Multivariate Clustering

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K-means Clustering

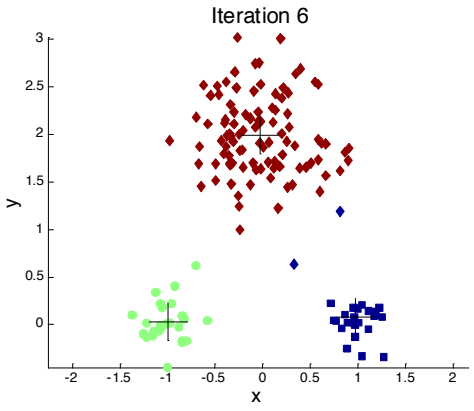
- Partitional clustering approach
- Number of clusters, K, must be specified
- Each cluster is associated with a centroid (center point)
- Each point is assigned to the cluster with the closest centroid

K-means Clustering

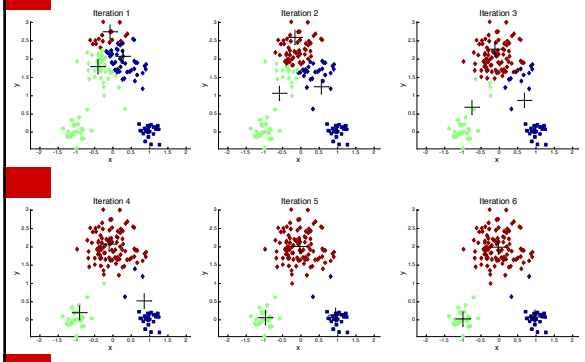
- The basic algorithm is very simple

1: Select K points as the initial centroids.
2: **repeat**
3: Form K clusters by assigning all points to the closest centroid.
4: Recompute the centroid of each cluster.
5: **until** The centroids don't change

Example of K-means Clustering



Example of K-means Clustering



K-means Clustering – Details

- Initial centroids are often chosen randomly.
  - Clusters produced vary from one run to another.
- The centroid is (typically) the mean of the points in the cluster.
- 'Closeness' is measured by Euclidean distance, cosine similarity, correlation, etc.
- K-means will converge for common similarity measures mentioned above.
- Most of the convergence happens in the first few iterations.
  - Often the stopping condition is changed to 'Until relatively few points change clusters'
- Complexity is O(n * K * I * d)
  - n = number of points, K = number of clusters, I = number of iterations, d = number of attributes

K-Means: Detailed Algorithm

K-MEANS $(\mathbf{D}, k, \epsilon)$:

$t = 0$
Randomly initialize k centroids: $\boldsymbol{\mu}_1^t, \boldsymbol{\mu}_2^t, \ldots, \boldsymbol{\mu}_k^t \in \mathbb{R}^d$
repeat
  $t \leftarrow t + 1$
  $C_j \leftarrow \emptyset$ for all $j = 1, \cdots, k$
  // Cluster Assignment Step
  foreach $\mathbf{x}_j \in \mathbf{D}$ **do**
    $j^* \leftarrow \arg\min_i \left\{ \left\| \mathbf{x}_j - \boldsymbol{\mu}_i^t \right\|^2 \right\}$ // Assign $\mathbf{x}_j$ to closest centroid
    $C_{j^*} \leftarrow C_{j^*} \cup \{\mathbf{x}_j\}$
  // Centroid Update Step
  foreach $i = 1$ *to* k **do**
    $\boldsymbol{\mu}_i^t \leftarrow \frac{1}{|C_i|} \sum_{\mathbf{x}_j \in C_i} \mathbf{x}_j$
until $\sum_{i=1}^k \left\| \boldsymbol{\mu}_i^t - \boldsymbol{\mu}_i^{t-1} \right\|^2 \leq \epsilon$

M. Zaki

K-Means: Basic Computations

- Compute new cluster centroid (mean)

$$m_k = \frac{\sum_{i:C(i)=k} x_i}{N_k}, k = 1,\ldots,K.$$

- Cluster assignment

$$C(i) = \arg\min_{1 \le k \le K} \left\| x_i - m_k \right\|^2, i = 1,\ldots,N$$

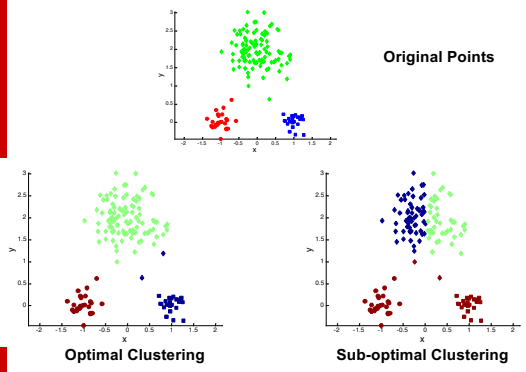
Evaluating K-means Clusters

- Most common measure is Sum of Squared Error (SSE)
  - For each point, the error is the distance to the nearest cluster
  - To get SSE, we square these errors and sum them.

