CSE 4621
Machine Learning

Lecture 14

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What is Cluster Analysis?

- Cluster: A collection of data objects
  - similar (or related) to one another within the same group
  - dissimilar (or unrelated) to the objects in other groups
- Cluster analysis (or *clustering, data segmentation, …*)
  - Finding similarities between data according to the characteristics found in the data and grouping similar data objects into clusters
- Unsupervised learning: no predefined classes (i.e., *learning by observations* vs. learning by examples: supervised)
- Typical applications
  - As a stand-alone tool to get insight into data distribution
  - As a preprocessing step for other algorithms

Clustering for Data Understanding and Applications

- Biology: taxonomy of living things: kingdom, phylum, class, order, family, genus and species
- Information retrieval: document clustering
- Land use: Identification of areas of similar land use in an earth observation database
- Marketing: Help marketers discover distinct groups in their customer bases, and then use this knowledge to develop targeted marketing programs
- City-planning: Identifying groups of houses according to their house type, value, and geographical location
- Earth-quake studies: Observed earth quake epicenters should be clustered along continent faults
- Web Search: Clustering can be used to organize the search results into groups and present the results in a concise and easily accessible way.
- Information Retrieval: Cluster documents into topics.

Clustering as a Preprocessing Tool (Utility)

- Summarization:
  - Preprocessing for regression, PCA, classification, and association analysis
- Compression:
  - Image processing: vector quantization
- Finding K-nearest Neighbors
  - Localizing search to one or a small number of clusters
- Outlier detection
  - Outliers are often viewed as those “far away” from any cluster

Quality: What Is Good Clustering?

- A good clustering method will produce high quality clusters
  - high intra-class similarity: cohesive within clusters
  - low inter-class similarity: distinctive between clusters
- The quality of a clustering method depends on
  - the similarity measure used by the method
  - its implementation, and
  - Its ability to discover some or all of the hidden patterns

Measure the Quality of Clustering

- Dissimilarity/Similarity metric
  - Similarity is expressed in terms of a distance function, typically metric: $d(i, j)$
  - The definitions of distance functions are usually rather different for interval-scaled, boolean, categorical, ordinal ratio, and vector variables
  - Weights should be associated with different variables based on applications and data semantics
- Quality of clustering:
  - There is usually a separate "quality" function that measures the "goodness" of a cluster.
  - It is hard to define "similar enough" or "good enough"
    - The answer is typically highly subjective

Considerations for Cluster Analysis

- Partitioning criteria
  - Single level vs. hierarchical partitioning (often, multi-level hierarchical partitioning is desirable). E.g. Politics, Sports: Football, Cricket, volleyball, etc.

- Separation of clusters
  - Exclusive (e.g., one customer belongs to only one region) vs. non-exclusive (e.g., one document may belong to more than one class)

- Similarity measure
  - Distance-based (e.g., Euclidian, road network, vector) vs. connectivity-based (e.g., density or contiguity)
  - Distance-based methods can often take advantage of optimization techniques, density- and continuity-based methods can often find clusters of arbitrary shape

- Clustering space
  - Full space (often when low dimensional) vs. subspaces (often in high-dimensional clustering)

Major Clustering Approaches

- Partitioning approach:
  - Construct various partitions and then evaluate them by some criterion, e.g., minimizing the sum of square errors
  - Typical methods: k-means, k-medoids, CLARANS
- Hierarchical approach:
  - Create a hierarchical decomposition of the set of data (or objects) using some criterion
  - Typical methods: Diana, Agnes, BIRCH, CAMELEON
- Density-based approach:
  - Based on connectivity and density functions
  - Typical methods: DBSACN, OPTICS, DenClue
- Grid-based approach:
  - based on a multiple-level granularity structure
  - quantize object space into a finite number of cells (grid structure)
  - Typical methods: STING, WaveCluster, CLIQUE

Overview of Clustering Methods

Method	General Characteristics
Partitioning methods	– Find mutually exclusive clusters of spherical shape – Distance-based – May use mean or medoid (etc.) to represent cluster center – Effective for small- to medium-size data sets
Hierarchical methods	– Clustering is a hierarchical decomposition (i.e., multiple levels) – Cannot correct erroneous merges or splits – May incorporate other techniques like microclustering or consider object "linkages"
Density-based methods	– Can find arbitrarily shaped clusters – Clusters are dense regions of objects in space that are separated by low-density regions – Cluster density: Each point must have a minimum number of points within its "neighborhood" – May filter out outliers
Grid-based methods	– Use a multiresolution grid data structure – Fast processing time (typically independent of the number of data objects, yet dependent on grid size)

Partitioning Algorithms: Basic Concept

- <u>Partitioning method:</u> Partitioning a database ***D*** of ***n*** objects into a set of ***k*** clusters, such that the sum of squared distances is minimized (where c_i is the centroid or medoid of cluster C_i)

$$E = \Sigma_{i=1}^{k} \Sigma_{p \in C_i} \| p - c_i \|^2$$

- Given *k <=n*, find a partition of *k clusters* that optimizes the chosen partitioning criterion
  - Global optimal: exhaustively enumerate all partitions
  - Heuristic methods: *k-means* and *k-medoids* algorithms
  - <u>*k-means*</u> (MacQueen'67, Lloyd'57/'82): Each cluster is represented by the center of the cluster
  - <u>*k-medoids*</u> or PAM (Partition around medoids) (Kaufman & Rousseeuw'87): Each cluster is represented by one of the objects in the cluster

The *K-Means* Clustering Method

- Given *k*, the *k-means* algorithm is implemented as

Algorithm: *k*-means. The *k*-means algorithm for partitioning, where each cluster's center is represented by the mean value of the objects in the cluster.

Input:

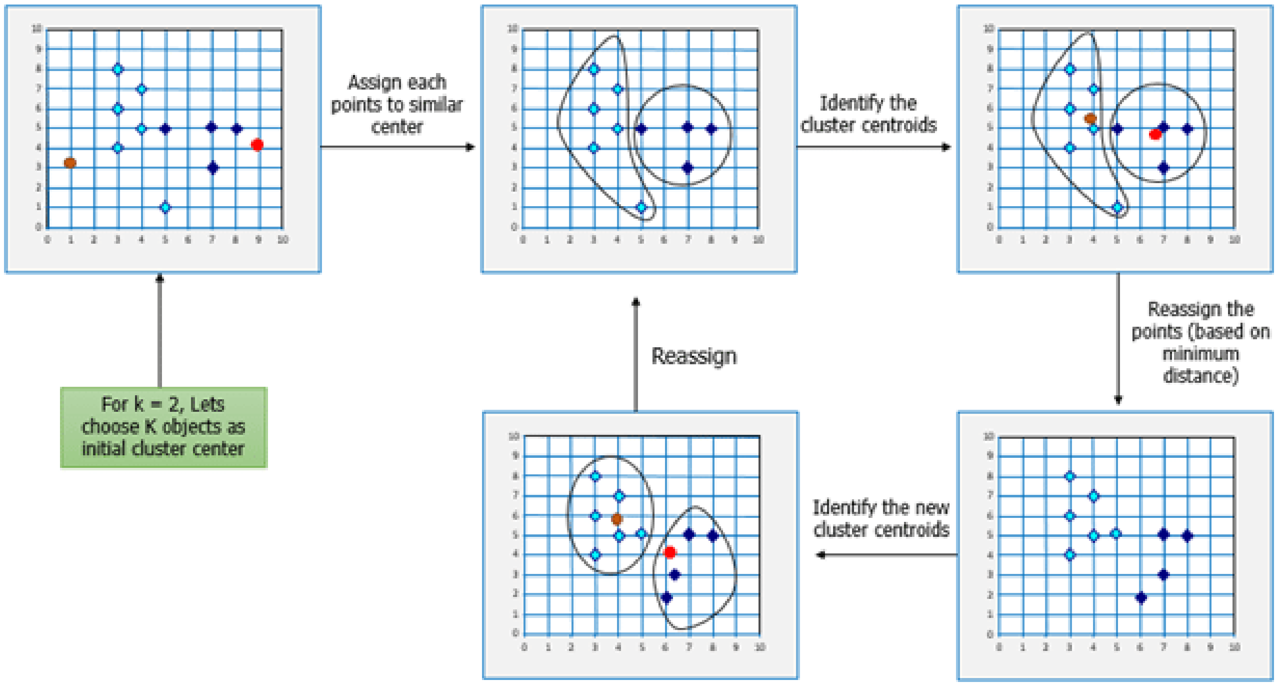
- *k*: the number of clusters,
- *D*: a data set containing *n* objects.

