K-means Clustering

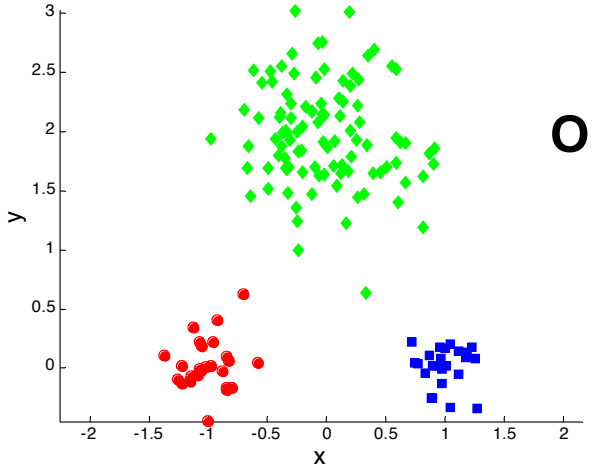
- Partitional clustering approach
- Each cluster is associated with a centroid (center point)
- Each point is assigned to the cluster with the closest centroid
- Number of clusters, K, must be specified
- The basic algorithm is very simple

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

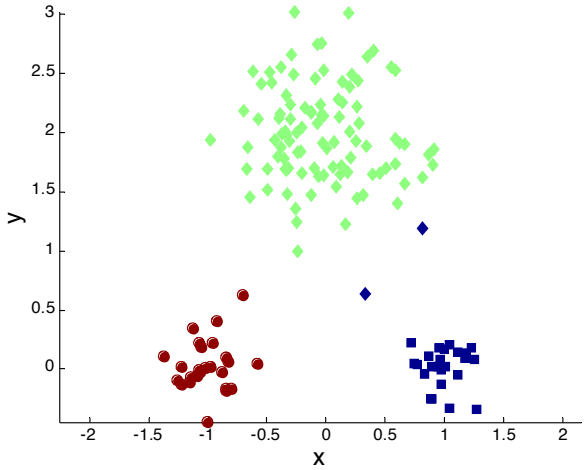
K-means Clustering – Details

- 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

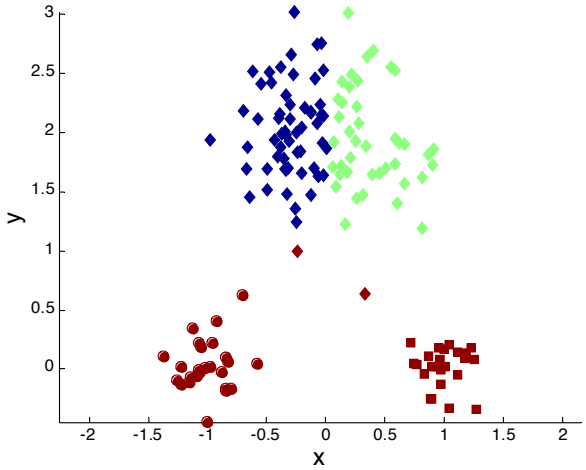
Two different K-means Clusterings



Original Points

