K-Means Overview

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Clustering: The Problem

We want to find subgroups (clusters) in our data set.

Contrast this to classification where we want to assign a class to each observation.

1. K-Means
2. Hierarchical Clustering

We will partition the data into distinct groups such that the observations within each group are similar to each other, while observations in different groups are different from each other.

We can cluster on either observations or features. (e.g. genome data)

- Cancer data
- Market Segmentation

The Goal

The goal is to partition the data into K cluster.

Disadvantage: we need to specify the number of clusters (contrast to hierarchical clustering)

- $C_1 \cup C_2 \cup \cdots \cup C_K = 1, \cdots, n$
- $C_i \cap C_j = \phi \; ; i \neq j$

We want to minimize within cluster variation:

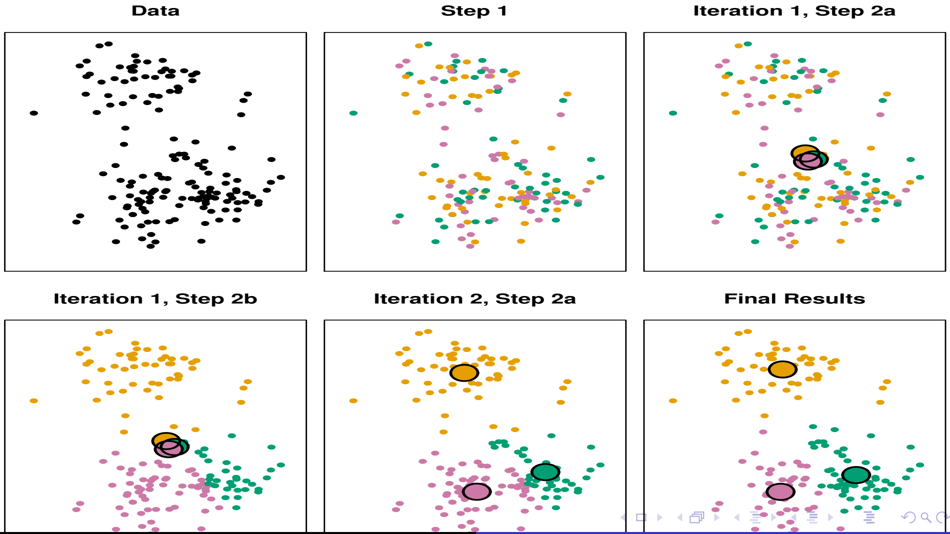
$$\min_{C_1,\cdots,C_K} \sum_{i=1}^{K} W(C_i)$$

For Euclidean distance:

$$W(C_k) = \frac{1}{|C_k|} \sum_{i,j \in C_k} \|\mathbf{x}_i - \mathbf{x}_j\|^2$$

- There are K^n ways to partition the data into K clusters.
- NP-Hard problem.

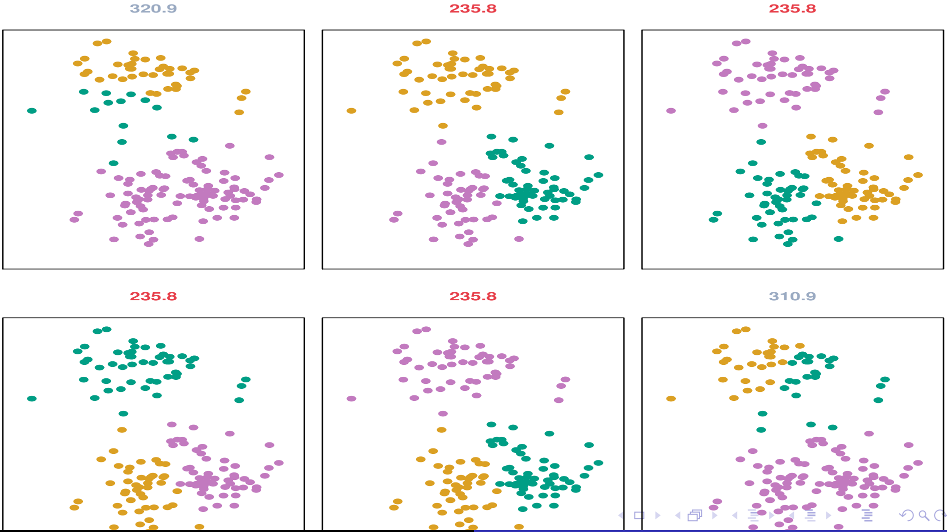
1. Randomly assign each observation to one of the K cluster.
2. Iterate until cluster assignment stop changing:
    a. For each of the K clusters, compute the cluster's centroid.
    b. Assign each obseration to the cluster with the closest centroid.

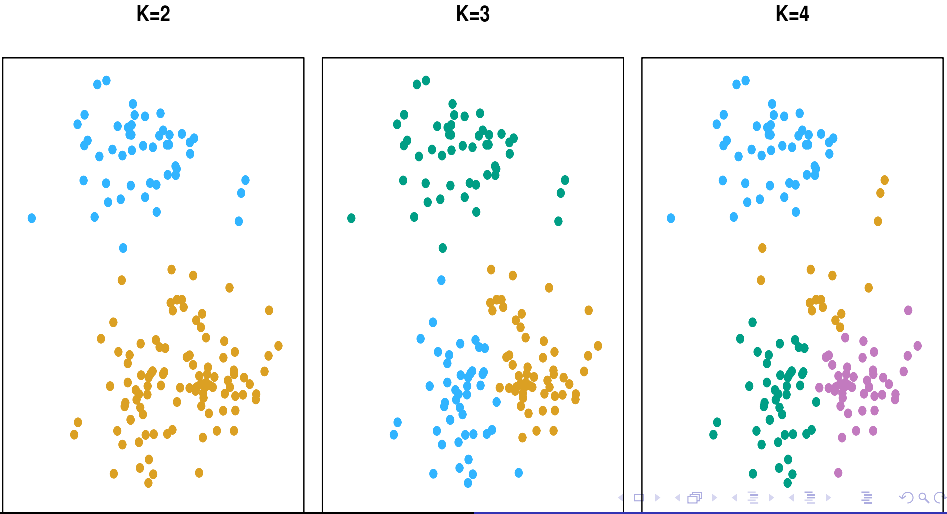

Data
Step 1
Iteration 1, Step 2a
Iteration 1, Step 2b
Iteration 2, Step 2a
Final Results

Local Optimum

It is important to run the algorithm several times with different initial cluster assignment.

We choose the solution with the smallest value to our objective function.


320.9
235.8
235.8
235.8
235.8
310.9


K=2
K=3
K=4

- Should we standardize observations (or features)?
- Validation: Are we clustering noise or are these true subgroups?
- K-means forces every observation into a cluster (Mixture models)
- Not robust to perturbation to the data

```
km.out = kmeans(data,number.of.clusters,num.start)
plot (data,col=(km.out$cluster+1))
```

Thank You For Listening

Questions and/or Comments

- Hastie, T., Tibshirani, R., Friedman, J. The Elements of Statistical Learning.
- James, G., Witten, D., Hastie, T., Tibshirani, R. An Introduction to Statistical Learnin