ITCS 6156/8156 Fall 2024
Machine Learning

Clustering

Instructor: Hongfei Xue
Email: hongfei.xue@charlotte.edu
Class Meeting: Tue & Thu, 4:00 PM – 5:15 PM, WWH 130

UNIVERSITY OF NORTH CAROLINA
CHARLOTTE

Some content in the slides is based on Dr. Raquel Urtasun’s lecture

Unsupervised Learning

- Supervised learning algorithms have a clear goal: produce desired outputs for given inputs.
  - You are given $\{(x^{(i)}, t^{(i)})\}$ during training (inputs and targets)
- Goal of unsupervised learning algorithms (no explicit feedback whether outputs of system are correct) less clear.
  - You are given the inputs $\{x^{(i)}\}$ during training, labels are unknown.
- Tasks to consider:
  - Reduce dimensionality
  - Find clusters
  - Model data density
  - Find hidden causes
- Key utility
  - Compress data
  - Detect outliers
  - Facilitate other learning

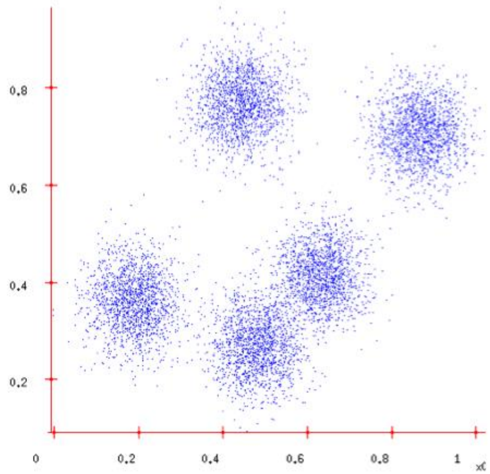
Major Types

- Primary problems, approaches in unsupervised learning fall into three classes:

  1. Dimensionality reduction: represent each input case using a small number of variables (e.g., principal components analysis, factor analysis, independent components analysis)
  2. Clustering: represent each input case using a prototype example (e.g., k-means, mixture models)
  3. Density estimation: estimating the probability distribution over the data space

Clustering

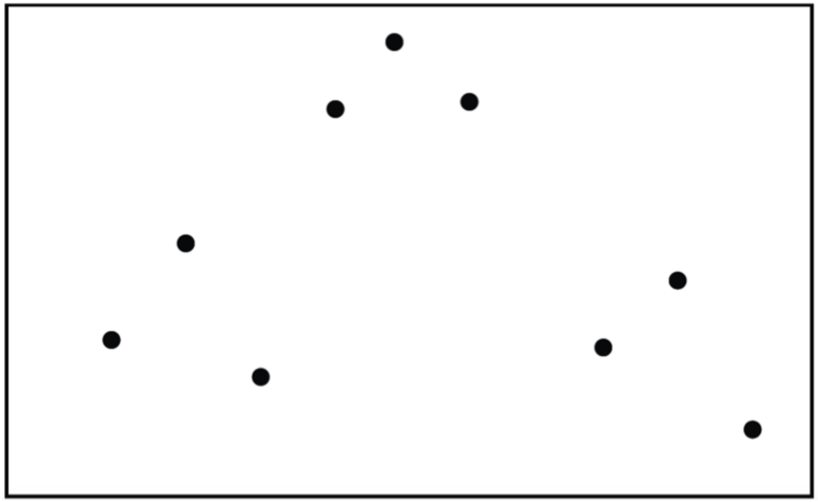
- Grouping N examples into K clusters one of canonical problems in unsupervised learning



Clustering is a task in machine learning and data analysis that involves grouping a set of **unlabeled** data points into subsets, or "clusters," such that data points within the same cluster are more **similar** to each other than to those in other clusters.

- Motivation: prediction; lossy compression; outlier detection
- We assume that the data was generated from a number of different classes. The aim is to cluster data from the same class together.
  - How many classes?
  - Why not put each datapoint into a separate class?
- What is the objective function that is optimized by sensible clustering?

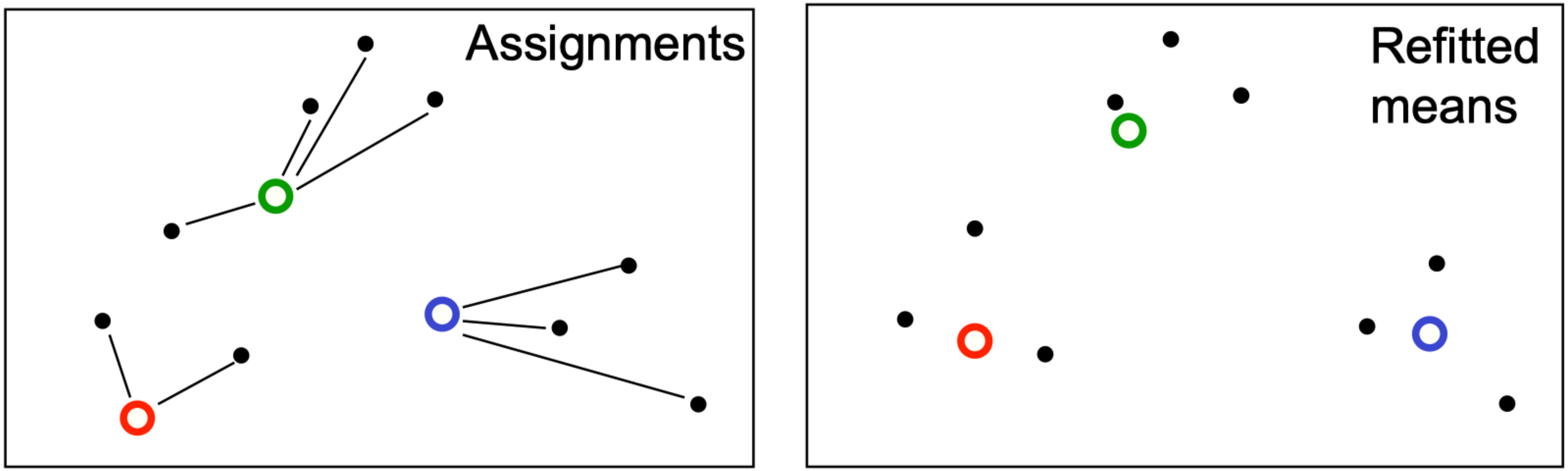
Clustering



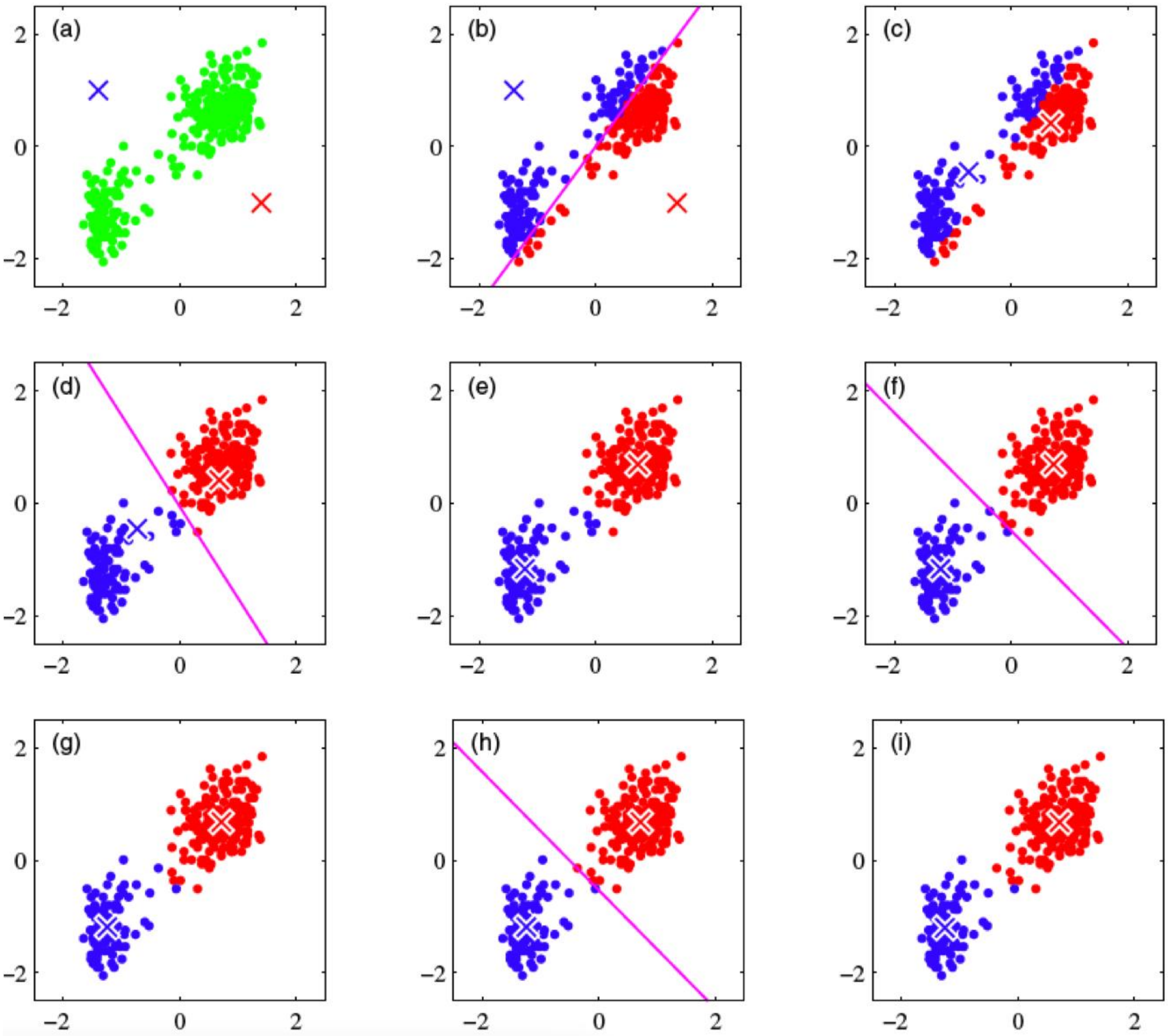
- Assume the data $\{\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(N)}\}$ lives in a Euclidean space, $\mathbf{x}^{(n)} \in \mathbb{R}^d$.
- Assume the data belongs to K classes (patterns)
- How can we identify those classes (data points that belong to each class)?

