UNSUPERVISED LEARNING IN R

Welcome to the course!

Chapter 1 overview

- Unsupervised learning
- Three major types of machine learning
- Execute one type of unsupervised learning using R

Types of machine learning

- Unsupervised learning
  - Finding structure in unlabeled data
- Supervised learning
  - Making predictions based on labeled data
  - Predictions like regression or classification
- Reinforcement learning

Labeled vs. unlabeled data

Features

Label

Observations

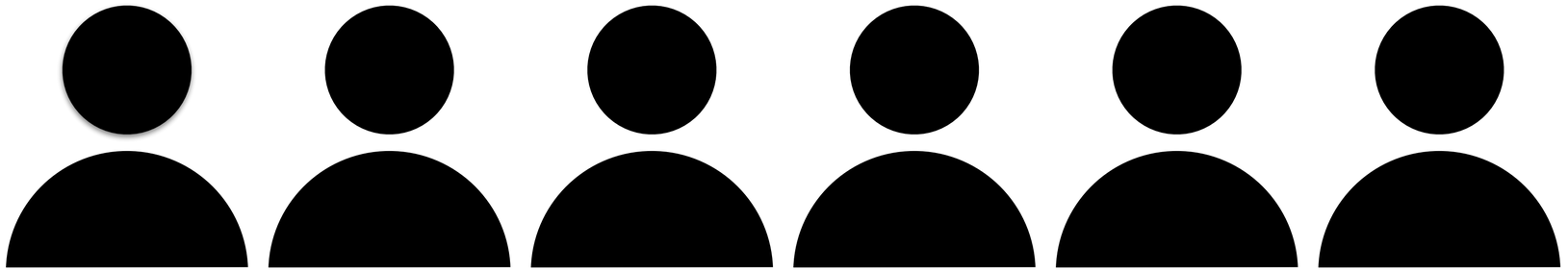
Color	Shape	Size (cm)	Group
Blue	Square	10	1
Red	Ellipse	2.4	1
Red	Ellipse	20.7	2

Unlabeled data

Sample from Murphy, Machine Learning: A Probabilistic Perspective

Unsupervised learning

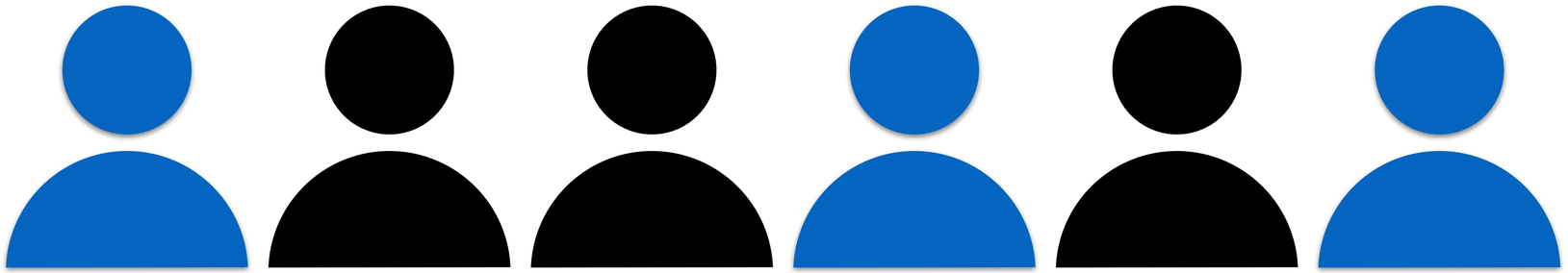
- Finding homogenous subgroups within larger group