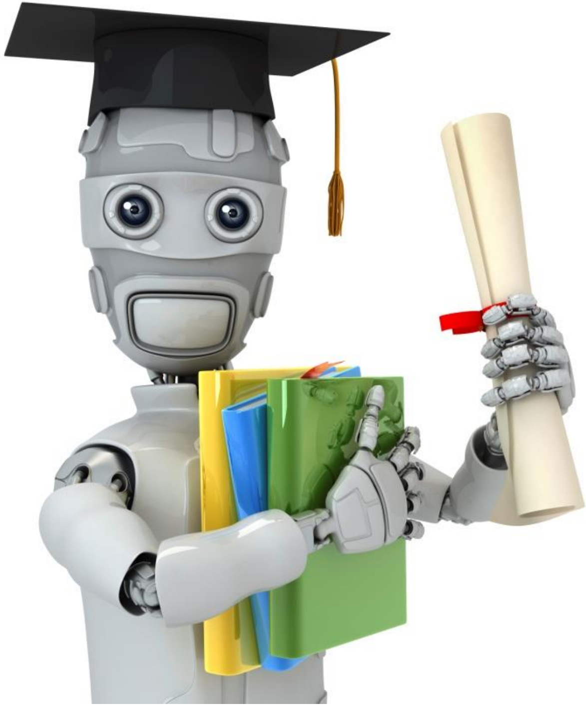
Output: A set of *k* clusters.

Method:

(1) arbitrarily choose *k* objects from *D* as the initial cluster centers;
(2) **repeat**
(3) (re)assign each object to the cluster to which the object is the most similar, based on the mean value of the objects in the cluster;
(4) update the cluster means, that is, calculate the mean value of the objects for each cluster;
(5) **until** no change;

An Example of *K-Means* Clustering

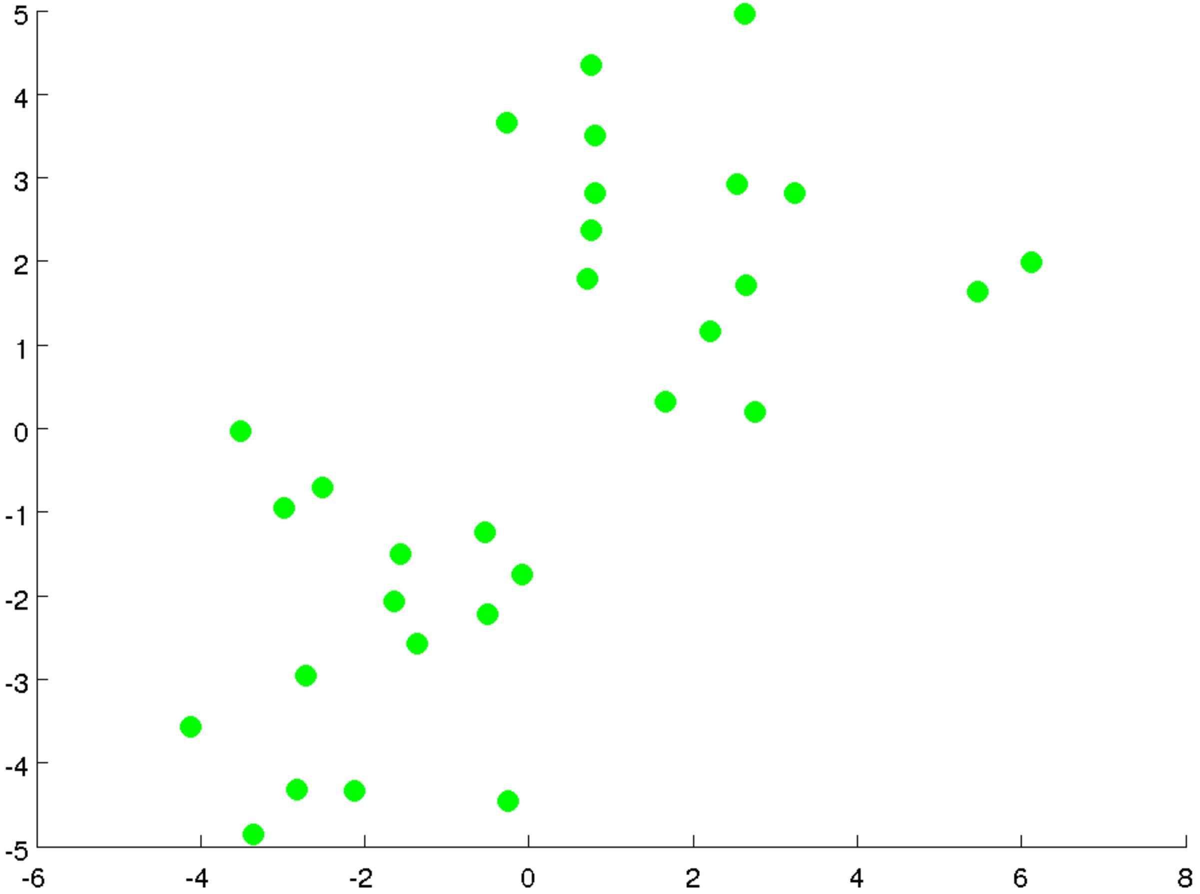




Machine Learning

Clustering

K-means Example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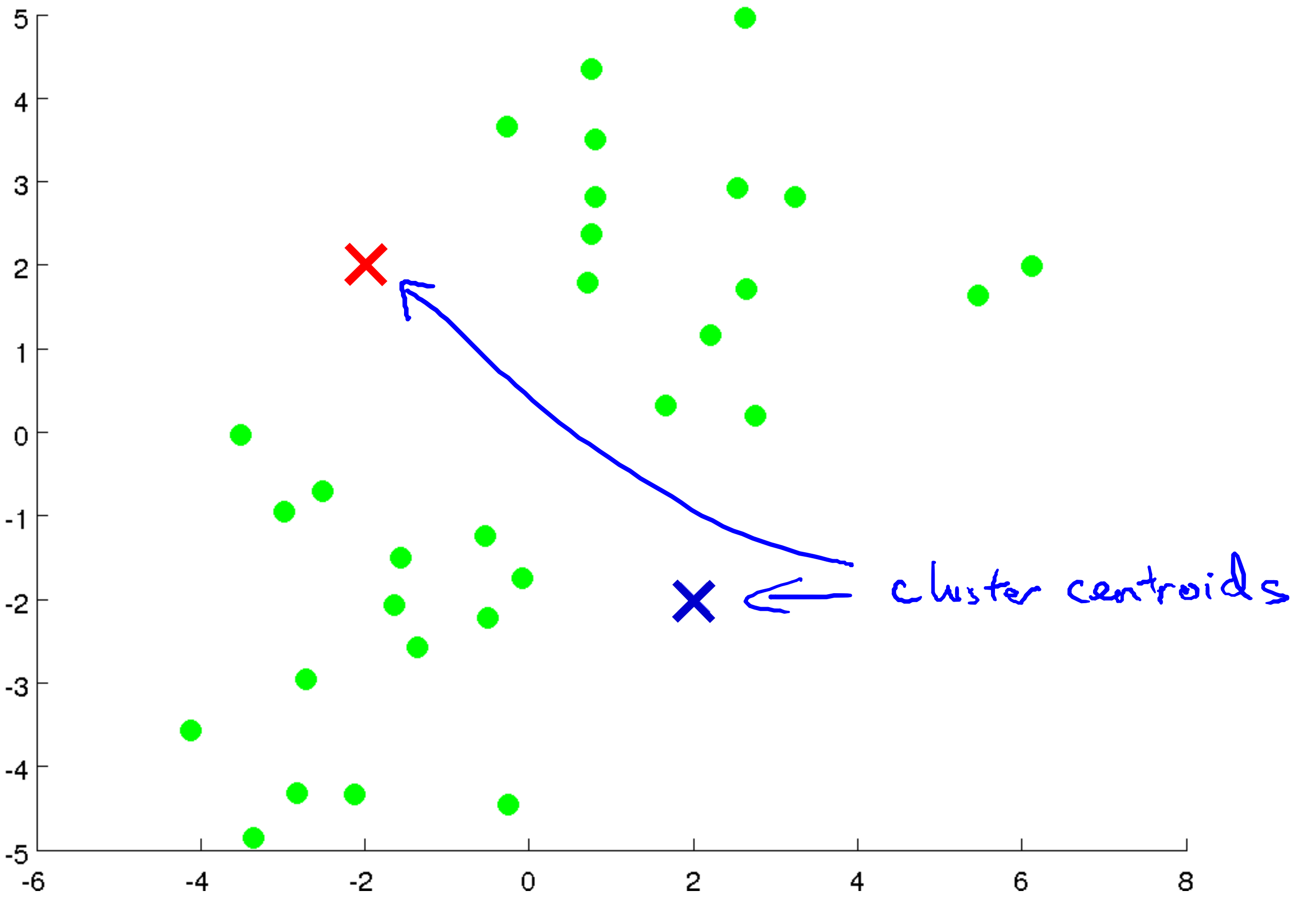