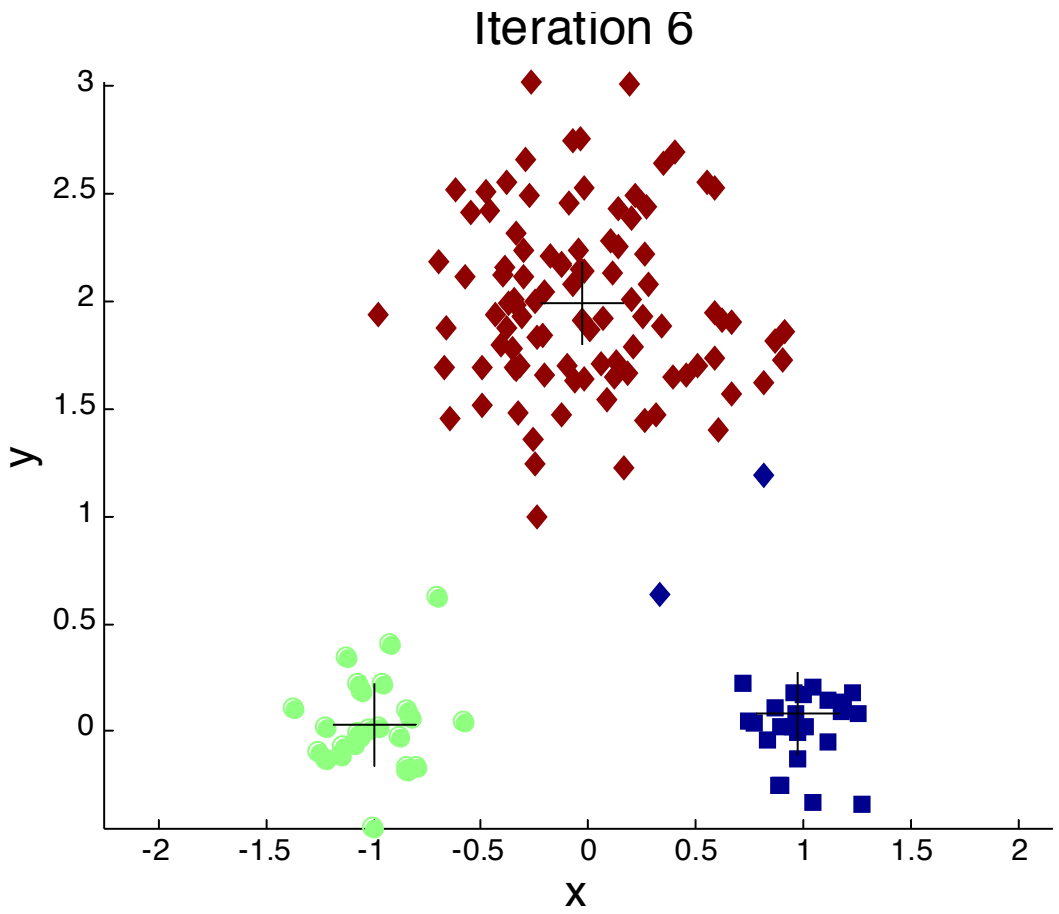


Optimal Clustering



Sub-optimal Clustering

Importance of Choosing Initial Centroids



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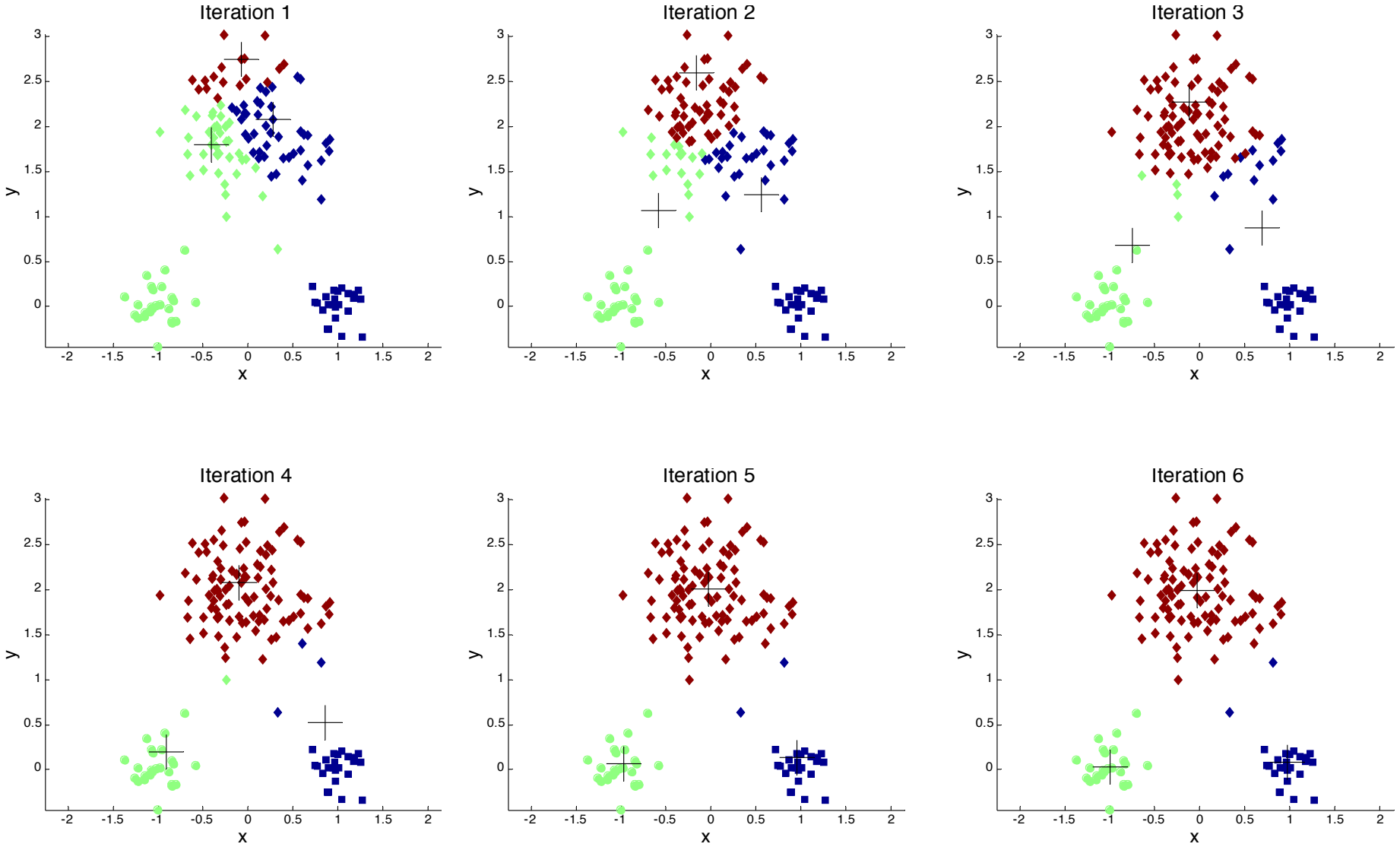
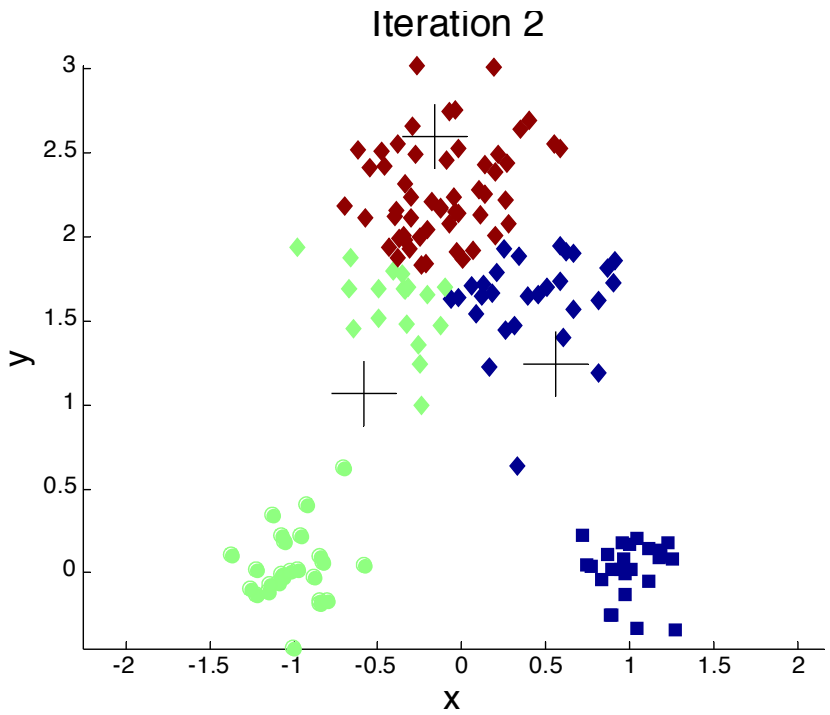
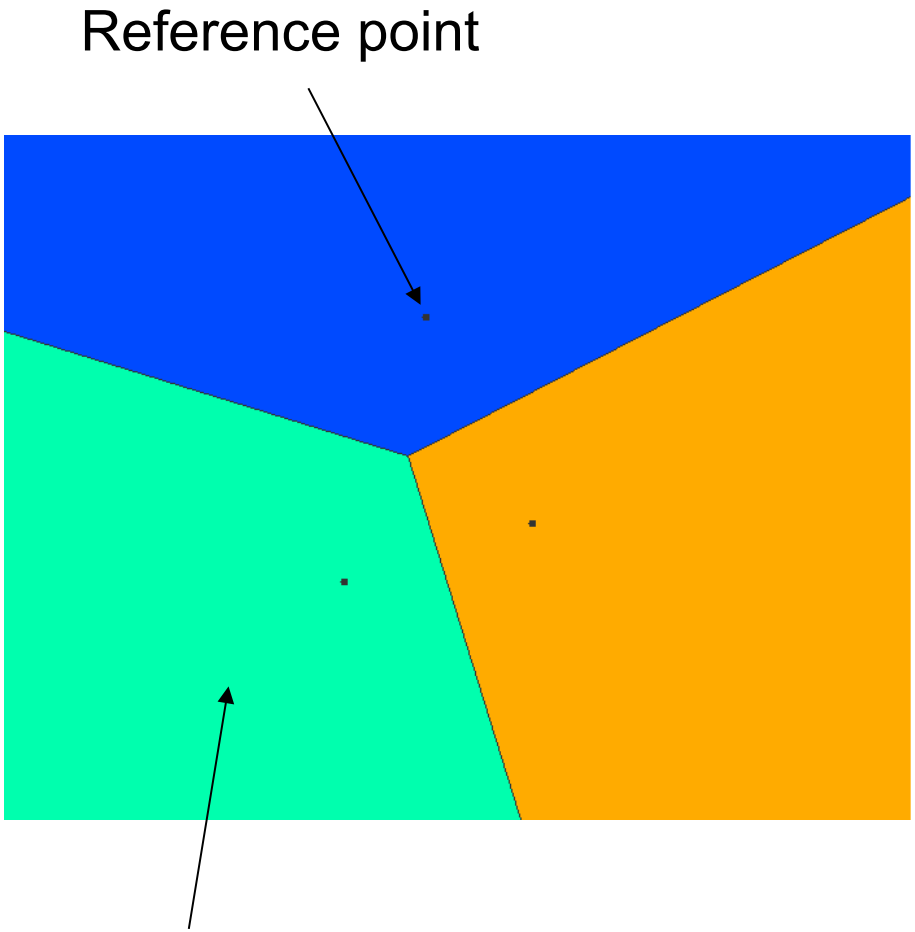


