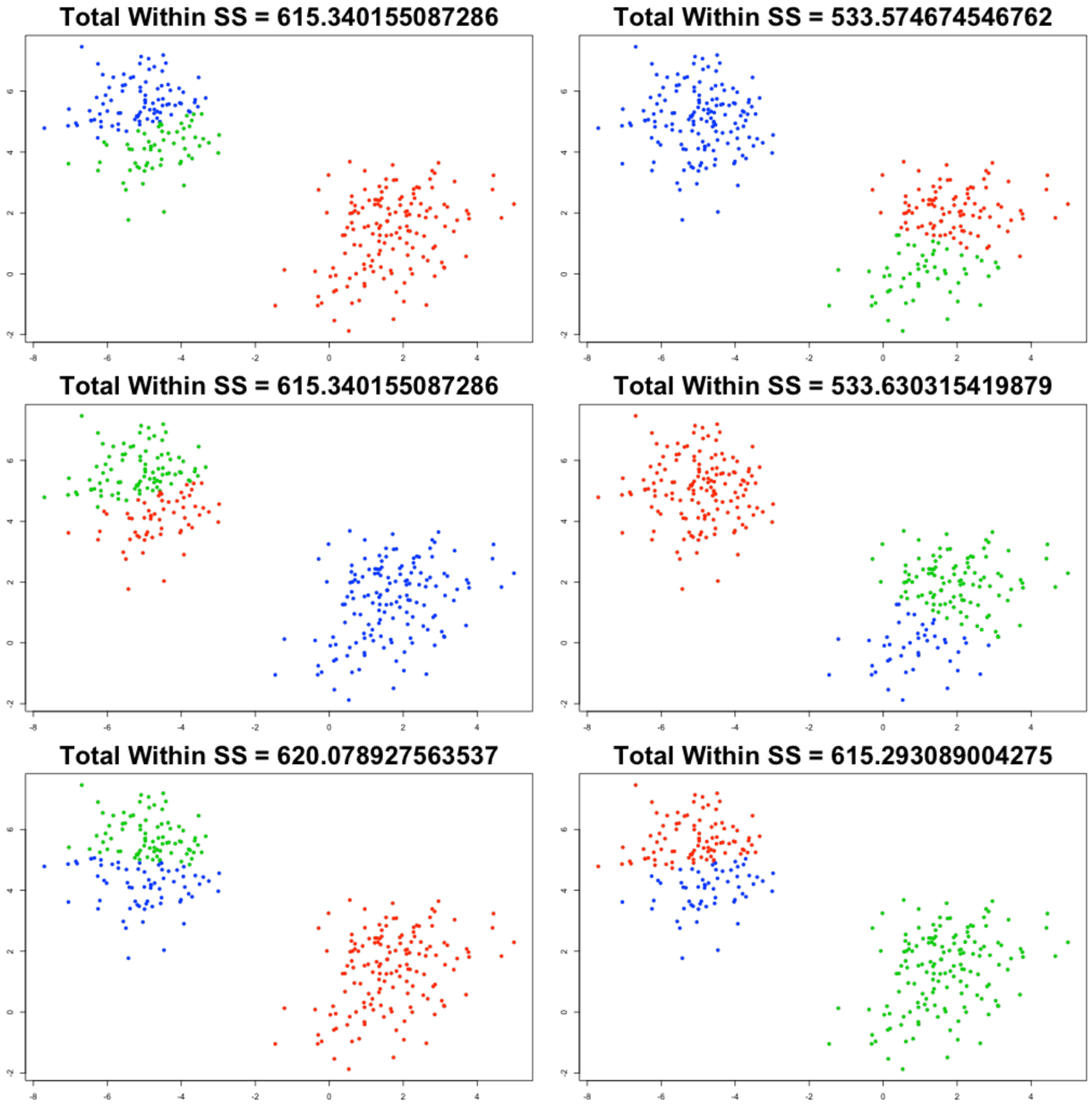
```

Dendrogram

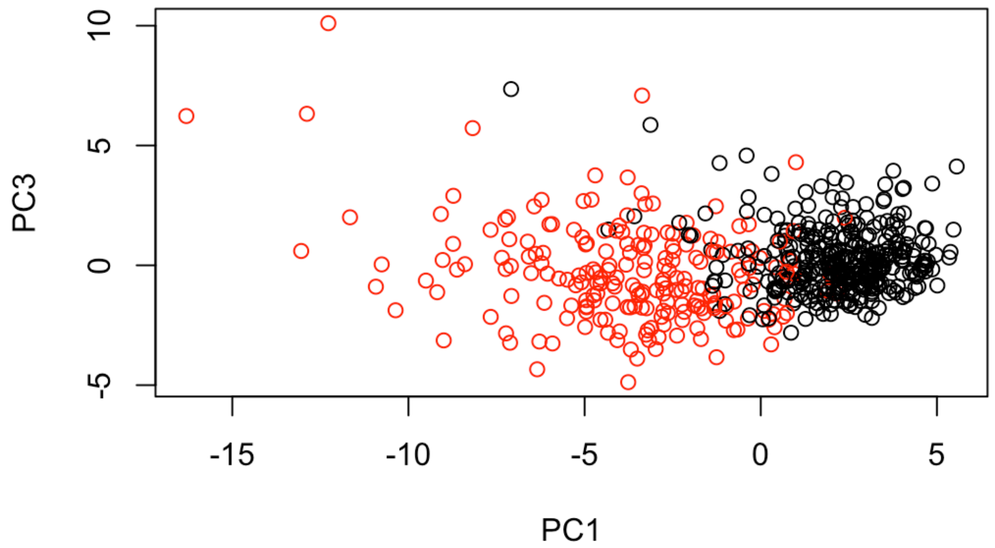





Total Within SS = 615.340155087286
Total Within SS = 533.574674546762
Total Within SS = 615.340155087286
Total Within SS = 533.630315419879
Total Within SS = 620.078927563537
Total Within SS = 615.293089004275

Course review

```
> # Repeat for components 1 and 3
> plot(wisc.pr$x[, c(1, 3)], col = (diagnosis + 1),
       xlab = "PC1", ylab = "PC3")
```



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Thanks!