

# Welcome to the course!

UNSUPERVISED LEARNING IN R



Hank Roark

Senior Data Scientist at Boeing

# 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

Observations	Features		
	Color	Shape	Size
	Blue	Square	10
	Red	Ellipse	2.4
	Red	Ellipse	20.7

*1 Unlabeled data*

<sup>1</sup> Sample from Murphy, Machine Learning: A Probabilistic Perspective

# Labeled vs. unlabeled data

The diagram illustrates labeled data as a table. At the top, a horizontal double-headed arrow is labeled "Features". To its left, a vertical double-headed arrow is labeled "Observations". The table itself has four columns: "Color", "Shape", "Size", and "Label". The first three columns represent features, while the last column represents the label. The data consists of three rows:

Color	Shape	Size	Label
Blue	Square	10	1
Red	Ellipse	2.4	1
Red	Ellipse	20.7	2

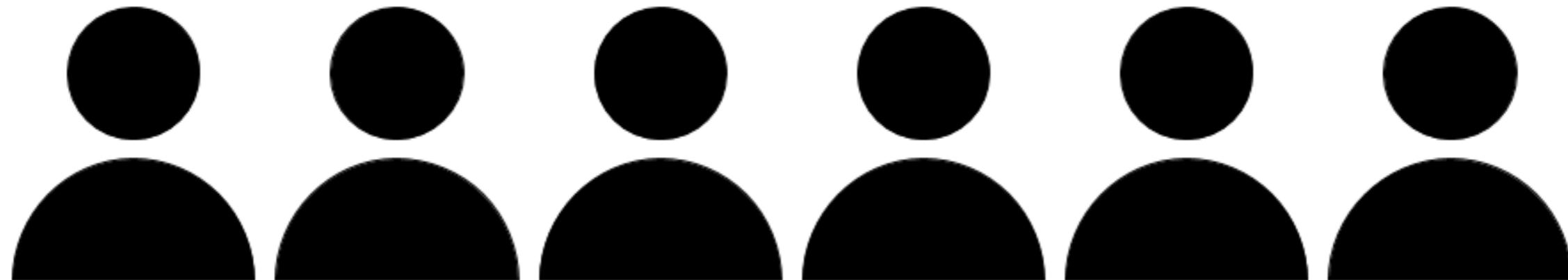
Labeled data

<sup>1</sup> Sample from Murphy, Machine Learning: A Probabilistic Perspective

# Unsupervised learning - clustering

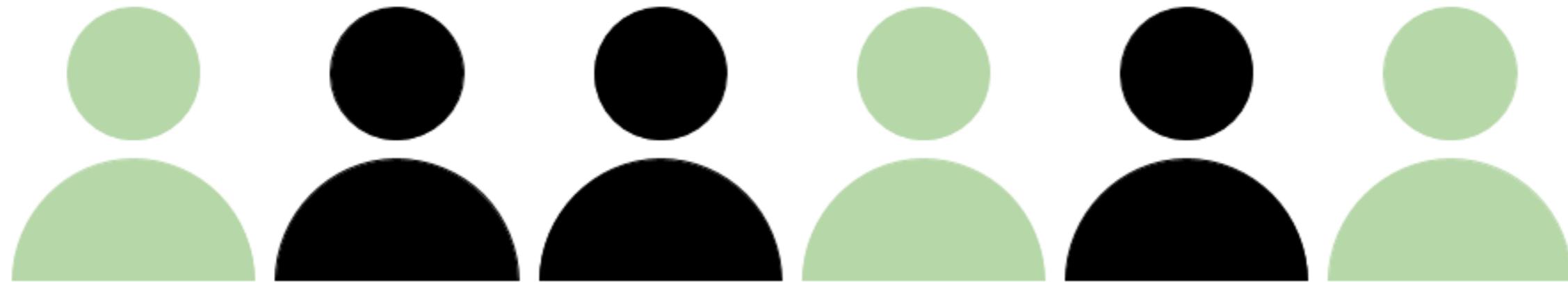
- Finding homogeneous subgroups within larger group

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



# Unsupervised learning - clustering

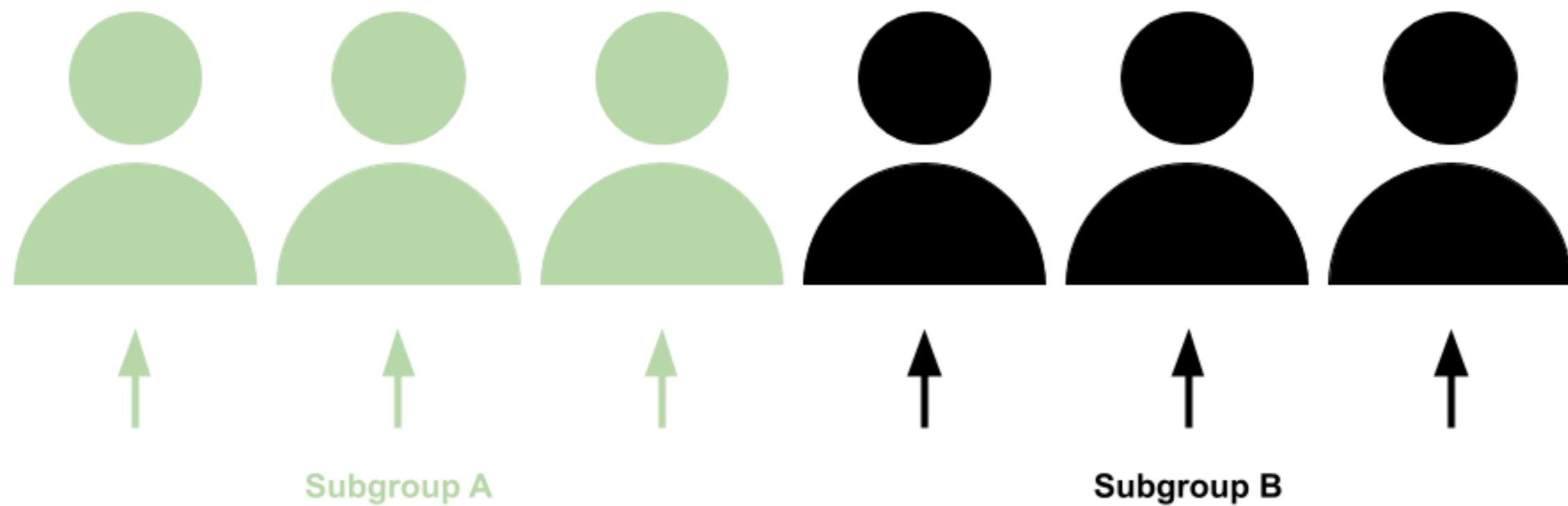
- Finding homogeneous subgroups within larger group