Clusters vs. Voronoi diagrams

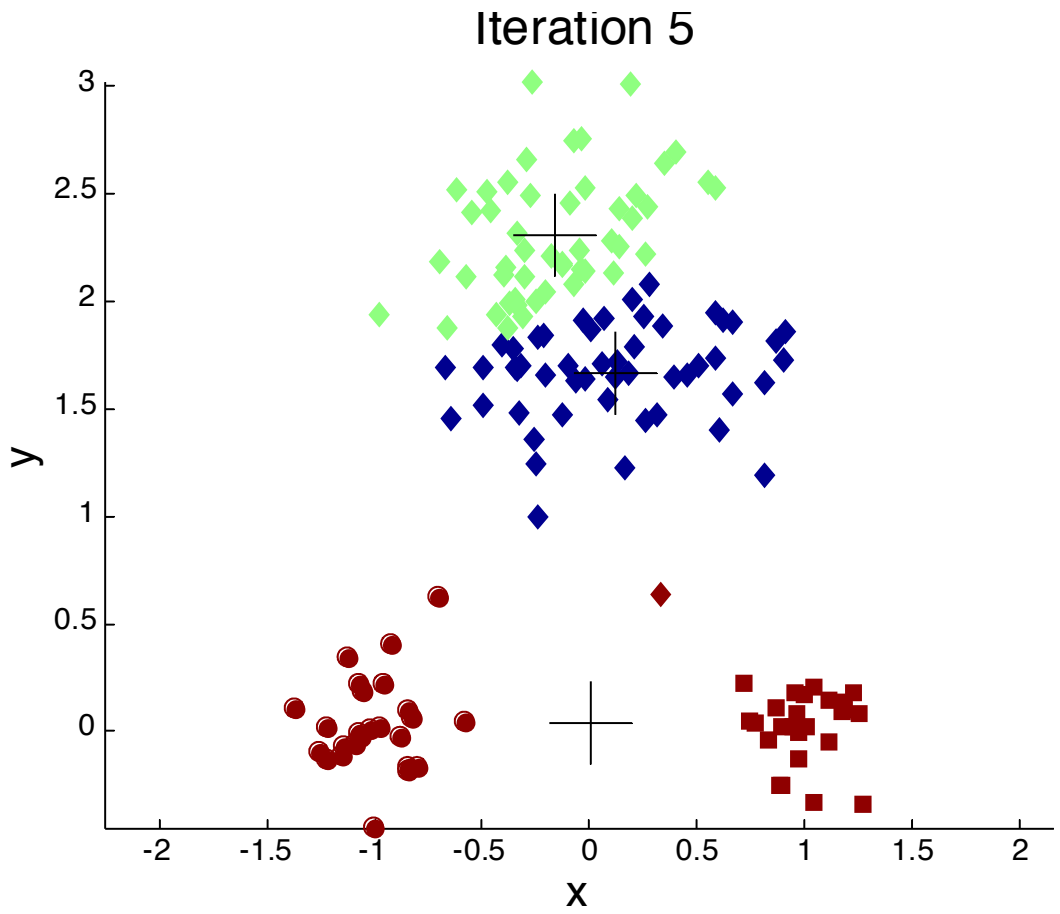




Voroni cell = set of points that are closer to a reference point than any other

`http://www.cs.cornell.edu/home/chew/Delaunay.html`

Importance of Choosing Initial Centroids …



