Data Mining
Cluster Analysis: Basic Concepts and Algorithms

Lecture Notes for Chapter 7

Introduction to Data Mining, 2nd Edition

by

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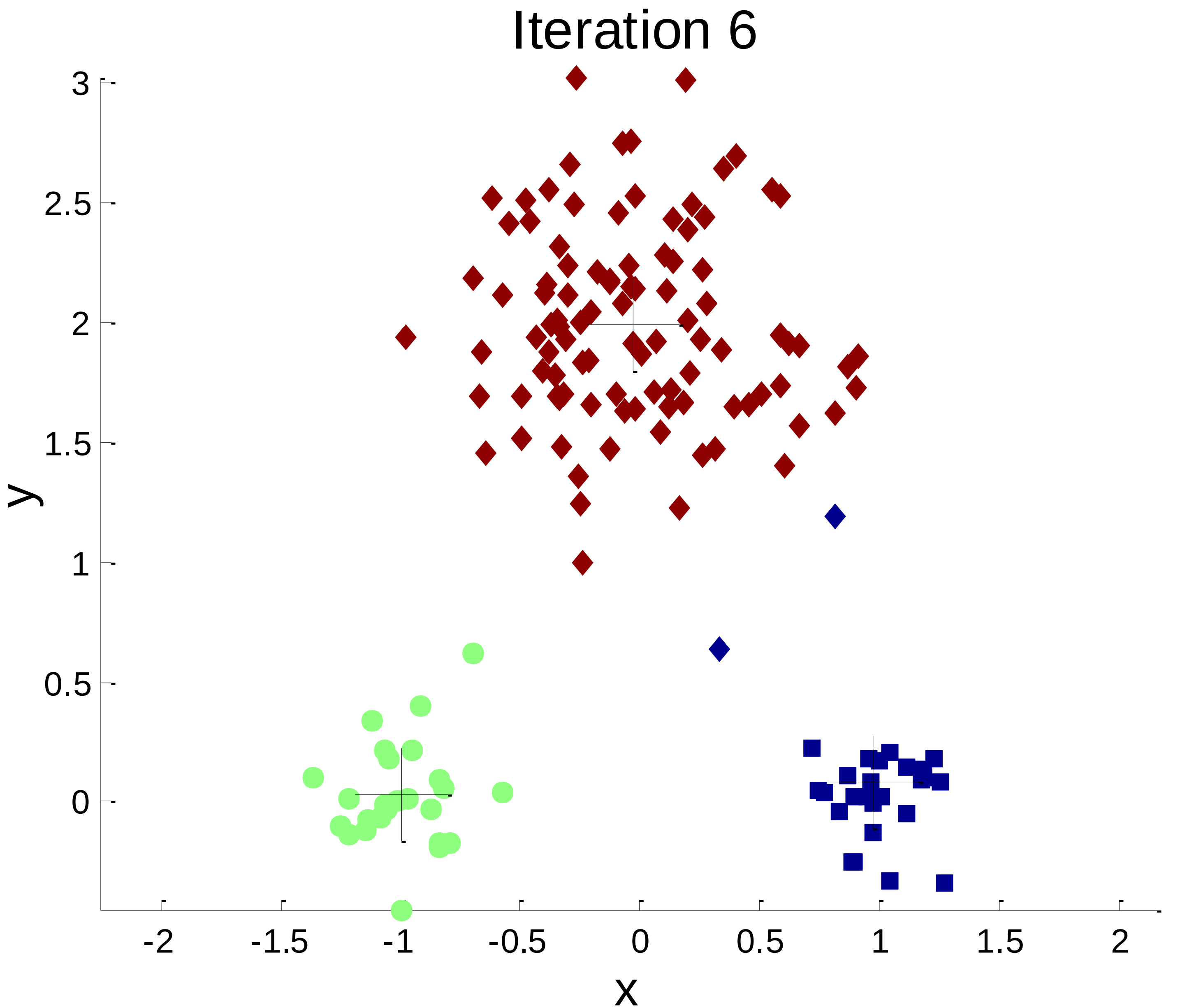
K-means

K-means Clustering

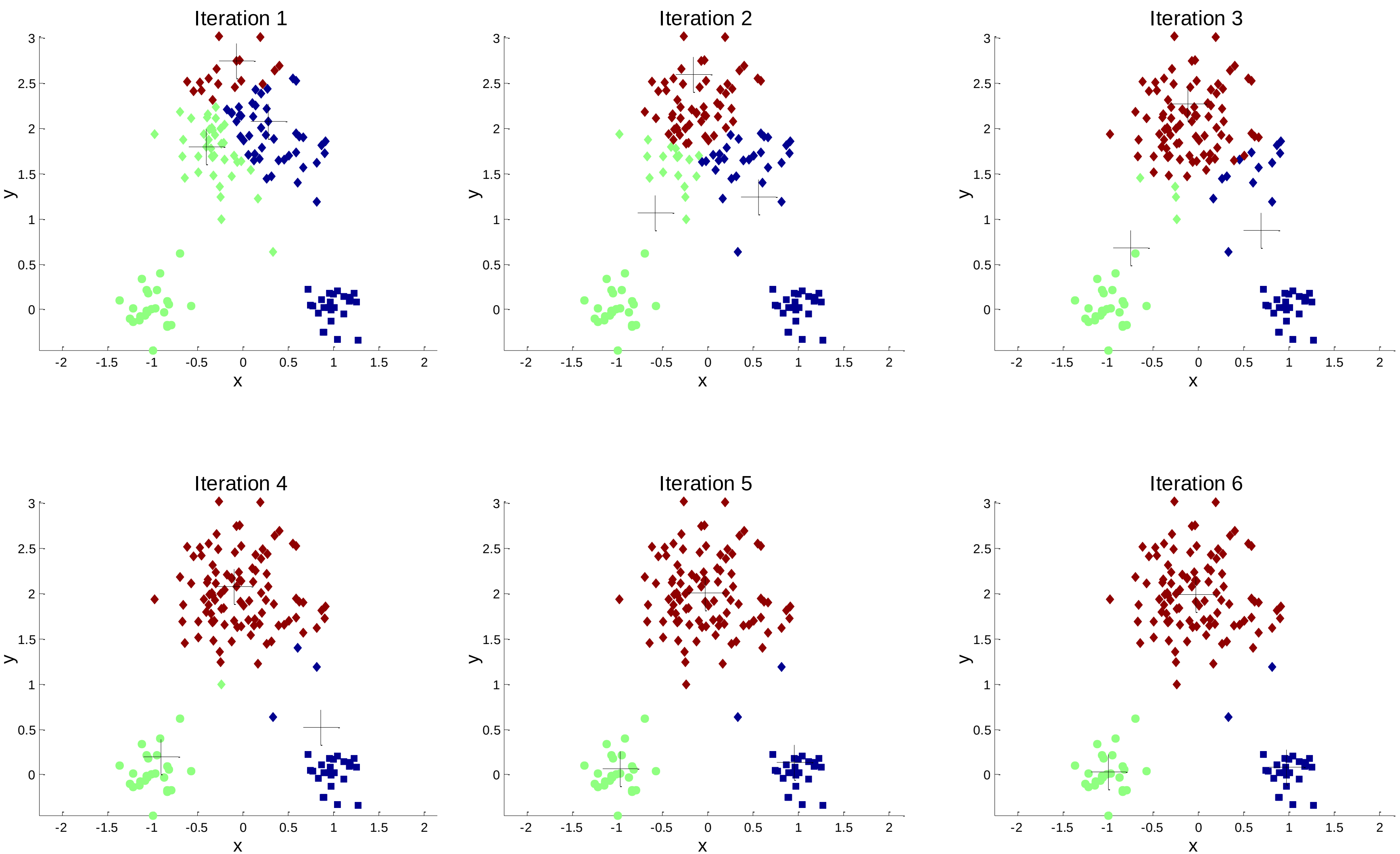
- Partitional clustering approach
- Number of clusters, K, must be specified
- Each cluster is associated with a **centroid** (center point)
- Each point is assigned to the cluster with the **closest centroid**
- The basic algorithm is very simple

Select K points as the initial centroids.
repeat
  Form K clusters by assigning all points to the closest centroid.
  Recompute the centroid of each cluster.
until The centroids don't change

