Unsupervised Learning with Clustering

K-means

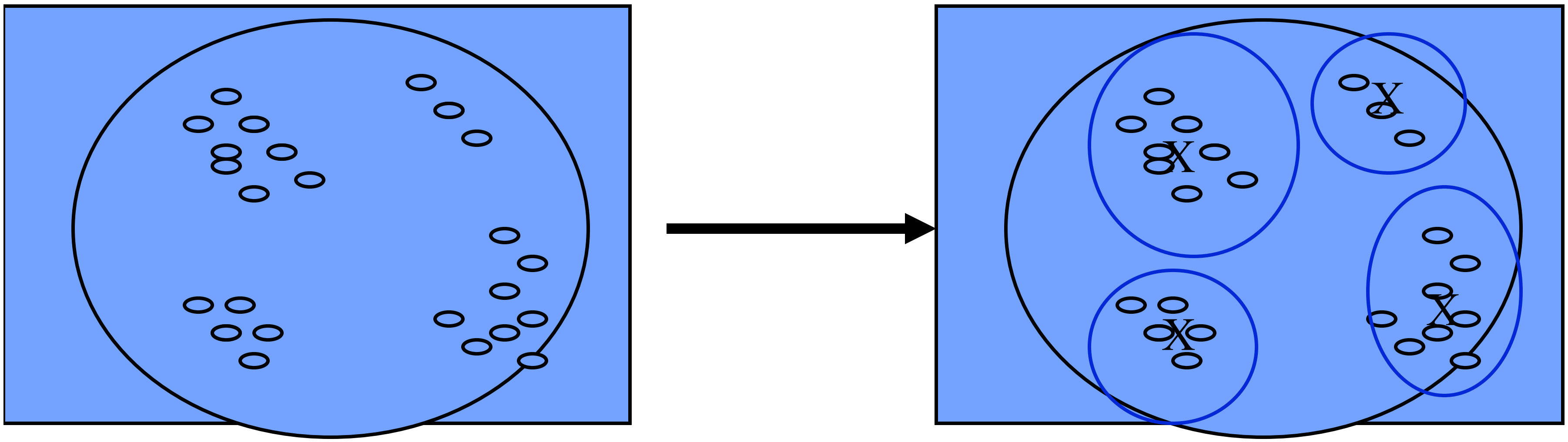
Why Clustering

- **A good grouping implies some structure**
- **In other words, given a good grouping, we can then:**
  - Interpret and label clusters
  - Identify important features
  - Characterize new points by the closest cluster (or nearest neighbors)
  - Use the cluster assignments as a compression or summary of the data

Clustering

- **Basic idea: Group similar things together**
- **Unsupervised Learning – Useful when no other info is available**
- **K-means**
  - Partitioning instances into k disjoint clusters
  - Measure of similarity

Clustering



Clustering Techniques

- **K-means clustering**
- **Hierarchical clustering**
- **Conceptual clustering**
- **Probability-based clustering**
- **Bayesian clustering**

Clustering Techniques

- K-means clustering
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- Bayesian clustering

Clustering Applications

- Example: Clustering of a large number of gene experiments
- Multiple sequence alignment of genes closely clustered together
- Search for metabolic pathways genes may be involved with
- Possible functional classification of genes in the same cluster
- Identifying co-regulated genes from expression arrays

Common uses of Clustering

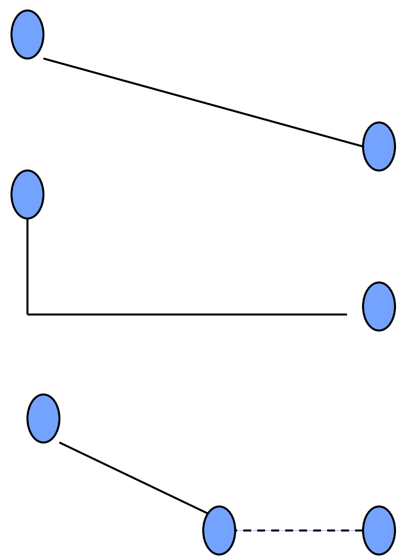
- Often used as an exploratory data analysis tool
- In one-dimension, a good way to quantify real-valued variables into k non-uniform buckets
- Used on acoustic data in speech understanding to convert waveforms into one of k categories (known as Vector Quantization)
- Also used for choosing color palettes on old fashioned graphical display devices
- Color Image Segmentation