People have features such as income, education attainment, and gender

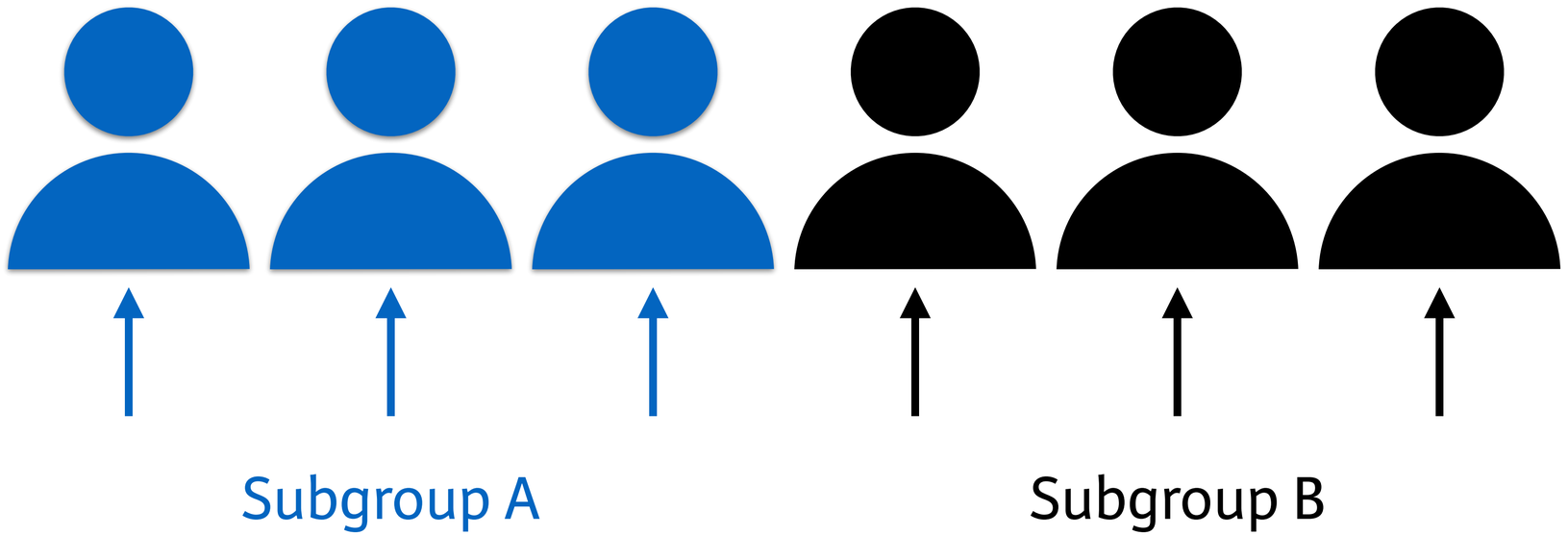
Unsupervised learning

- Finding homogenous subgroups within larger group



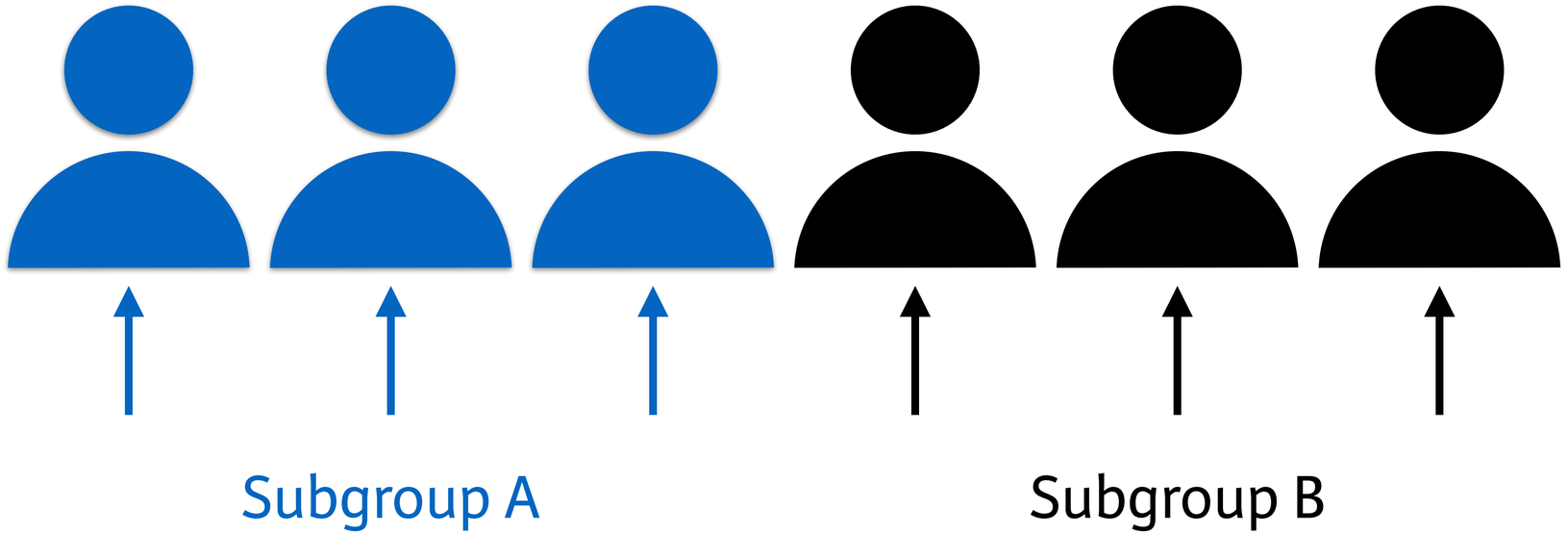
Unsupervised learning

- Finding homogenous subgroups within larger group



Unsupervised learning

- Finding homogenous subgroups within larger group
  - Clustering



Clustering examples

Unsupervised learning

- Finding homogenous subgroups within larger group
  - Clustering
- Finding patterns in the features of the data
  - Dimensionality reduction

Dimensionality reduction

- Find patterns in the features of the data
- Visualization of high dimensional data
- Pre-processing before supervised learning

Challenges and benefits

- No single goal of analysis
- Requires more creativity
- Much more unlabeled data available than cleanly labeled data

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Let’s practice!

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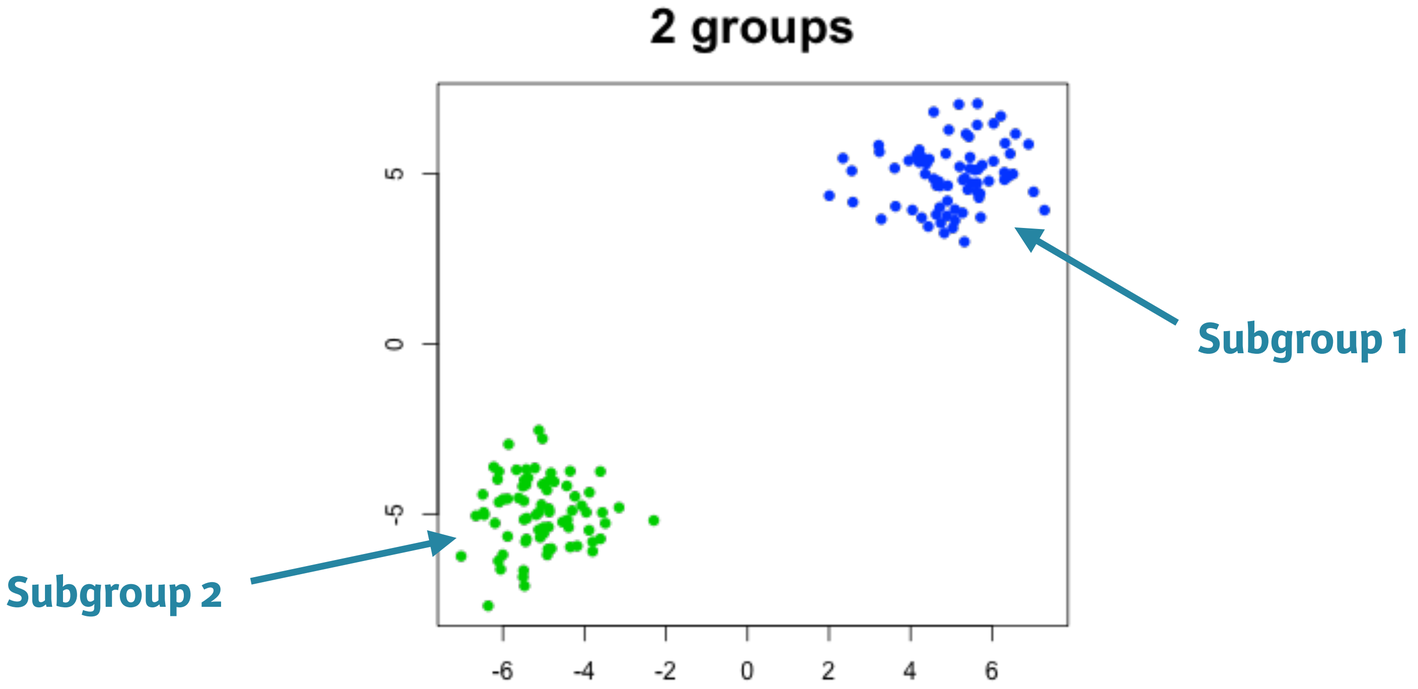
Introduction to k-means clustering

k-means clustering algorithm

- First of two clustering algorithms covered in this course
- Breaks observations into pre-defined number of clusters



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

First exercises

- First exercise uses synthetic data
- Synthetic data generated from 3 subgroups
- Selecting the best number of subgroups for k-means
- Example with more fun data later in the chapter

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Let’s practice!