Example of K-means Clustering



Example of K-means Clustering



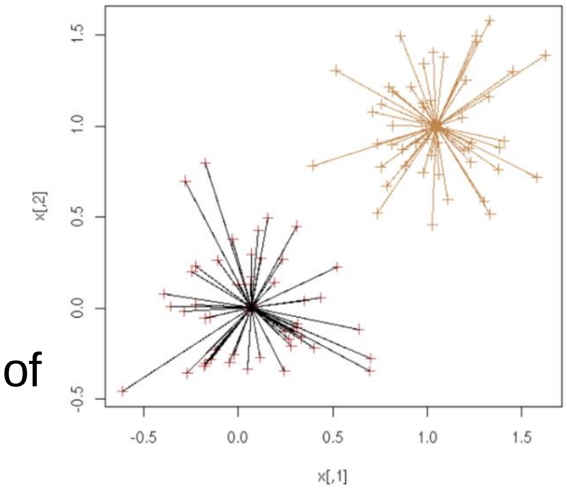
K-means Clustering – Details

- 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

Evaluating K-means Clusters

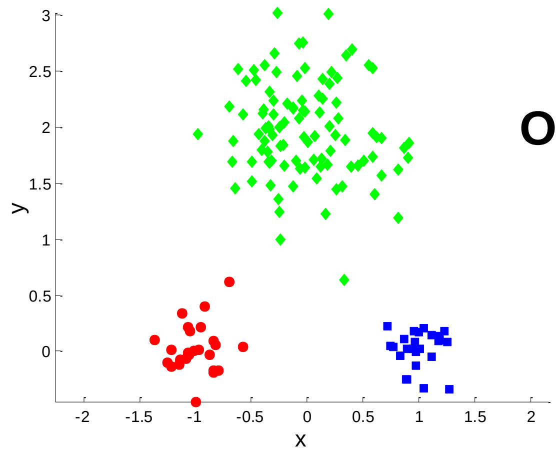
- Most common measure is Sum of Squared Error (SSE)
  - For each point, the error is the distance to the nearest cluster
  - To get SSE, we square these errors and sum them.

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

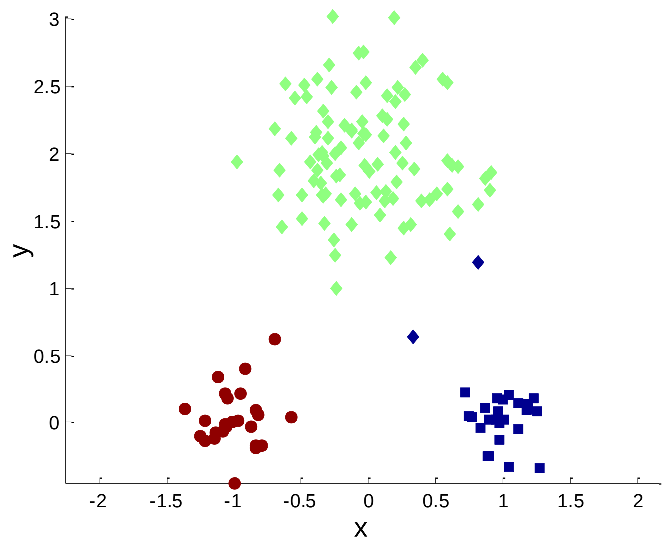


- x is a data point in cluster C_i and m_i is the representative point for cluster Ci
  - can show that mi corresponds to the center (mean) of the cluster
- Given two sets of clusters, we prefer the one with the smallest error
- One easy way to reduce SSE is to increase K, the number of clusters
- A good clustering with smaller K can have a lower SSE than a poor clustering with higher K

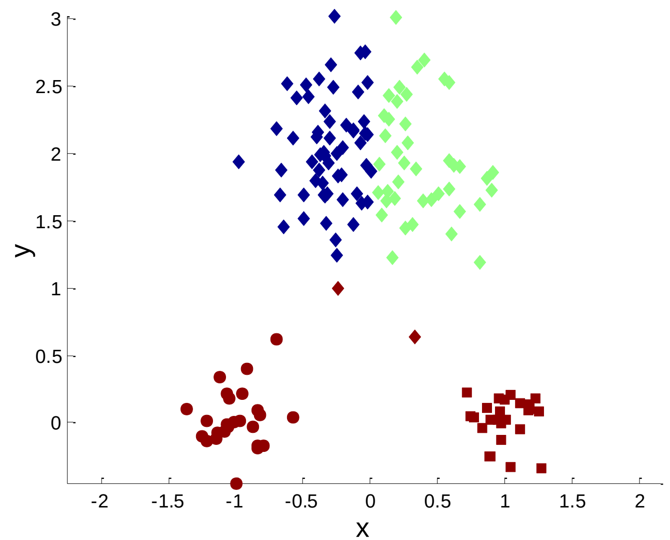
Two different K-means Clusterings



Original Points



Optimal Clustering



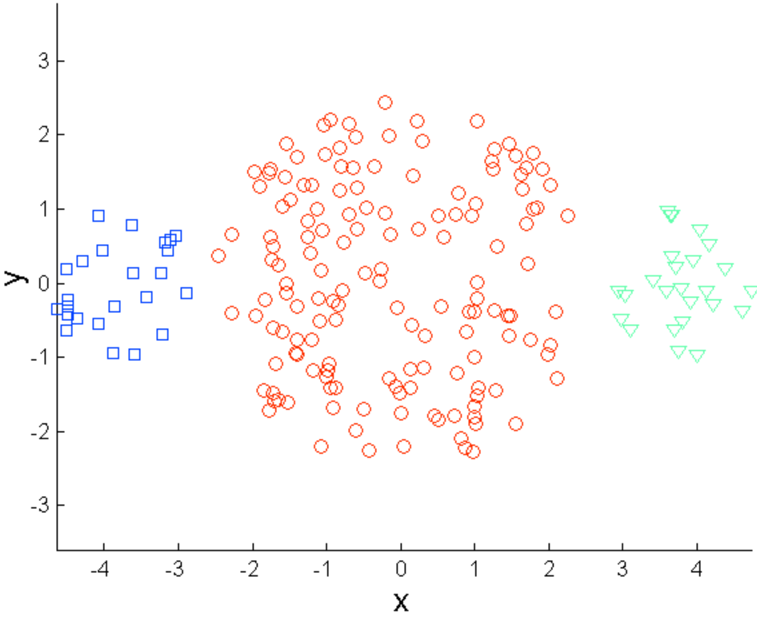
Sub-optimal Clustering

Limitations of K-means

- 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: Differing Sizes



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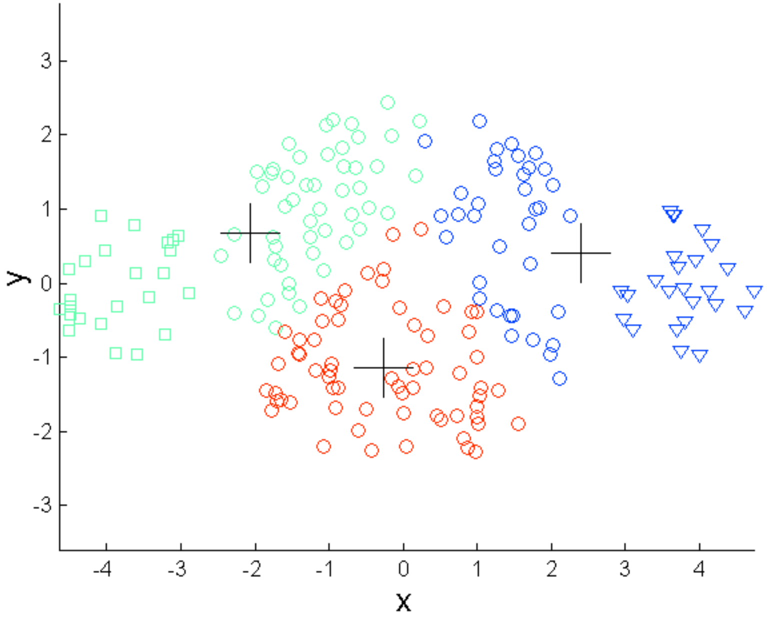
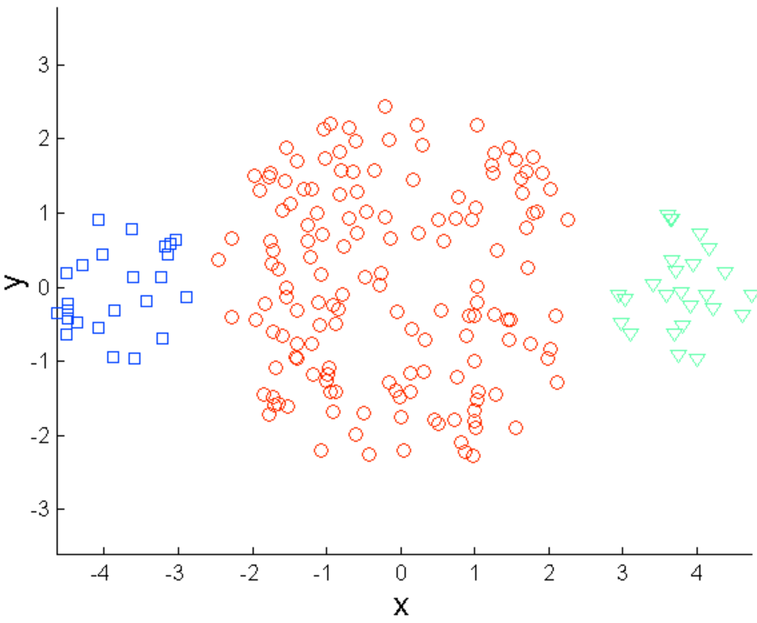