K-means

- Initialization: randomly initialize cluster centers
- The algorithm iteratively alternates between two steps:
  - Assignment step: Assign each data point to the closest cluster
  - Refitting step: Move each cluster center to the center of gravity of the data assigned to it



K-means



K-means Objective

What is actually being optimized?

K-means Objective:
Find cluster centers $\mathbf{m}$ and assignments $\mathbf{r}$ to minimize the sum of squared distances of data points $\{\mathbf{x}^{(n)}\}$ to their assigned cluster centers

$$\min_{\{\mathbf{m}\},\{\mathbf{r}\}} J(\{\mathbf{m}\},\{\mathbf{r}\}) = \min_{\{\mathbf{m}\},\{\mathbf{r}\}} \sum_{n=1}^{N} \sum_{k=1}^{K} r_k^{(n)} ||\mathbf{m}_k - \mathbf{x}^{(n)}||^2$$

$$\text{s.t.} \sum_k r_k^{(n)} = 1, \forall n, \quad \text{where} \quad r_k^{(n)} \in \{0,1\}, \forall k, n$$

where $r_k^{(n)} = 1$ means that $\mathbf{x}^{(n)}$ is assigned to cluster k (with center $\mathbf{m}_k$)

- Optimization method is a form of coordinate descent ("block coordinate descent")
  - Fix centers, optimize assignments (choose cluster whose mean is closest)
  - Fix assignments, optimize means (average of assigned datapoints)

The K-means Algorithm

- Initialization: Set K cluster means $\mathbf{m}_1, \ldots, \mathbf{m}_K$ to random values
- Repeat until convergence (until assignments do not change):
  - Assignment: Each data point $\mathbf{x}^{(n)}$ assigned to nearest mean

$$\hat{k}^n = arg \min_k d(\mathbf{m}_k, \mathbf{x}^{(n)})$$

(with, for example, L2 norm: $\hat{k}^n = arg \min_k ||\mathbf{m}_k - \mathbf{x}^{(n)}||^2$)

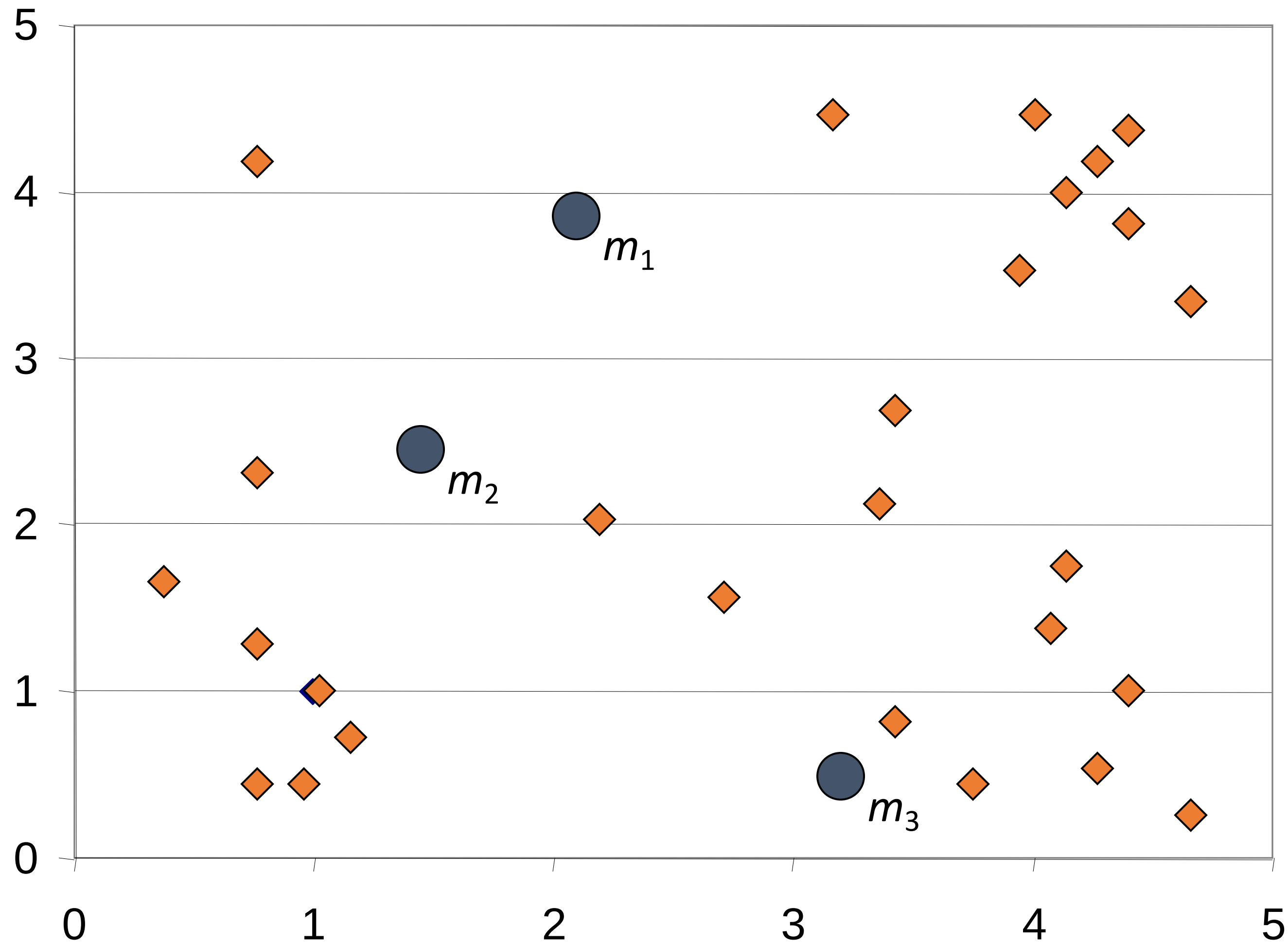
and Responsibilities (1 of k encoding)

$$r_k^{(n)} = 1 \longleftrightarrow \hat{k}^{(n)} = k$$

  - Update: Model parameters, means are adjusted to match sample means of data points they are responsible for:

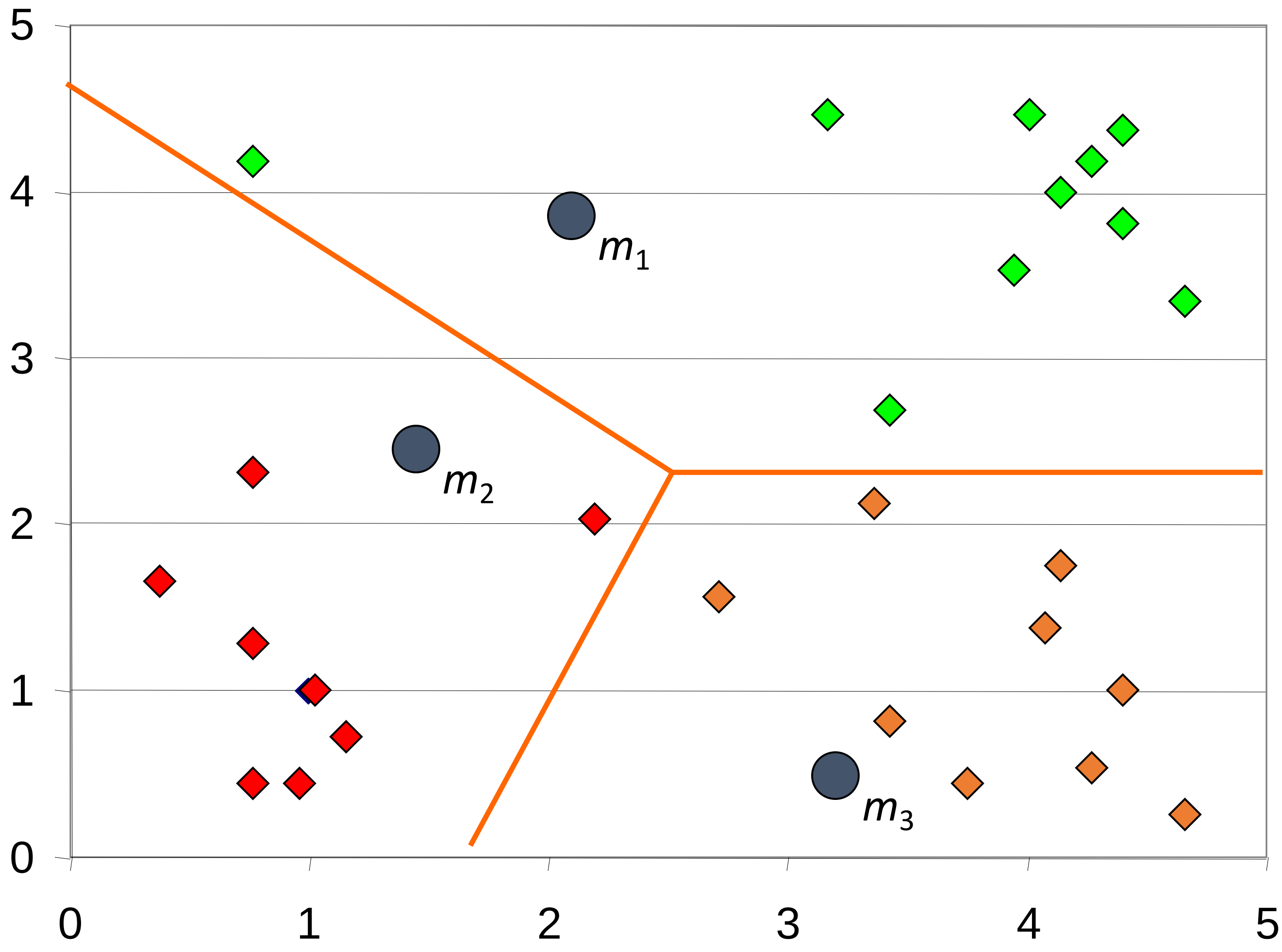
$$\mathbf{m}_k = \frac{\sum_n r_k^{(n)} \mathbf{x}^{(n)}}{\sum_n r_k^{(n)}}$$