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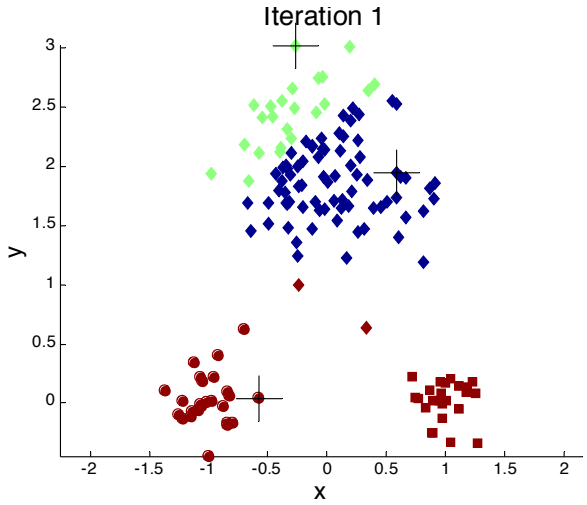
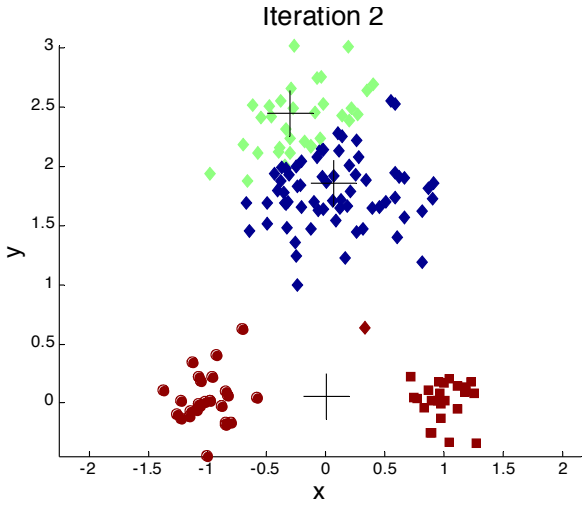
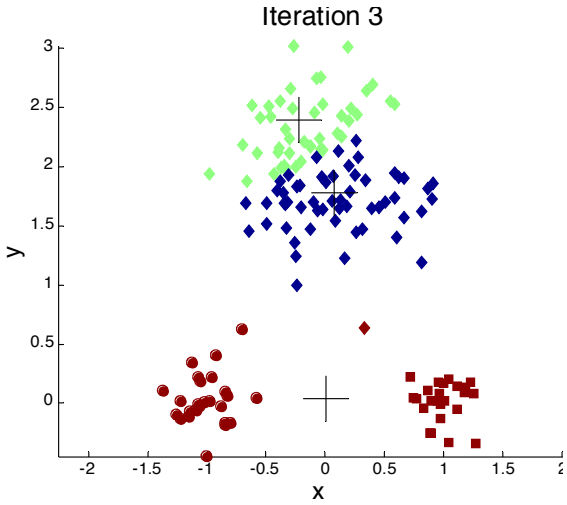
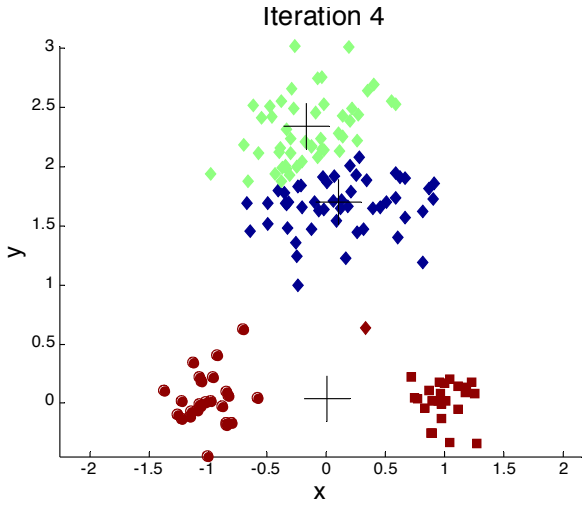
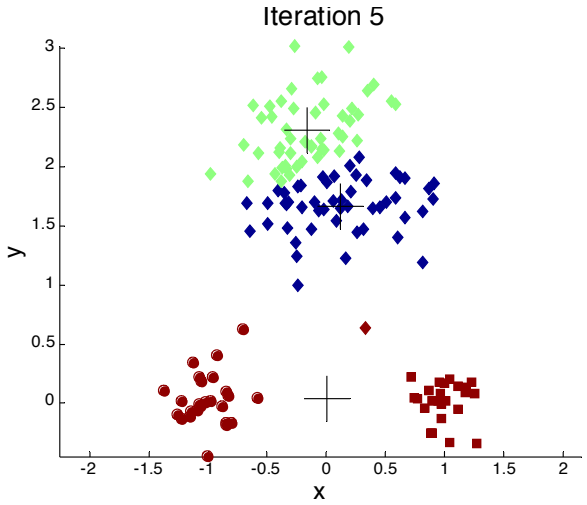