K-means (3 Clusters)

Overcoming K-means Limitations



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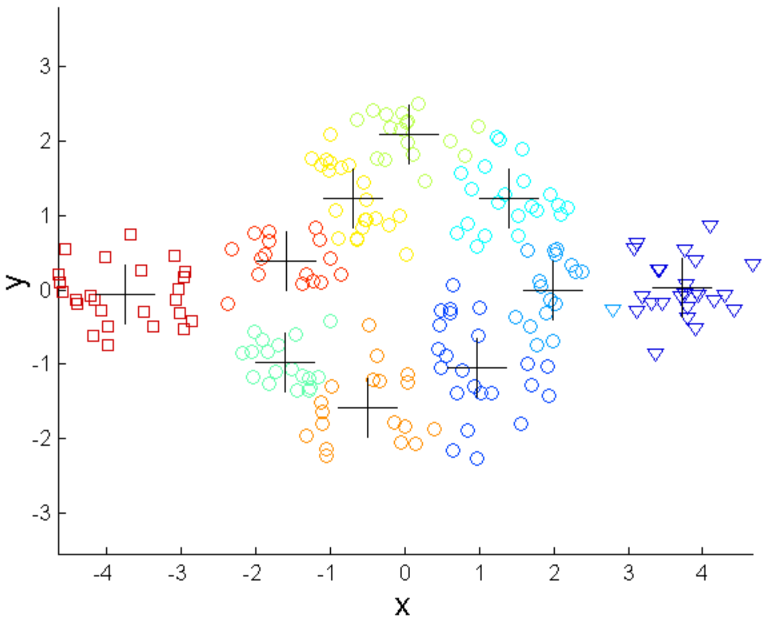
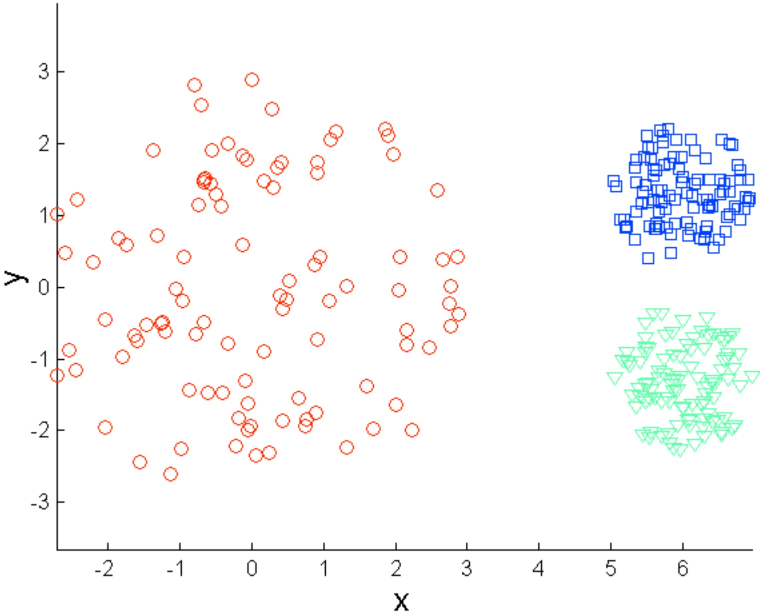


K-means Clusters

One solution is to use many clusters.

Find parts of clusters, but need to put together.

Limitations of K-means: Differing Density



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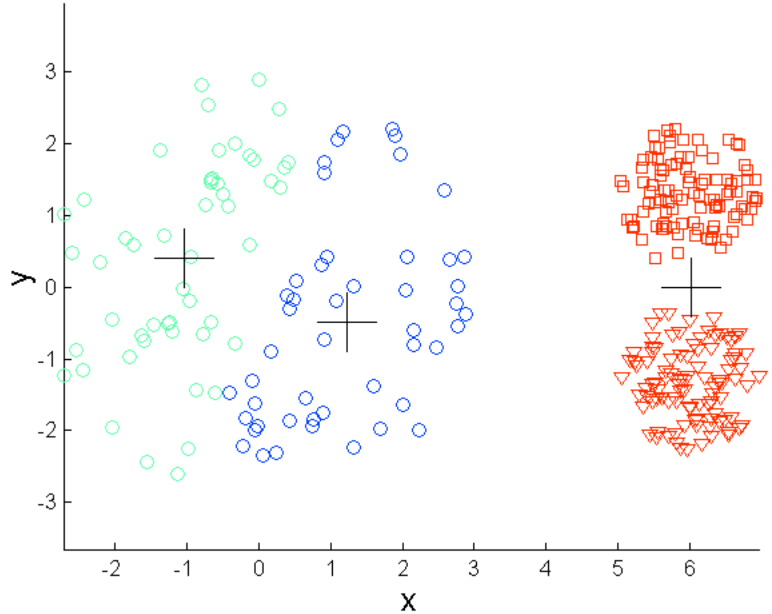
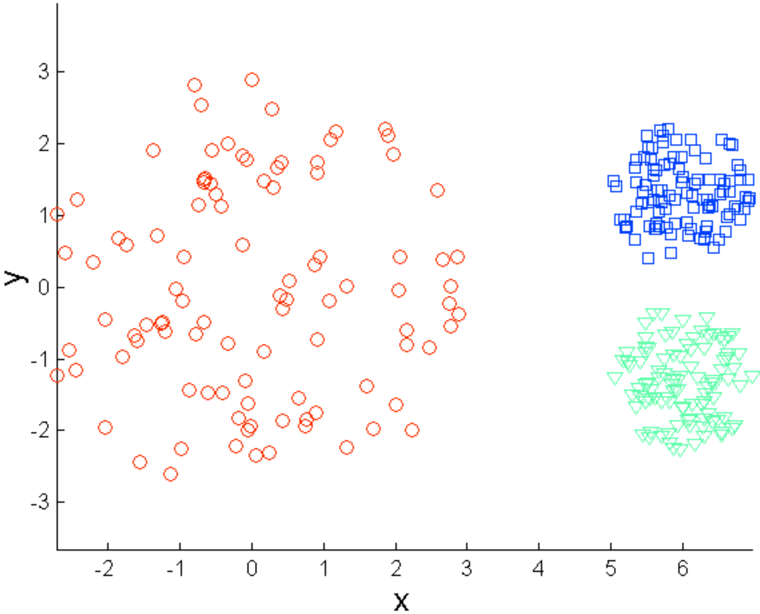
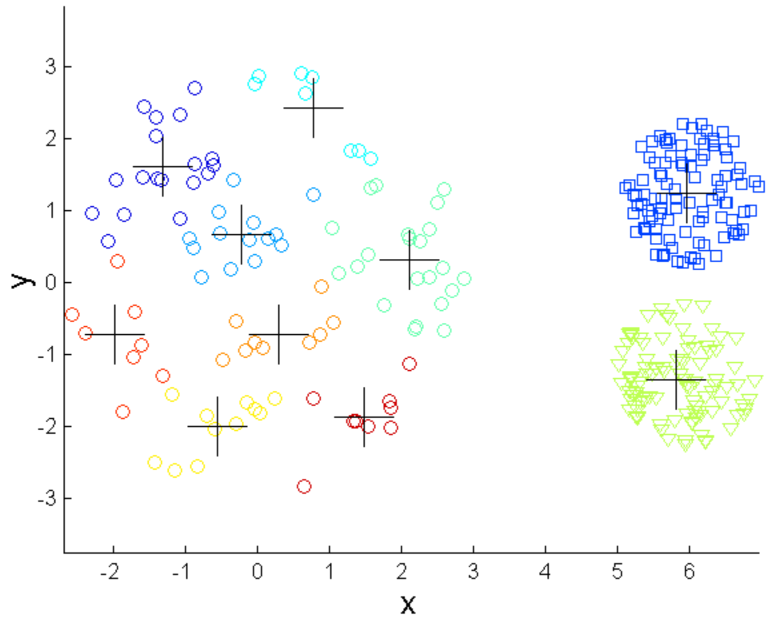