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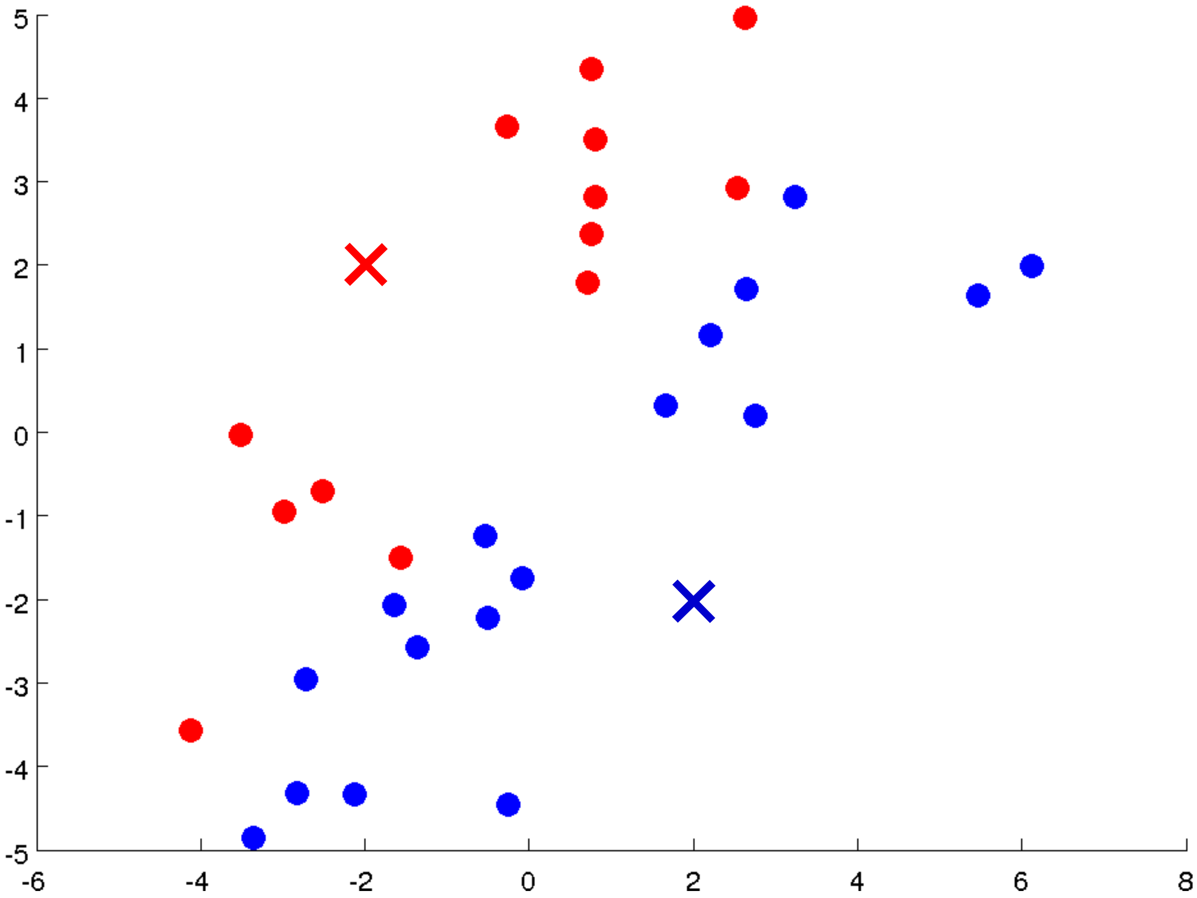

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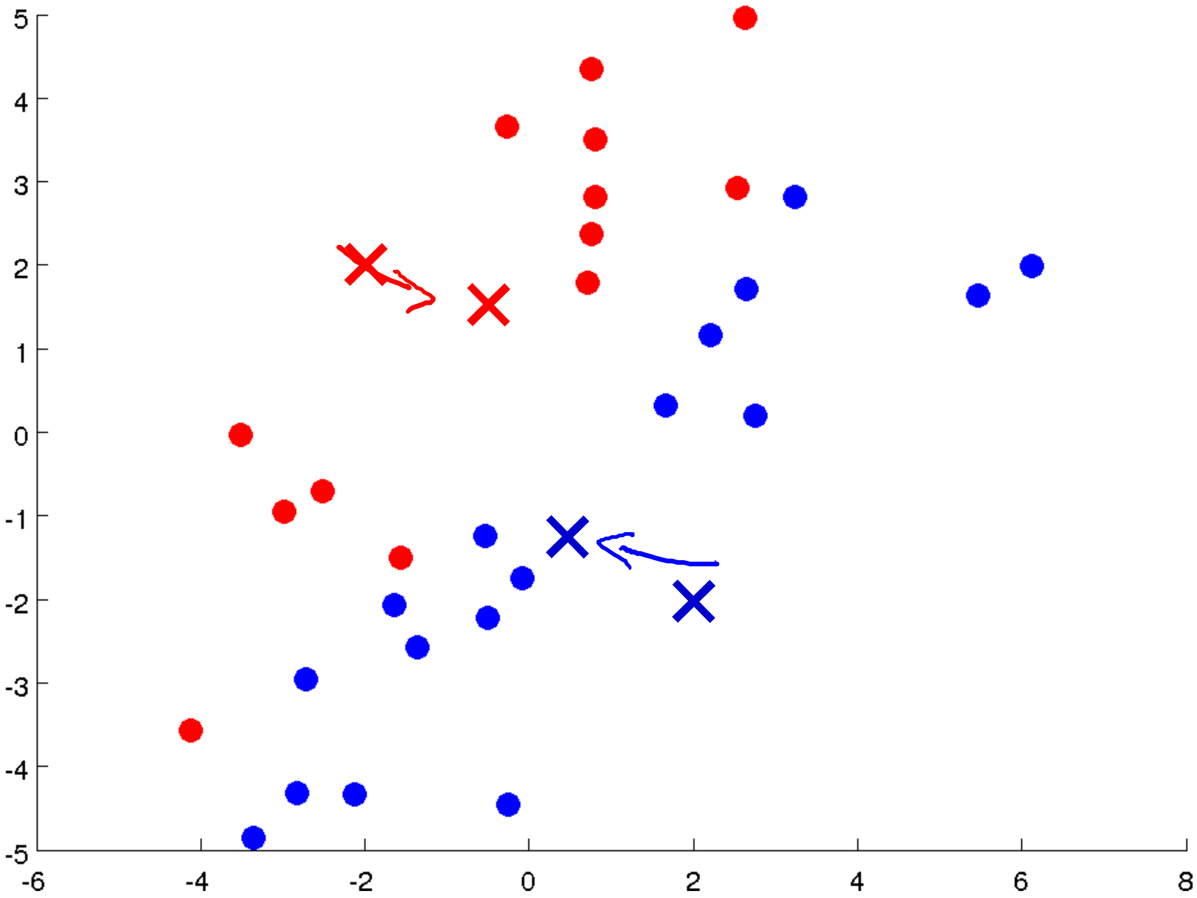