# Unsupervised learning - clustering

- Finding homogeneous subgroups within larger group

## *Clustering*



# Clustering examples



# Clustering examples



# Unsupervised learning - dimensionality reduction

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

# Unsupervised learning - 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

# **Let's practice!**

## **UNSUPERVISED LEARNING IN R**

# Introduction to k-means clustering

UNSUPERVISED LEARNING IN R

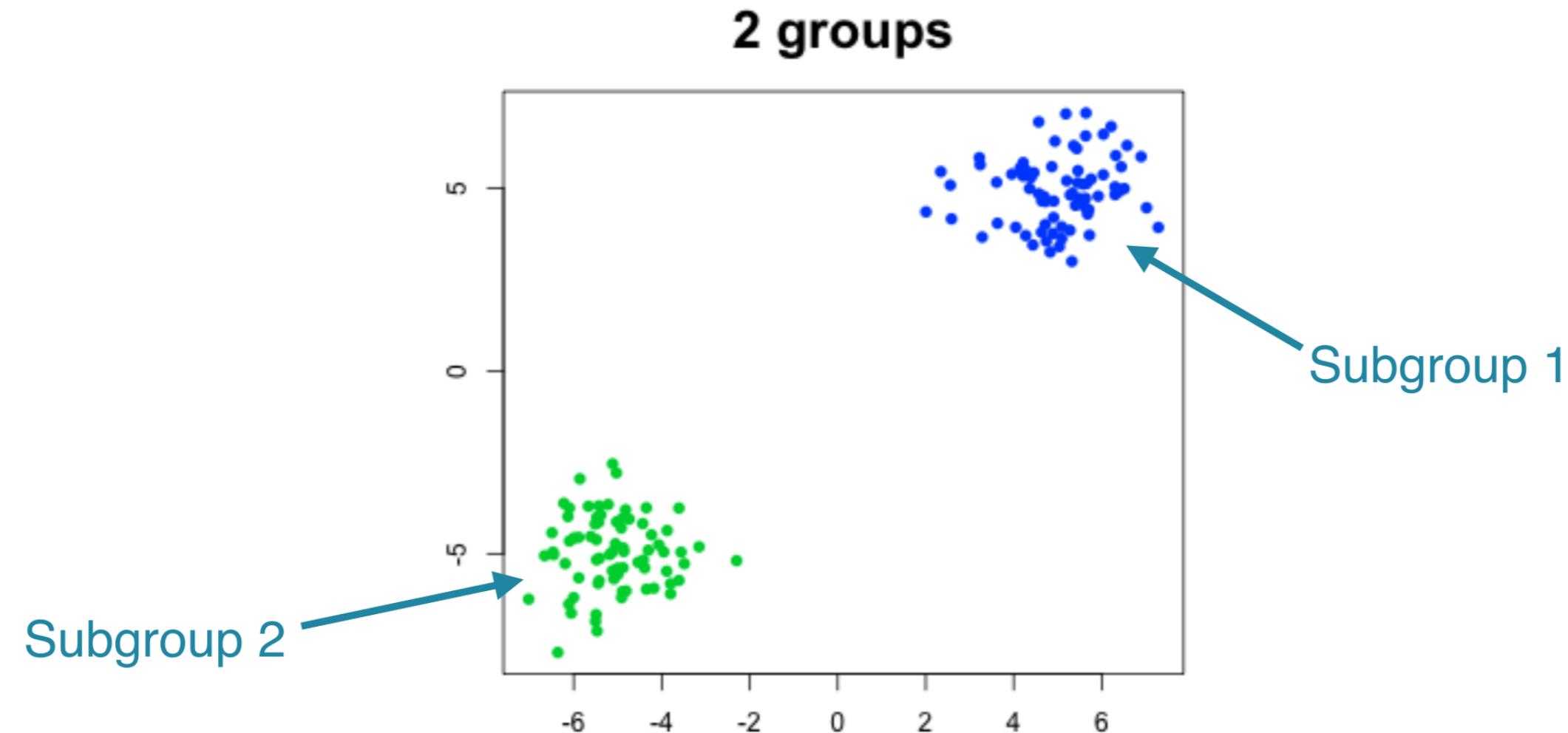


Hank Roark

Senior Data Scientist at Boeing

# 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

# **Let's practice!**

## **UNSUPERVISED LEARNING IN R**

# How k-means works and practical matters

UNSUPERVISED LEARNING IN R



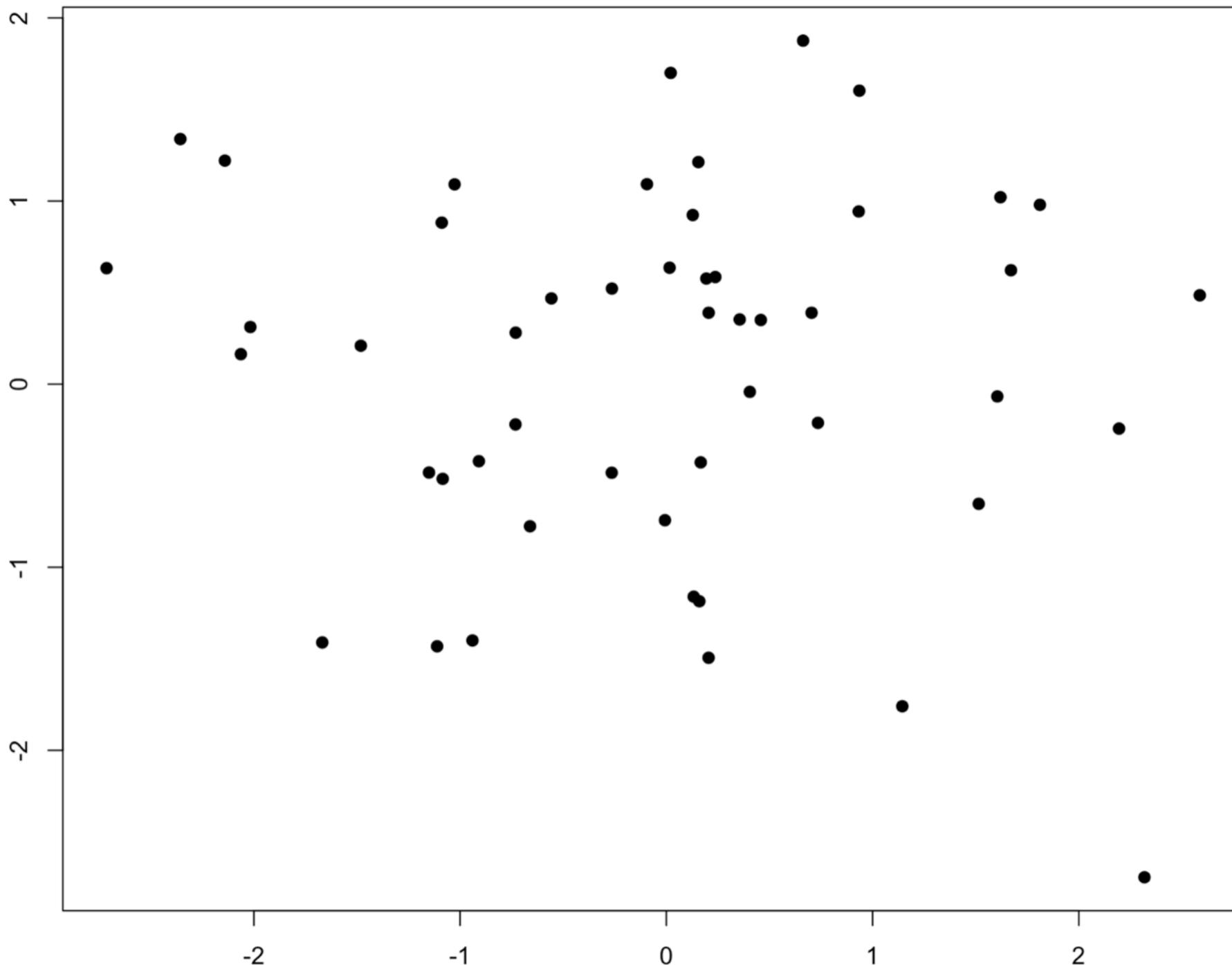