K-means (3 Clusters)

Overcoming K-means Limitations

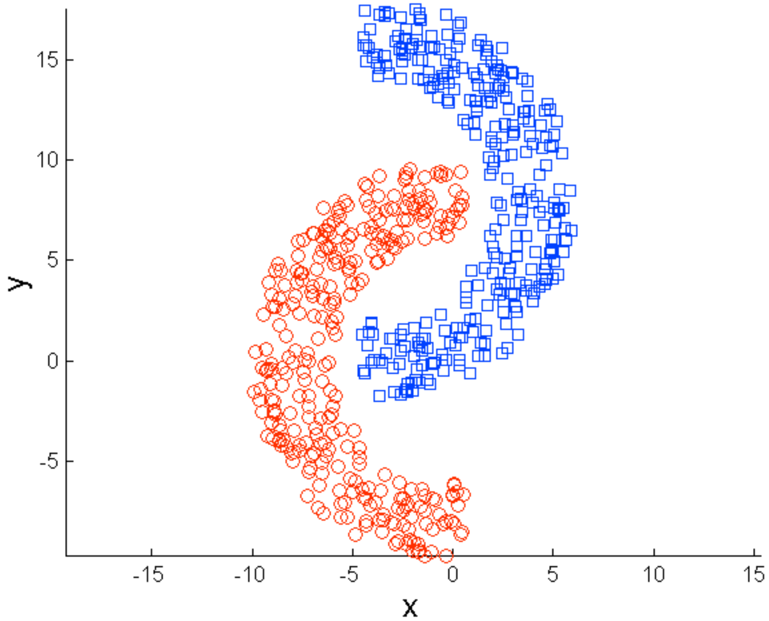




Original Points

K-means Clusters

Limitations of K-means: Non-globular Shapes



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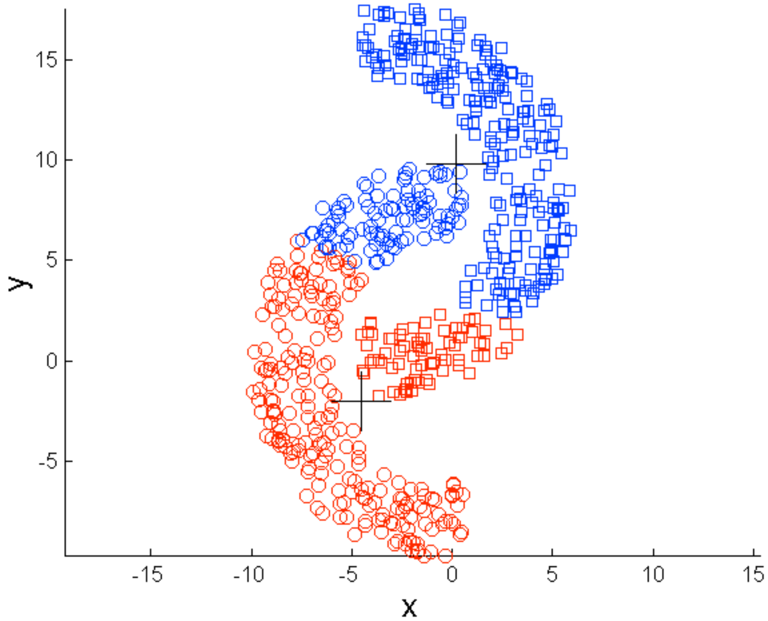
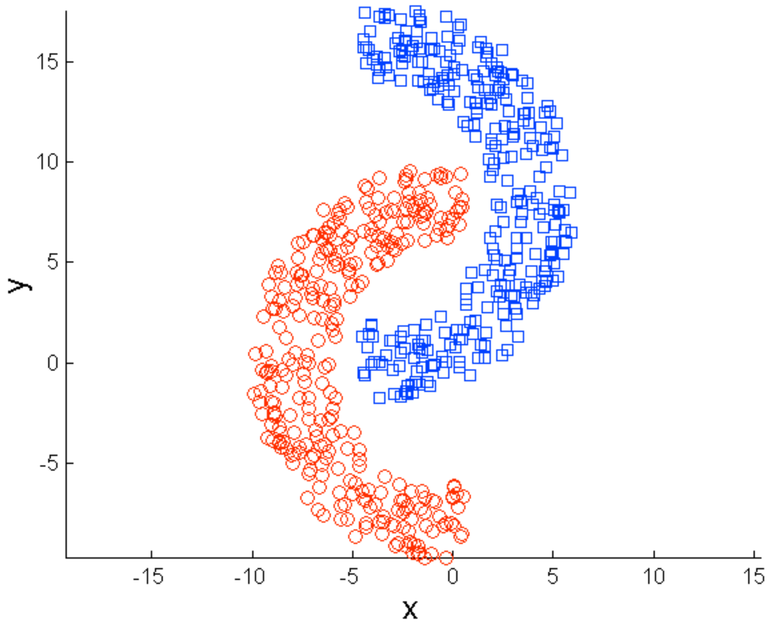
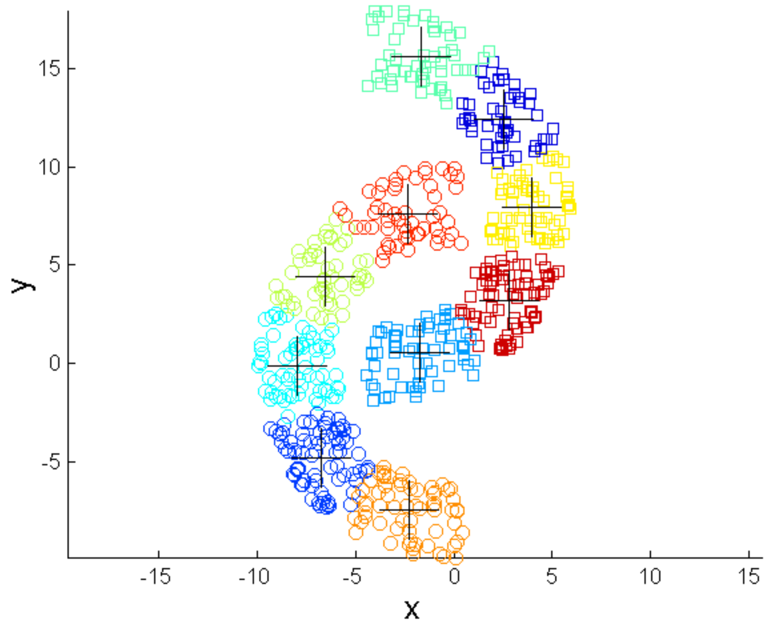


K-means (2 Clusters)