Why K-means Converges



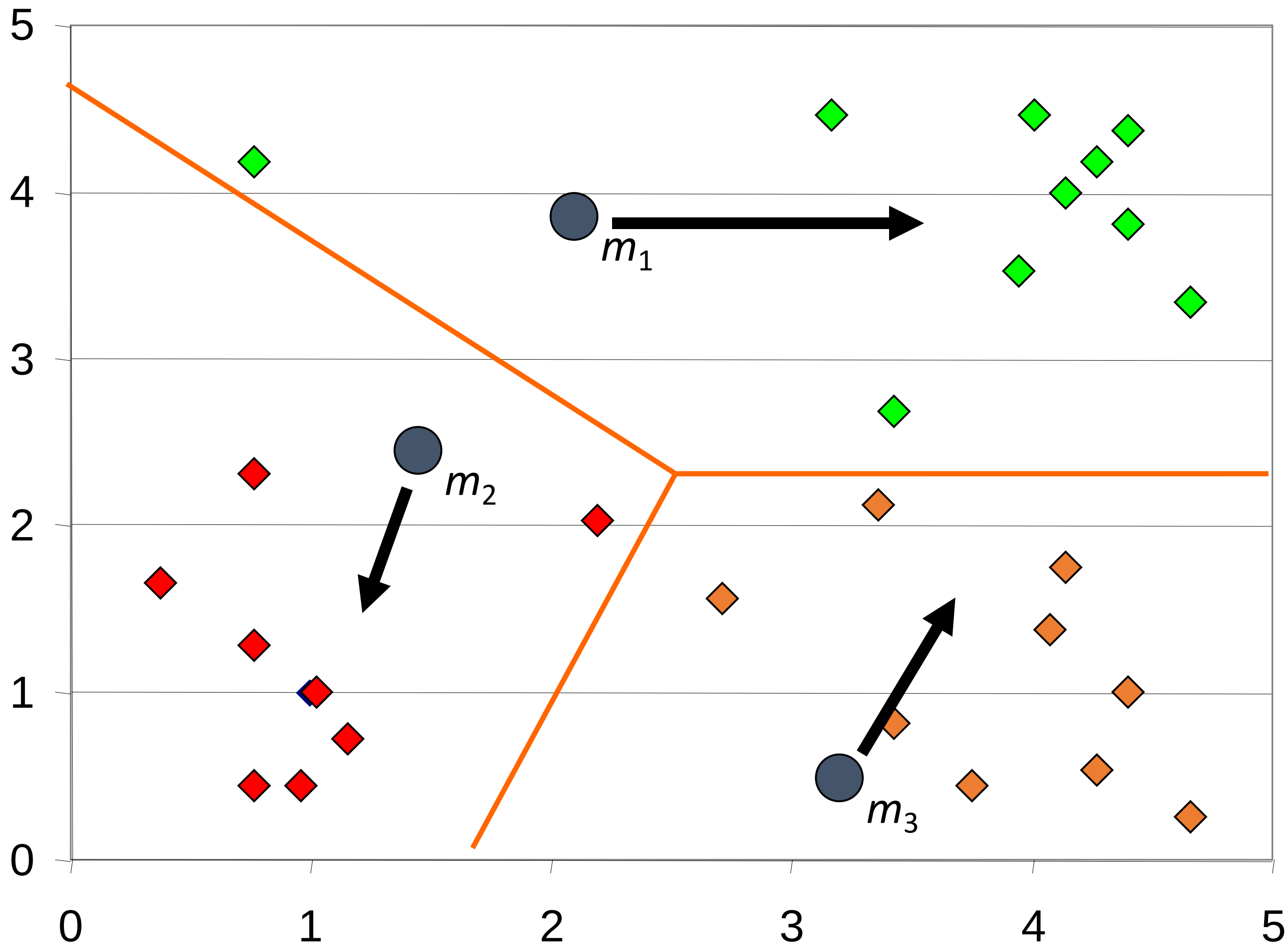
- Initialize

Why K-means Converges



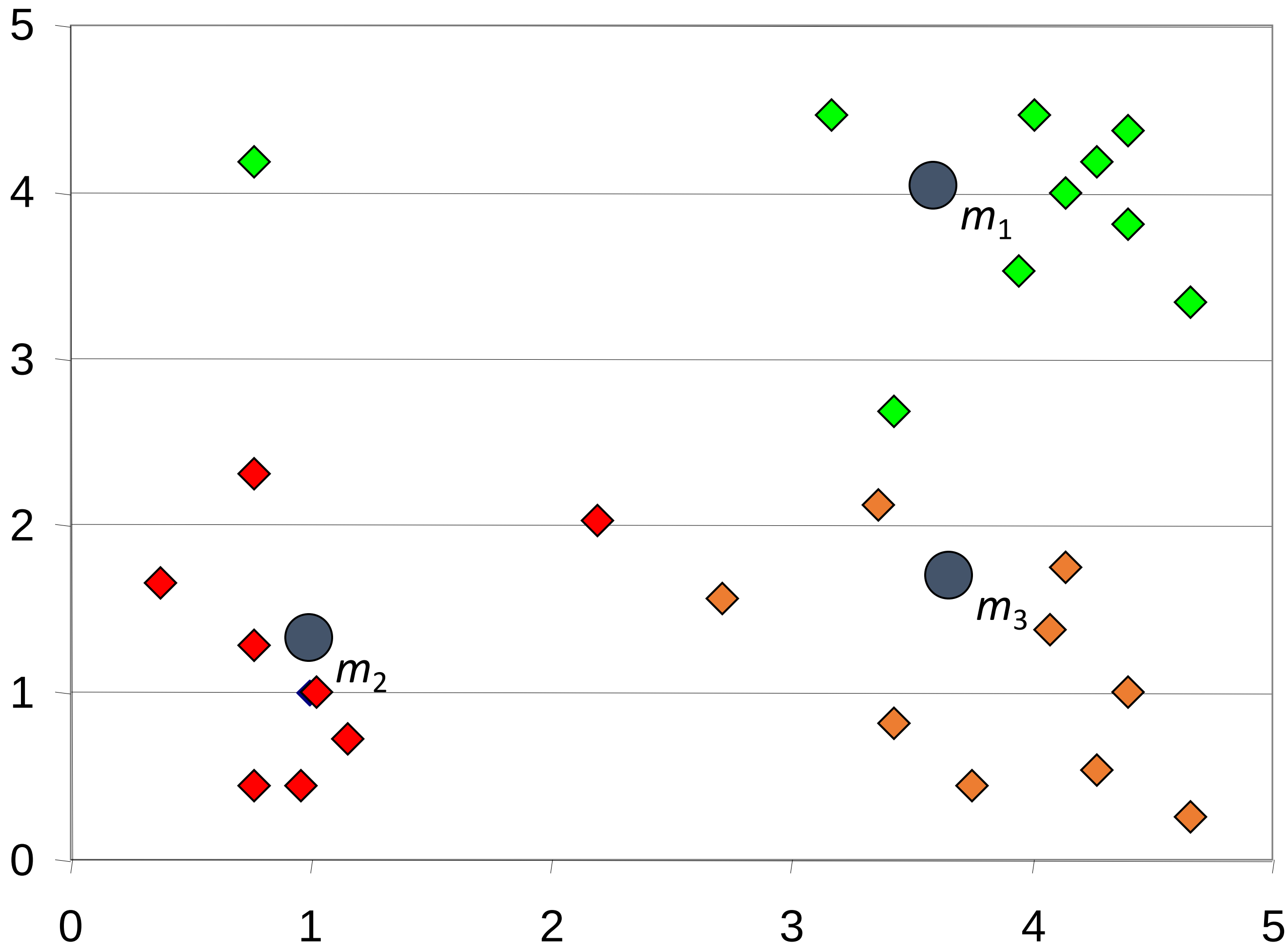
- Split into clusters.