Clustering

- **Unsupervised: no target value to be predicted**
- **Differences ways clustering results can be produced/represented/learned**
  - Exclusive vs. overlapping
  - Deterministic vs. probabilistic
  - Hierarchical vs. flat
  - Incremental vs. batch learning

Clustering Objective

- **Objective: find subsets that are similar within cluster and dissimilar between clusters**
- **Similarity defined by distance measures**



  - Euclidean distance
  - Manhattan distance
  - Mahalanobis (Euclidean w/dimensions rescaled by variance)

Clustering Objective

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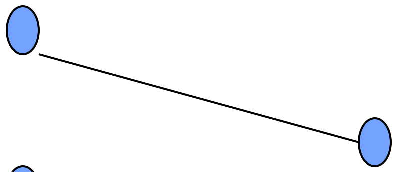
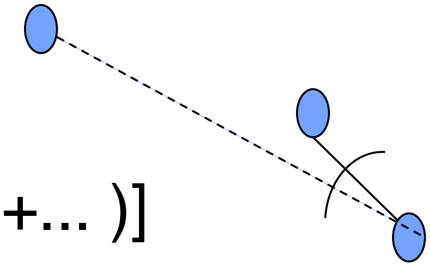


  - Euclidean distance =

    $\mathrm{sqrt}[(a1 - b1)^2 + (a2 - b2)^2 + \ldots)]$

  - Manhattan distance

    $[|a1 - b1| + |a2 - b2| + \ldots)]$

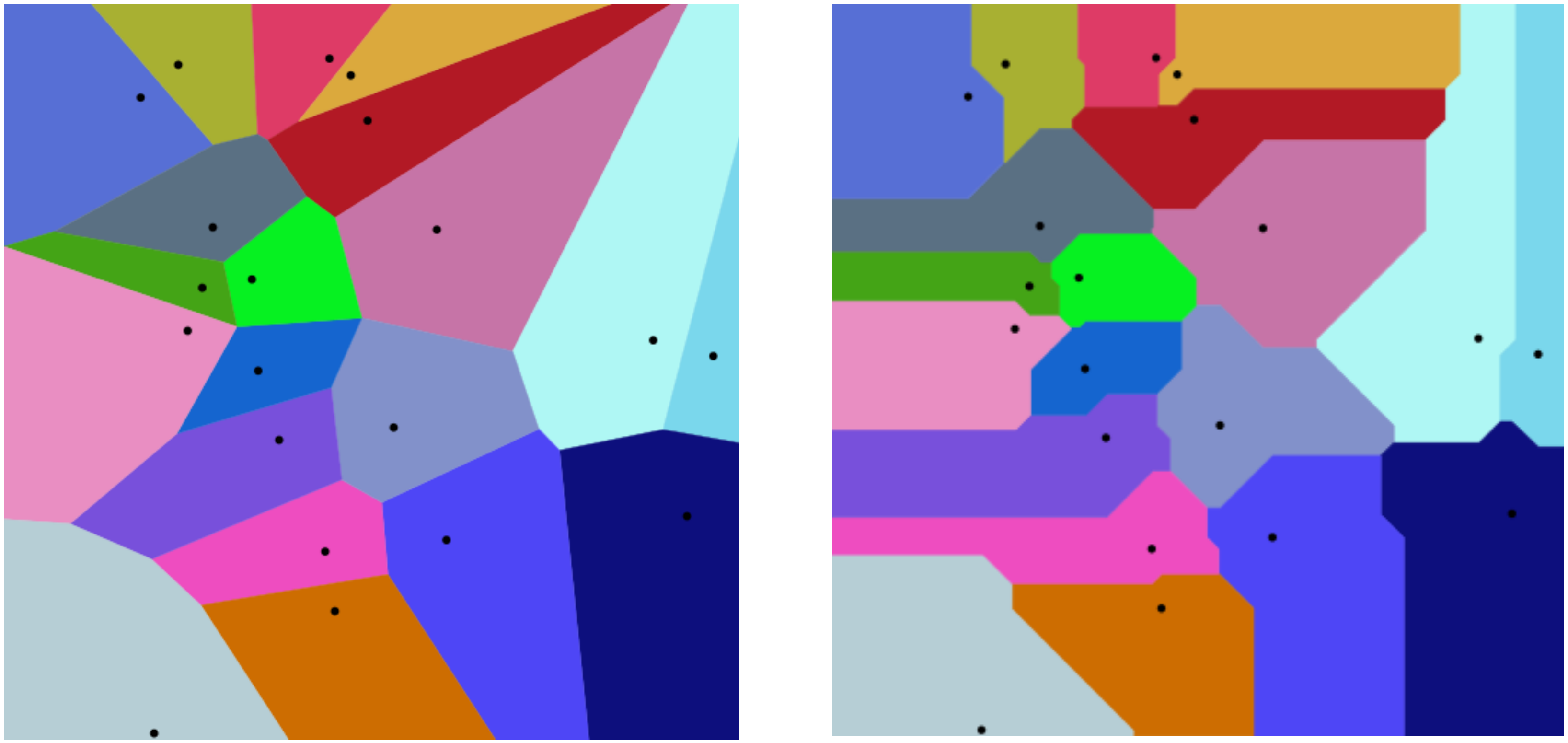


  - Cosine (insensitive to size)

    Euc Dist/

    $\mathrm{sqrt}[(a1)^2 + (a2)^2 ..] * \mathrm{sqrt}[(b1)^2 + \ldots)]$

Euclidean Vs. Manhattan



"Euclidean and Manhattan Voronoi diagram" by Balu Ertl - Own work. Licensed under CC BY-SA 4.0 via Wikimedia Commons - http://commons.wikimedia.org/wiki/File:Euclidean_Voronoi_diagram.svg#/media/File:Euclidean_Voronoi_diagram.svg

The k-means Algorithm
Iterative Distance Based Clustering

- **Clusters the data into k groups where k is specified in advance**
  1. Cluster centers are chosen at random
  2. Instances are assigned to clusters based on their distance to the cluster centers
  3. Centroids of clusters are computed – “means”
  4. Go to 1st step until convergence