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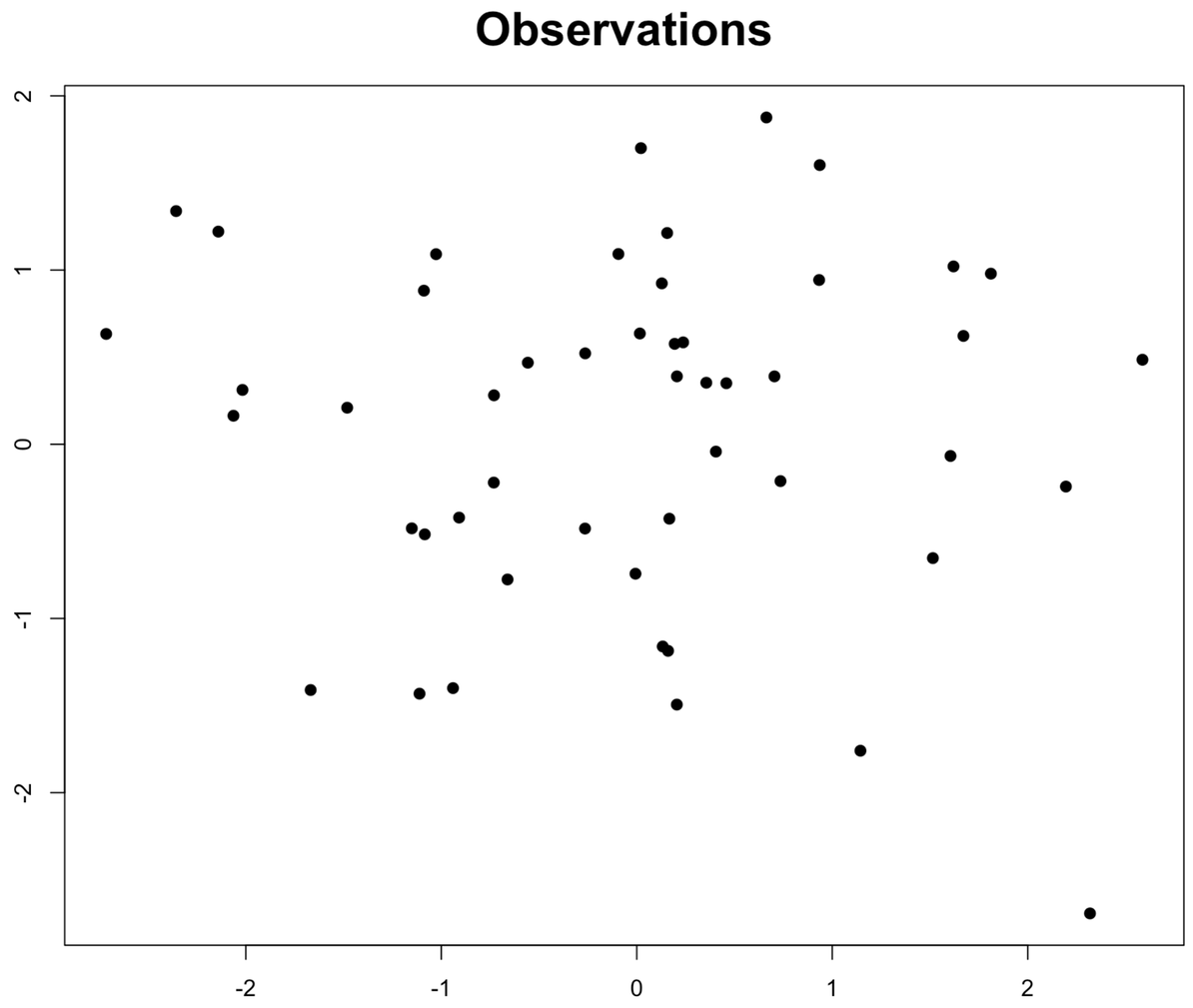
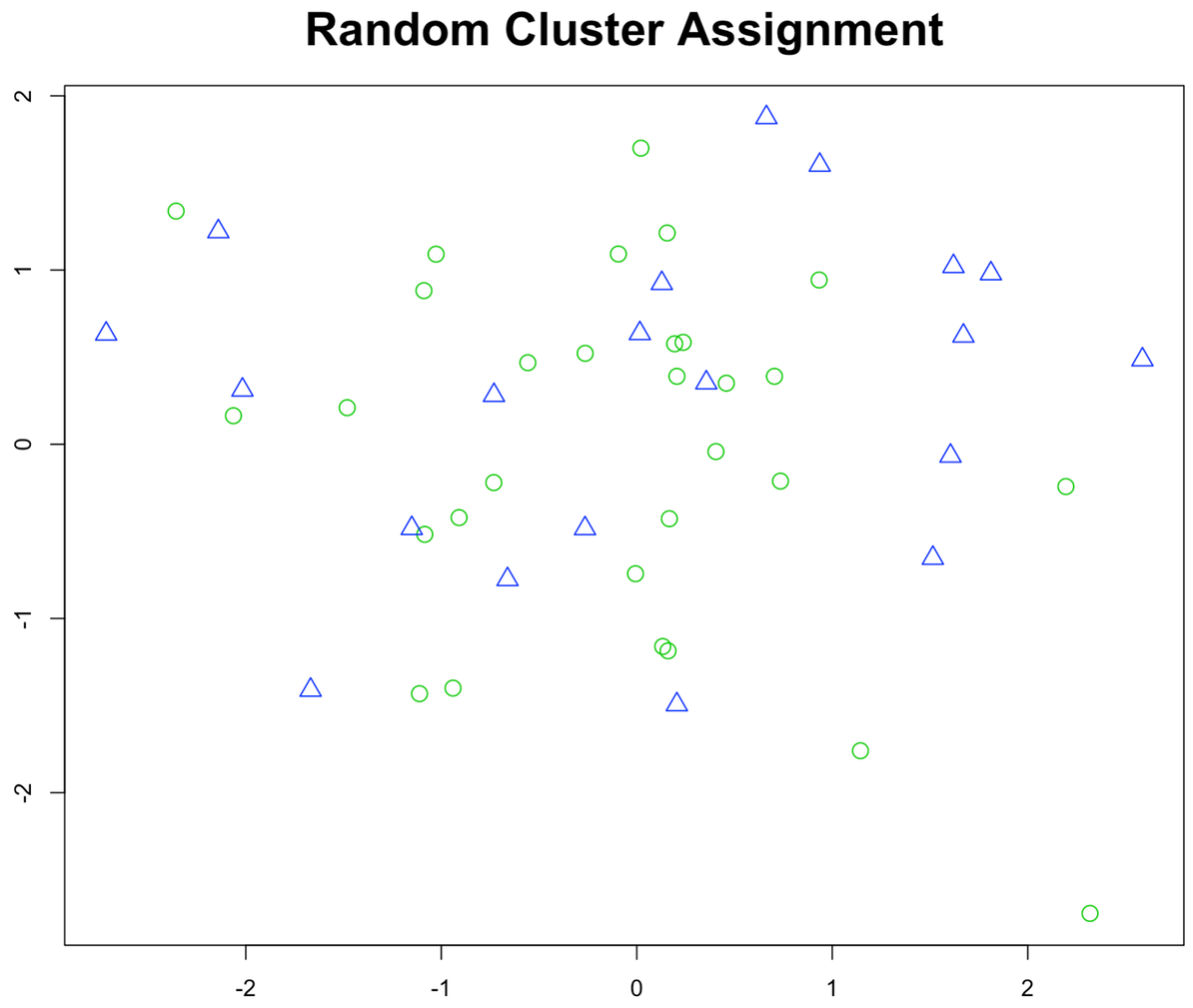
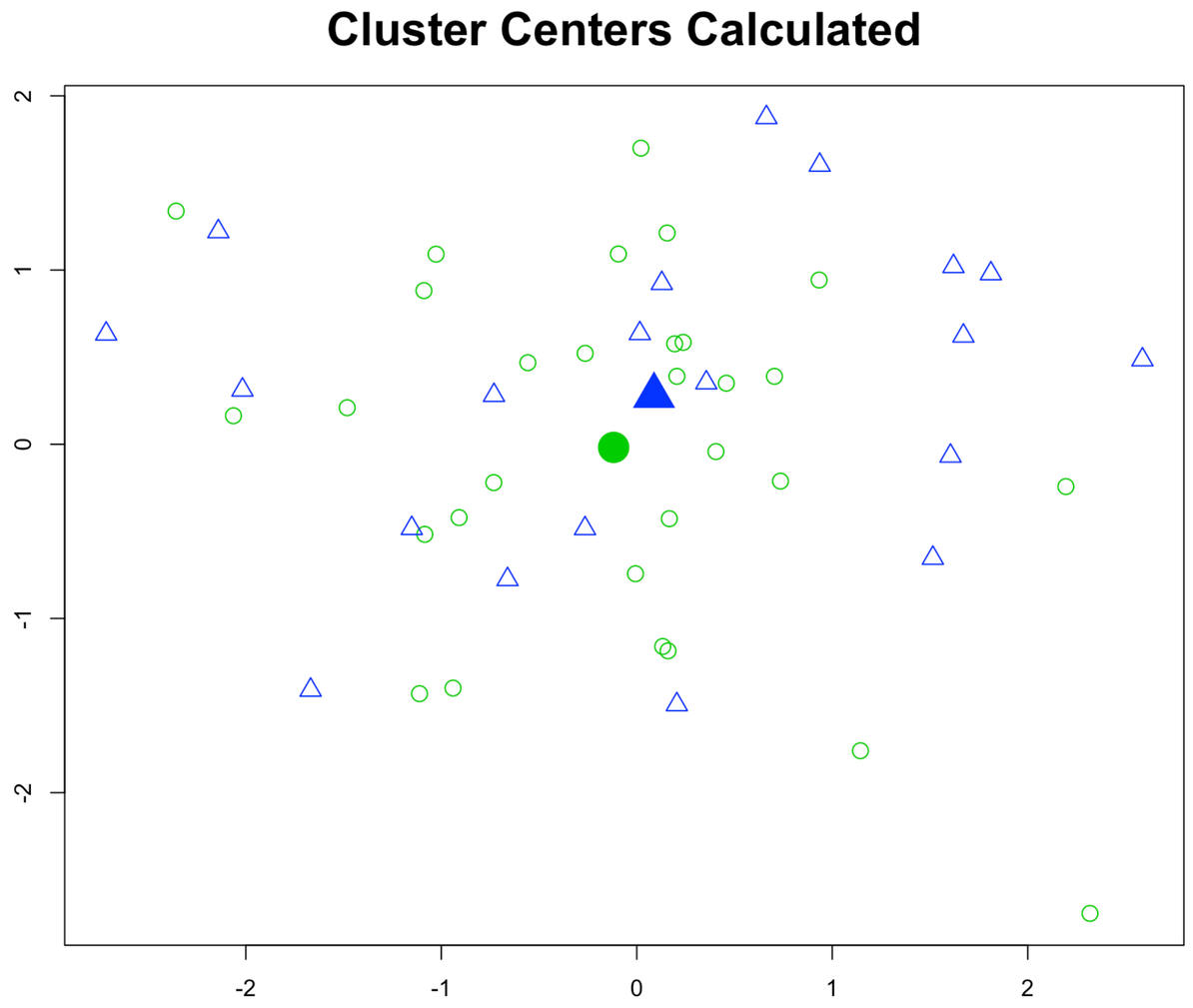
How kmeans() works and practical matters