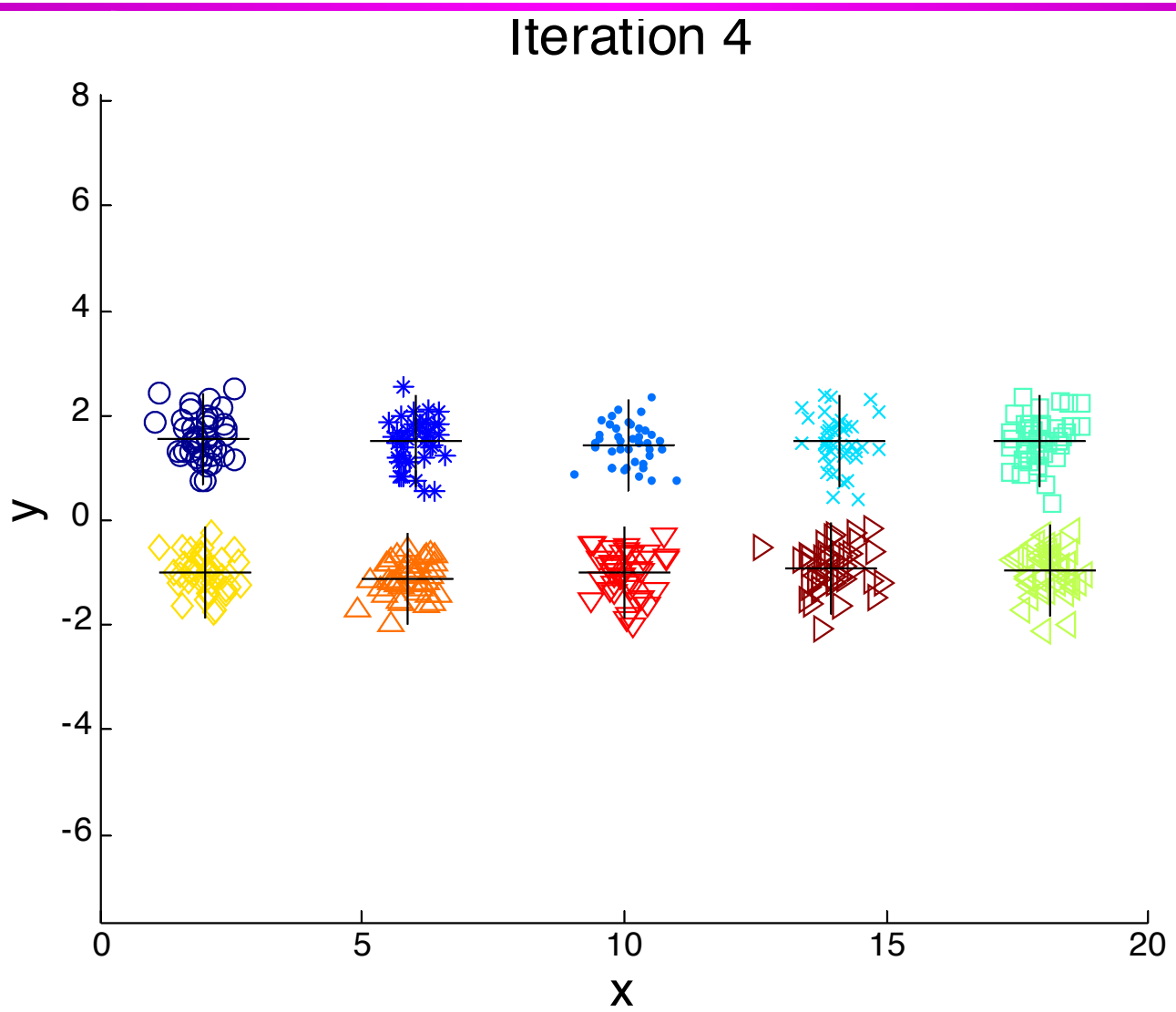
Problems with Selecting Initial Points

- 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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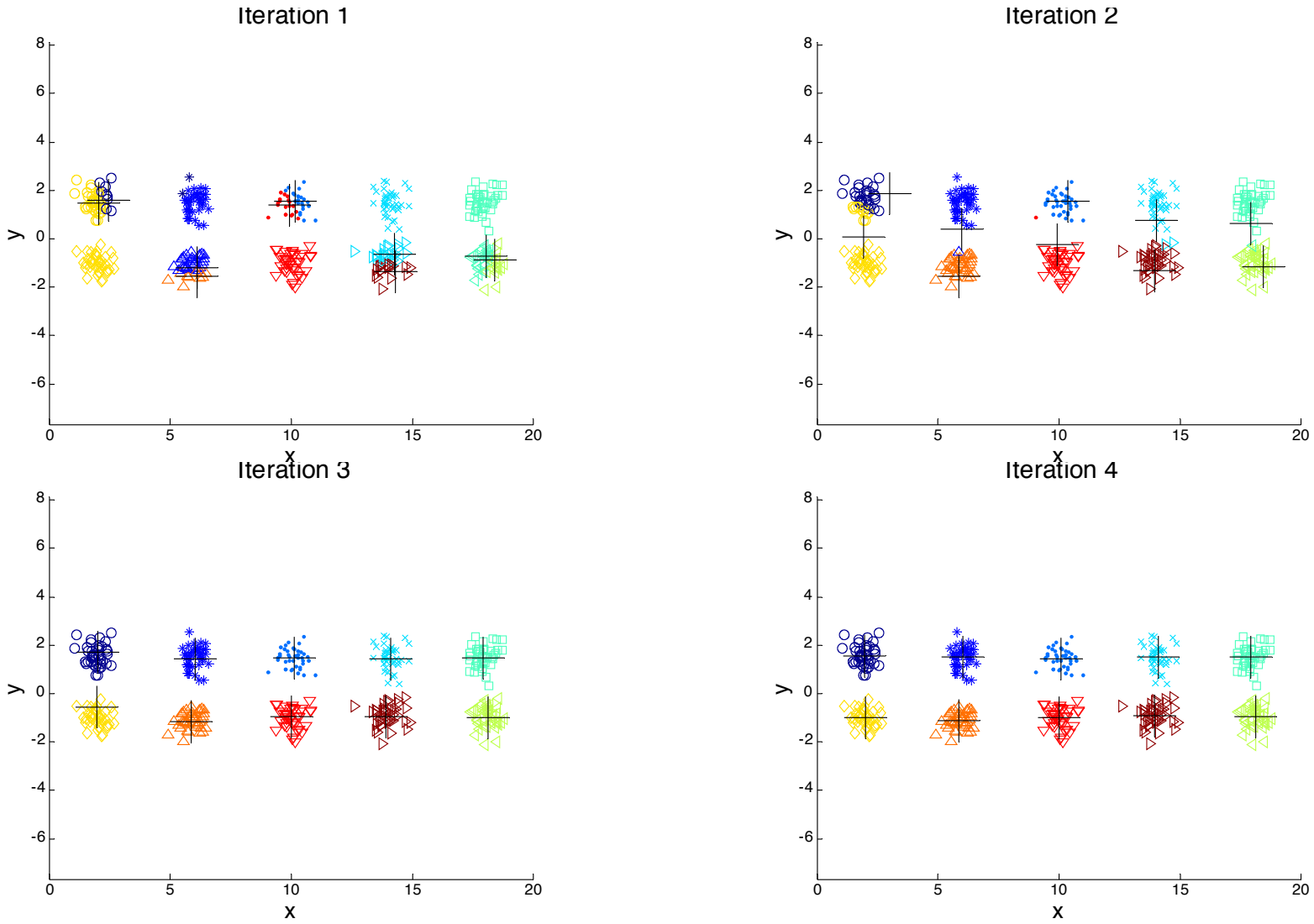