K-means Clustering

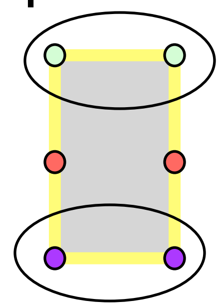
- **A simple, effective, and standard method**
  - Start with K initial cluster centers
  - Loop:
    - Assign each data point to nearest cluster center
    - Calculate mean of cluster for new center
  - Stop when assignments don't change
- **Issues:**
  - How to choose K?
  - How to choose initial centers?
  - Will it always stop?

K-Means Clustering Pros & Cons

- **Simple and reasonably effective**
- **The final cluster centers do not represent a global minimum but only a local one**
- **Result can vary significantly based on initial choice of seeds**
  - Completely different final clusters can arise from differences in the initial randomly chosen cluster centers
- **Algorithm can easily fail to find a reasonable clustering**

Getting Trapped in a Local Minimum

- **Example: four instances at the vertices of a two-dimensional rectangle**
  - Local minimum: two cluster centers at the midpoints of the rectangle's long sides



- **Simple way to increase chance of finding a global optimum: restart with different random seeds**

Clustering

- **Partition unlabeled examples into disjoint subsets of *clusters*, such that:**
  - Examples within a cluster are very similar
  - Examples in different clusters are very different
- **Discover new categories in an *unsupervised* manner (no sample category labels provided)**

K-Means Algorithm

Let d be the distance measure between instances.
Select k random instances $\{s_1, s_2, \ldots s_k\}$ as seeds.
Until clustering converges or other stopping criterion:

For each instance x_i:

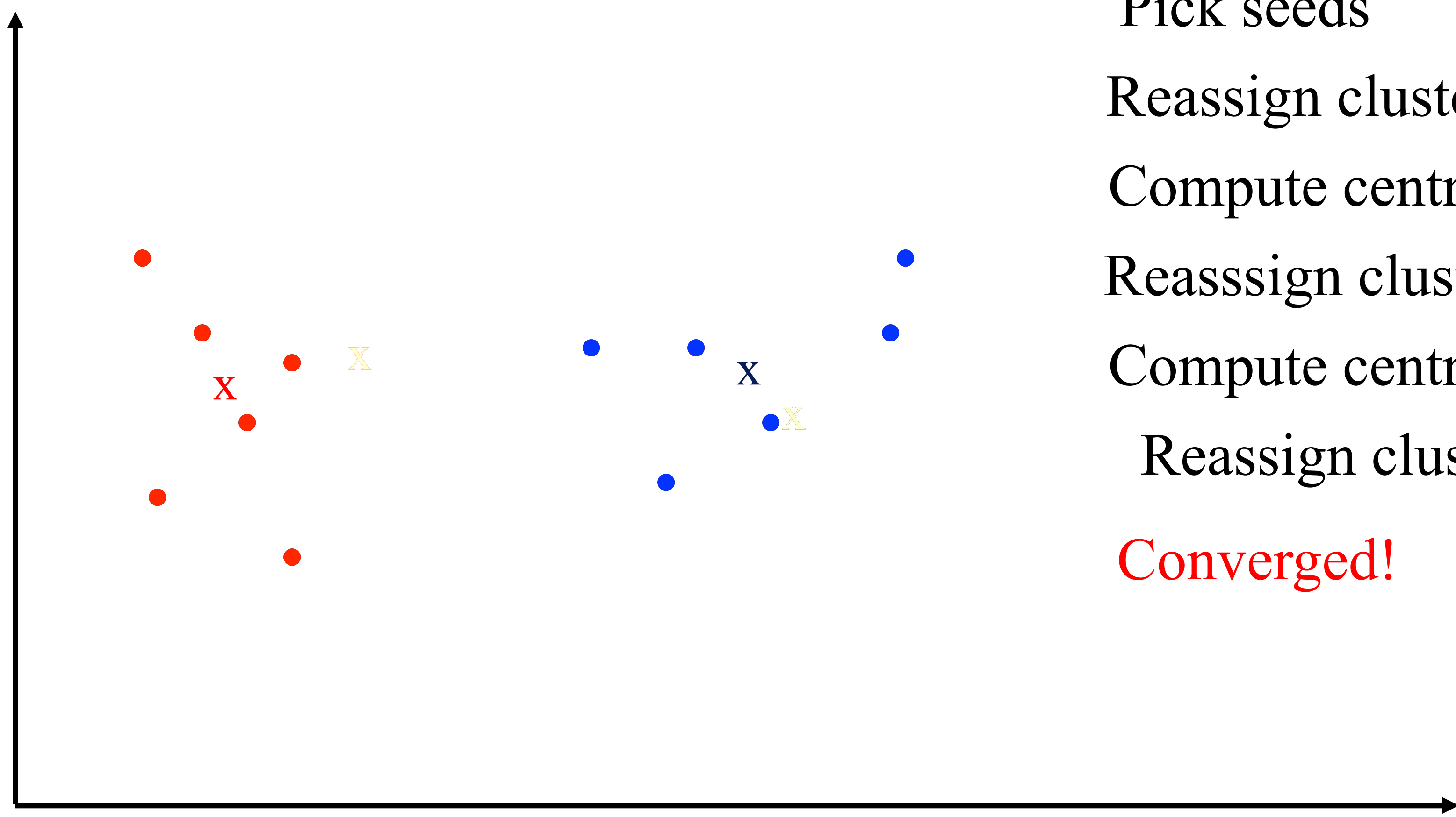
Assign x_i to the cluster c_j such that $d(x_i, s_j)$ is minimal.

(Update the seeds to the centroid of each cluster)

For each cluster c_j

$$s_j = \square(c_j)$$

K Means Example (K=2)