Why K-means Converges

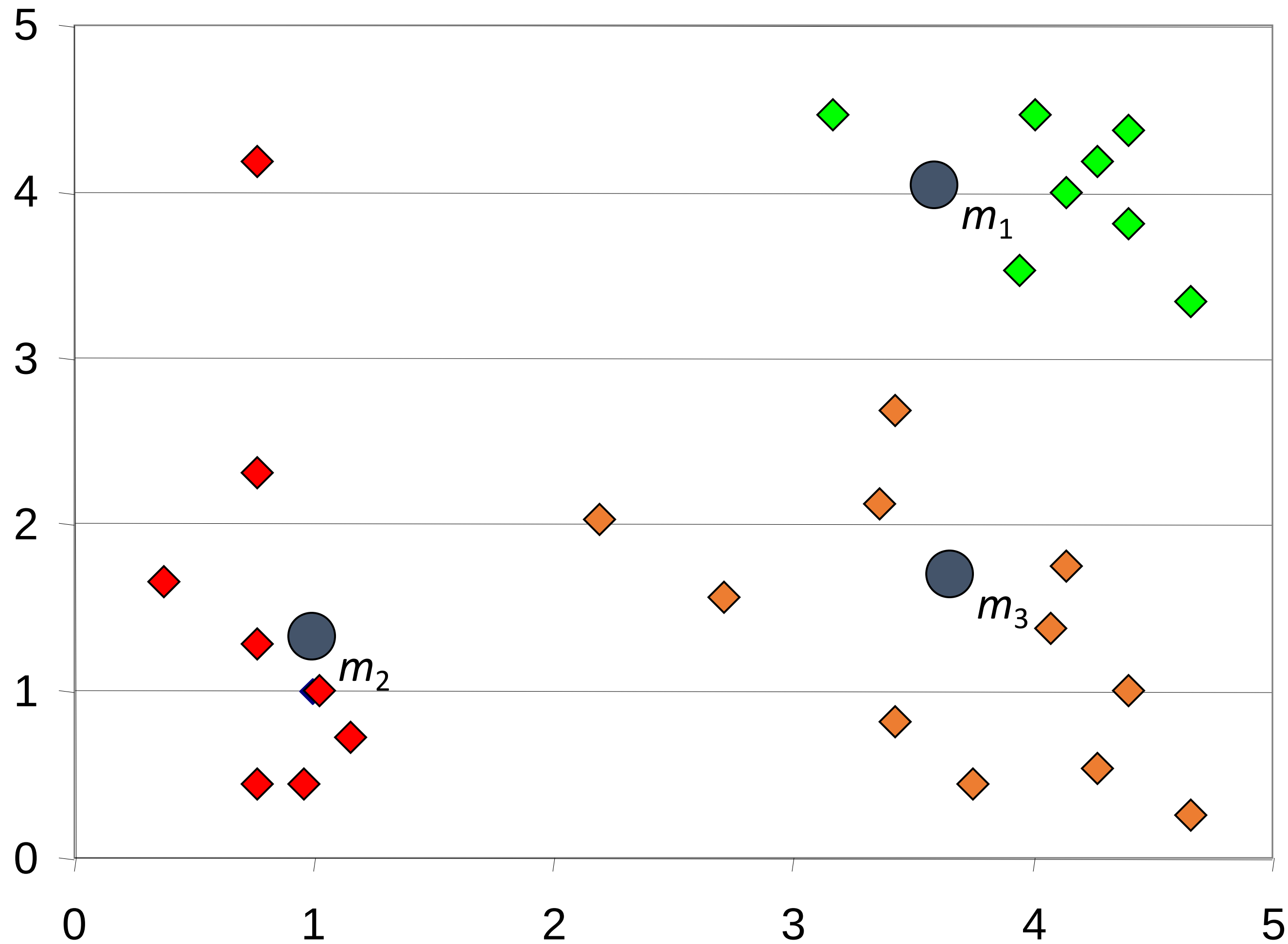


- Overall distances are reduced since the distances in each cluster is reduced.

Why K-means Converges

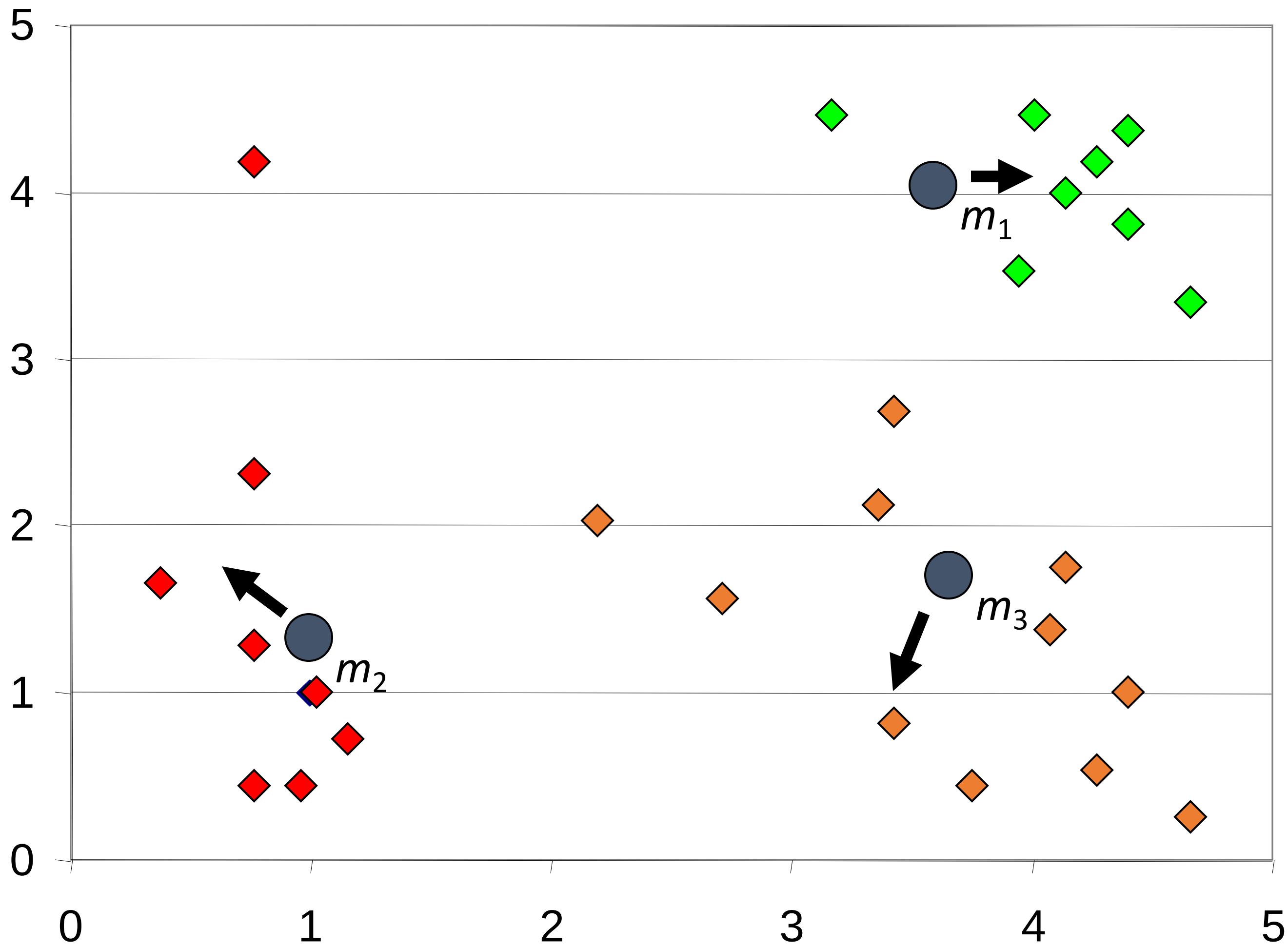


Why K-means Converges



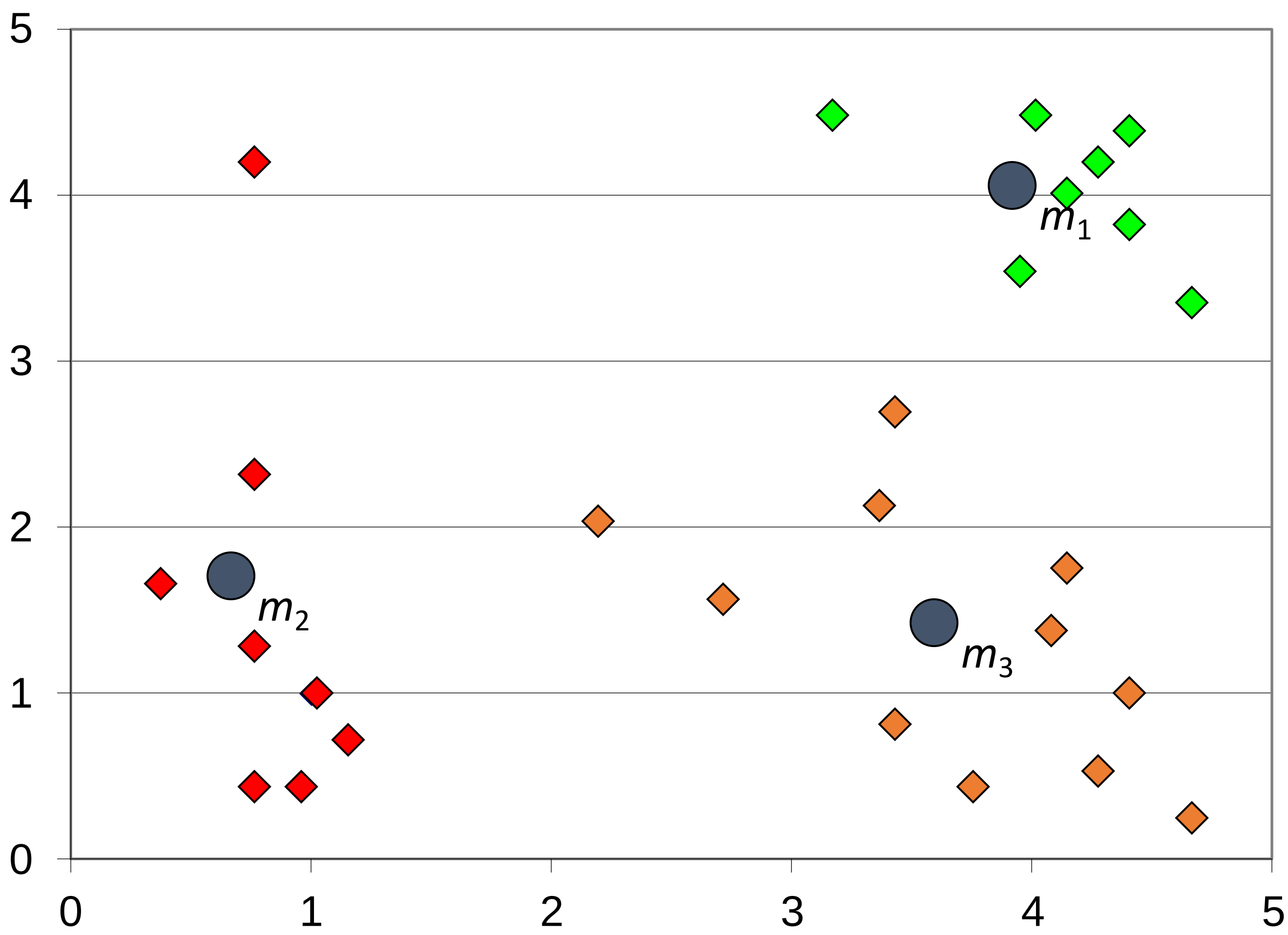
- Overall distances are reduced since the points are assigned to closer centroids.