$$SSE = \sum_{i=1}^{K} \sum_{x \in C_i} dist(m_i, x)^2$$

  - x is a data point in cluster C_i and m_i is the representative point for cluster C_i
    - show that m_i corresponds to the center (mean) of the cluster
  - Given two sets of clusters, we prefer the one with the smallest error
  - One easy way to reduce SSE is to increase K, the number of clusters
    - But may not lead to better clustering!

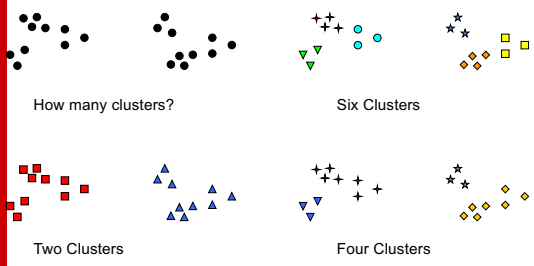
Two different K-means Clusterings



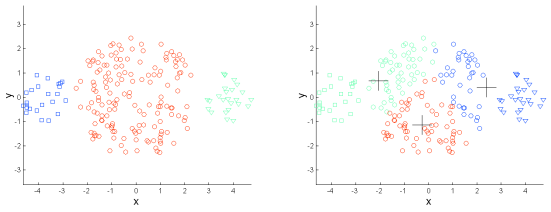
Limitations of K-means

- What is appropriate "K"
- K-means has problems when clusters are of differing
  - Sizes
  - Densities
  - Non-globular shapes
- K-means has problems when the data contains outliers.

Limitations of K-Means: What "K"



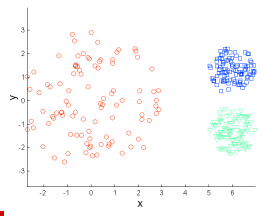
Limitations of K-means: Differing Sizes



Original Points

K-means (3 Clusters)

Limitations of K-means: Differing Density



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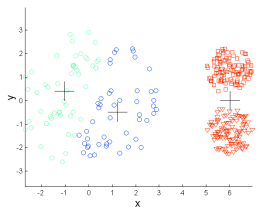
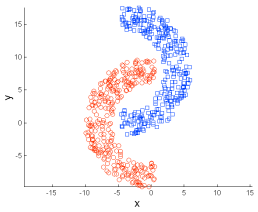


K-means (3 Clusters)

Limitations of K-means: Non-globular Shapes



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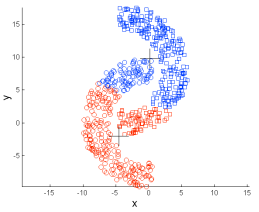
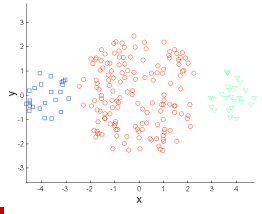


K-means (2 Clusters)

Overcoming K-means Limitations



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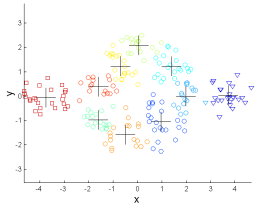
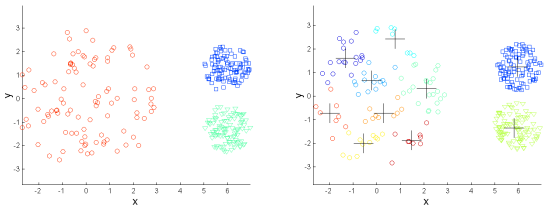


K-means Clusters

One solution is to use many clusters.
Find parts of clusters, but need to put together.