Pick seeds

Reassign clusters

Compute centroids

Reasssign clusters

Compute centroids

Reassign clusters

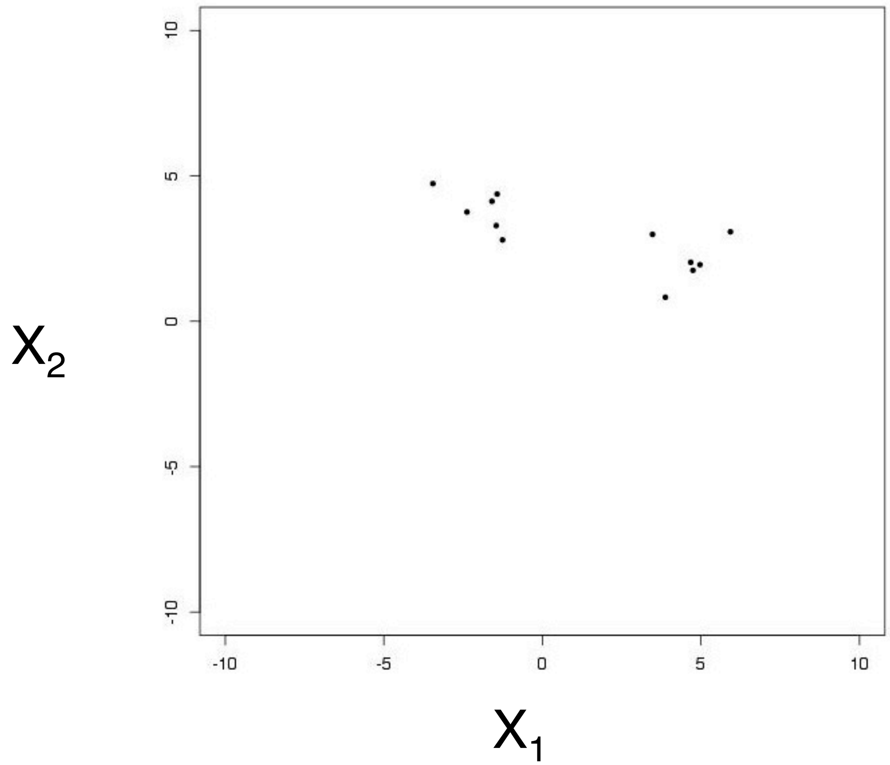
Converged!

Seed Choice

- Results can vary based on random seed selection
- Some seeds can result in poor convergence rate, or convergence to sub-optimal clusters
- Select good seeds using a heuristic or the results of another method