Hank Roark

Senior Data Scientist at Boeing

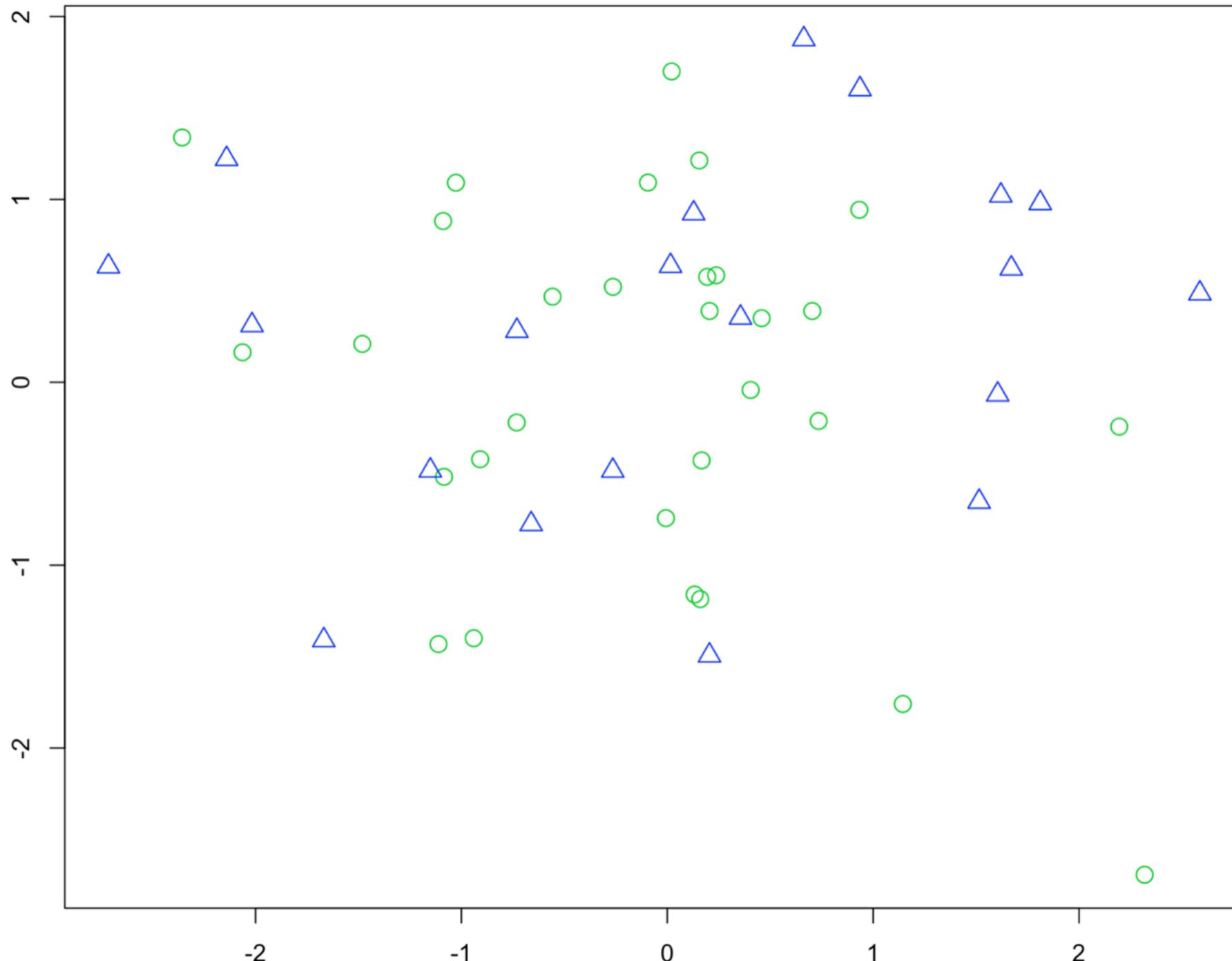
# Objectives

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

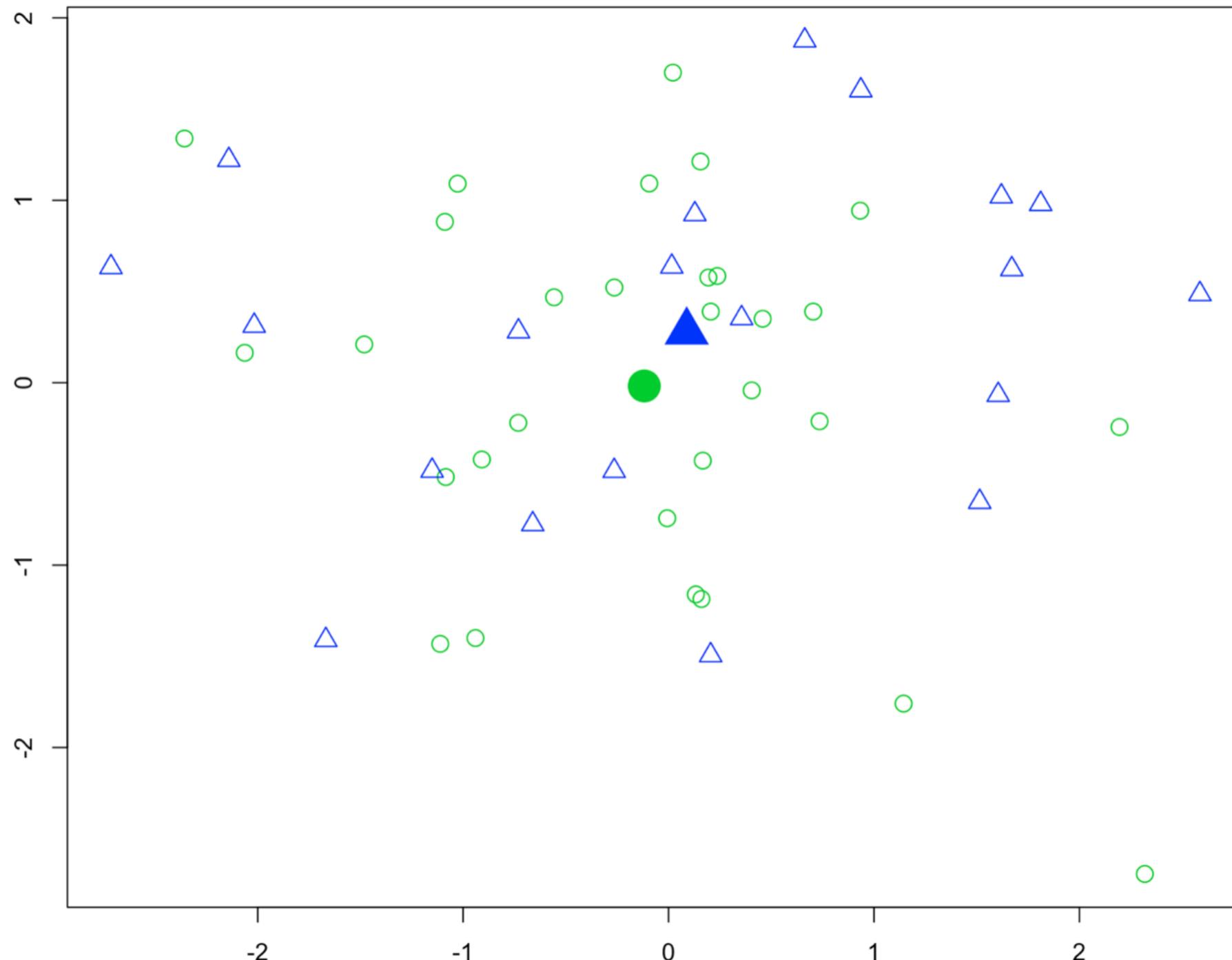
## Observations



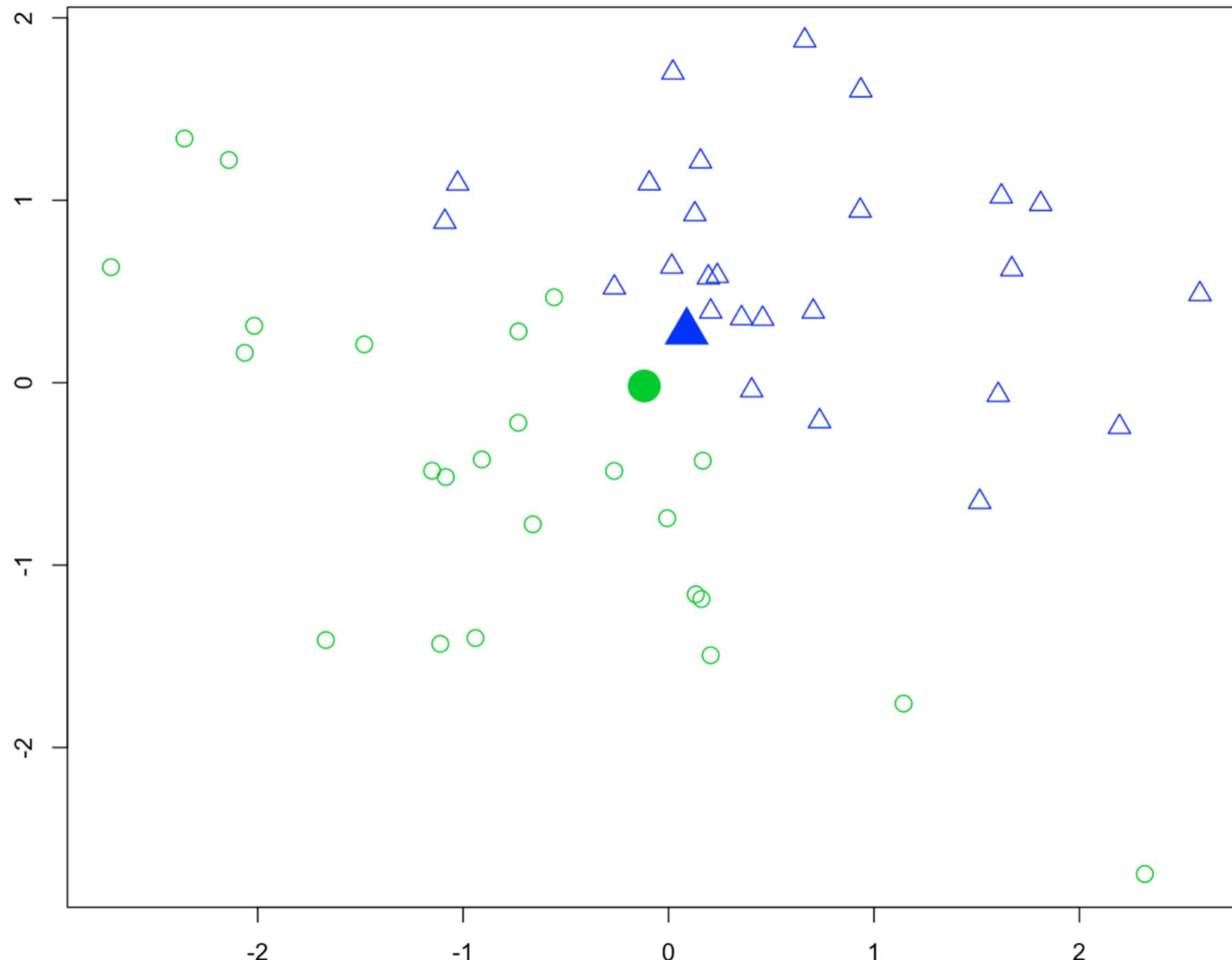
# Random Cluster Assignment



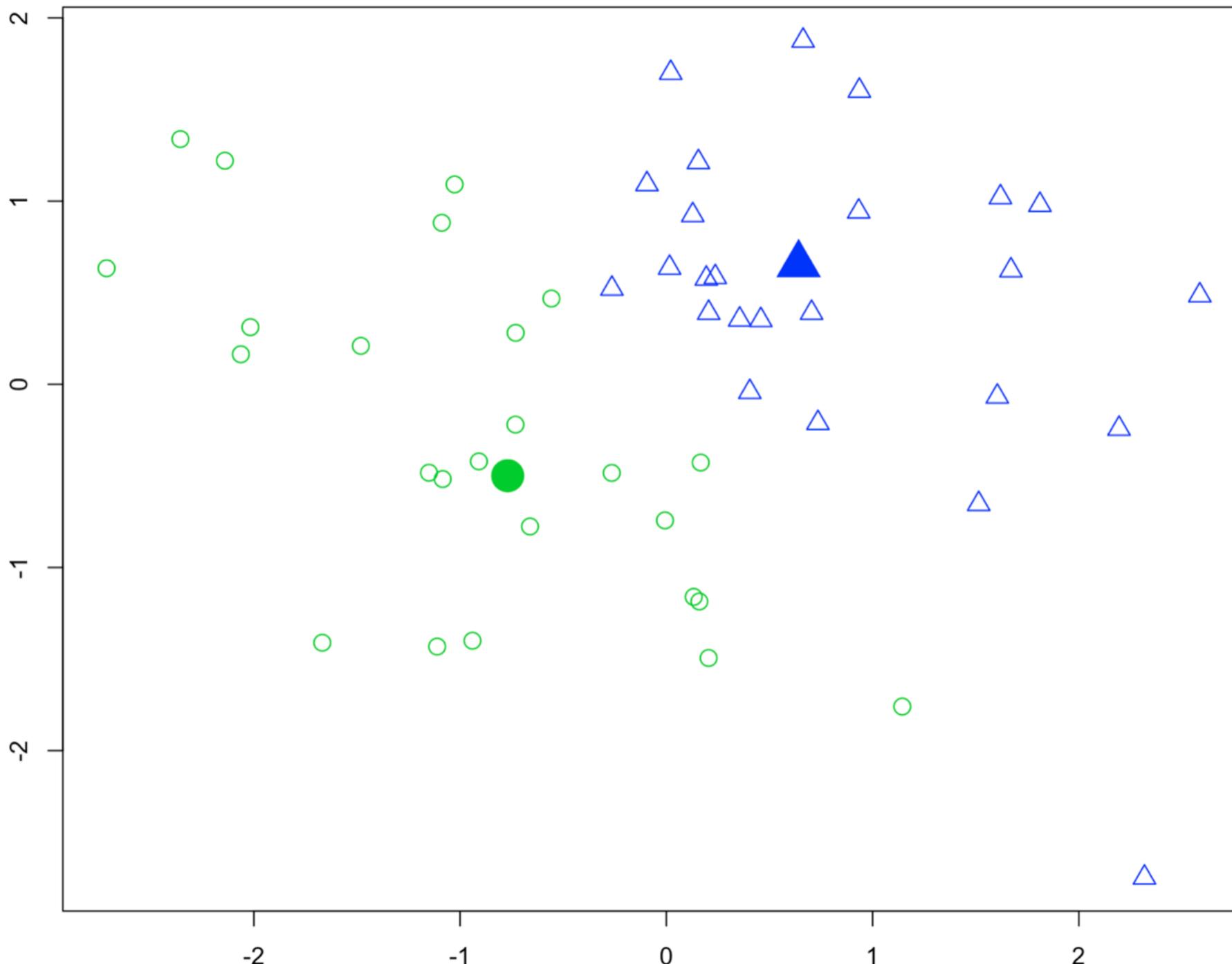
## Cluster Centers Calculated



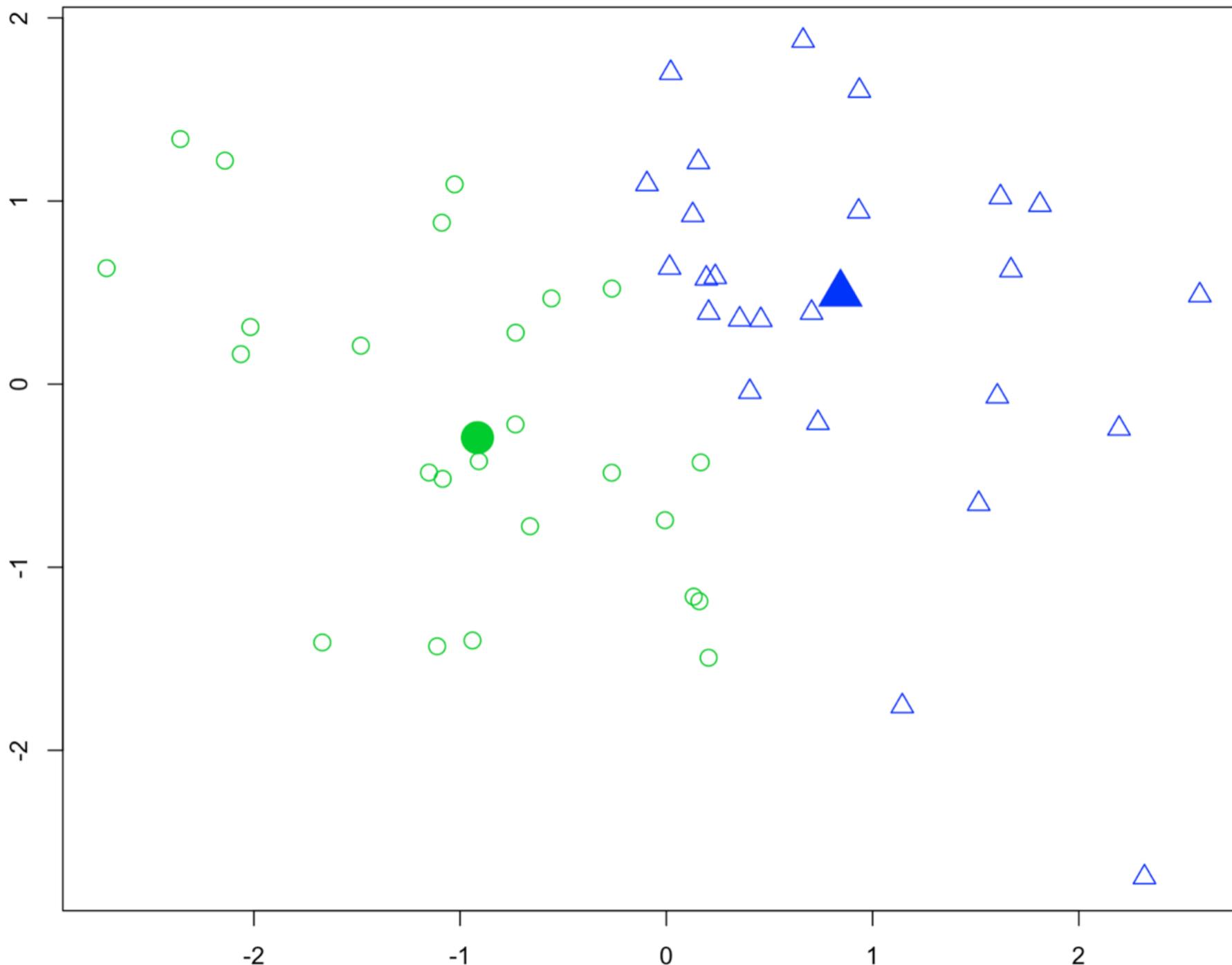