Overcoming K-means Limitations



Original Points K-means Clusters

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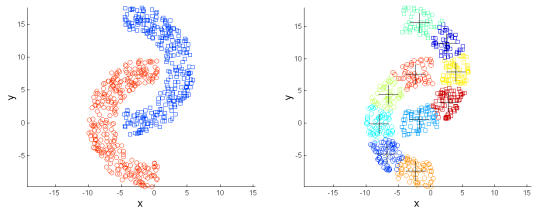
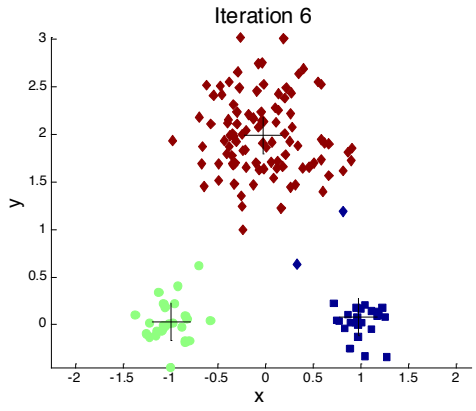


Original Points K-means Clusters

Importance of Choosing Initial Centroids



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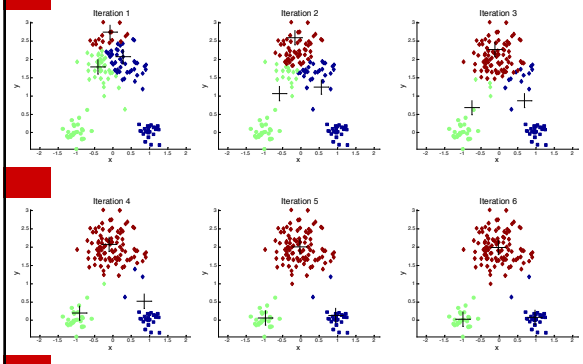

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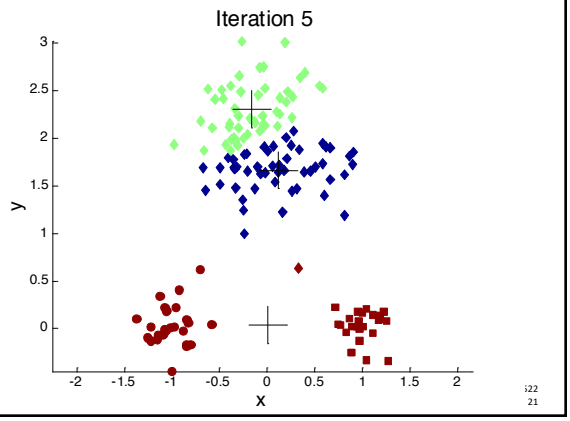

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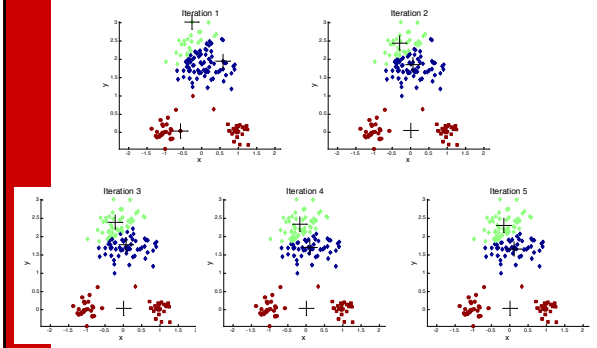


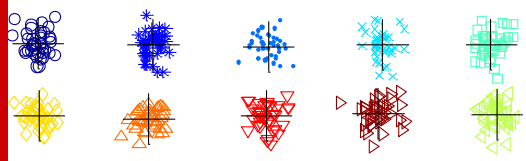
Problems with Selecting Initial Points

- If there are K 'real' clusters then the chance of selecting one centroid from each cluster is small.
  - Chance is relatively small when K is large
  - If clusters are the same size, n, then

$$P = \frac{\text{number of ways to select one centroid from each cluster}}{\text{number of ways to select } K \text{ centroids}} = \frac{K! n^K}{(Kn)^K} = \frac{K!}{K^K}$$

  - For example, if K = 10, then probability = $10!/10^{10}$ = 0.00036
  - Sometimes the initial centroids will readjust themselves in 'right' way, and sometimes they don't
  - Consider an example of five pairs of clusters

10 Clusters Example



Starting with two initial centroids in one cluster of each pair of clusters

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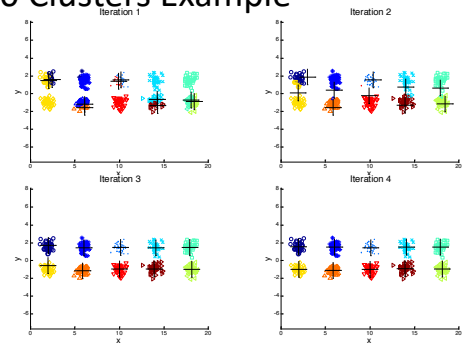

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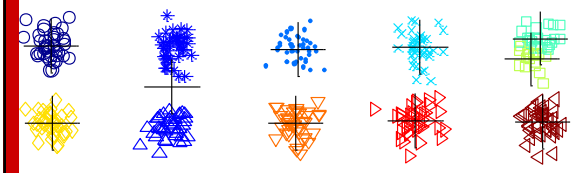

Starting with some pairs of clusters having three initial centroids, while other have only one.