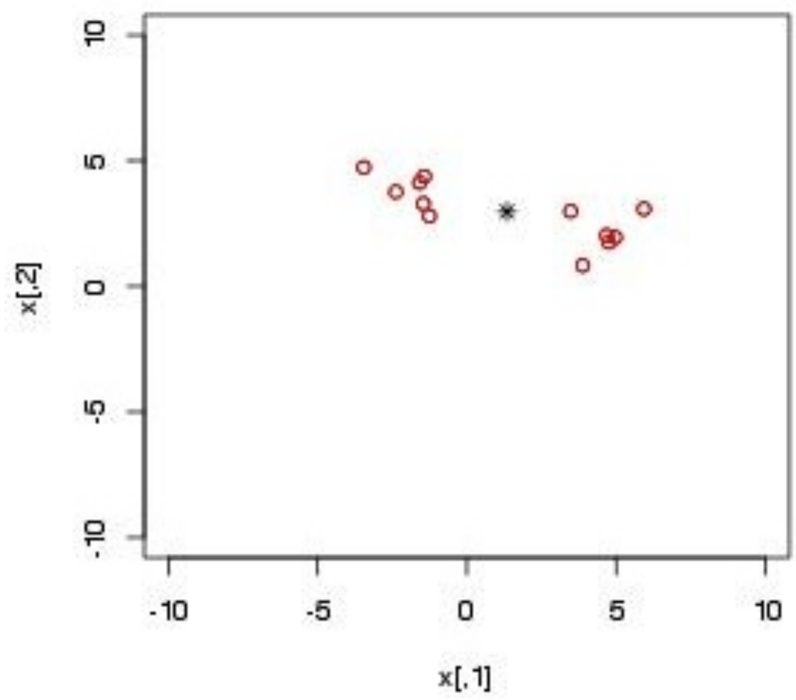
K-means Example

- **For K=1, using Euclidean distance, where will the cluster center be?**



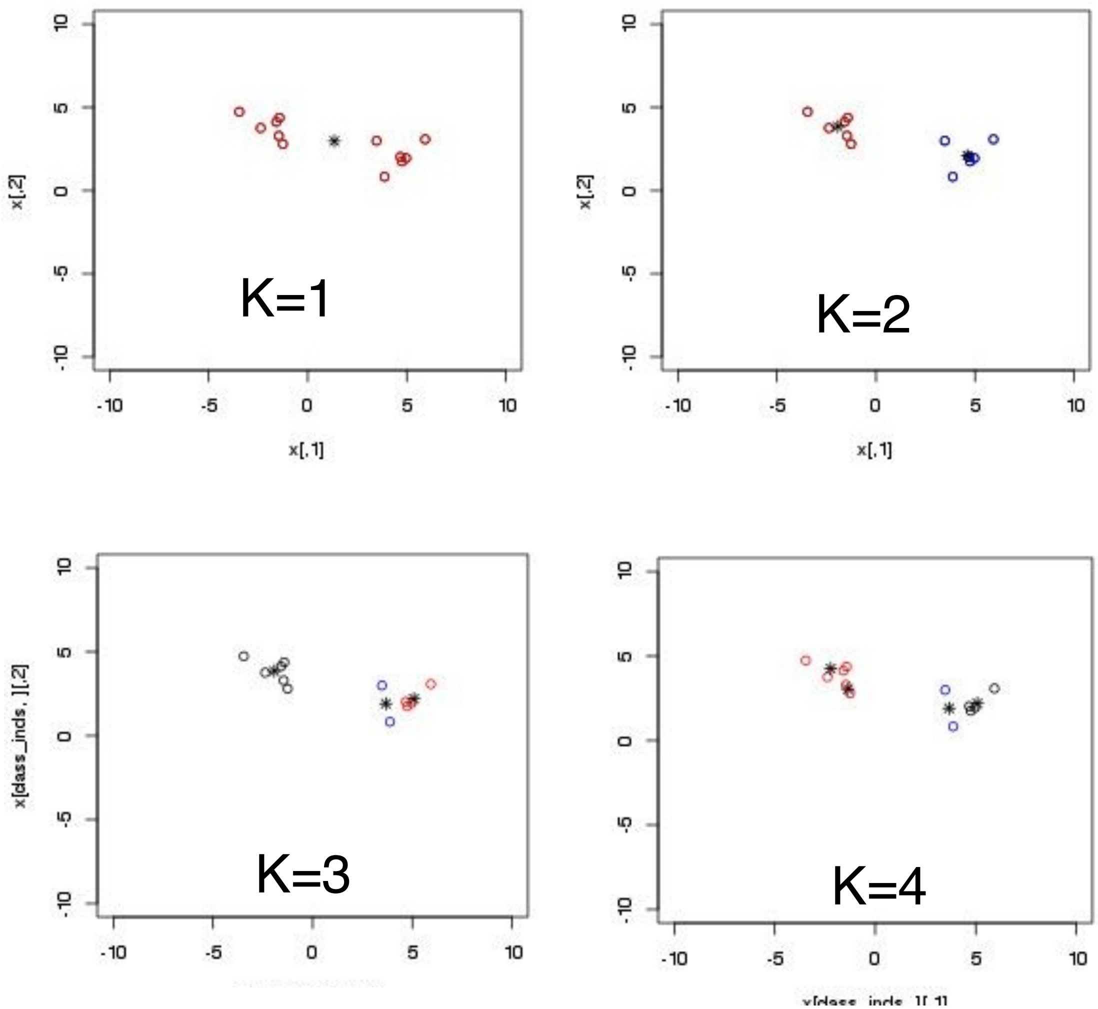
K-means Example

- **For K=1, the overall mean minimizes Sum Squared Error (SSE), aka Euclidean distance**