## Iteration 1 - After Reassignment



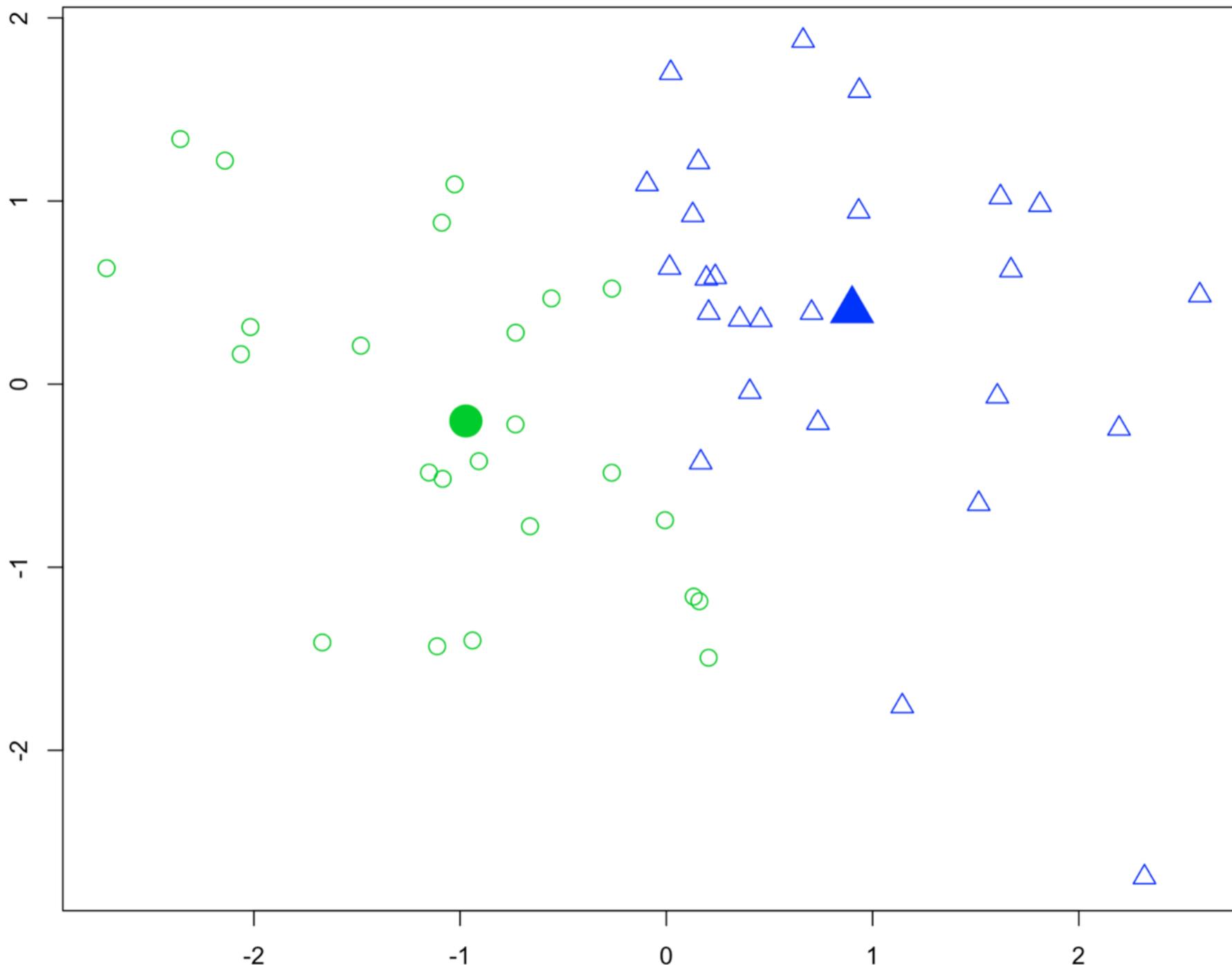
## Iteration 2



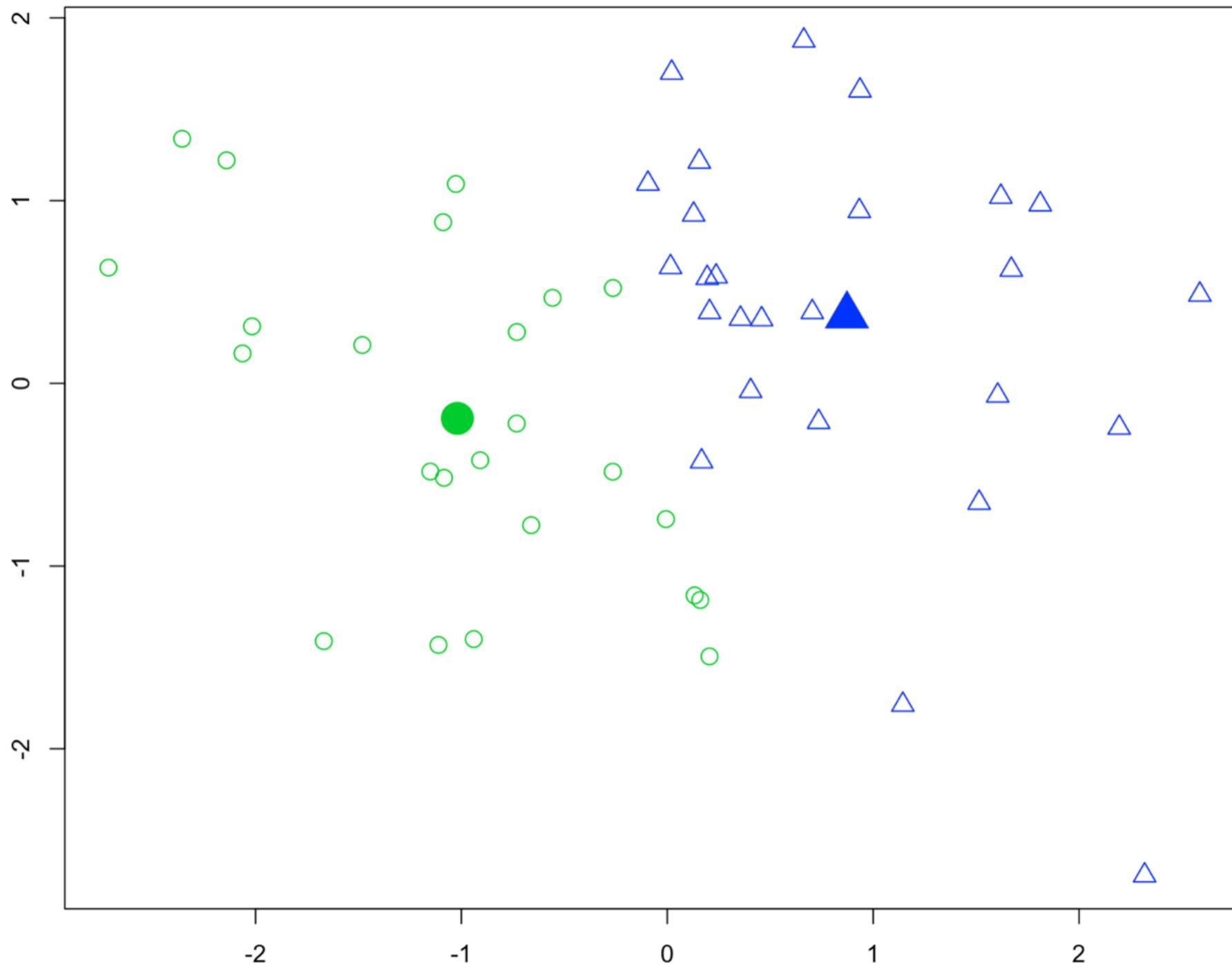
## Iteration 3



## Iteration 4



## Iteration 5



# Model selection

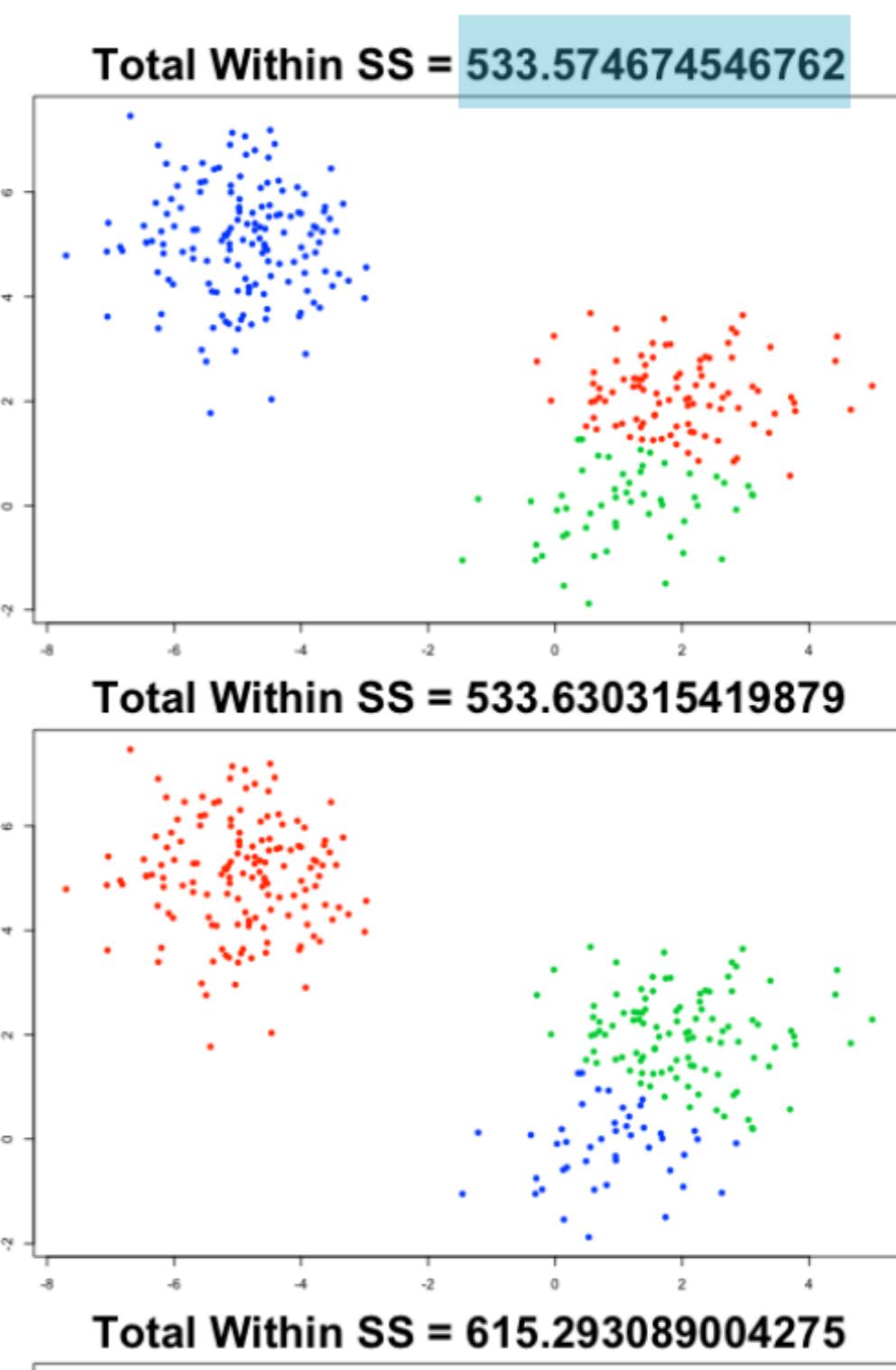
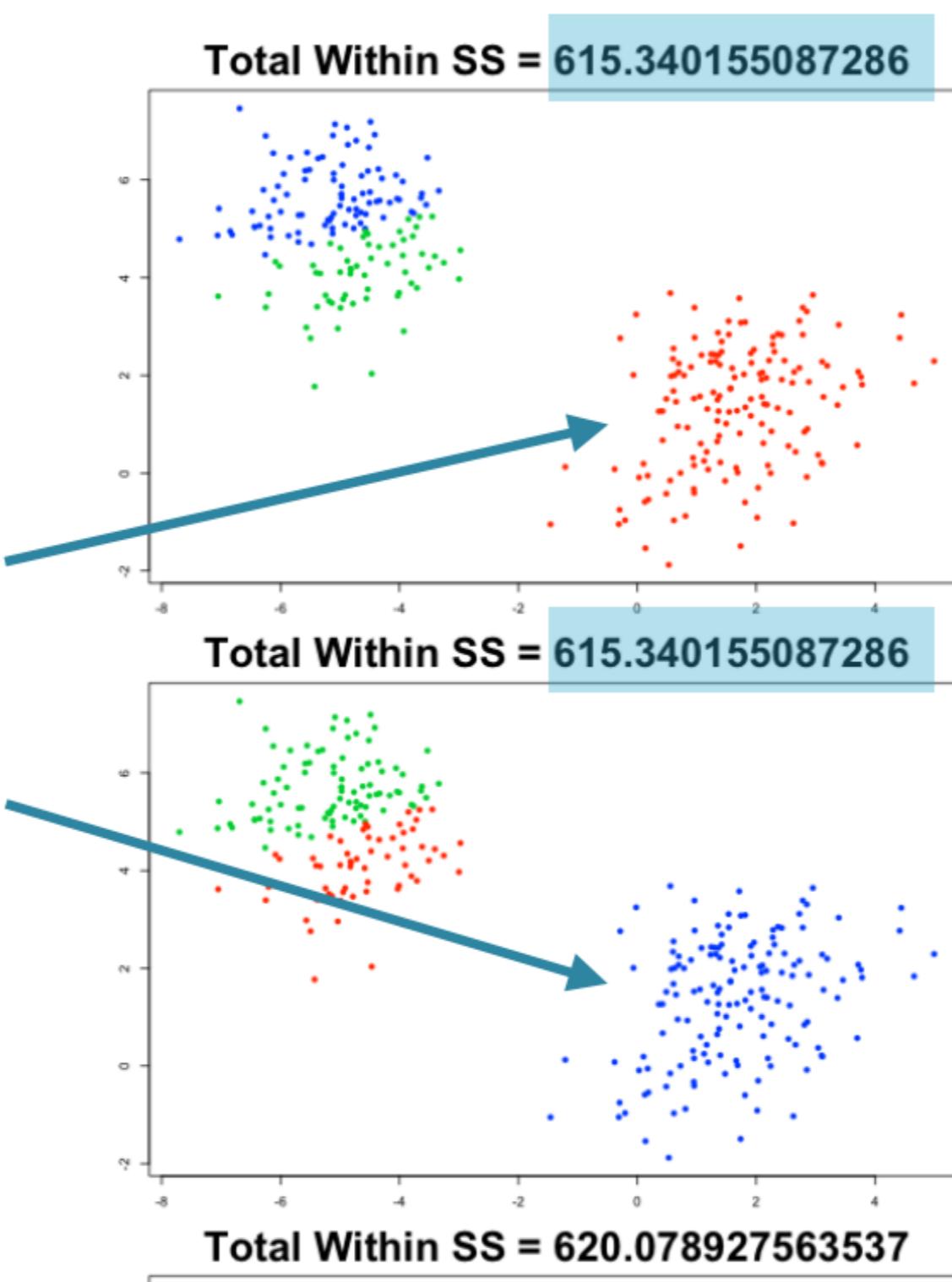
- Recall k-means has a random component