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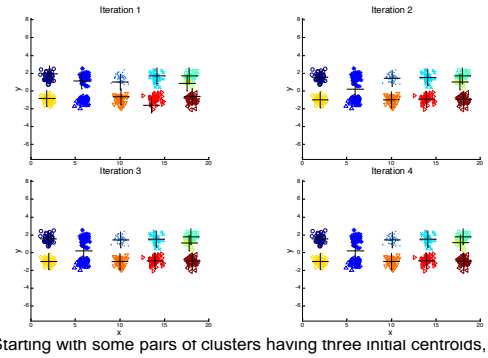


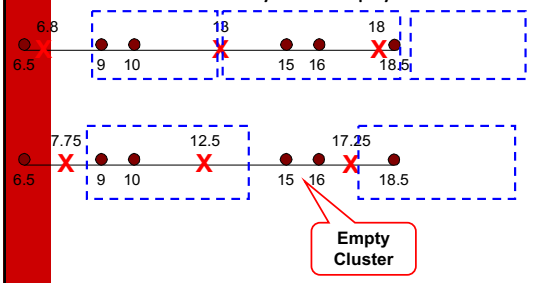
Starting with some pairs of clusters having three initial centroids, while other have only one.

Solutions to Initial Centroids Problem

- Multiple runs
  - Helps, but probability is not on your side
- Sample and use hierarchical clustering to determine initial centroids
- Select more than K initial centroids and then select among these initial centroids
  - Select most widely separated
- Post processing
- Generate a larger number of clusters and then perform a hierarchical clustering
- Bisecting K-means
  - Not as susceptible to initialization issues

Empty Clusters

- K-means can yield empty clusters



Handling Empty Clusters

- Basic K-means algorithm can yield empty clusters
- Several strategies
  - Choose the point that contributes most to SSE
  - Choose a replacement centroid from the cluster with the highest SSE
  - If there are several empty clusters, the above can be repeated several times.

Updating Centers Incrementally

- In the basic K-means algorithm, centroids are updated after all points are assigned to a centroid
- An alternative is to update the centroids after each assignment (incremental approach)
  - Each assignment updates zero or two centroids
  - More expensive
  - Introduces an order dependency
  - Never get an empty cluster
  - Relative weight of the point being added may be adjusted (decreased as clustering proceeds)

Pre-processing and Post-processing

- Pre-processing
  - Normalize the data
  - Eliminate outliers
- Post-processing
  - Eliminate small clusters that may represent outliers
  - Split 'loose' clusters, i.e., clusters with relatively high SSE
  - Merge clusters that are 'close' and that have relatively low SSE
  - Can use these steps during the clustering process
    - ISODATA

Bisecting K-means

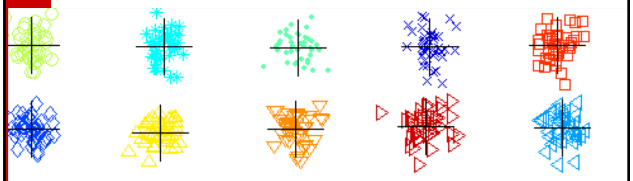
- Bisecting K-means algorithm
  - Variant of K-means that can produce a partitional or a hierarchical clustering

Algorithm 8.2 Bisecting K-means algorithm.

```
1: Initialize the list of clusters to contain the cluster consisting of all points.
2: repeat
3:    Remove a cluster from the list of clusters.
4:    {Perform several "trial" bisections of the chosen cluster.}
5:    for i = 1 to number of trials do
6:       Bisect the selected cluster using basic K-means.
7:    end for
8:    Select the two clusters from the bisection with the lowest total SSE.
9:    Add these two clusters to the list of clusters.
10: until Until the list of clusters contains K clusters.
```

CLUTO: http://glaros.dtc.umn.edu/gkhome/cluto/cluto/overview

Bisecting K-means Example



Acknowledgements

- Slides are customized from: Introduction to Data Mining by Tan, Steinbach, Kumar