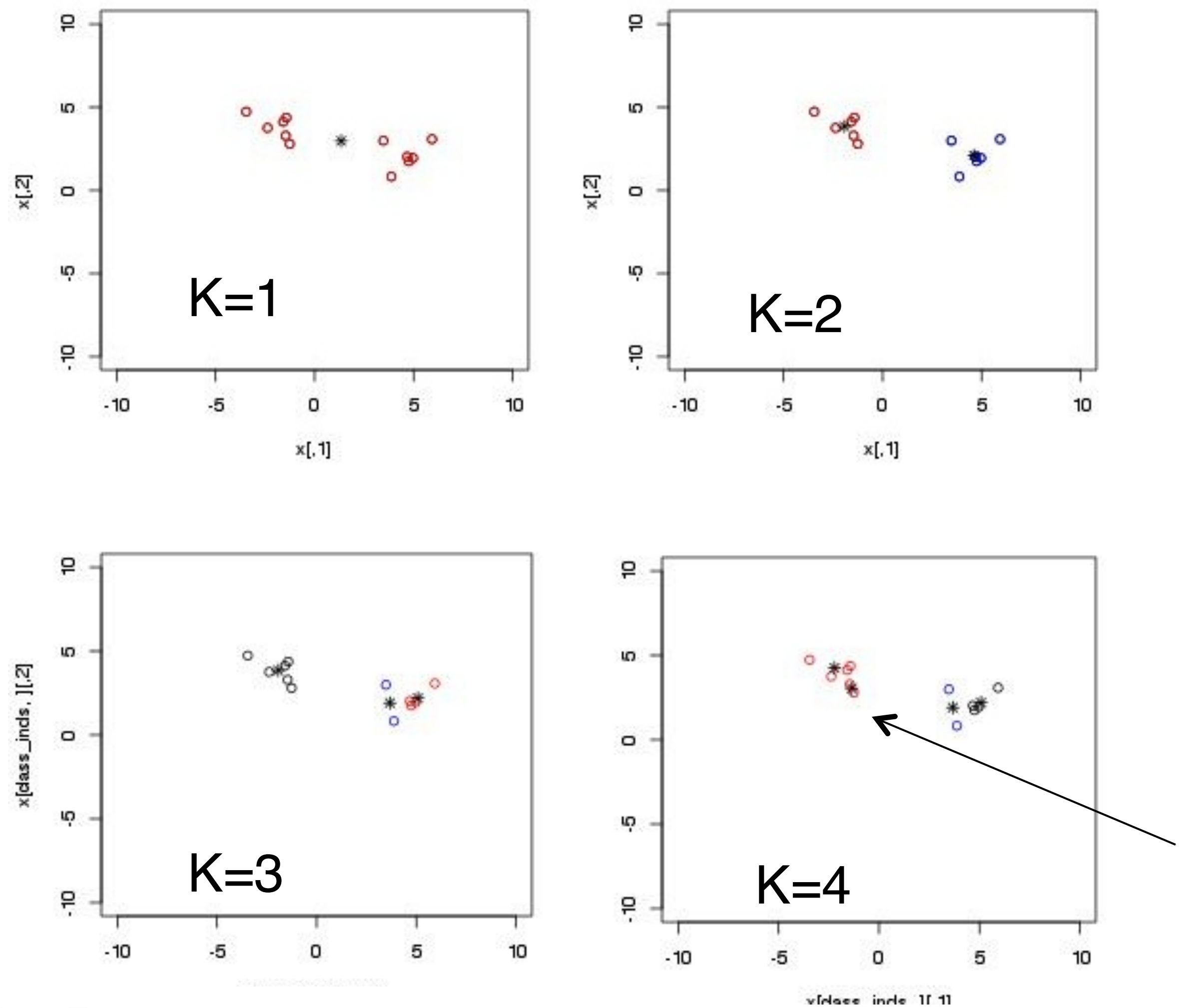


Simple example:
#choose 1 data point as initial K centers
#10 is max loop iterations
#1 is number of initial sets to try