Why K-means Converges



- Overall distances are reduced since the distances in each cluster is reduced.

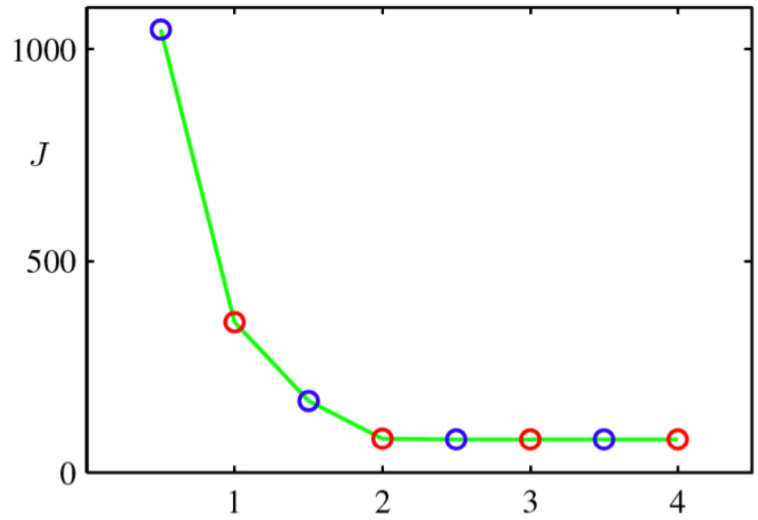
Why K-means Converges



- Converge

Why K-means Converges

- Whenever an assignment is changed, the sum squared distances J of data points from their assigned cluster centers is reduced.
- Whenever a cluster center is moved, J is reduced.
- Test for convergence: If the assignments do not change in the assignment step, we have converged (to at least a local minimum).

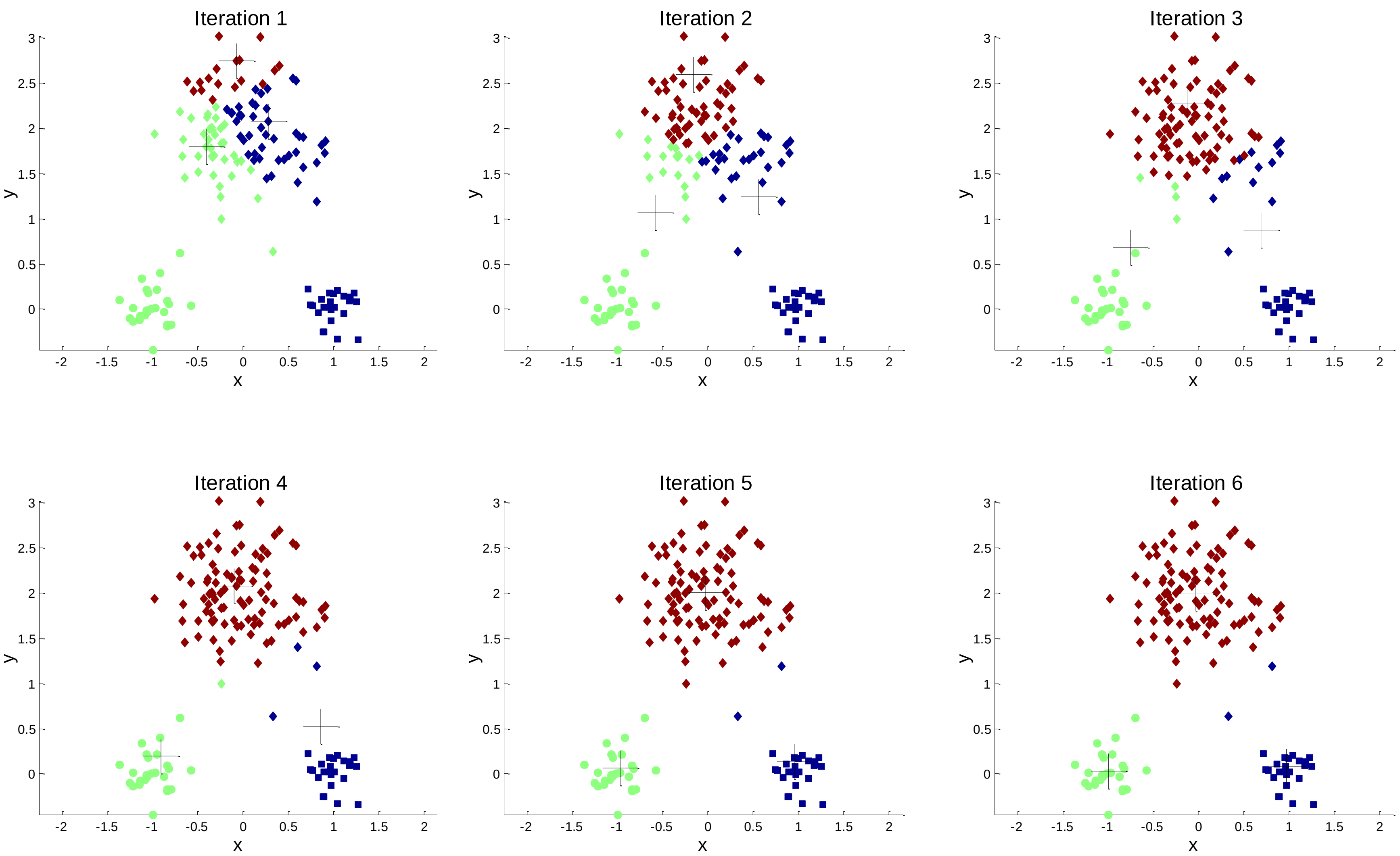


- K-means cost function after each E step (blue) and M step (red). The algorithm has converged after the third M step

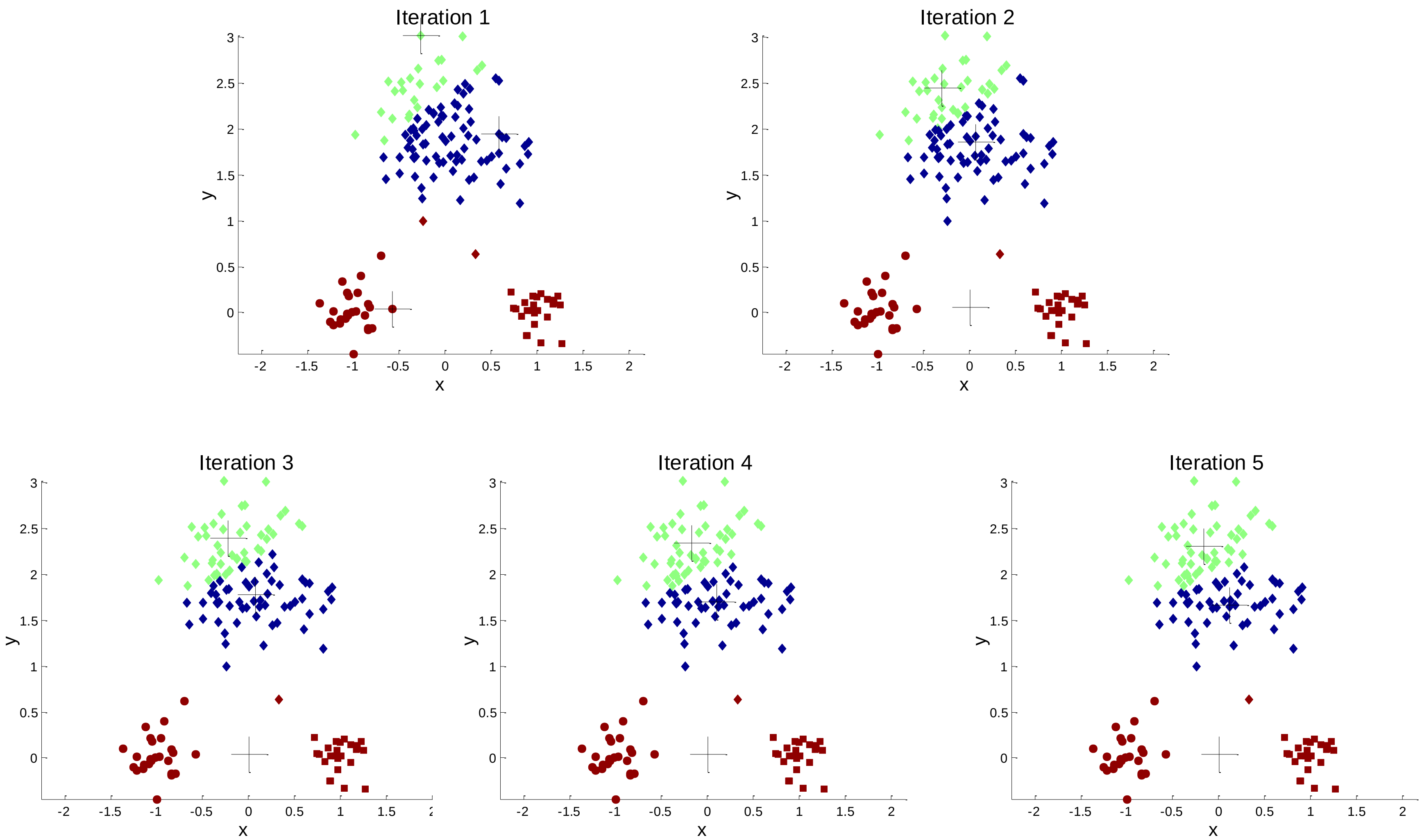
Comments on the K-Means Method

- **Strength**
  - Efficient: O(*tkn*), where *n* is # objects, *k* is # clusters, and *t* is # iterations. Normally, *k*, *t* << *n*
  - Easy to implement
- **Issues**
  - Need to specify *K*, the number of clusters
  - Local minimum– Initialization matters
  - Empty clusters may appear