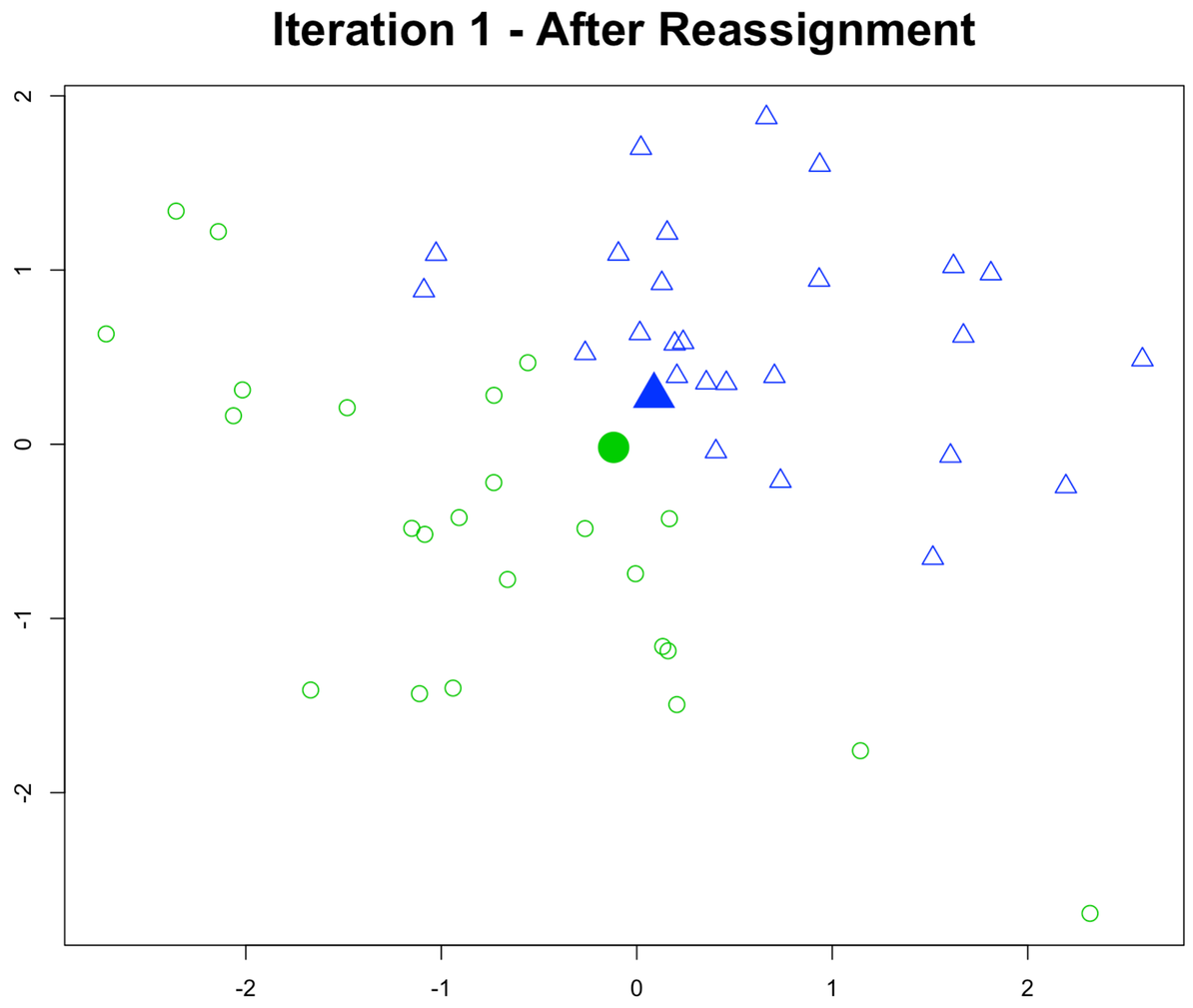
Objectives

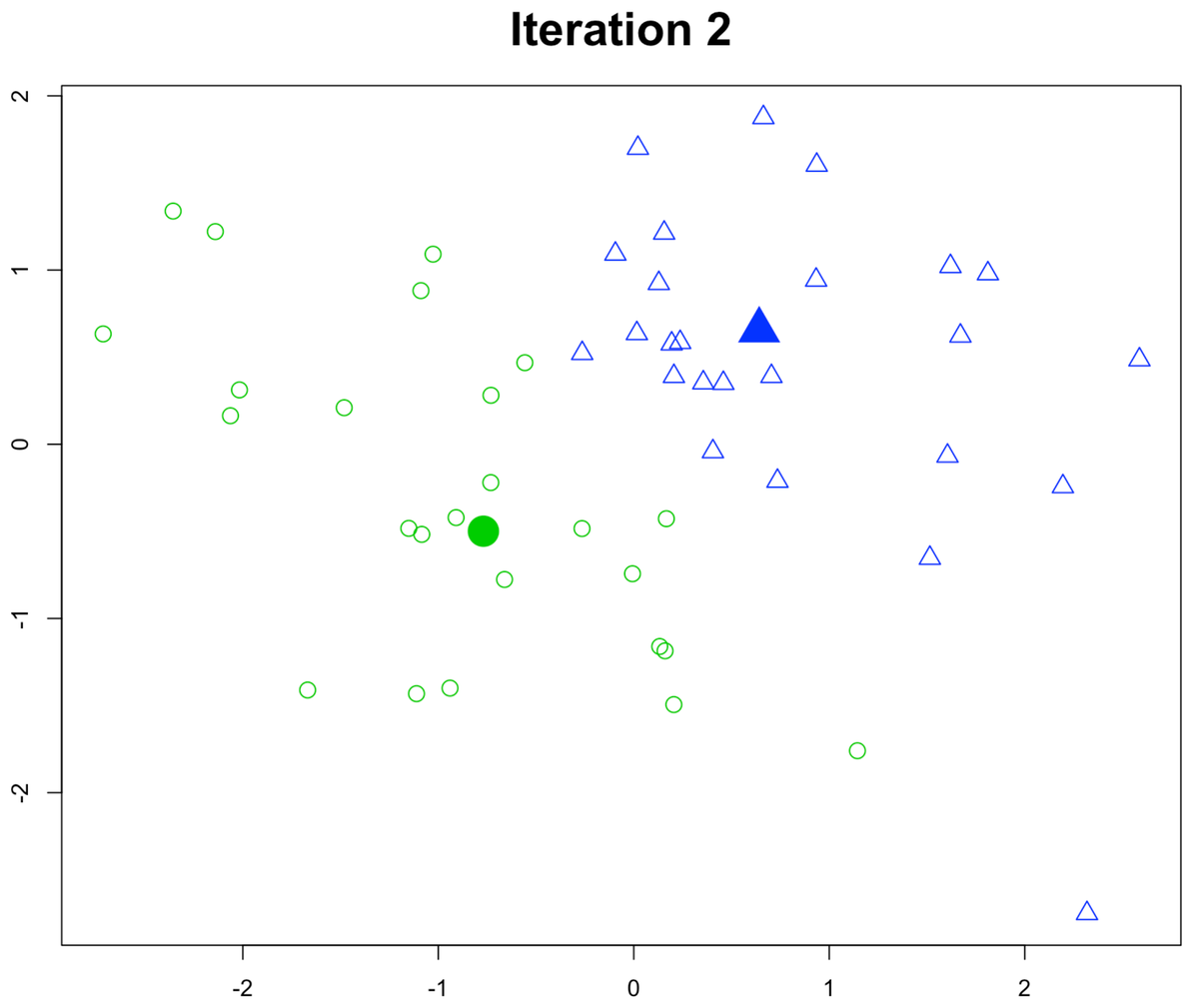
- Explain how k-means algorithm is implemented visually
- Model selection: determining number of clusters