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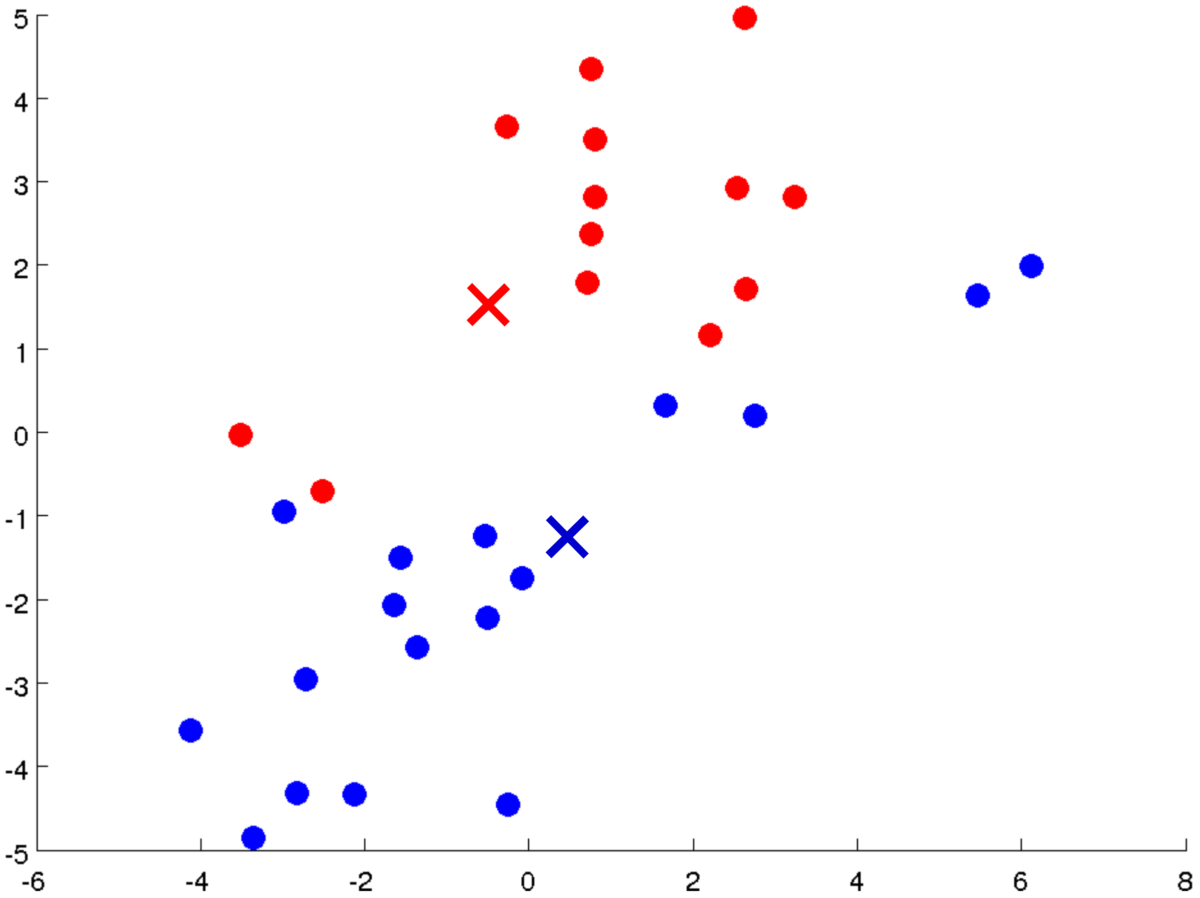

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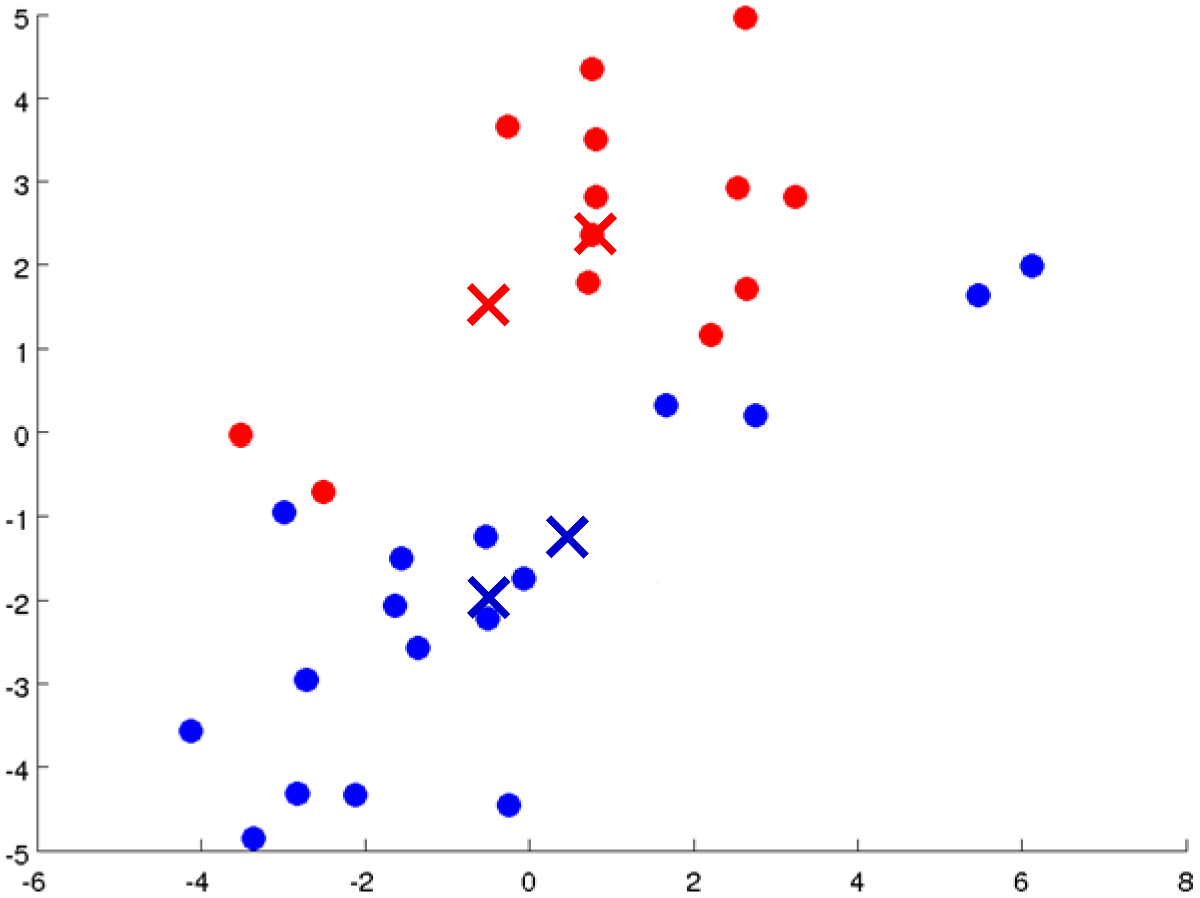
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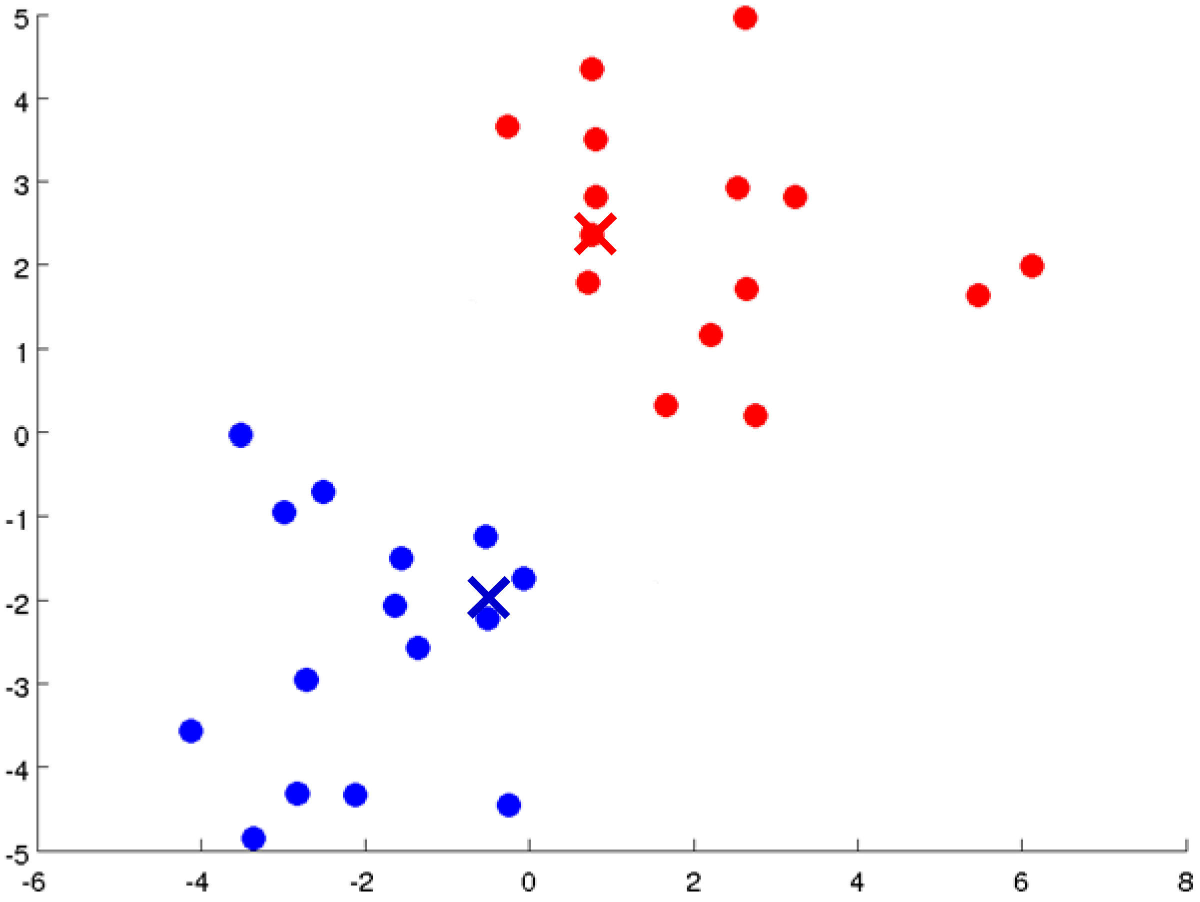