Problems with Selecting Initial Points



Problems with Selecting Initial Points



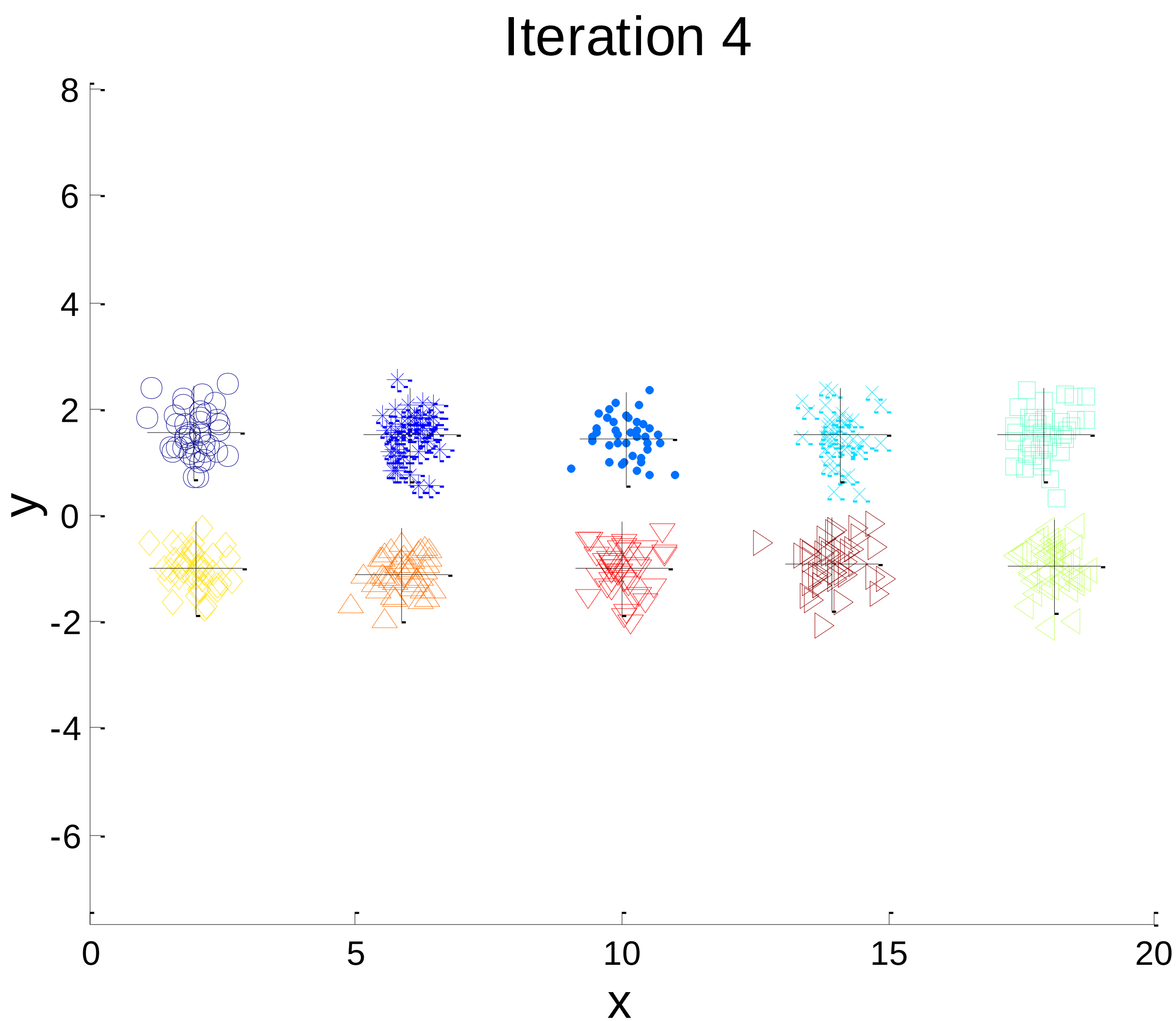
Problems with Selecting Initial Points

- 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

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

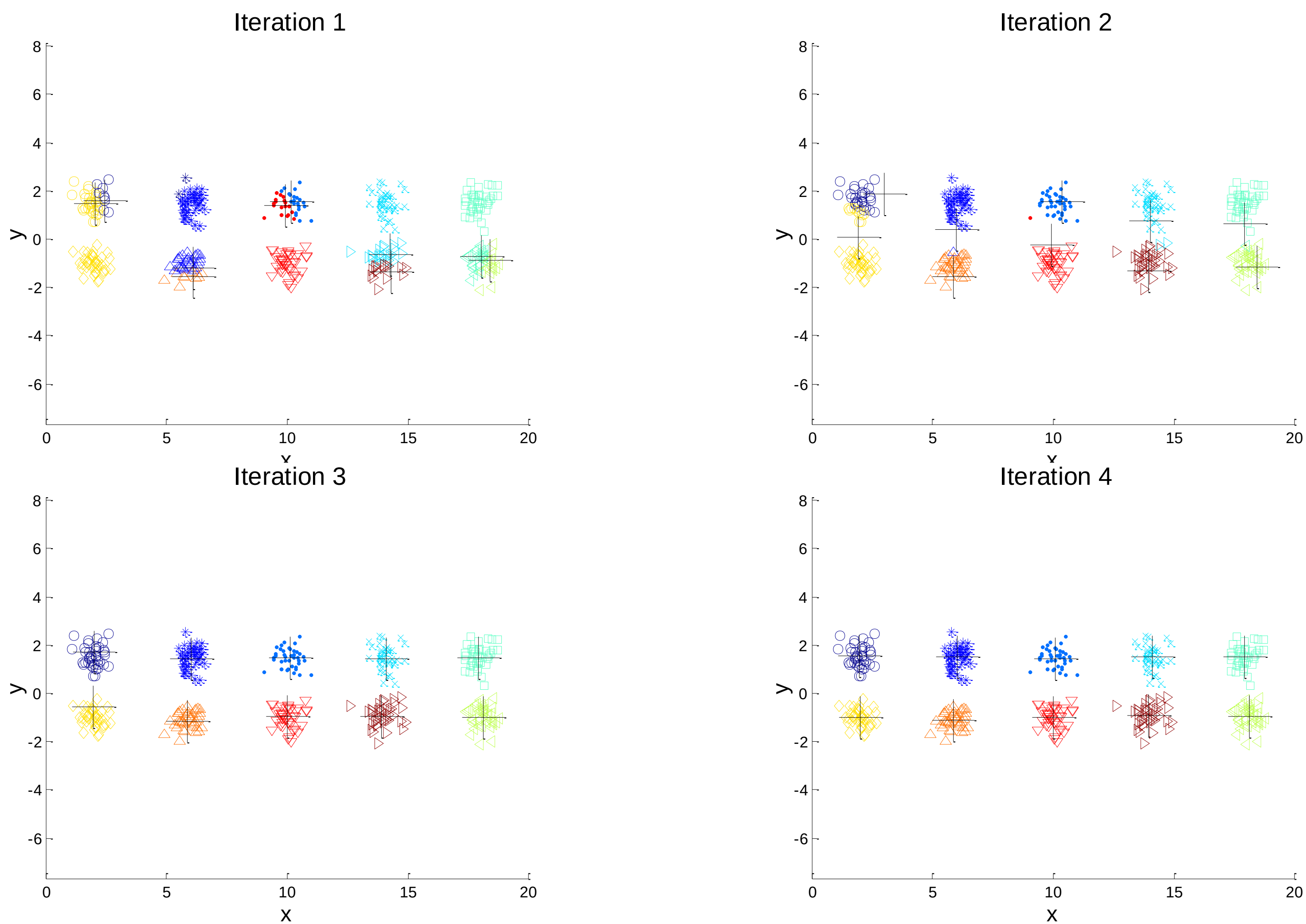
  - For example, if K = 10, then probability = $10!/10^{10}$ = 0.00036
  - Sometimes the initial centroids will readjust themselves in 'right' way, and sometimes they don't