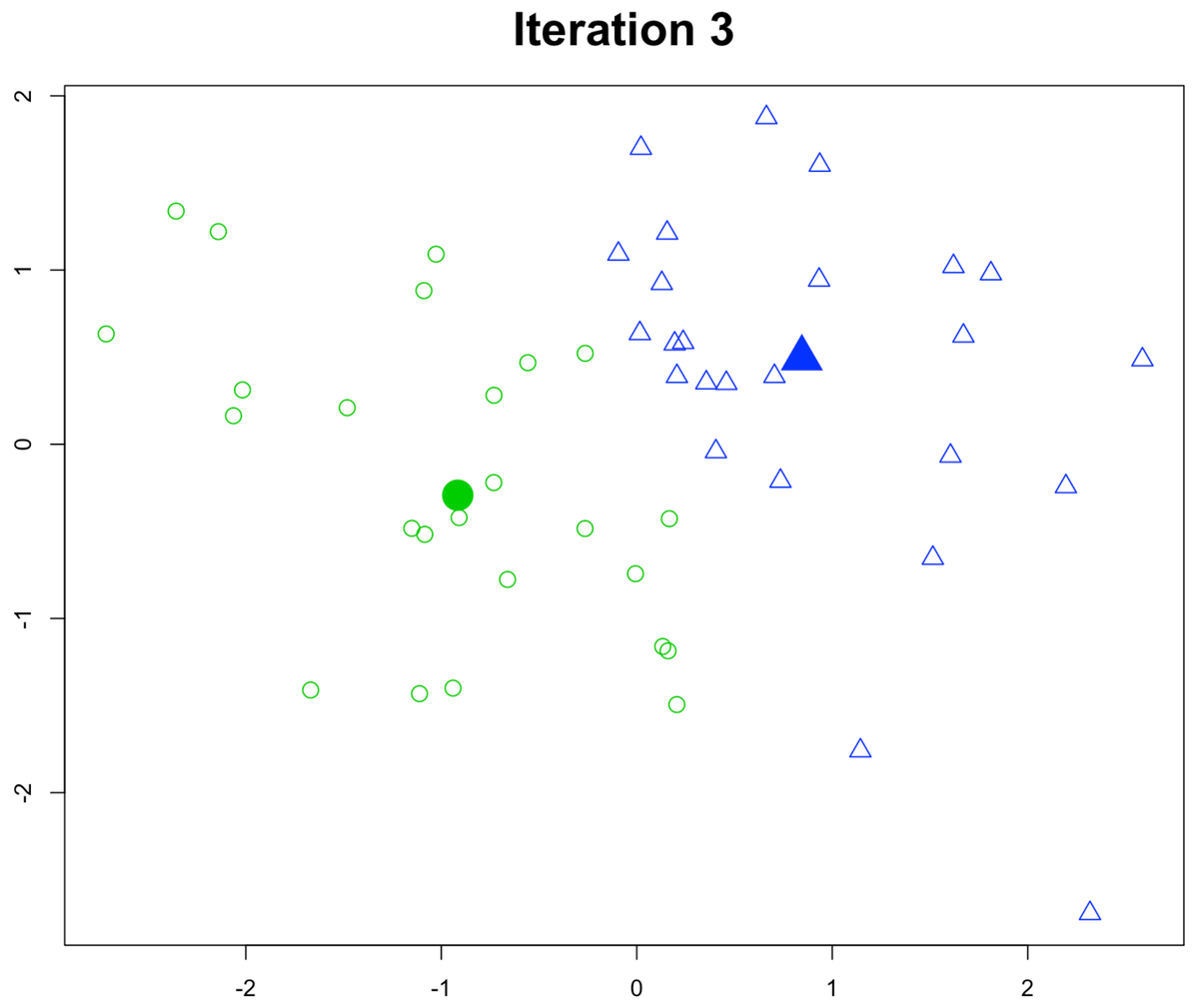

Observations
2
1
0
-1
-2
-2
-1
0
1
2

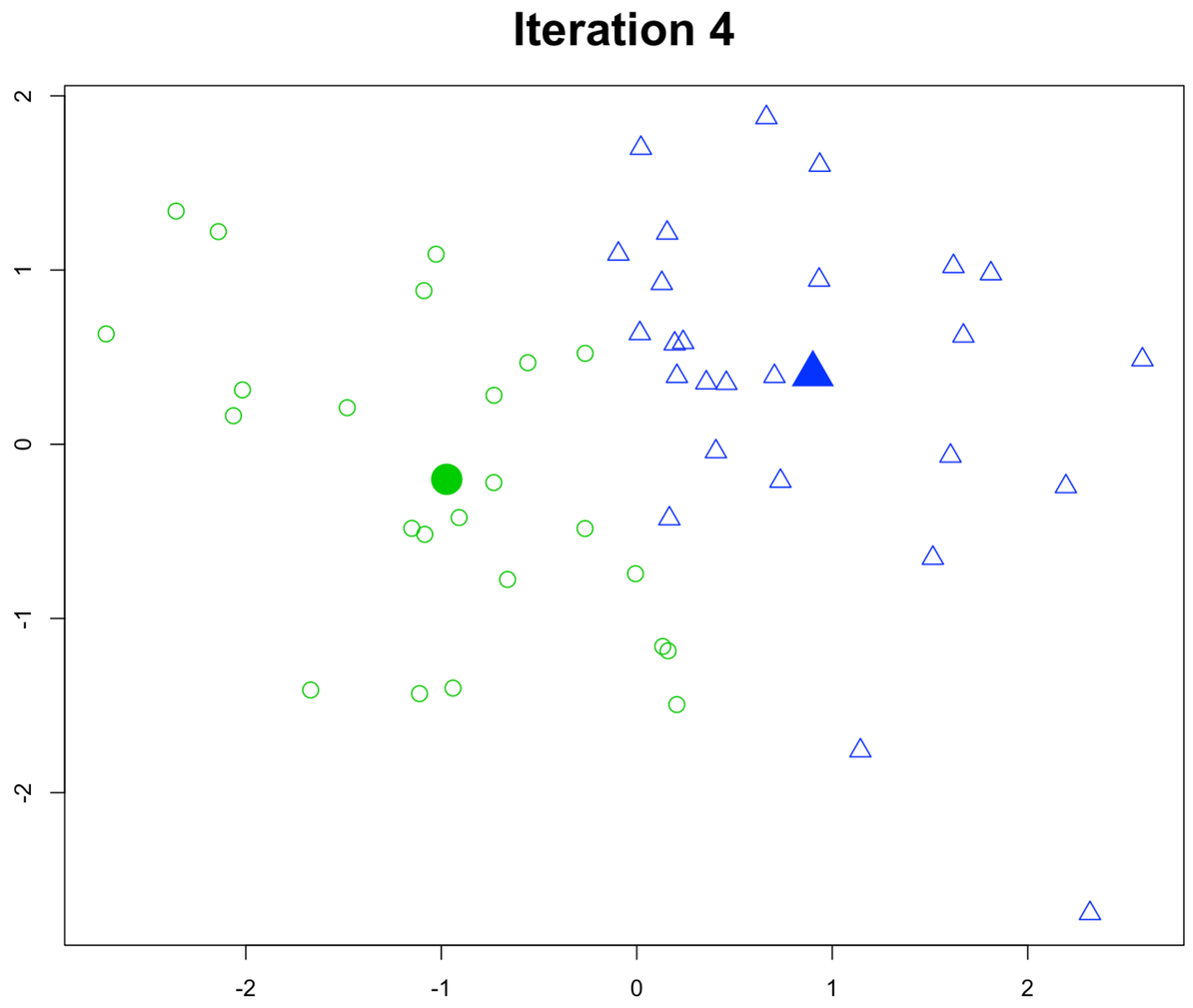

Random Cluster Assignment
2
1
0
-1
-2
-2
-1
0
1
2

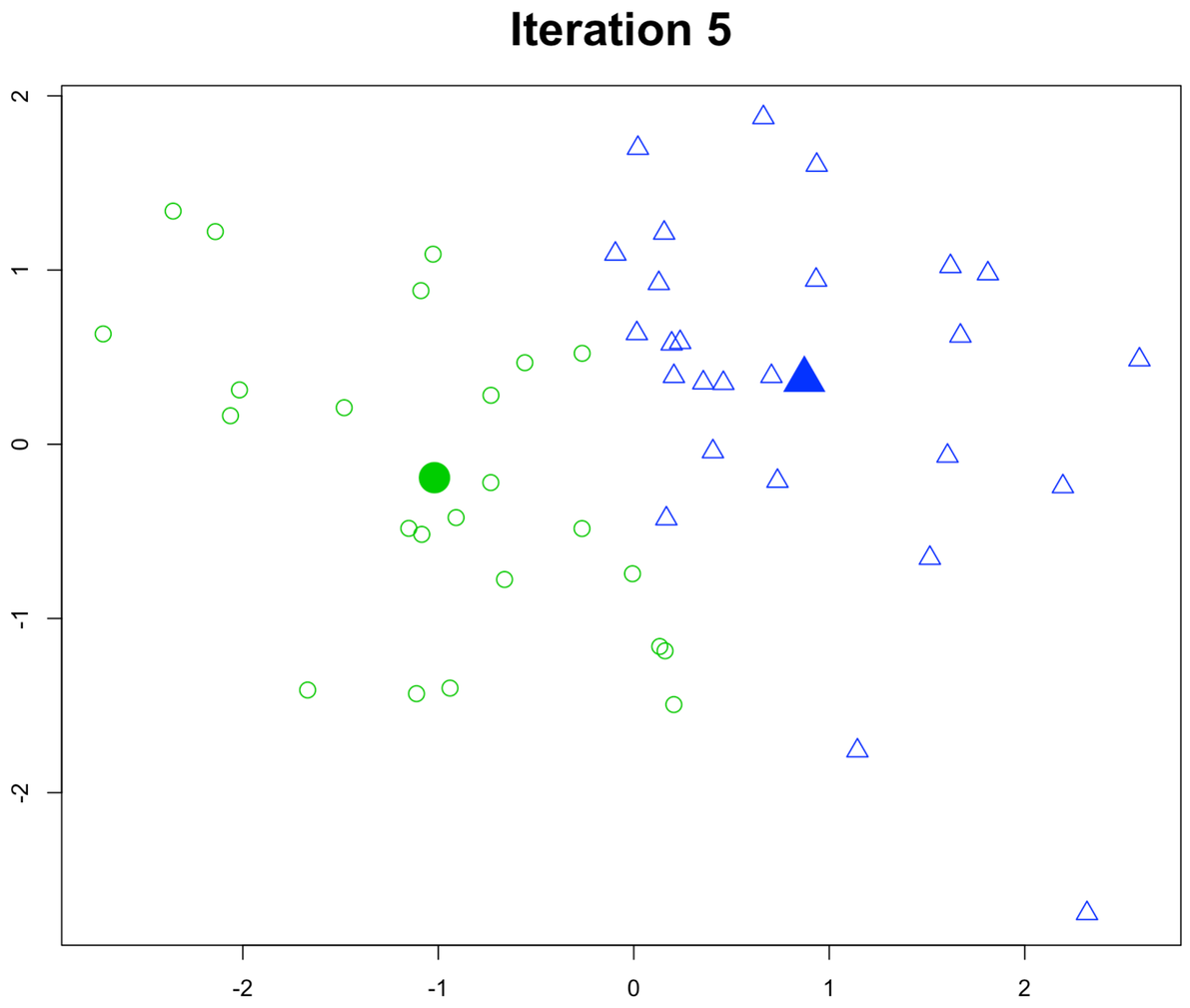

Cluster Centers Calculated
2
1
0
-1
-2
-2
-1
0
1
2


Iteration 1 - After Reassignment
2
1
0
-1
-2
-2
-1
0
1
2


Iteration 2
2
1
0
-1
-2
-2
-1
0
1
2


Iteration 3
2
1
0
-1
-2
-2
-1
0
1
2


Iteration 4
2
1
0
-1
-2