- Best outcome is based on total within cluster sum of squares:
  - For each cluster
    - For each observation in the cluster
      - Determine squared distance from observation to cluster center
      - Sum all of them together

# 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

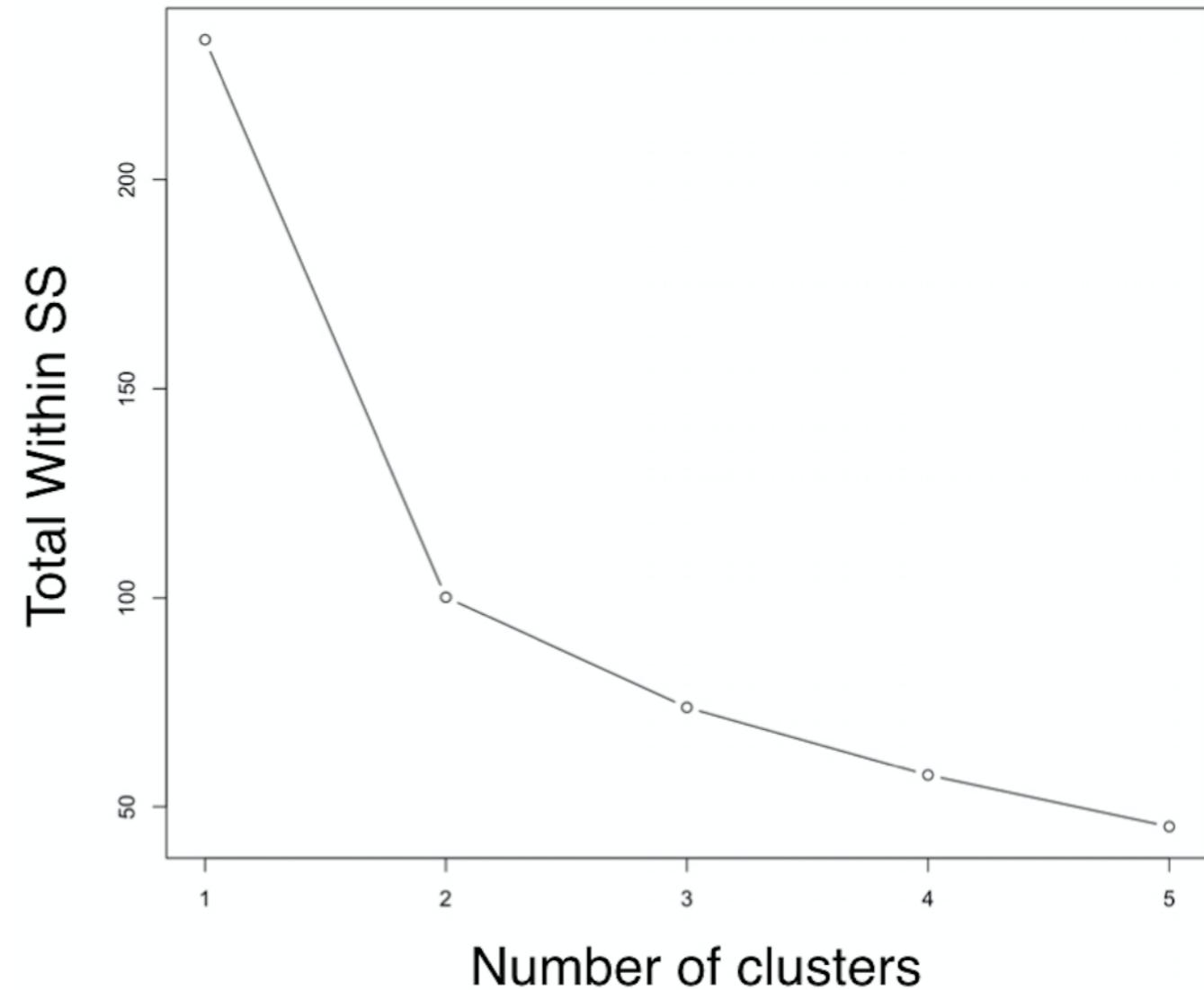
Identical groupings  
and Total Within SS,  
but different cluster  
labels