Overcoming K-means Limitations

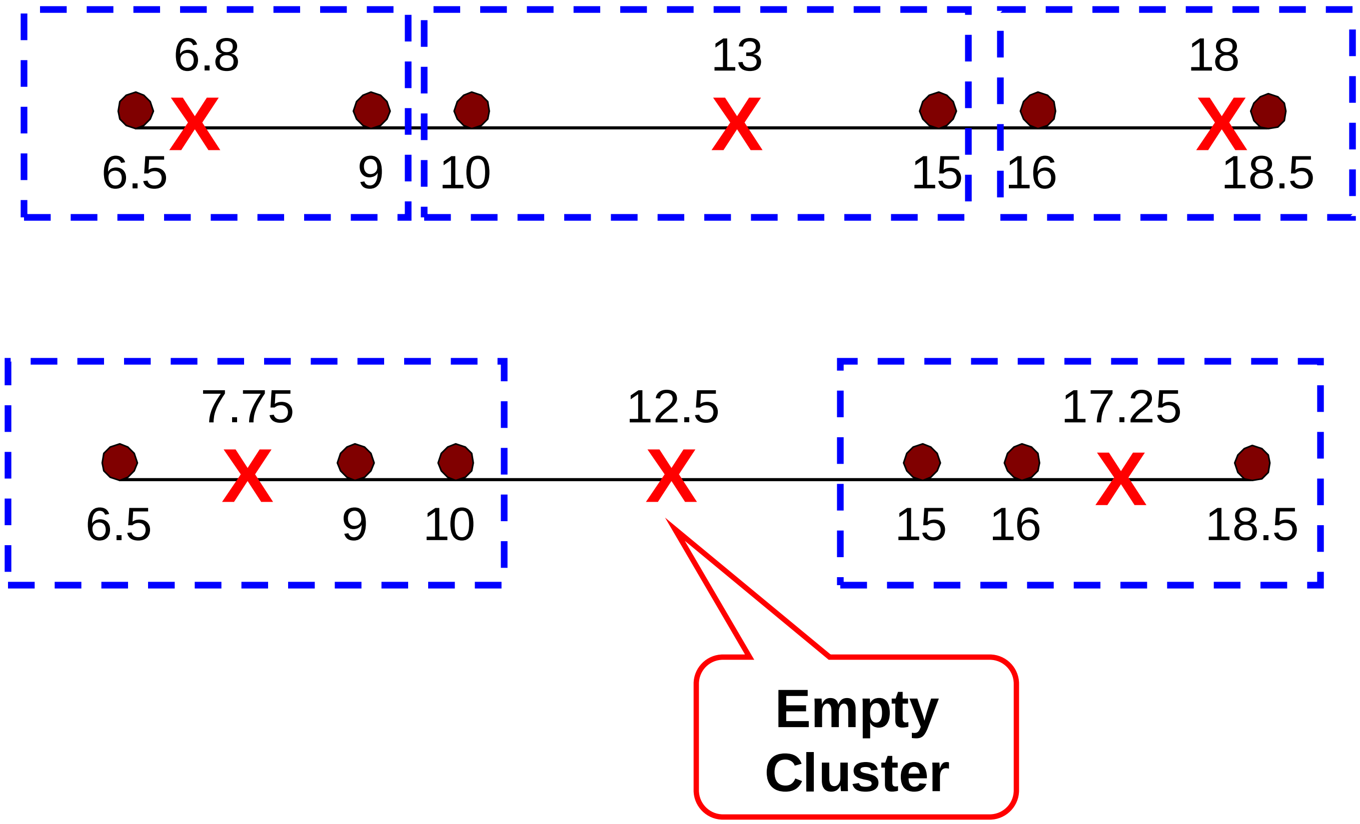




Original Points **K-means Clusters**

Empty Clusters

- K-means can yield empty clusters



Handling Empty Clusters

- Basic K-means algorithm can yield empty clusters

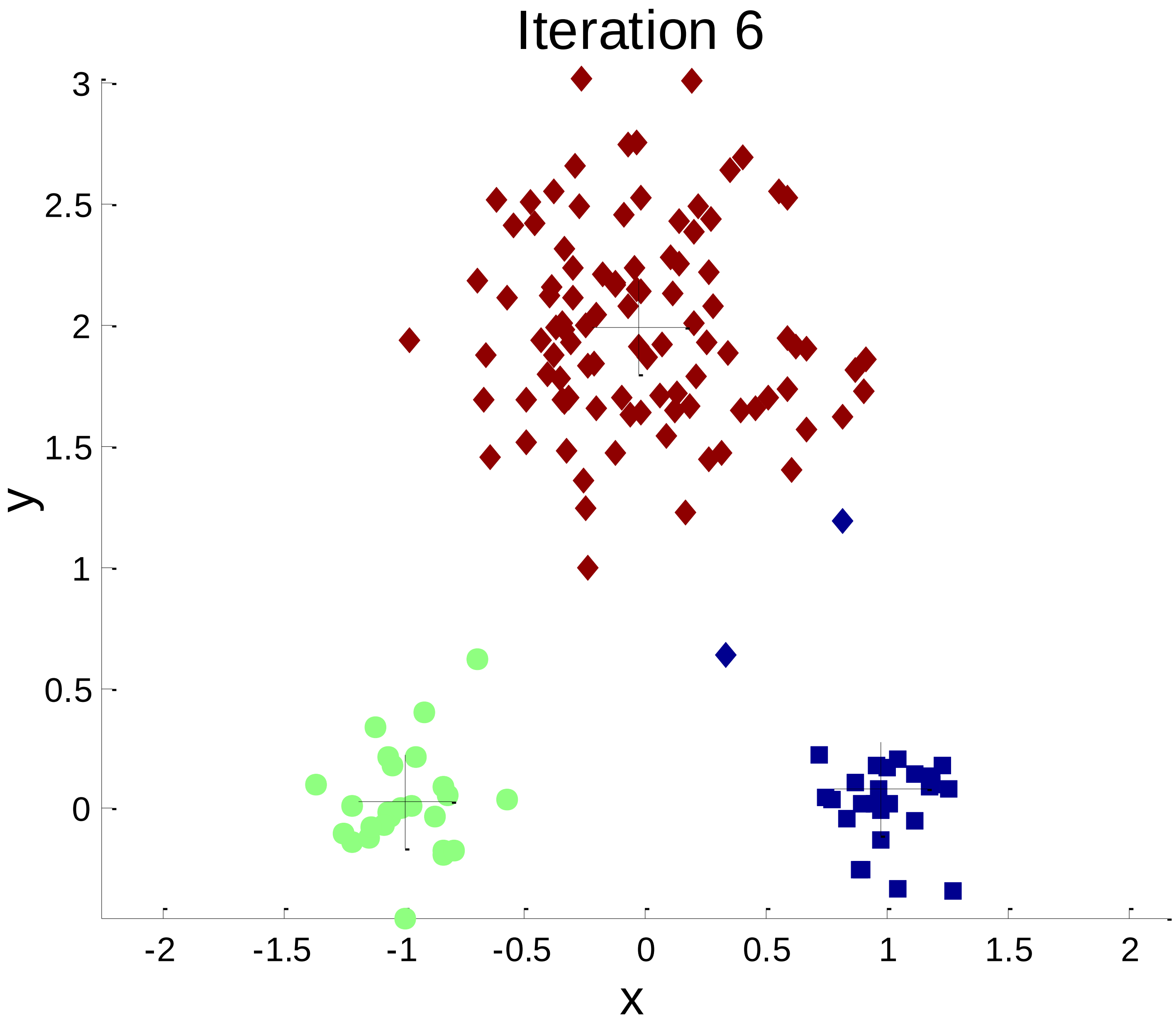
- Several strategies
  - Choose a point and assign it to the cluster
    - Choose the point that contributes most to SSE
    - Choose a point from the cluster with the highest SSE