-2
-1
0
1
2


Iteration 5
2
1
0
-1
-2
-2
-1
0
1
2

Model selection

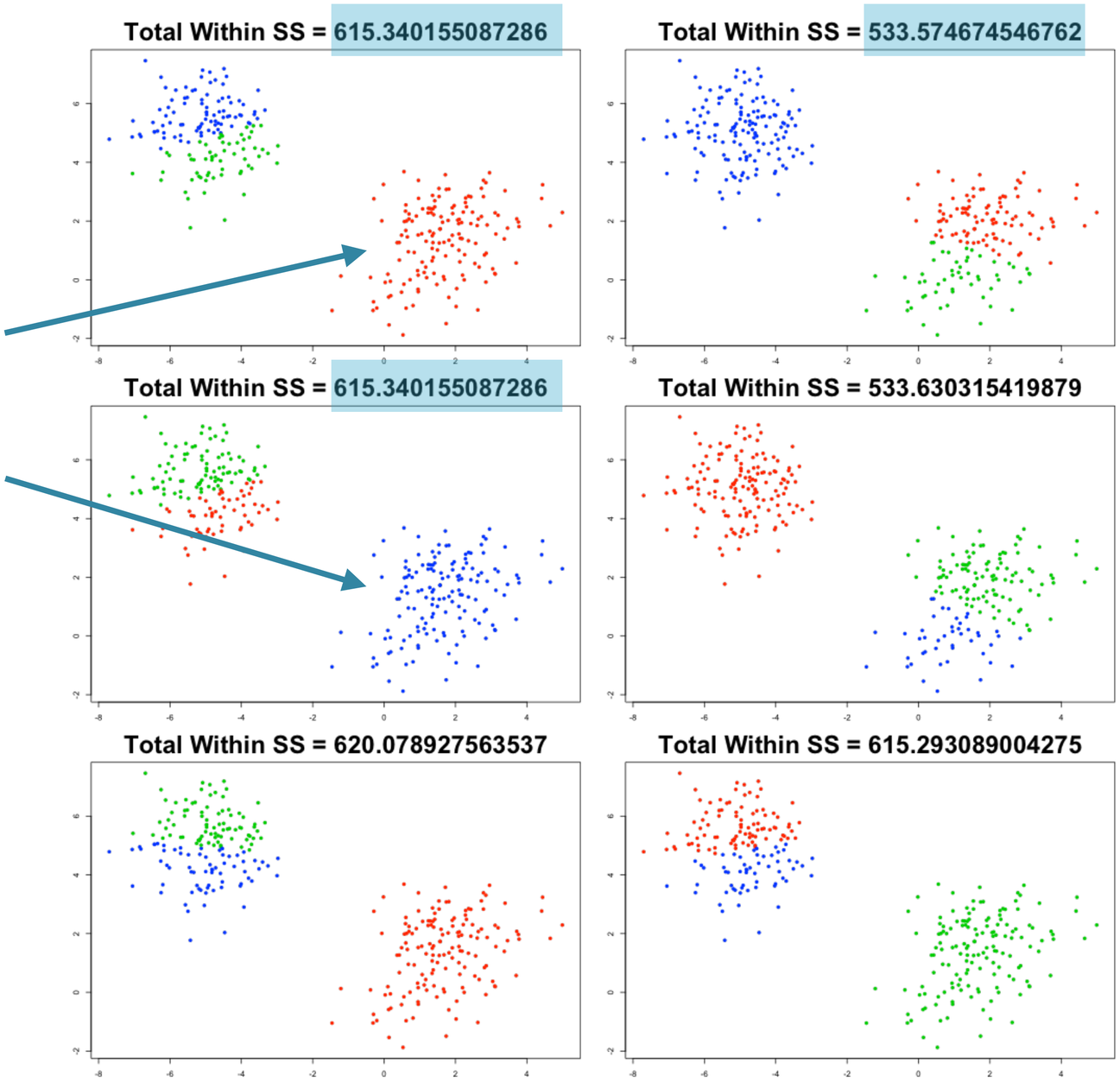
- Recall k-means has a random component
- Best outcome is based on *total within cluster sum of squares:*
  - For each cluster
    - For each observation in the cluster
      - Determine squared distance from observation to cluster center
    - Sum all of them together

Model selection

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