# Determining the best number of clusters

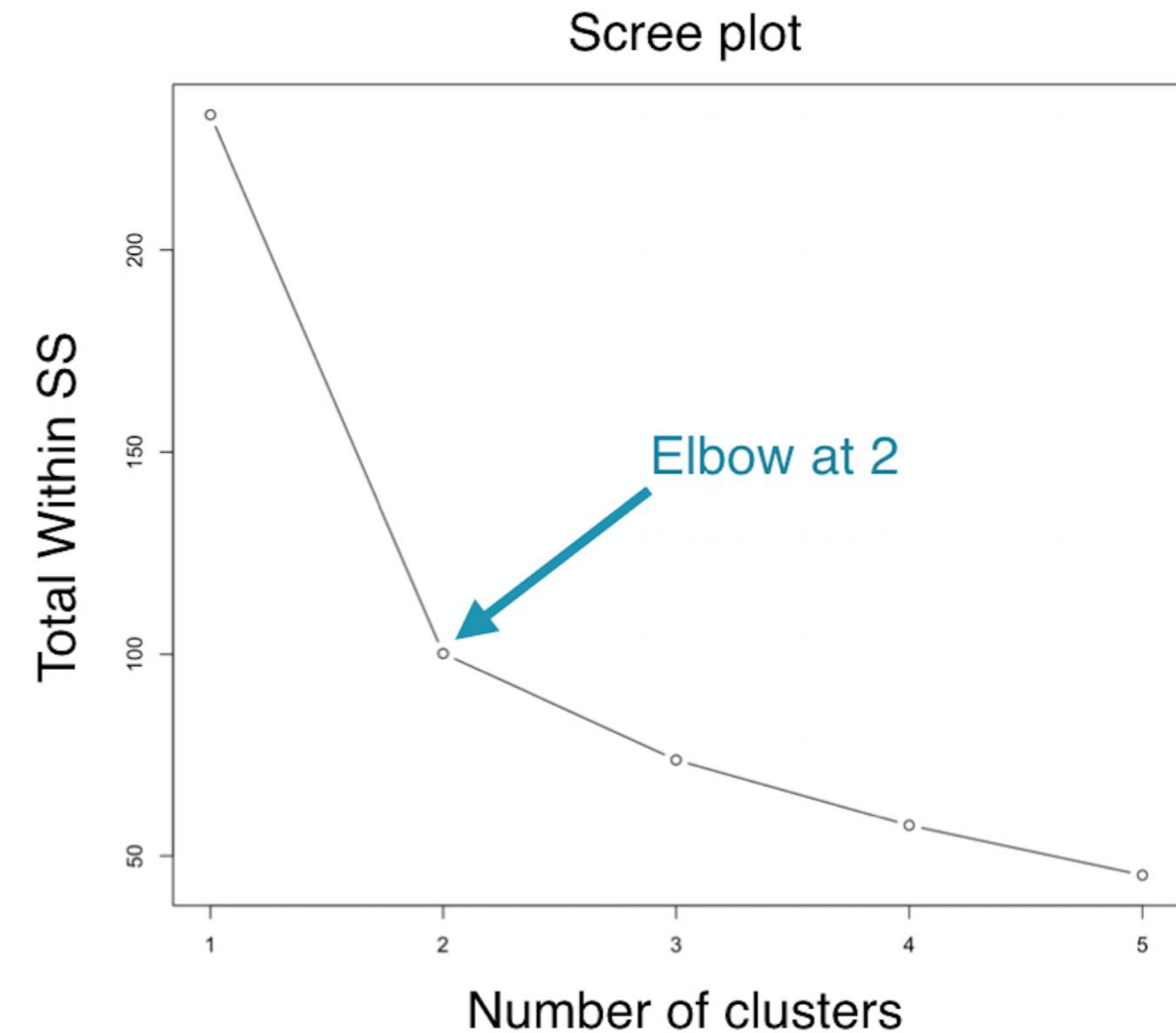
- Trial and error is not the best approach

Scree plot



# Determining the best number of clusters

- Trial and error is not the best approach



# **Let's practice!**

## **UNSUPERVISED LEARNING IN R**

# Introduction to the Pokemon data

UNSUPERVISED LEARNING IN R



Hank Roark

Senior Data Scientist at Boeing

# "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

<sup>1</sup> <https://www.kaggle.com/abcsds/pokemon> <sup>2</sup> <https://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