- 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

Importance of Choosing Initial Centroids



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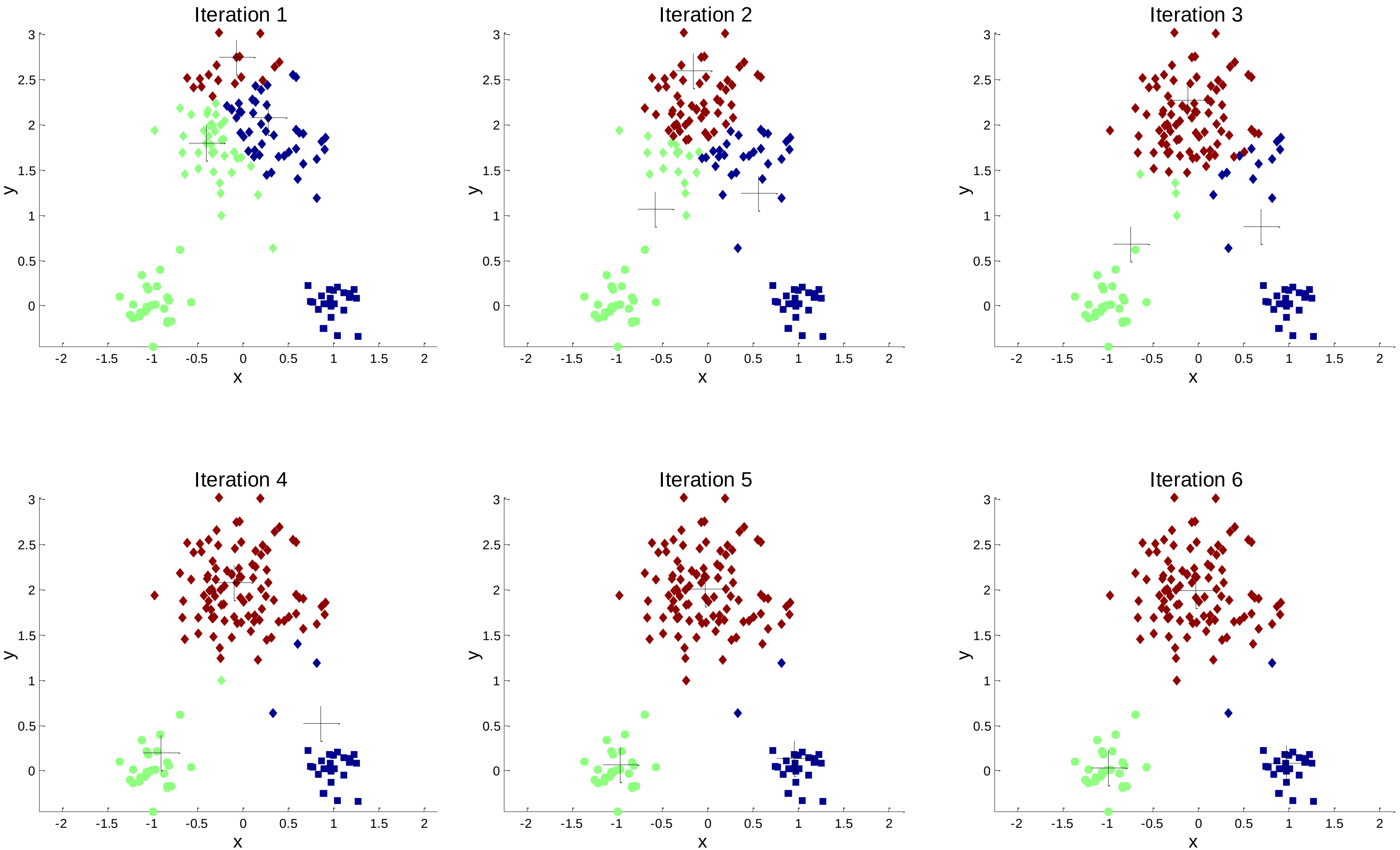

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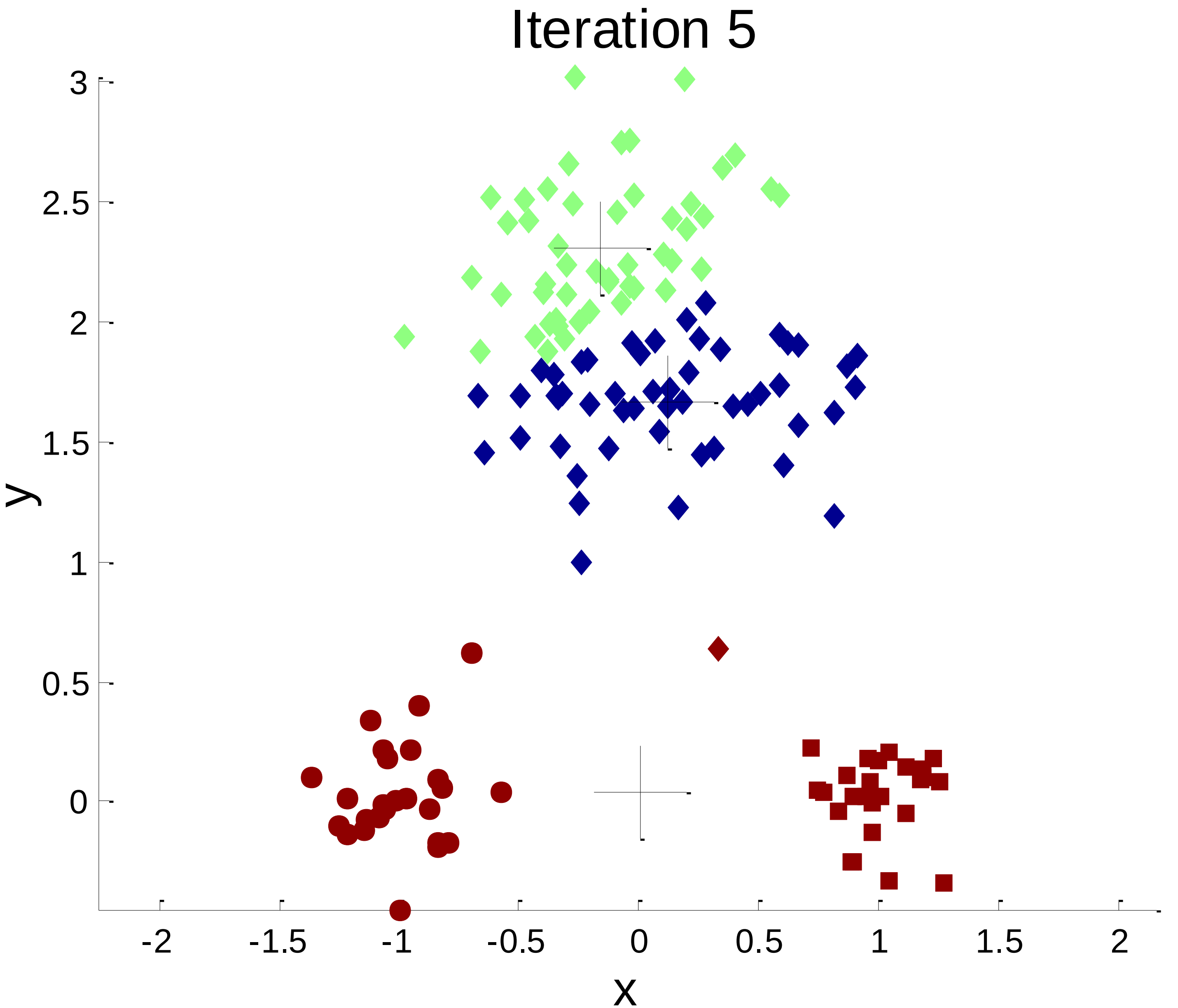

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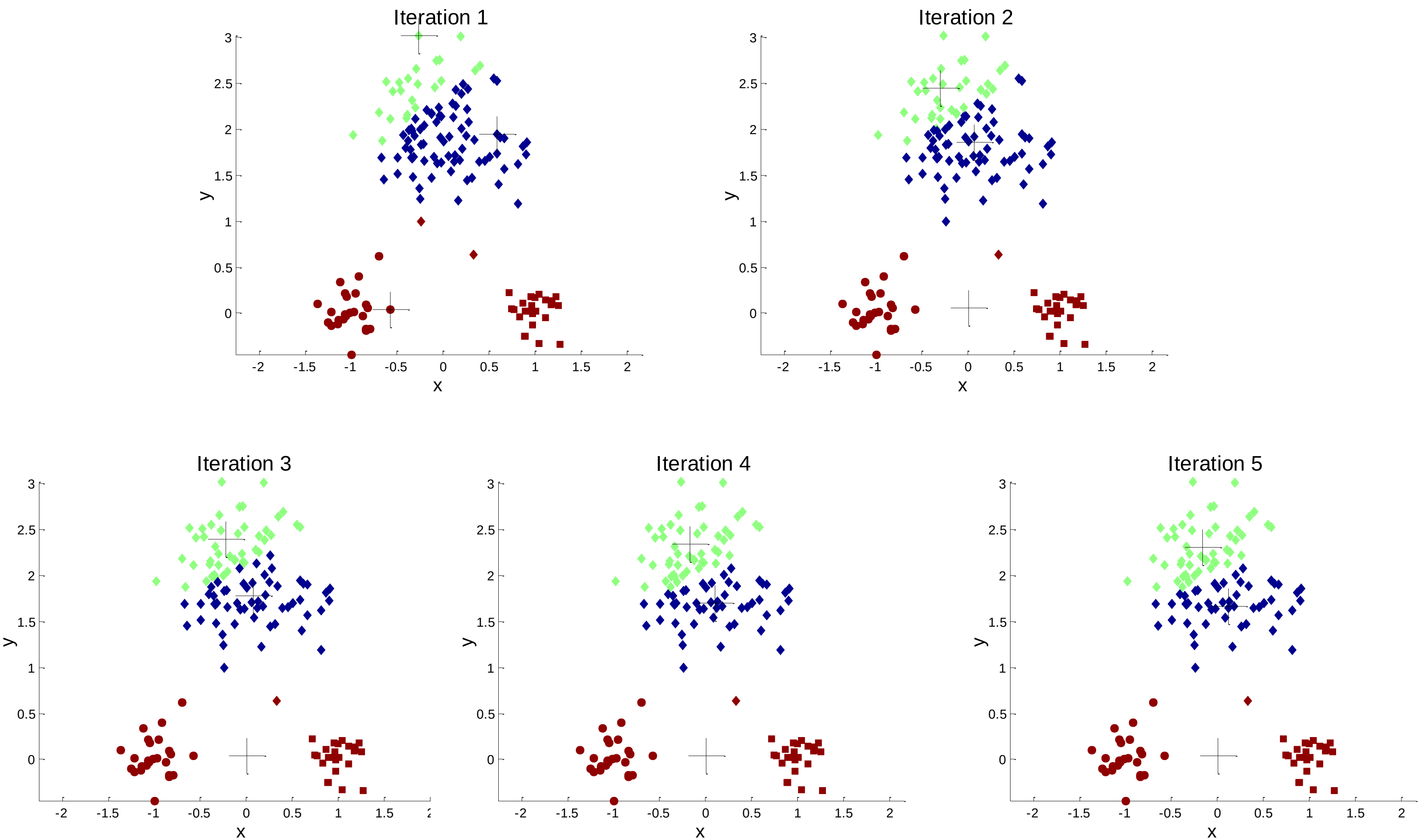