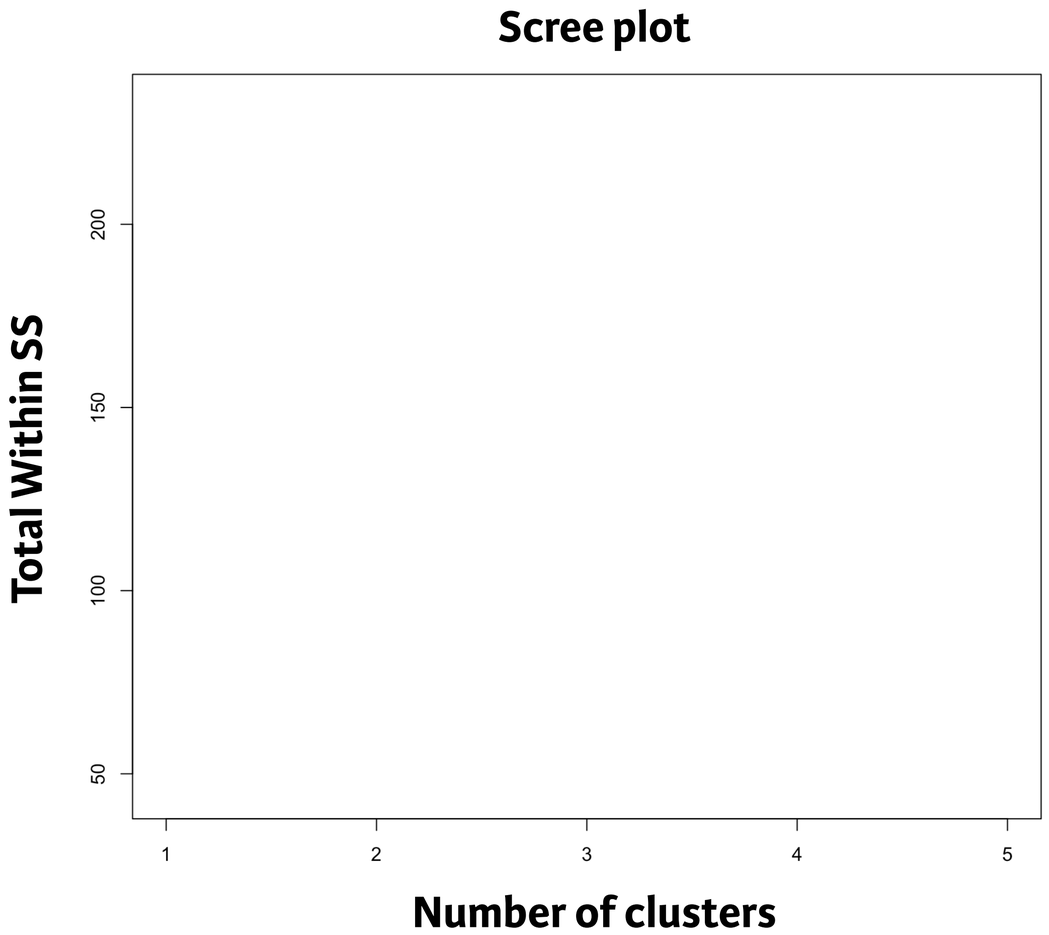
- Running algorithm multiple times helps find the global minimum total within cluster sum of squares
- You'll see an example in the exercises

Identical groupings and Total Within SS, but different cluster labels



Determining number of clusters

- Trial and error is not the best approach



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Let’s practice!