10 Clusters Example



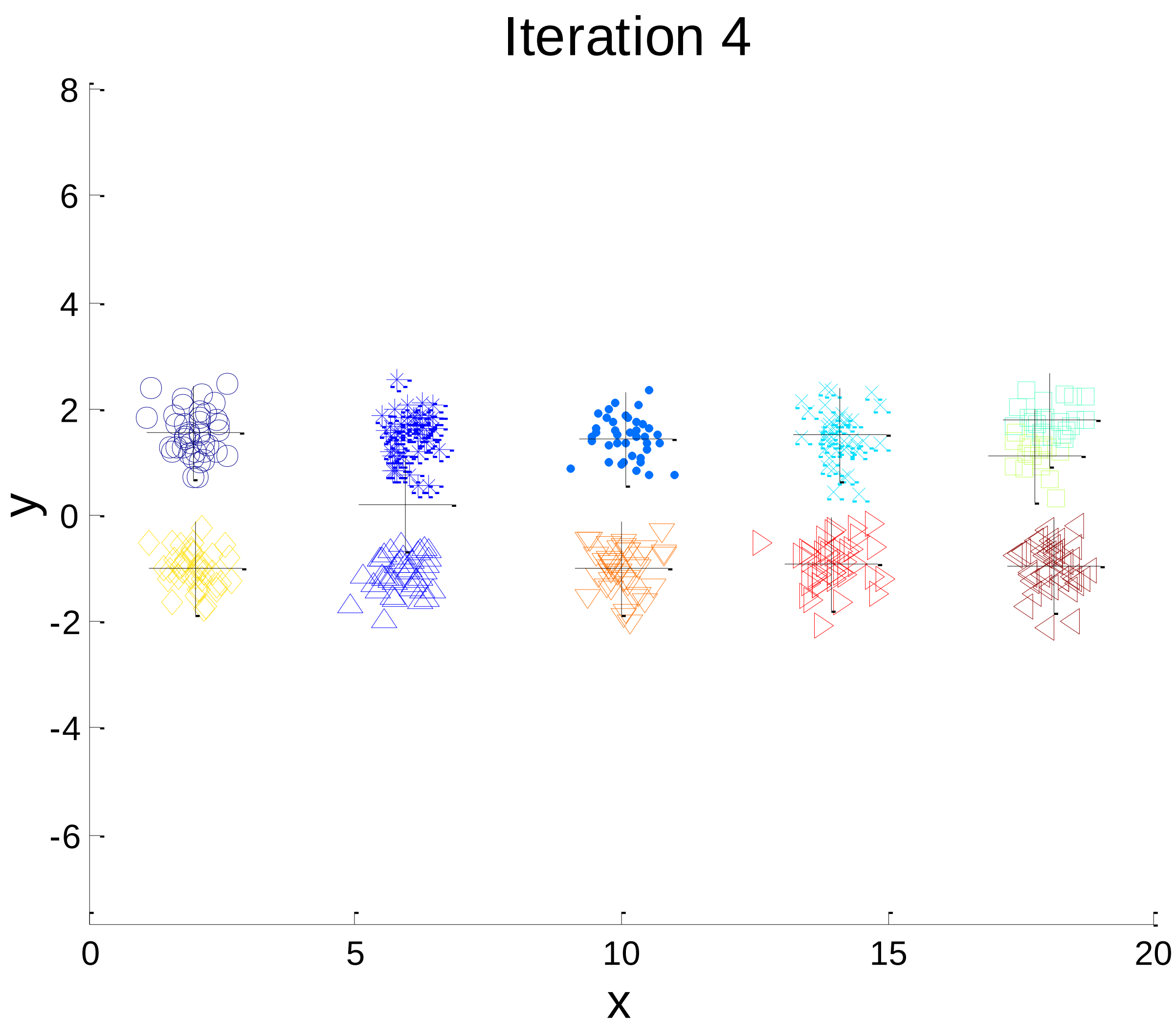
- Starting with two initial centroids in one cluster of each pair of clusters

10 Clusters Example



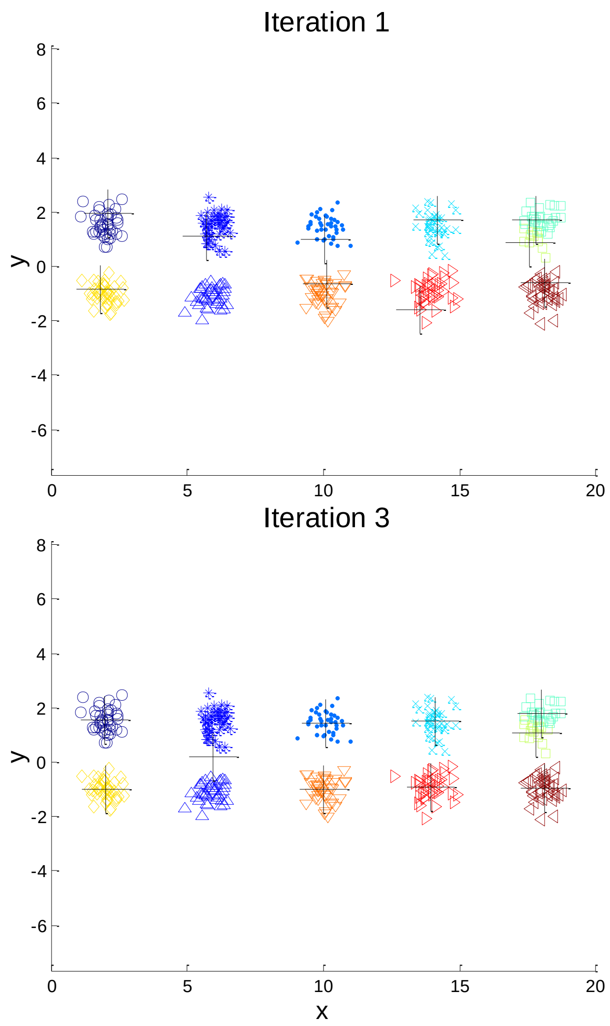
- Starting with two initial centroids in one cluster of each pair of clusters

10 Clusters Example



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

10 Clusters Example

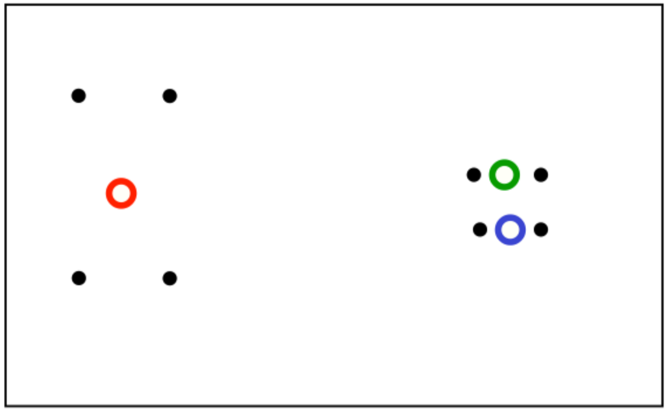


- Starting with some pairs of clusters having three initial centroids, while other have only one.

Local Minima

- The objective J is non-convex (so coordinate descent on J is not guaranteed to converge to the global minimum)
- There is nothing to prevent k-means getting stuck at local minima.
- We could try many random starting points
- We could try non-local split-and-merge moves:
  - Simultaneously merge two nearby clusters
  - and split a big cluster into two

A bad local optimum



Handling Empty Clusters

- Basic K-means algorithm can yield empty clusters
- Several strategies:
  - Choose a point that has the highest distance to a cluster center, set the point as the centroid of the empty cluster.
  - Split a cluster with the highest overall distance by assigning the centroid of the empty cluster within that cluster

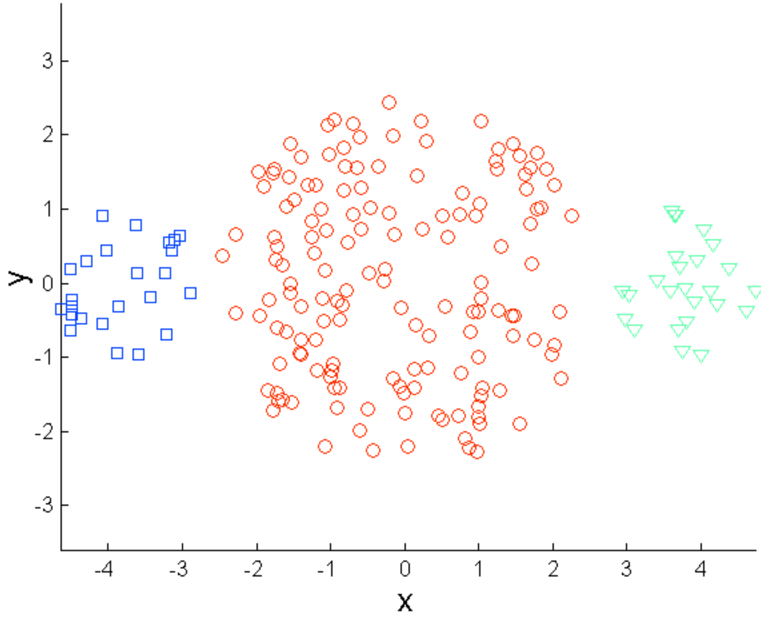
Pre-processing and Post-processing

- **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 error
  - Merge clusters that are ‘close’ and that have relatively low error

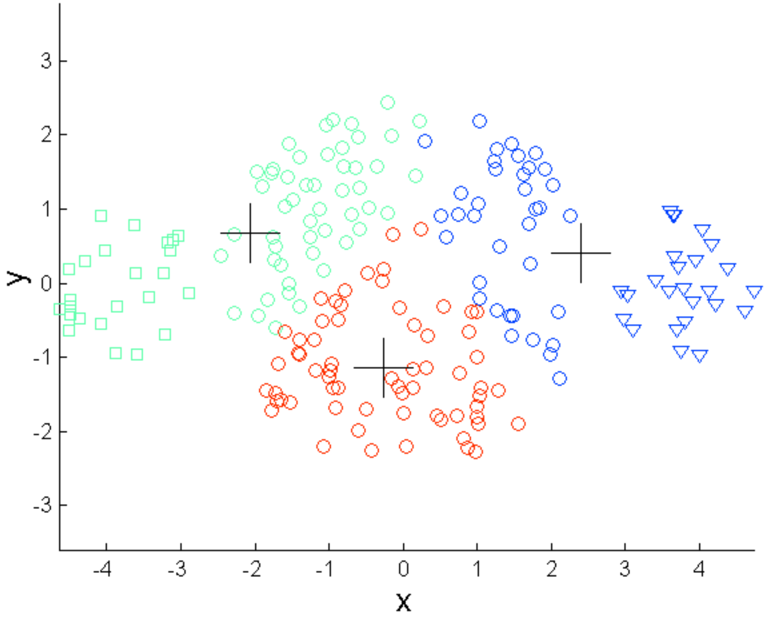
Limitations of K-means

- K-means has problems when clusters are of differing
  - Sizes
  - Densities
  - Irregular shapes