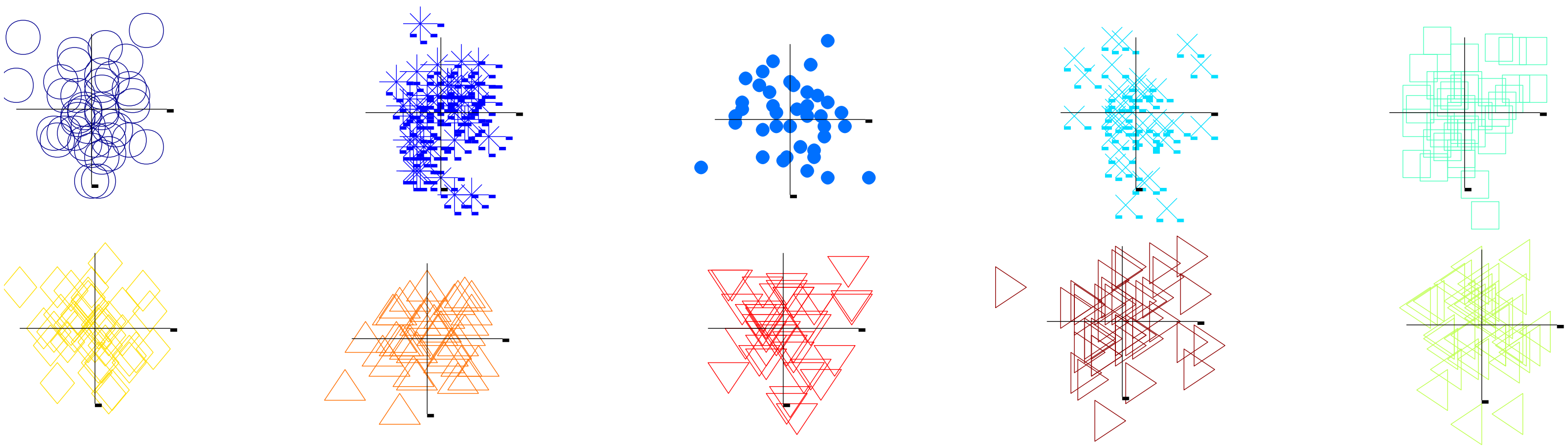
Problems with Selecting Initial Points

- 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

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

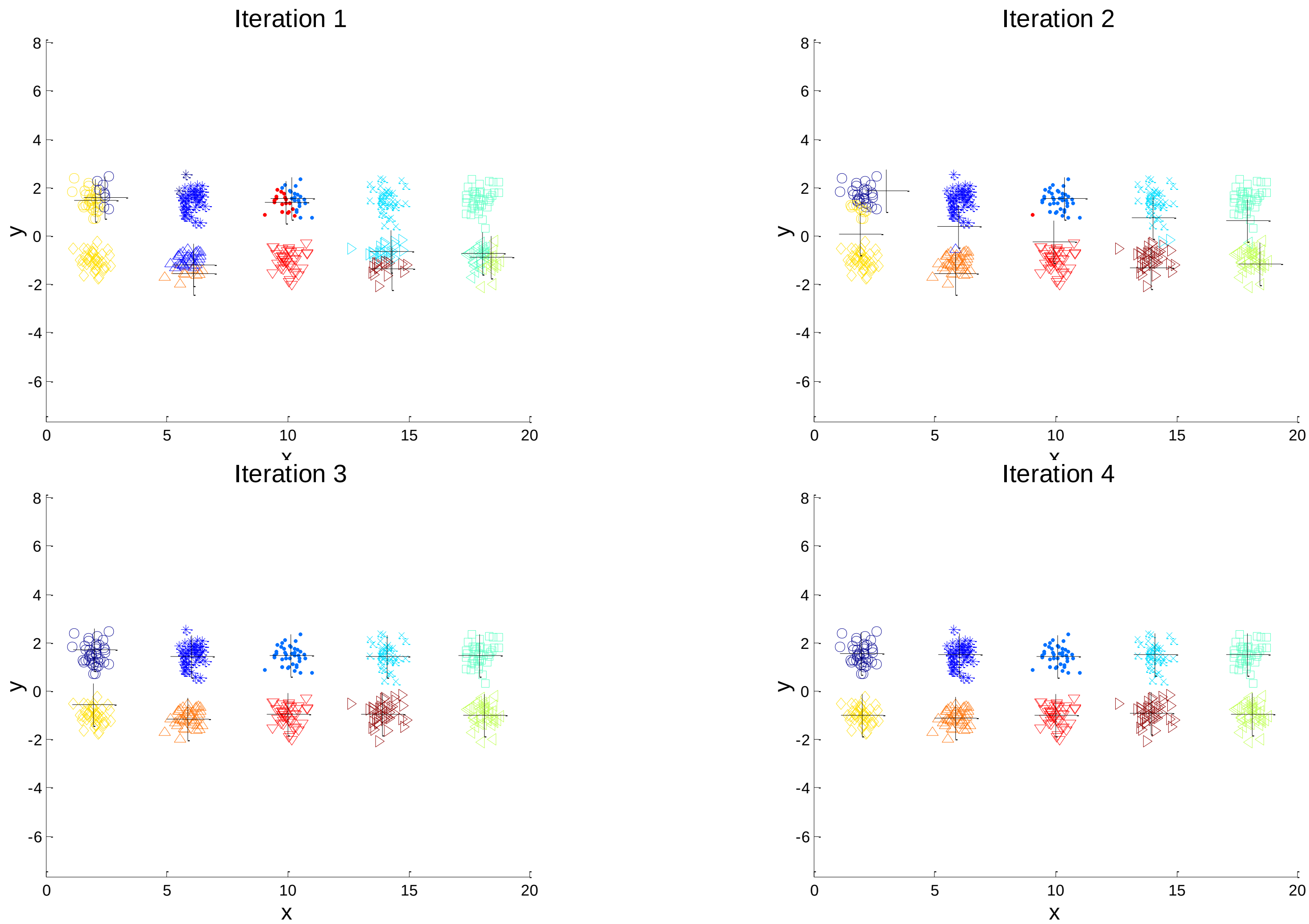
  - For example, if K = 10, then probability = $10!/10^{10} = 0.00036$
  - Sometimes the initial centroids will readjust themselves in ‘right’ way, and sometimes they don’t
  - Consider an example of five pairs of clusters