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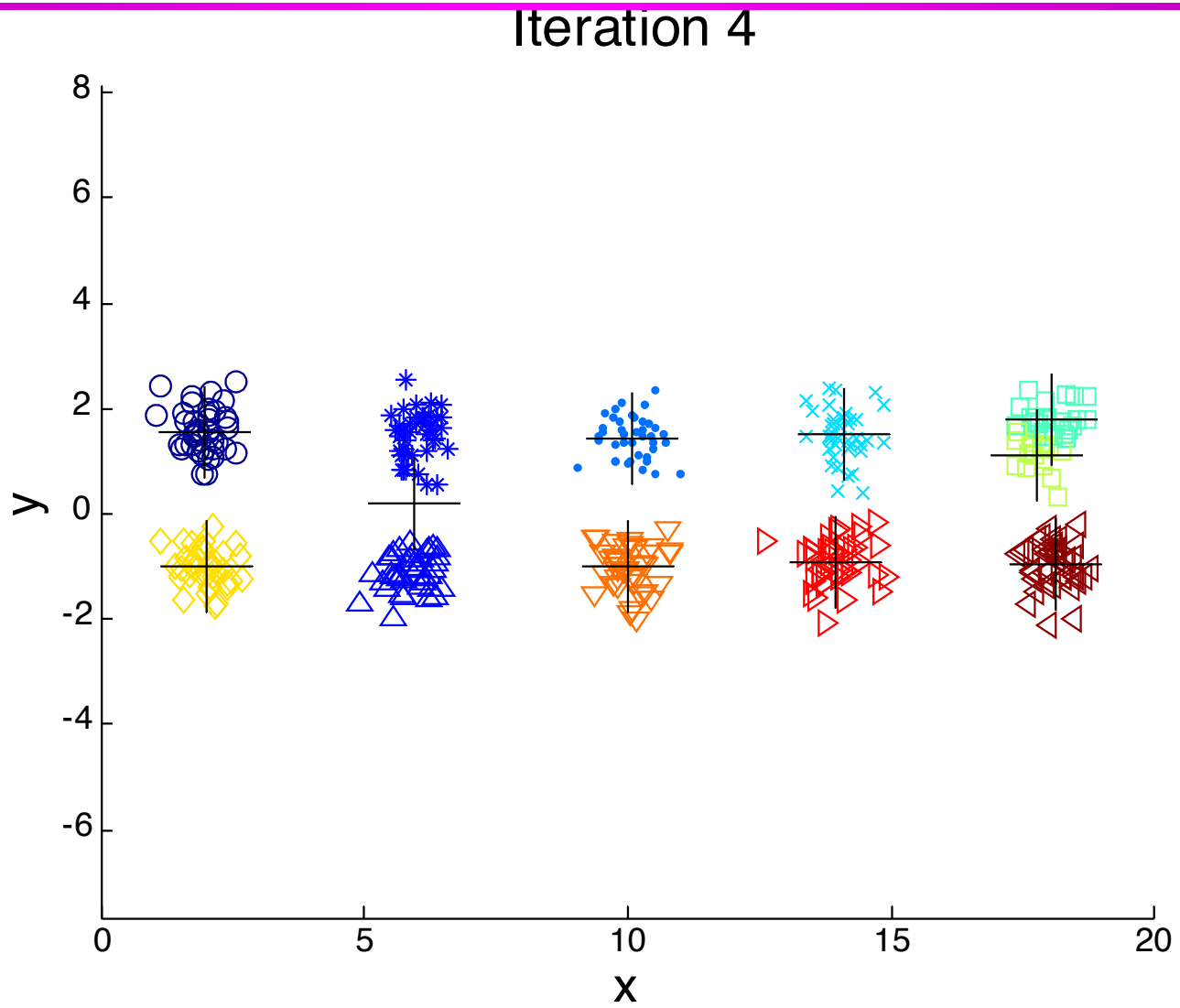

Starting with some pairs of clusters having three initial centroids, while other have only one.