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Introduction to Pokemon data

"Real" data exercise

The Pokemon dataset

```
> head(pokemon)
     HitPoints Attack Defense SpecialAttack SpecialDefense Speed
[1,]        45     49      49            65             65    45
[2,]        60     62      63            80             80    60
[3,]        80     82      83           100            100    80
[4,]        80    100     123           122            120    80
[5,]        39     52      43            60             50    65
[6,]        58     64      58            80             65    80
```

- Hosted at https://www.kaggle.com/abcsds/pokemon
- More information on Pokemon and these features can be found at http://pokemondb.net/pokedex

Data challenges

- Selecting the variables to cluster upon
- Scaling the data (will handle in last chapter)
- Determining the number of clusters
  - Often no clean "elbow" in scree plot
  - This will be a core part of the exercises
- Visualize the results for interpretation

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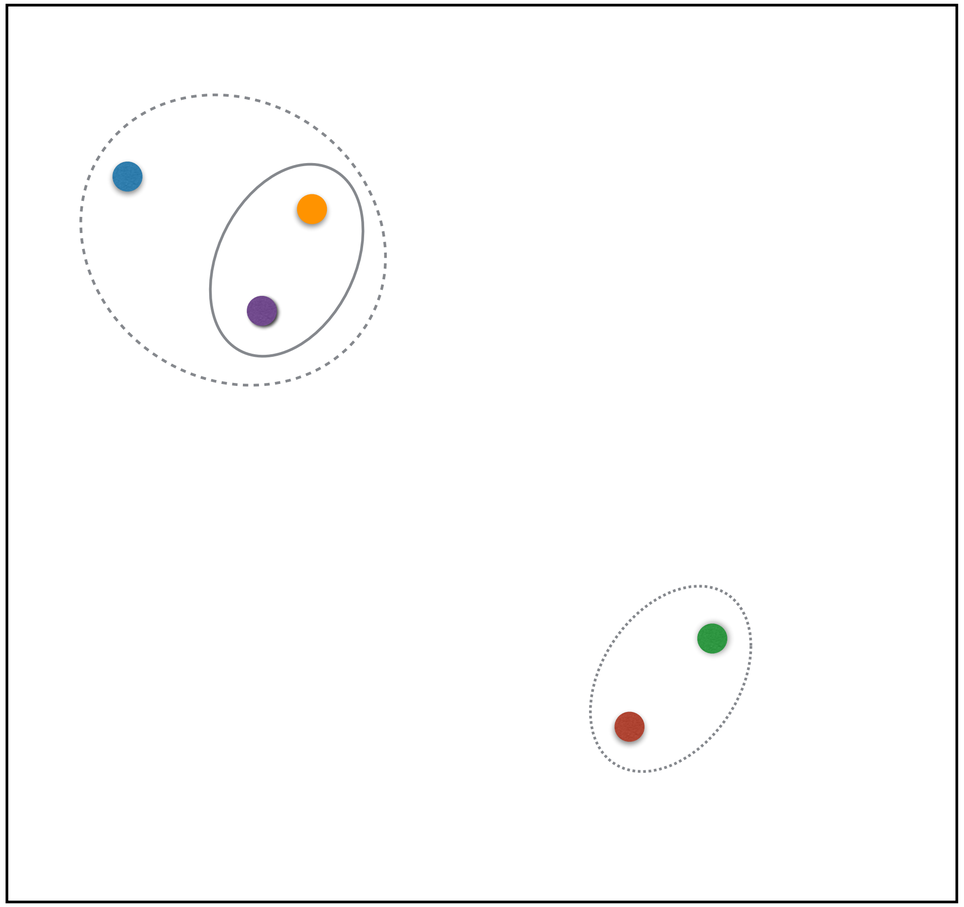
Review of k-means clustering

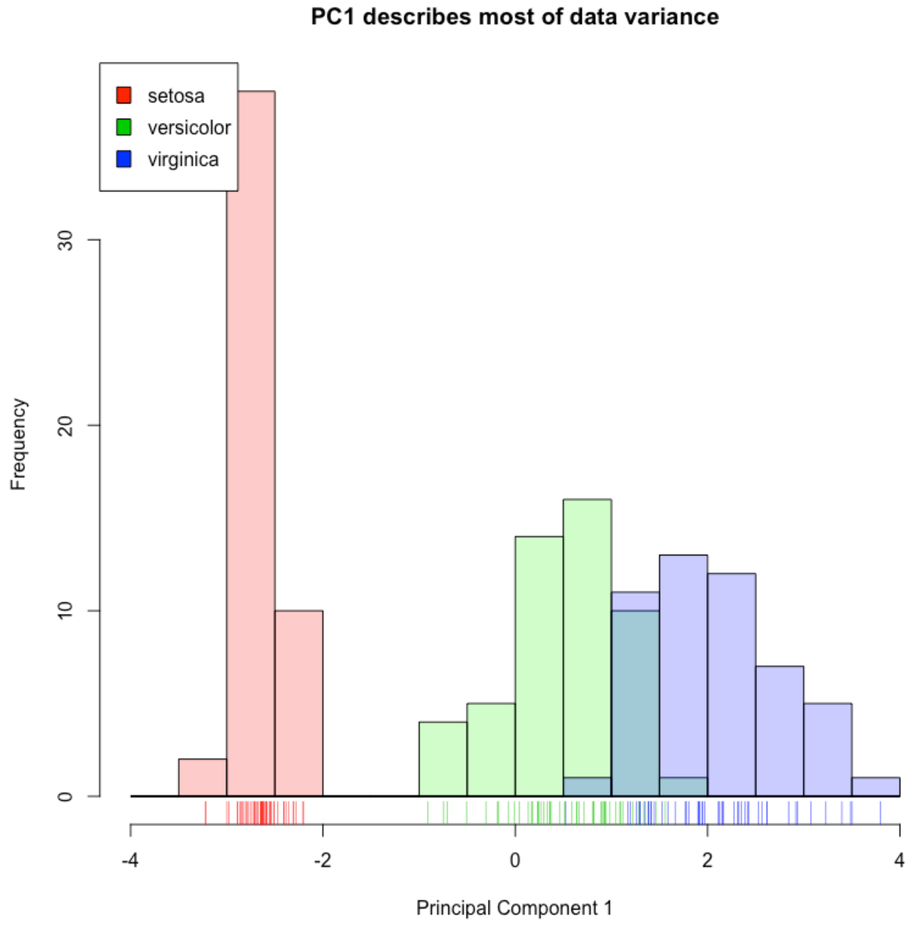
Chapter review

- Unsupervised vs. supervised learning
- How to create k-means cluster model in R
- How k-means algorithm works
- Model selection
- Application to "real" (and hopefully fun) dataset

Coming up: chapter 2

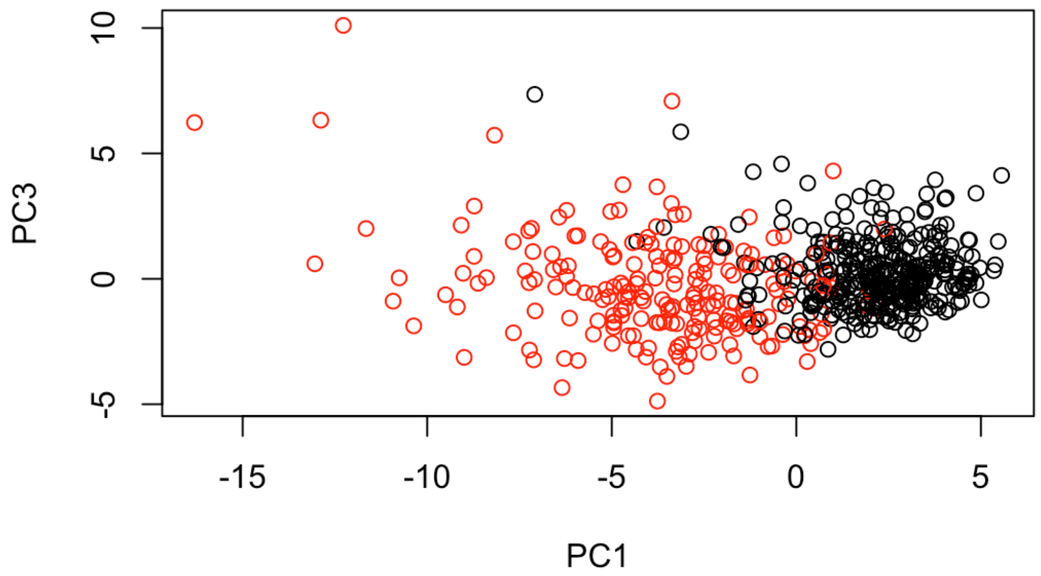


Coming up: chapter 3



Coming up: chapter 4

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



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