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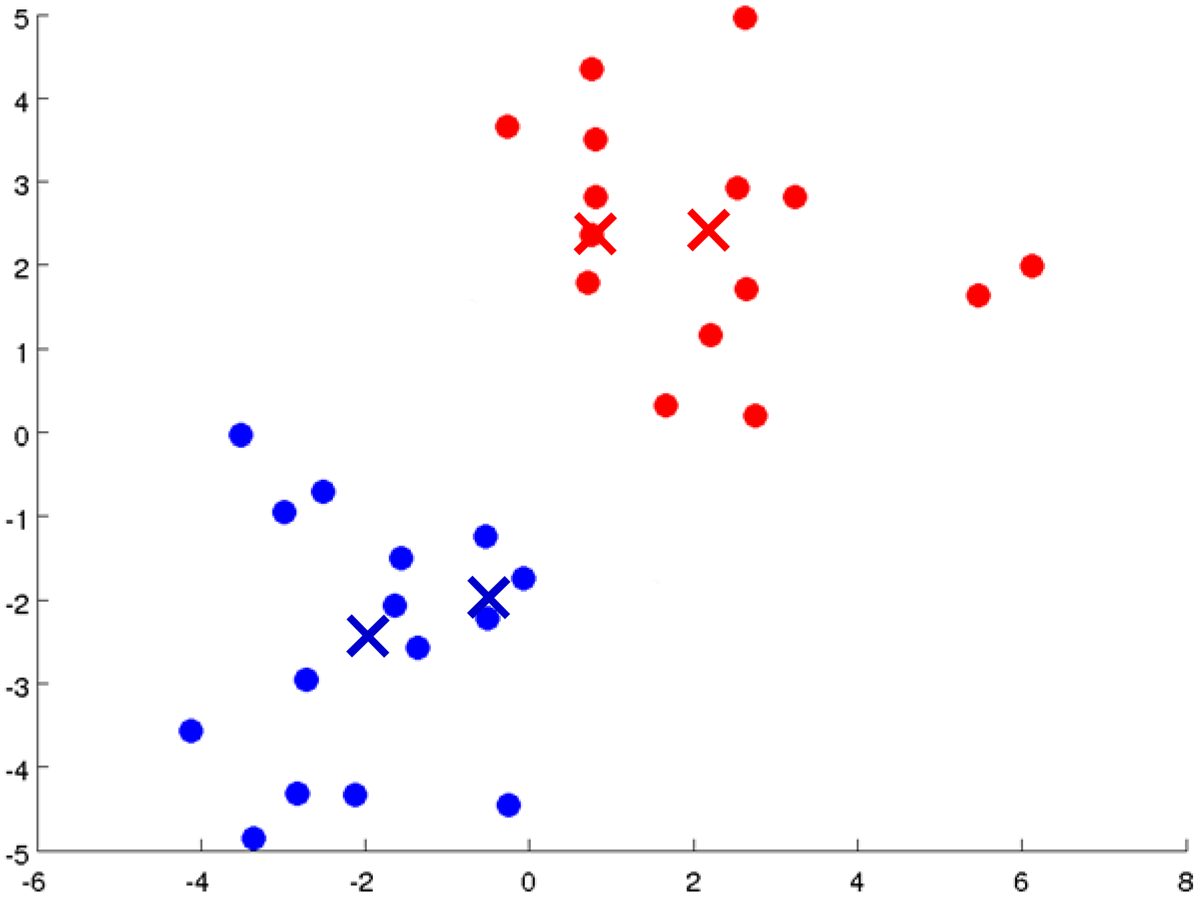

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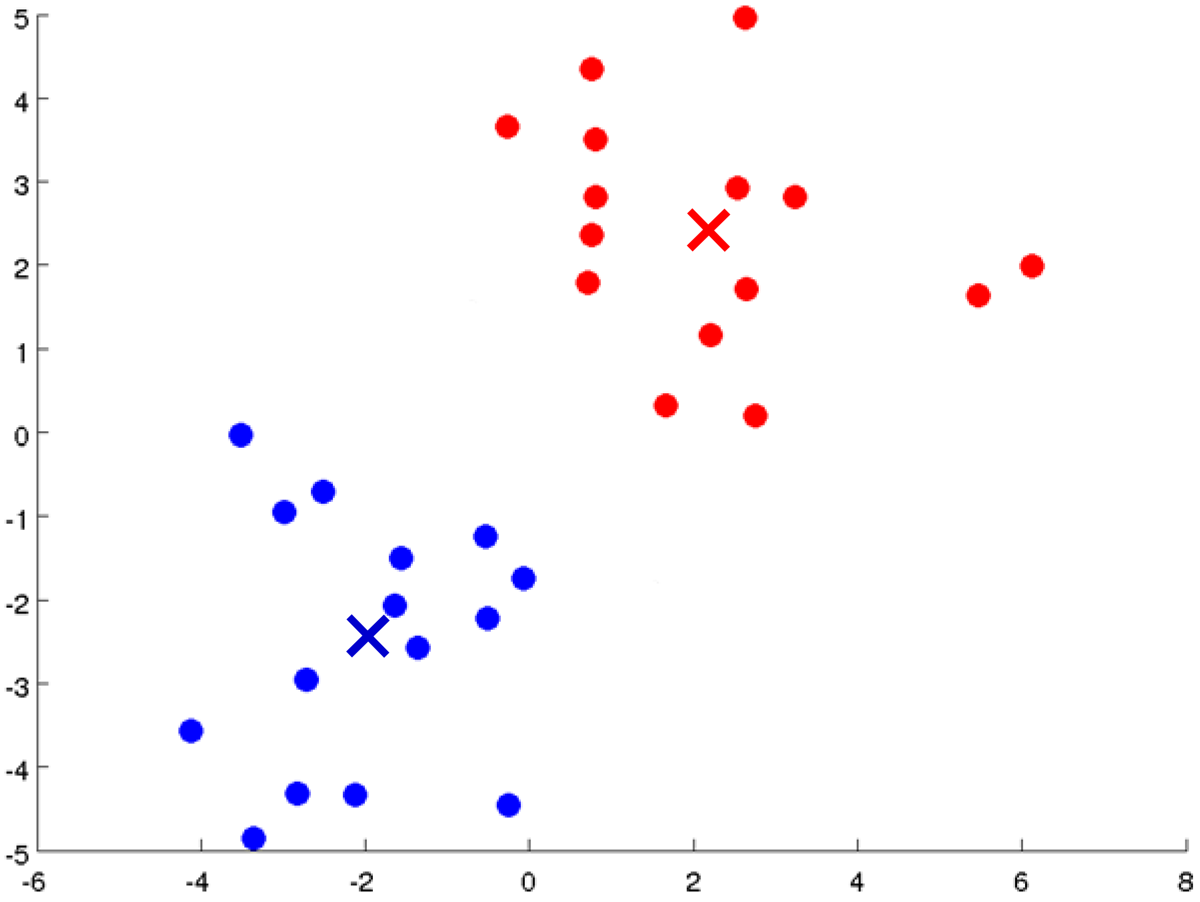