K-means Example



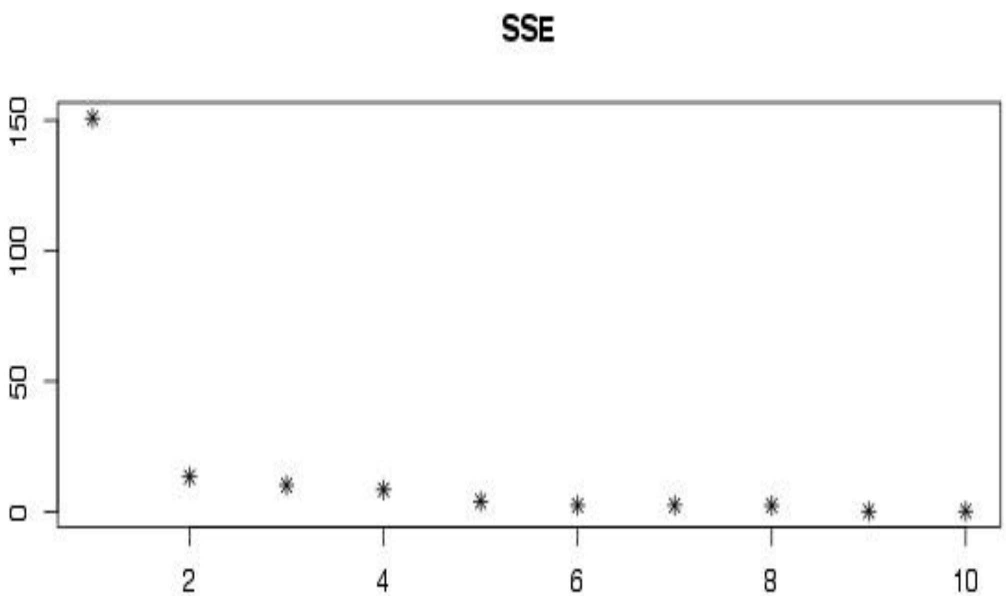
K-means Example



As K increases individual points get a cluster

Choosing K for K-means

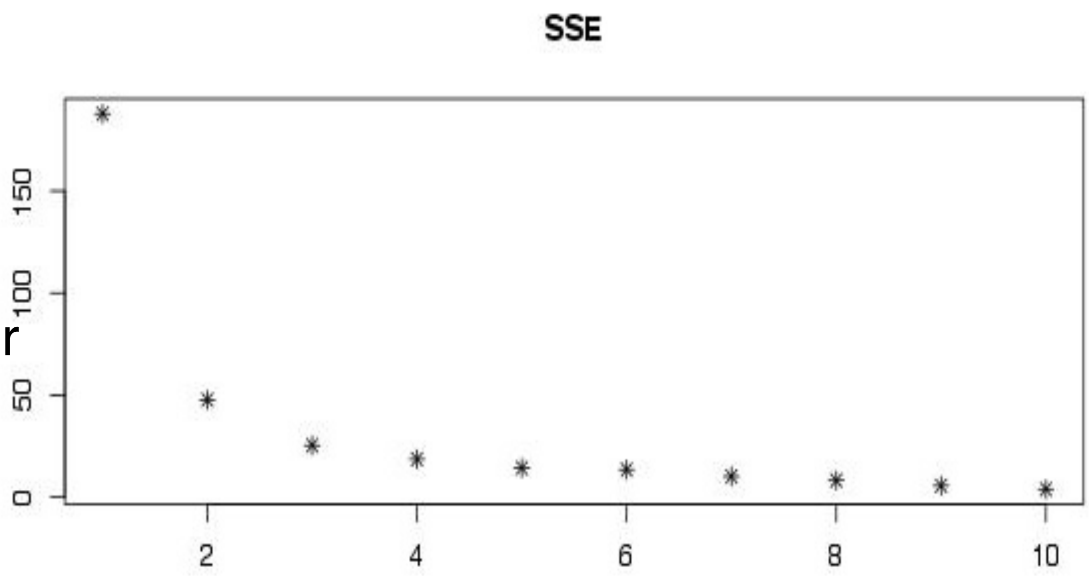
Total Within Cluster SSE



K=1 to 10

- Not much improvement after K=2 (“elbow”)

Choosing K for K-means



Total Within Cluster SSE

K=1 to 10

- Smooth decrease at K $\geq$ 2, harder to choose
- In general, smoother decrease => less structure

K-means Guidelines

- **Choosing K:**
  - “Elbow” in total-within-cluster SSE as K=1…N
  - Cross-validation: hold out points, compare fit as K=1…N
- **Choosing initial starting points:**
  - take K random data points, do several K-means, take best fit
- **Stopping:**
  - may converge to sub-optimal clusters
  - may get stuck or have slow convergence (point assignments bounce around), 10 iterations is often good

K-means Clustering Issues

- **Scale:**
  - Dimensions with large numbers may dominate distance metrics

- **Outliers:**
  - Outliers can pull cluster mean, K-mediods uses median instead of mean

Summary

- **Labeled clusters can be interpreted by using supervised learning - train a tree or learn rules**
- **Can be used to fill in missing attribute values**
- **All methods have a basic assumption of independence between the attributes**
  - Some methods allow the user to specify in advanced that two of more attributes are dependent and should be modeled with a joint probability

K-Means Exercise

Download the Bank data set: http://facweb.cs.depaul.edu/mobasher/classes/ect584/WEKA/k-means.html