10 Clusters Example



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

10 Clusters Example



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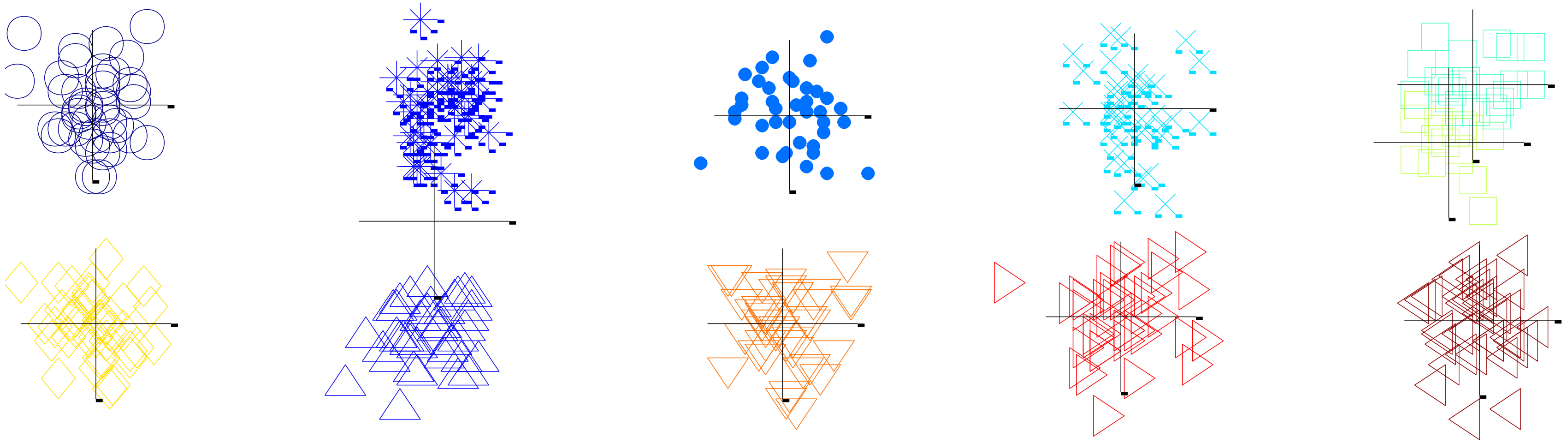

Starting with some pairs of clusters having three initial centroids, while other have only one.

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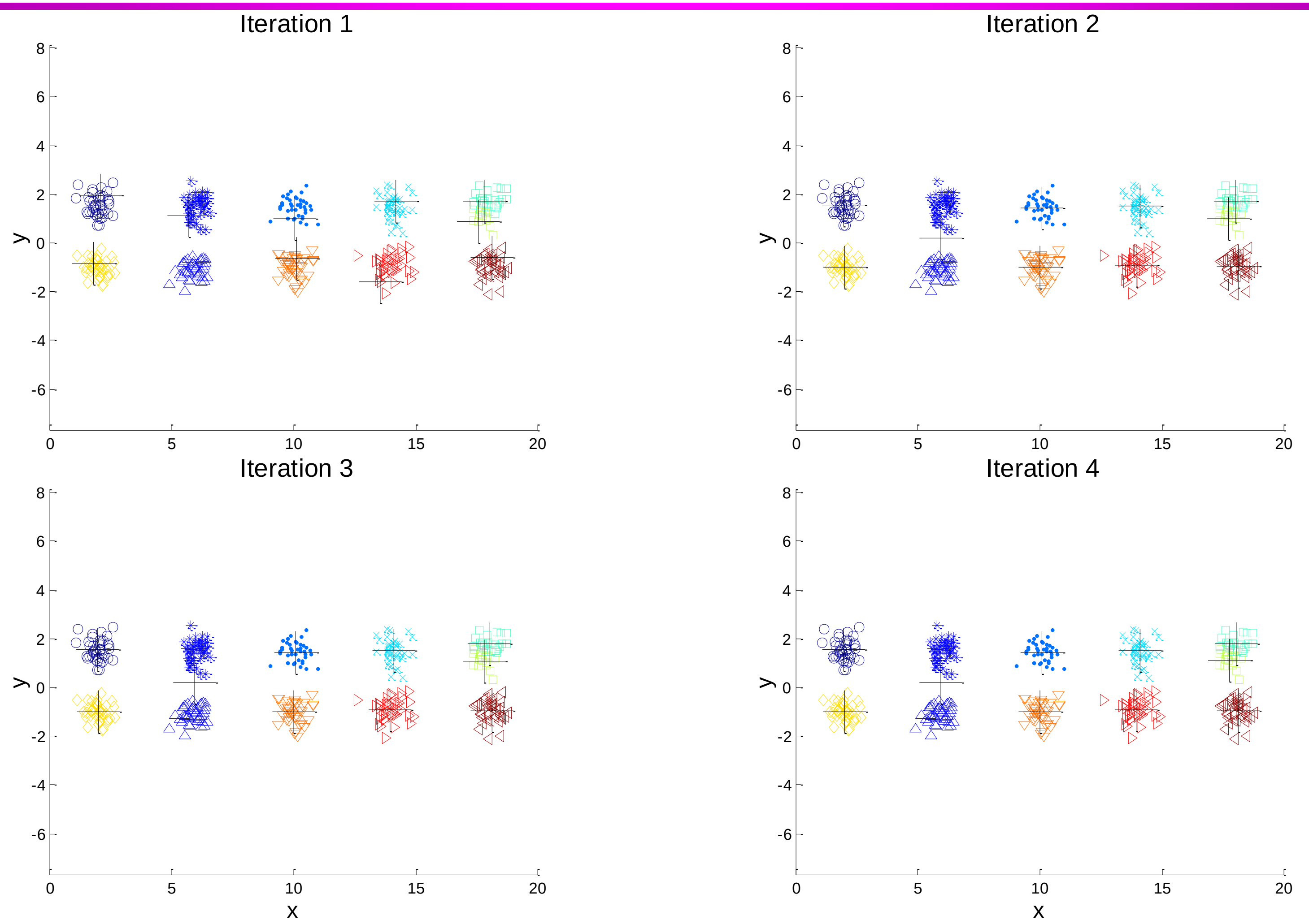


Starting with some pairs of clusters having three initial centroids, while other have only one.

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
- Postprocessing
- Generate a larger number of clusters and then perform a hierarchical clustering
- Bisecting K-means
  - Not as susceptible to initialization issues

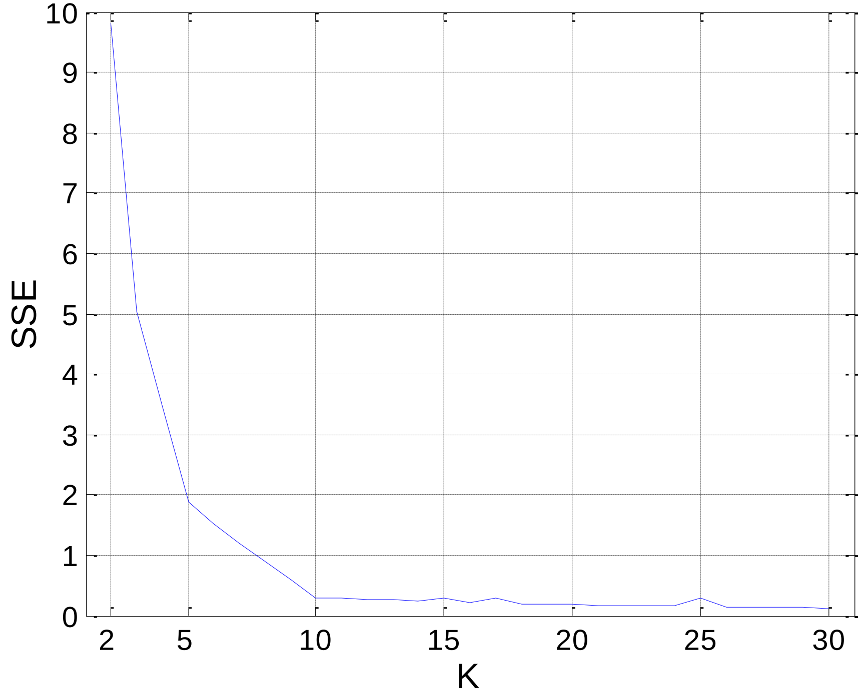
Updating Centers Incrementally

- 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
  - Can use “weights” to change the impact

Finding the best number of clusters

- In k-means the number of clusters *K* is given
  - Partition *n* objects into predetermined number of clusters
  - **Finding the "right" number of clusters is part of the problem**



Convergence of *K*-Means

- Define goodness measure of cluster c as sum of squared distances from cluster centroid:
  - $SSE_c(c,s) = \Sigma_i (d_i - s_c)^2$ (sum over all d_i in cluster c)
  - $G(C,s) = \Sigma_c SSE_c(c,s)$
- Re-assignment monotonically decreases G
  - It is a coordinate descent algorithm (**opt one component at a time**)
- At any step we have some value for G(C,s)

1) Fix s, optimize C → assign d to the closest centroid → G(C',s) <= G(C,s)

2) Fix C', optimize s → take the new centroids → G(C',s') <= G(C',s) <= G(C,s)

The new cost is smaller than the original one → local minimum