Limitations of K-means: Differing Sizes

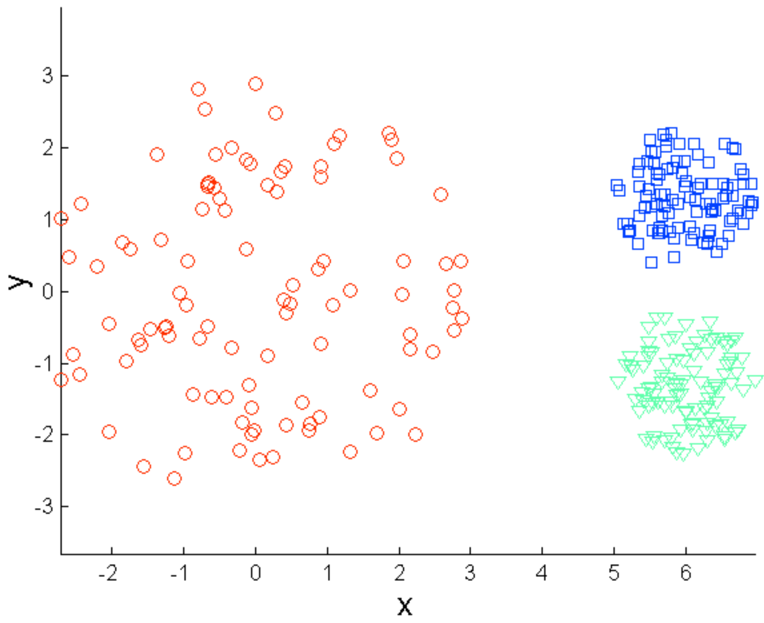


Original Points

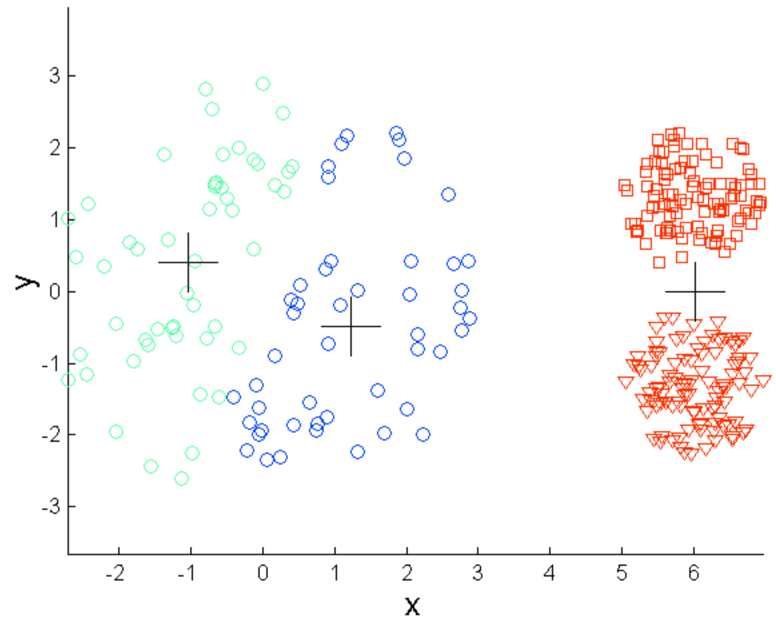


K-means (3 Clusters)

Limitations of K-means: Differing Density

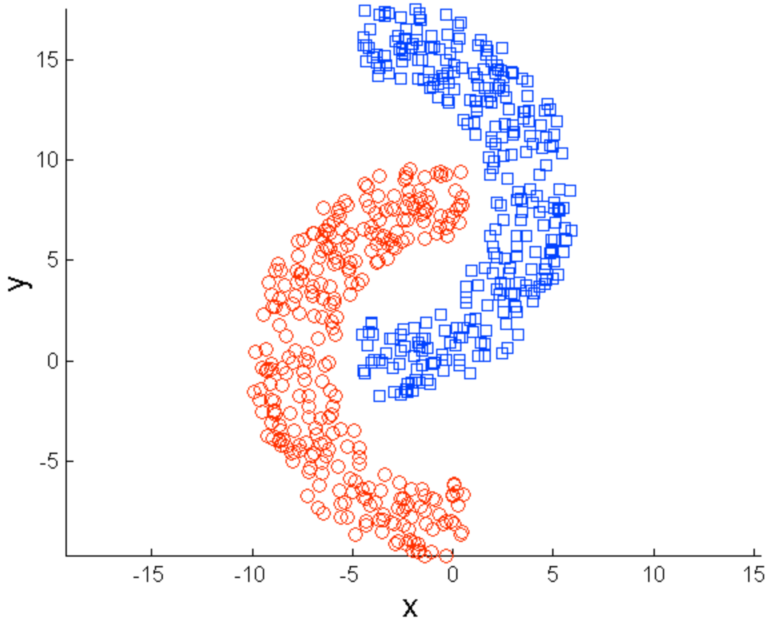


Original Points

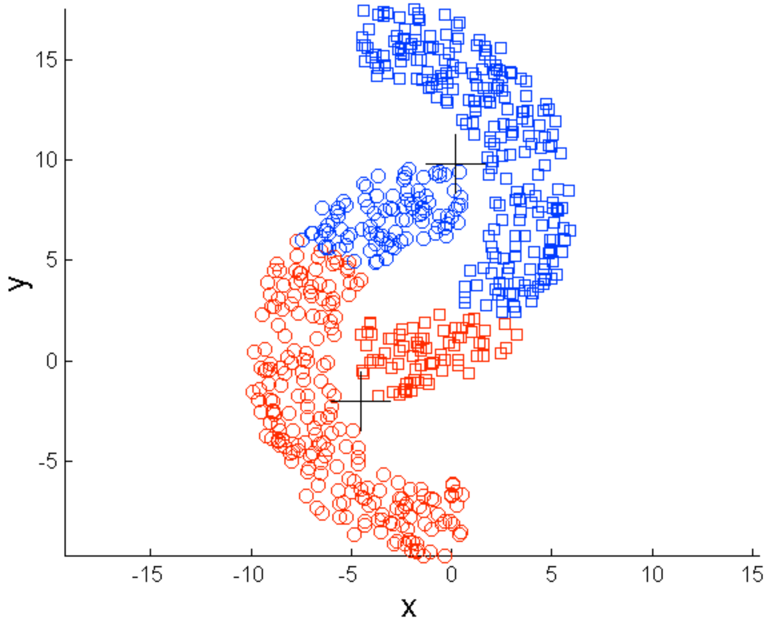


K-means (3 Clusters)

Limitations of K-means: Irregular Shapes



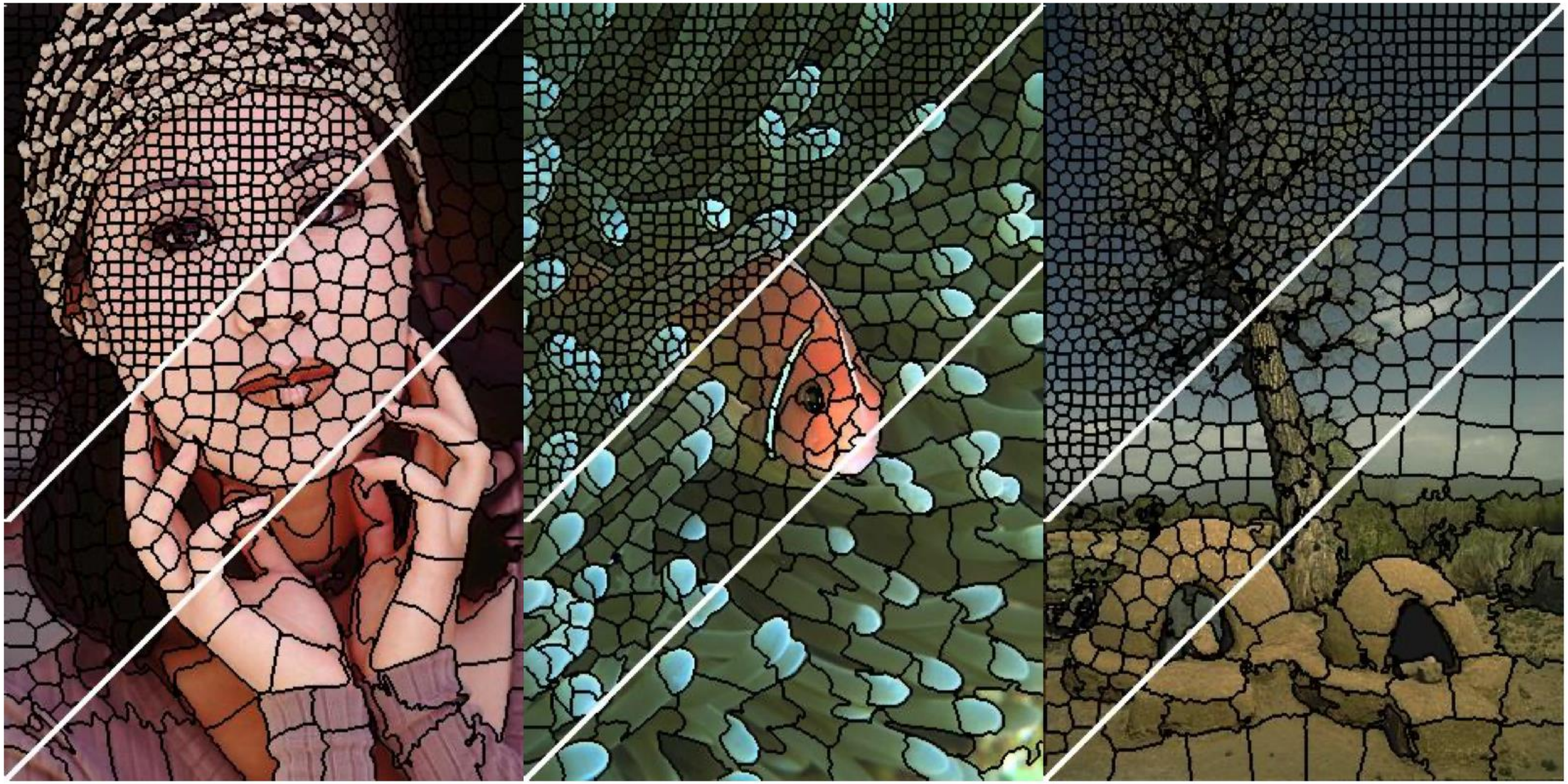
Original Points



K-means (2 Clusters)

K-means for Vector Quantization

K-means for Image Segmentation



- How would you modify k-means to get super pixels?

Questions?