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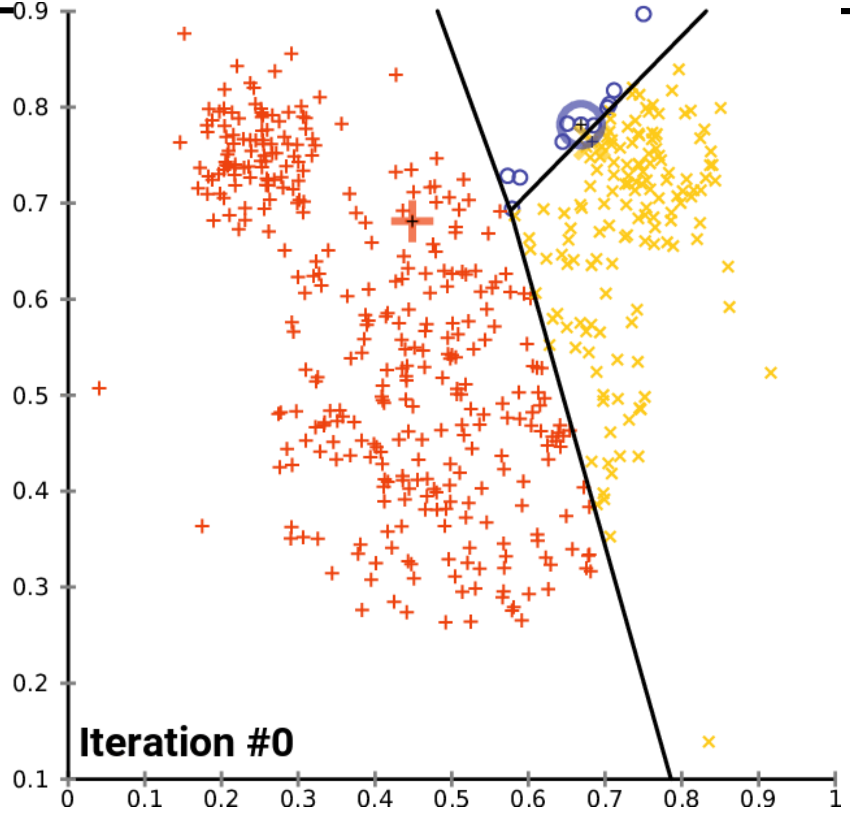
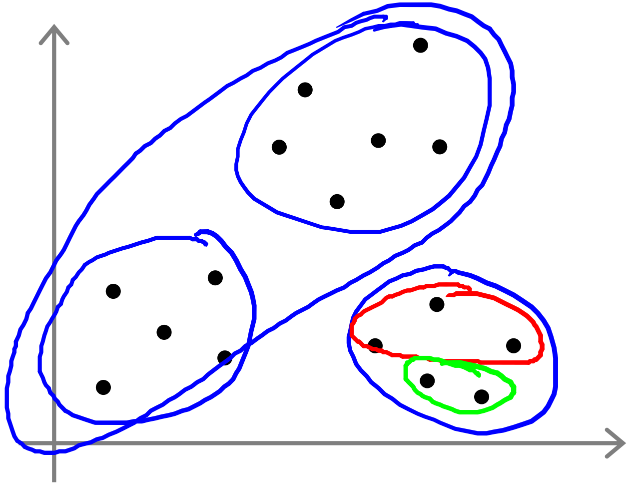
Graphical Example of *K-Means* Clustering

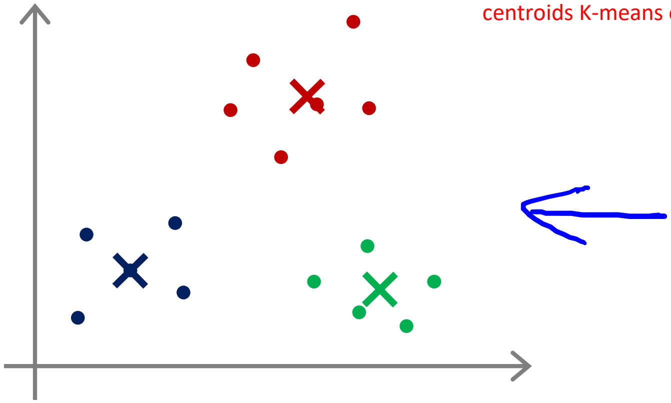


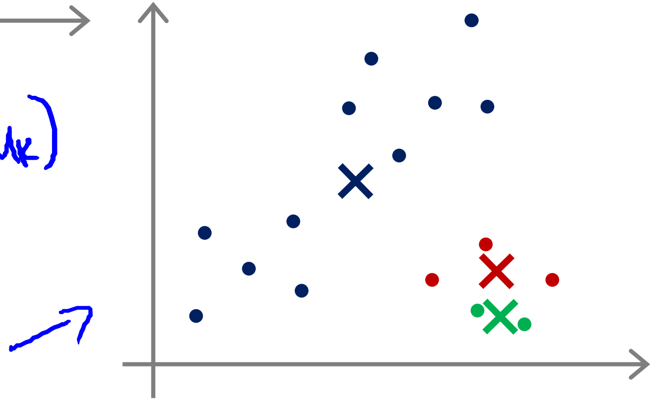
Local optima

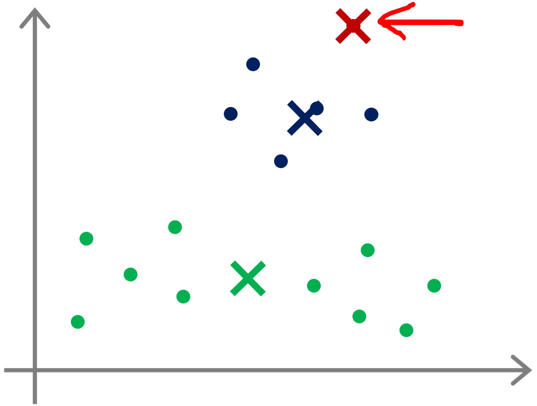
Depending on the initialization of cluster centroids K-means can produce different results



$$J(c^{(1)},\dots,c^{(m)},\mu_1,\dots,\mu_K)$$







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Random initialization

For i = 1 to 100 {

Randomly initialize K-means.

Run K-means. Get $(c_1, c_2, \ldots, c_K)$.

Compute cost function (distortion)

$$E(c_1, c_2, \ldots, c_K)$$

}

Pick clustering that gave lowest cost $E(c_1, c_2, \ldots, c_K)$

Comments on the *K-Means* Method

- <u>Strength:</u> *Efficient*: *O*(*tkn*), where *n* is # objects, *k* is # clusters, and *t* is # iterations. Normally, *k*, *t* << *n*.
    - Comparing: PAM: $O(k(n-k)^2)$, CLARA: $O(ks^2 + k(n-k))$
- <u>Comment:</u> Often terminates at a *local optimal*.
- <u>Weakness</u>
    - Applicable only to objects in a continuous n-dimensional space
        - Using the k-modes method for categorical data
        - In comparison, k-medoids can be applied to a wide range of data
    - Need to specify *k,* the *number* of clusters, in advance (there are ways to automatically determine the best k (see Hastie et al., 2009)
    - Sensitive to ***noisy data and outliers***
    - Not suitable to discover clusters with *non-convex shapes*