# **Let's practice!**

## **UNSUPERVISED LEARNING IN R**

# Review of k-means clustering

UNSUPERVISED LEARNING IN R



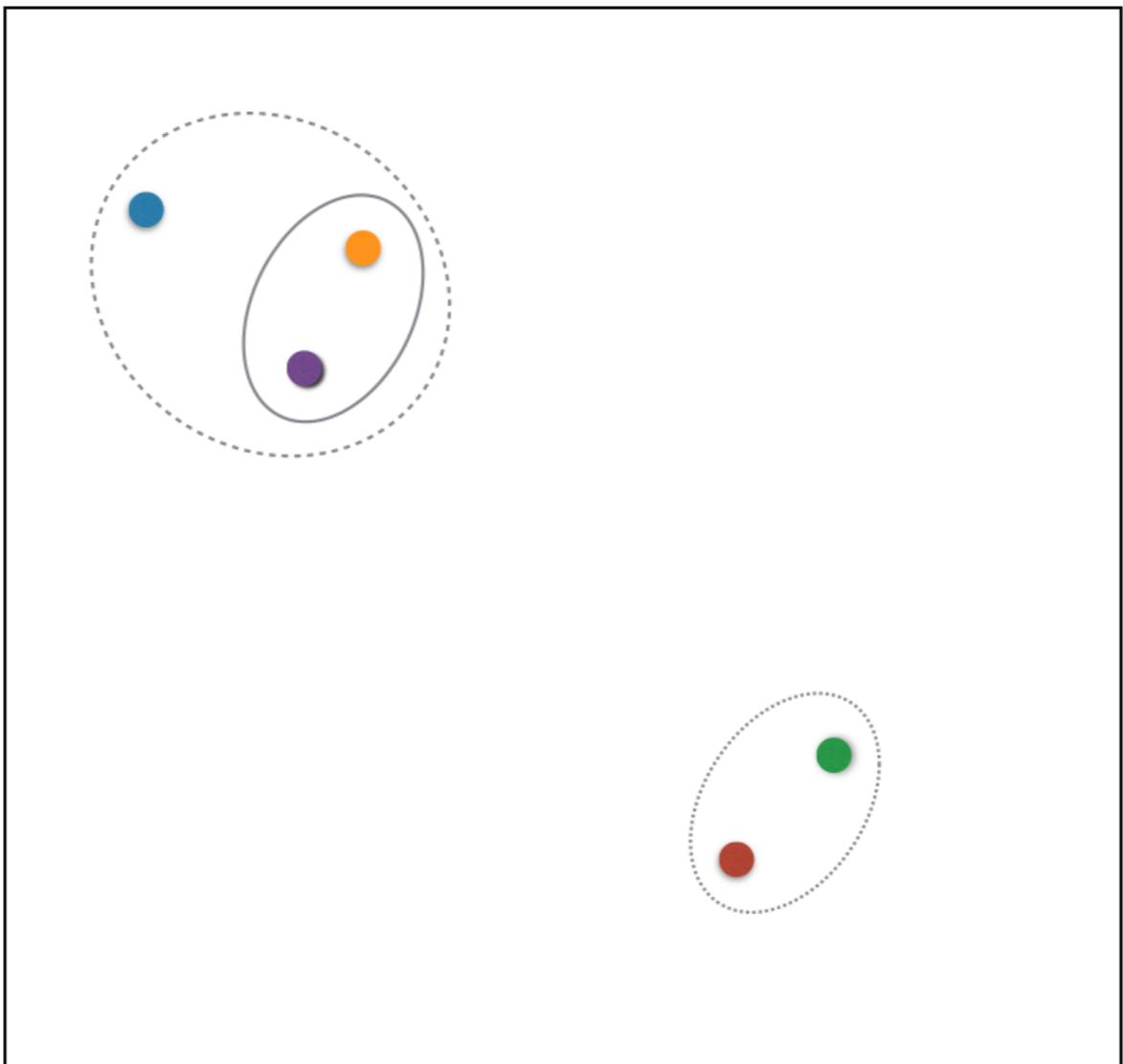
Hank Roark

Senior Data Scientist at Boeing

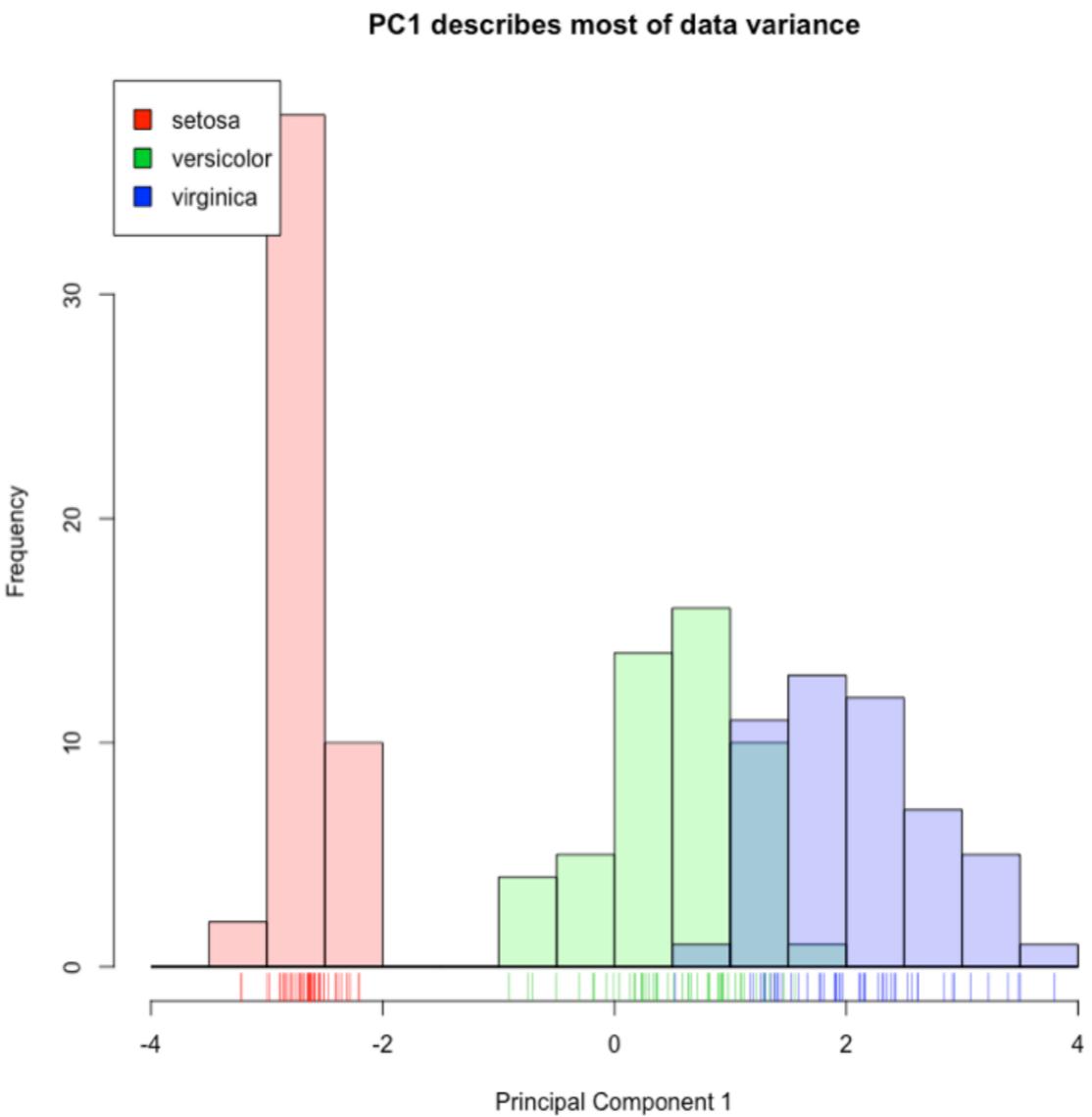
# Chapter review

- 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

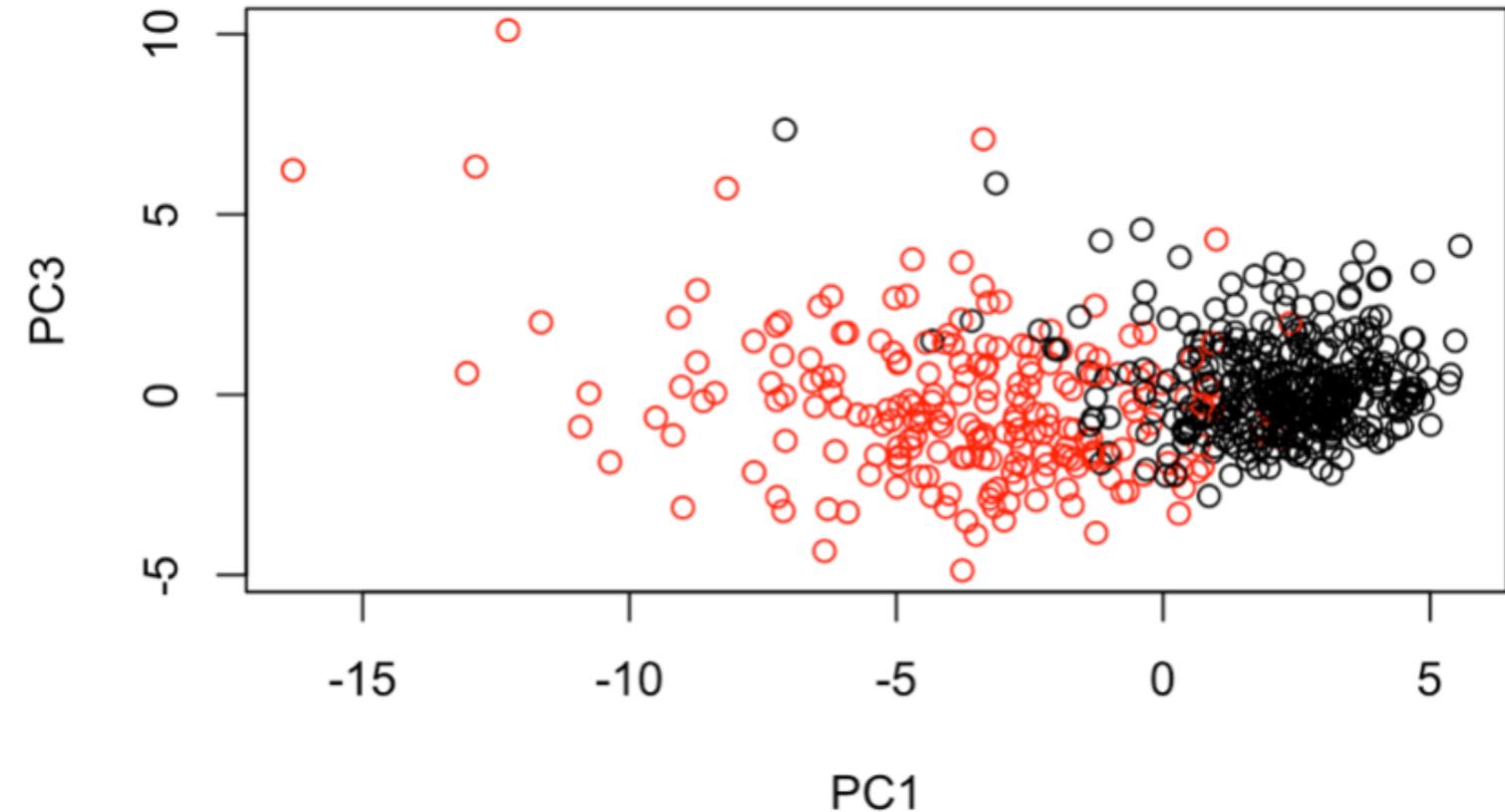


# Coming up: chapter 3



# Coming up: chapter 4

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



**See you in the next  
chapter!**

**UNSUPERVISED LEARNING IN R**