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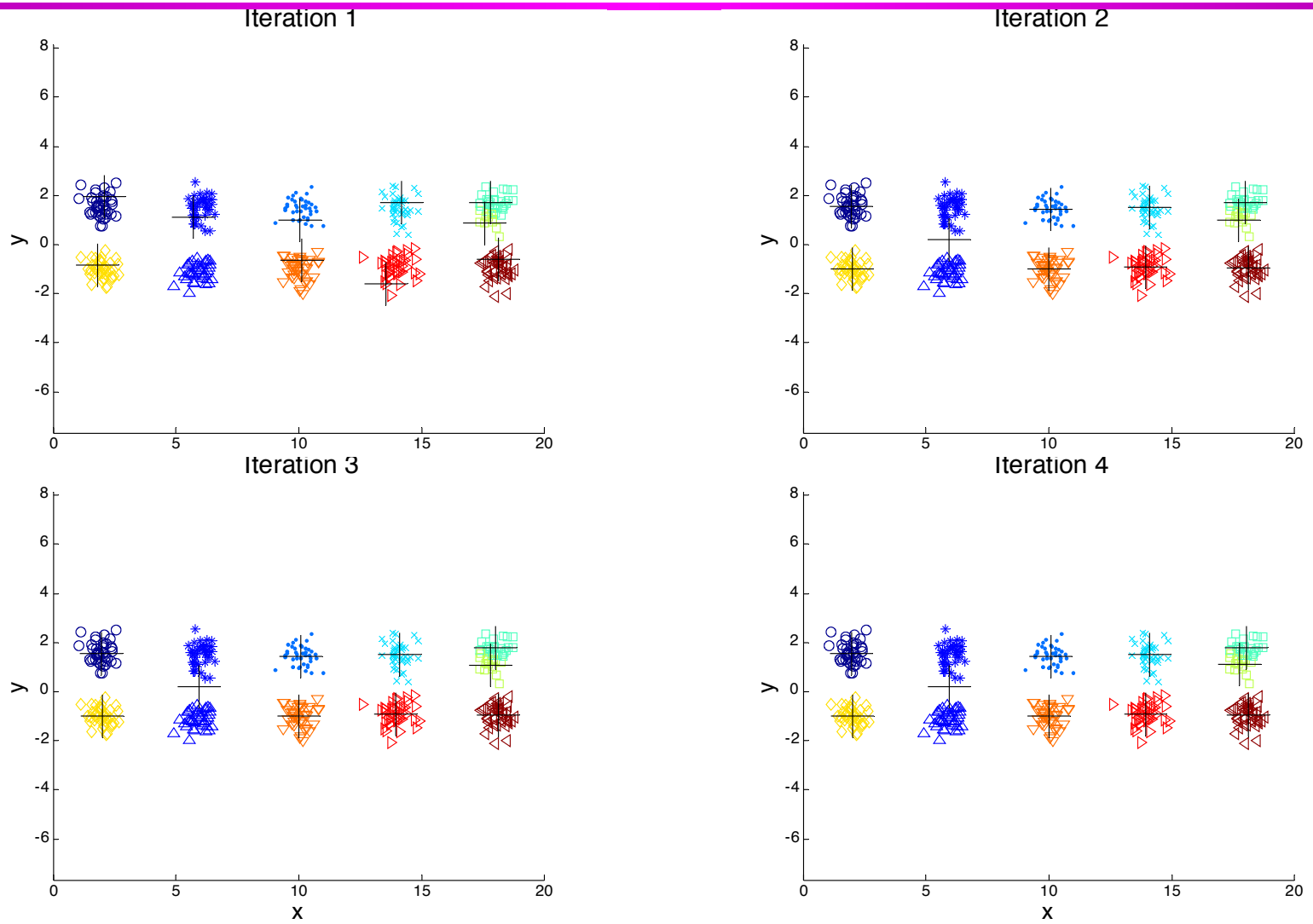

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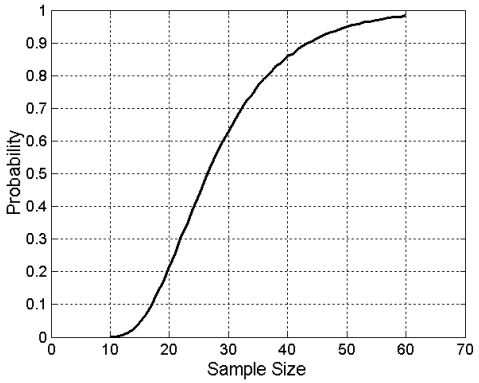
Solutions to Initial Centroids Problem

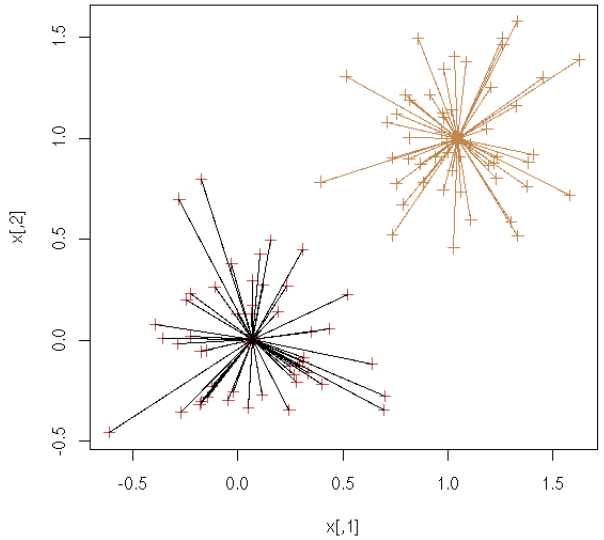
- Multiple runs
  - Helps, but probability is not on your side
- Sample and use hierarchical clustering to determine initial centroids
- Select more than k initial centroids and then select among these initial centroids
  - Select most widely separated
- Postprocessing
- Bisecting K-means
  - Not as susceptible to initialization issues



Evaluating K-means Clusters

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

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



  - x is a data point in cluster C_i and m_i is the representative point for cluster C_i
  - Given two clusters, we can choose the one with the smallest error
  - One easy way to reduce SSE is to increase K, the number of clusters
    - A good clustering with smaller K can have a lower SSE than a poor clustering with higher K

Handling Empty Clusters

- Basic K-means algorithm can yield empty clusters

- Several strategies
  - Choose a point and assign it to the cluster
    - The point that contributes most to SSE
    - A random point from the cluster with highest SSE
  - If there are several empty clusters, the above can be repeated several times.

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