k-means cannot represent density-based clusters

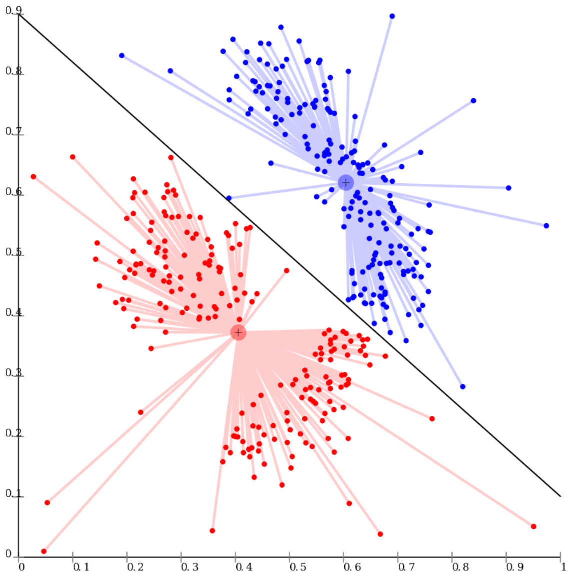


Fig: Convex Shaped

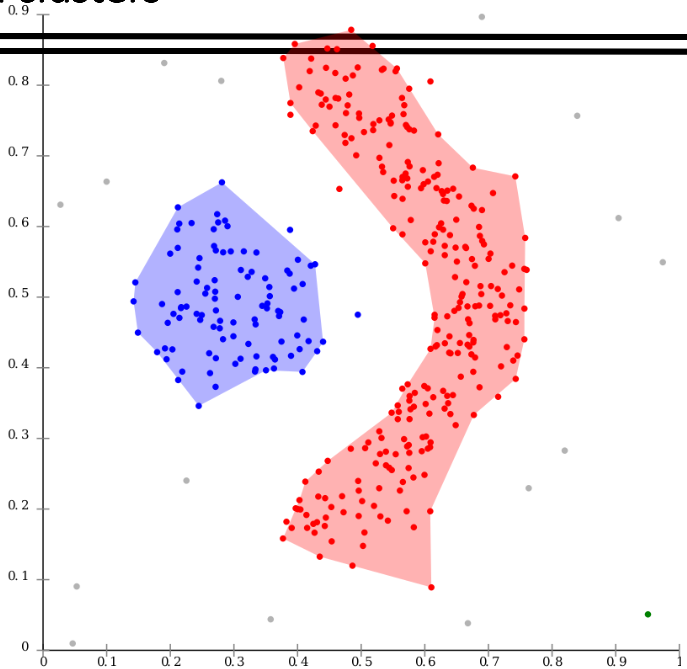
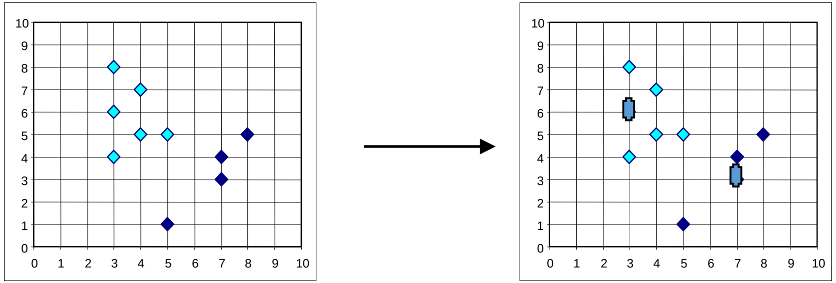


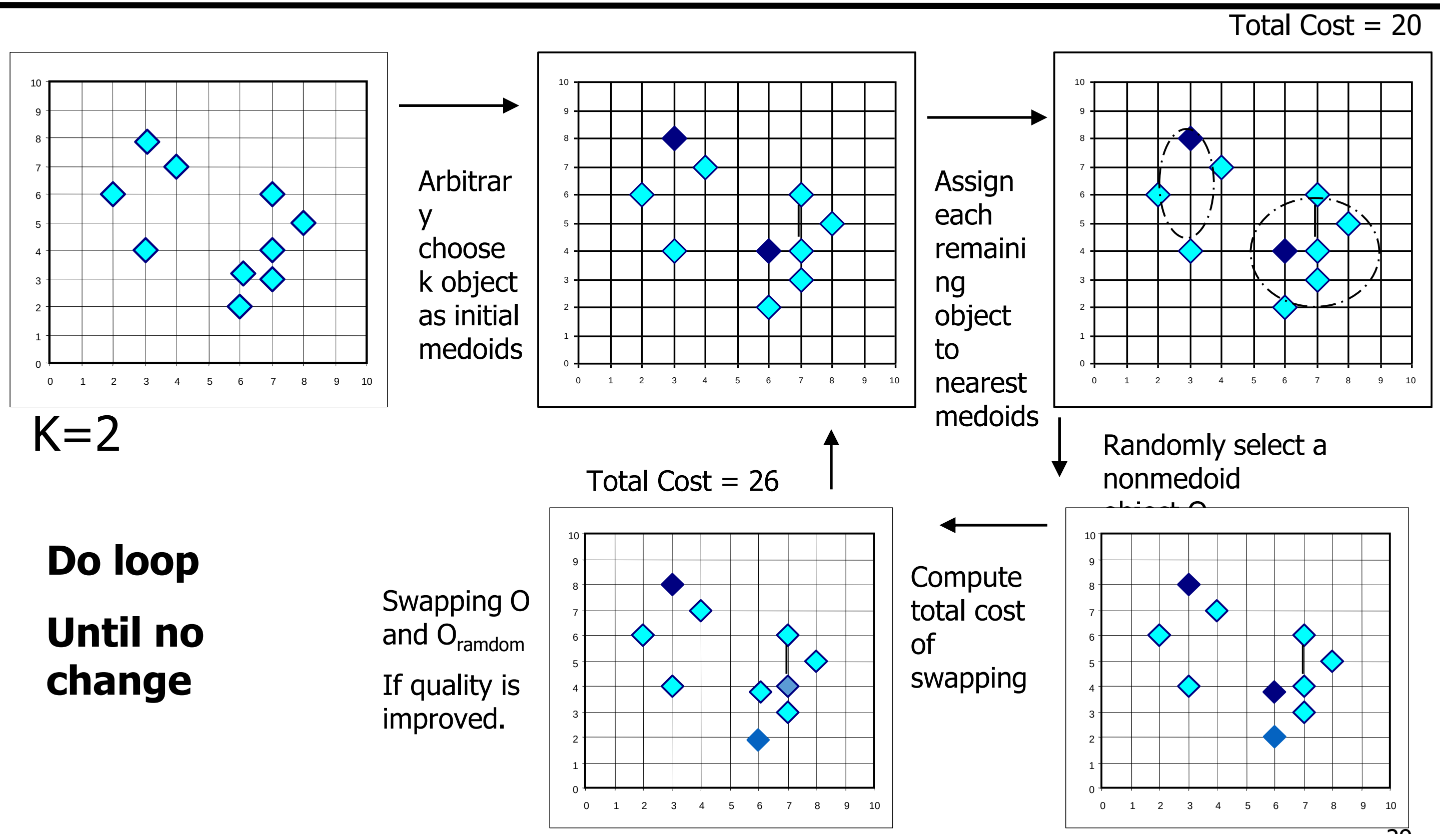
Fig: Non-Convex Shaped

What Is the Problem of the K-Means Method?

- The k-means algorithm is sensitive to outliers !
  - Since an object with an extremely large value may substantially distort the distribution of the data
- K-Medoids: Instead of taking the **mean** value of the object in a cluster as a reference point, **medoids** can be used, which is the **most centrally located** object in a cluster



PAM: A Typical K-Medoids Algorithm



Do loop

Until no change

The *K-Medoids* Clustering Method

Algorithm: ***k*-medoids.** PAM, a k-medoids algorithm for partitioning based on medoid or central objects.

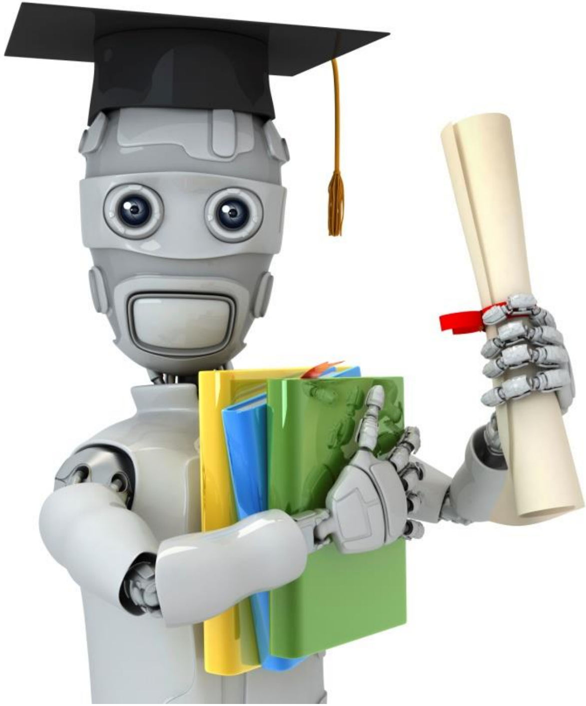
Input:

- k: the number of clusters,
- D: a data set containing n objects.

Output: A set of k clusters.

Method:

(1) arbitrarily choose k objects in D as the initial representative objects or seeds;
(2) **repeat**
(3)   assign each remaining object to the cluster with the nearest representative object;
(4)   randomly select a nonrepresentative object, $\boldsymbol{o}_{random}$;
(5)   compute the total cost, S, of swapping representative object, $\boldsymbol{o}_j$, with $\boldsymbol{o}_{random}$;
(6)   **if** $S < 0$ **then** swap $\boldsymbol{o}_j$ with $\boldsymbol{o}_{random}$ to form the new set of k representative objects;
(7) **until** no change;



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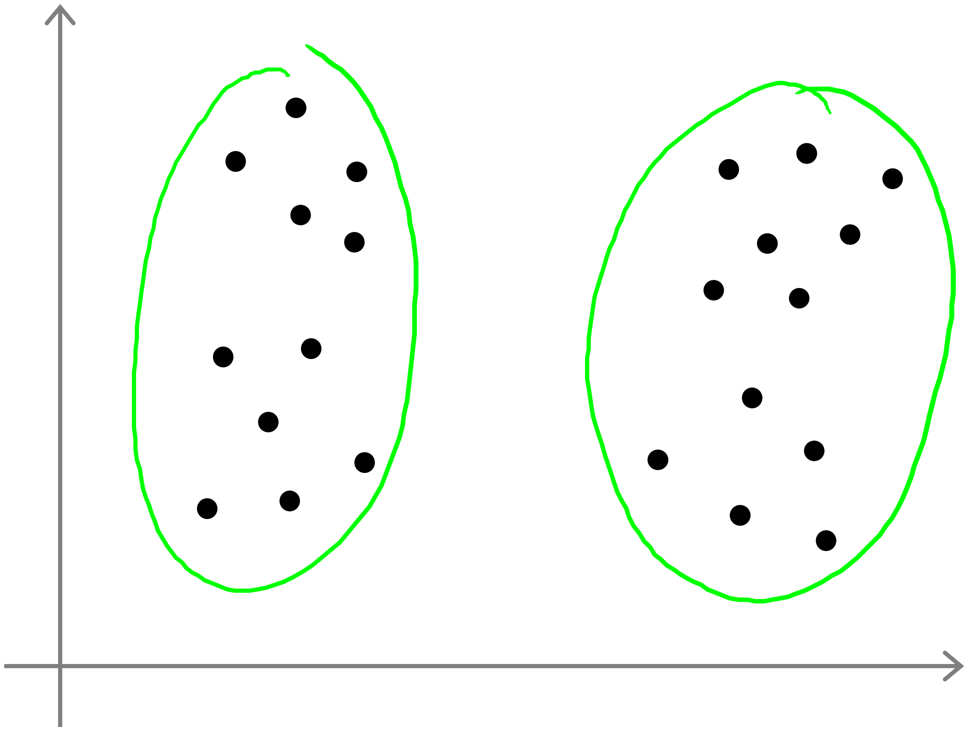
Clustering

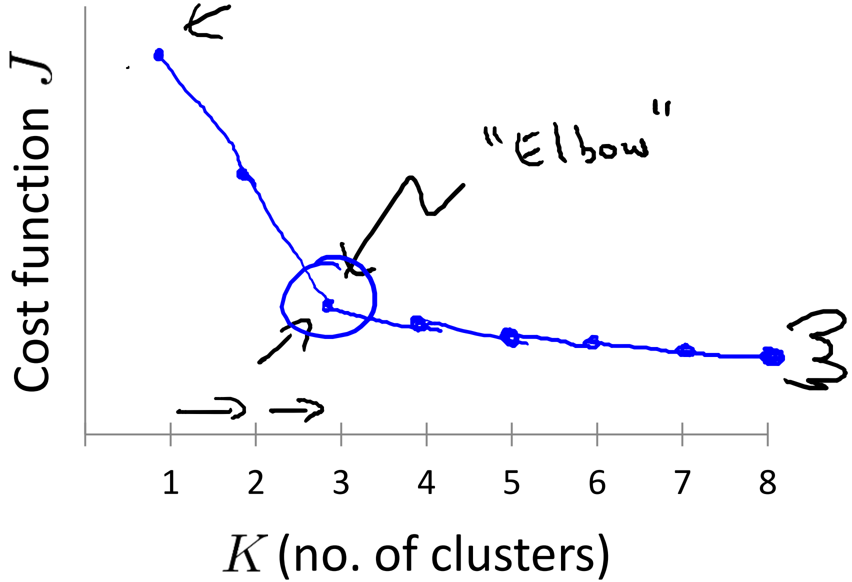
Choosing the number of clusters

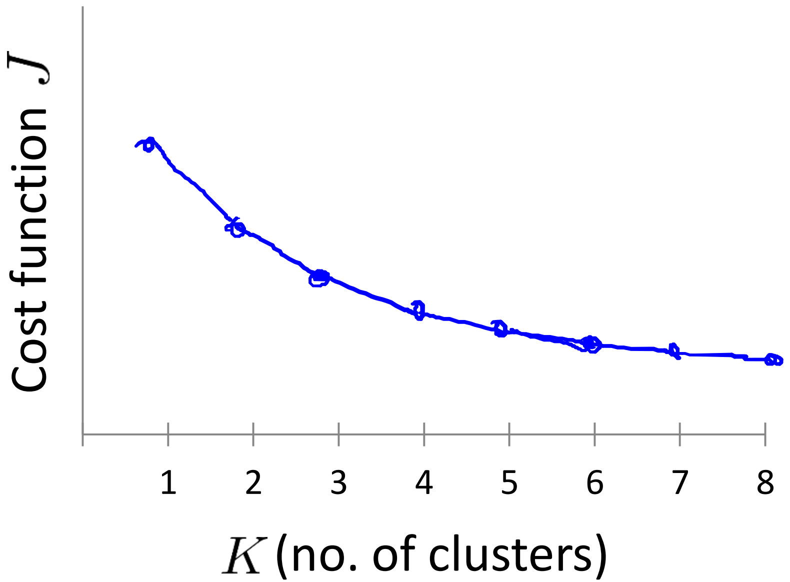
What is the right value of K?



Choosing the value of K

Elbow method:





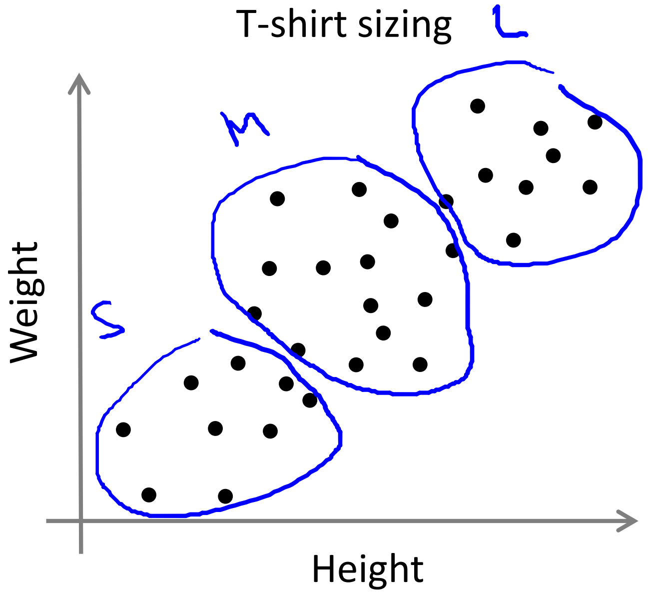
Choosing the value of K

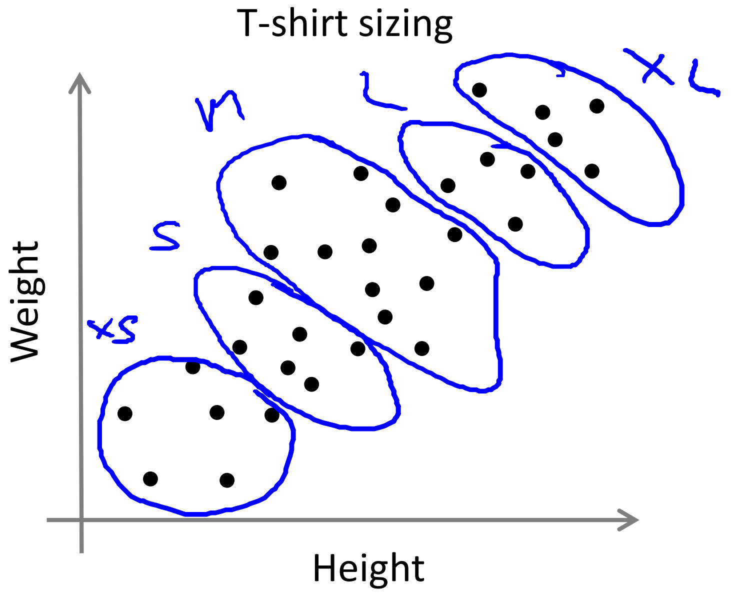
Sometimes, you're running K-means to get clusters to use for some later/downstream purpose. Evaluate K-means based on a metric for how well it performs for that later purpose.

K=3 S, M, L

K=5 XS, S, M, L, XL

E.g.





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