K-means

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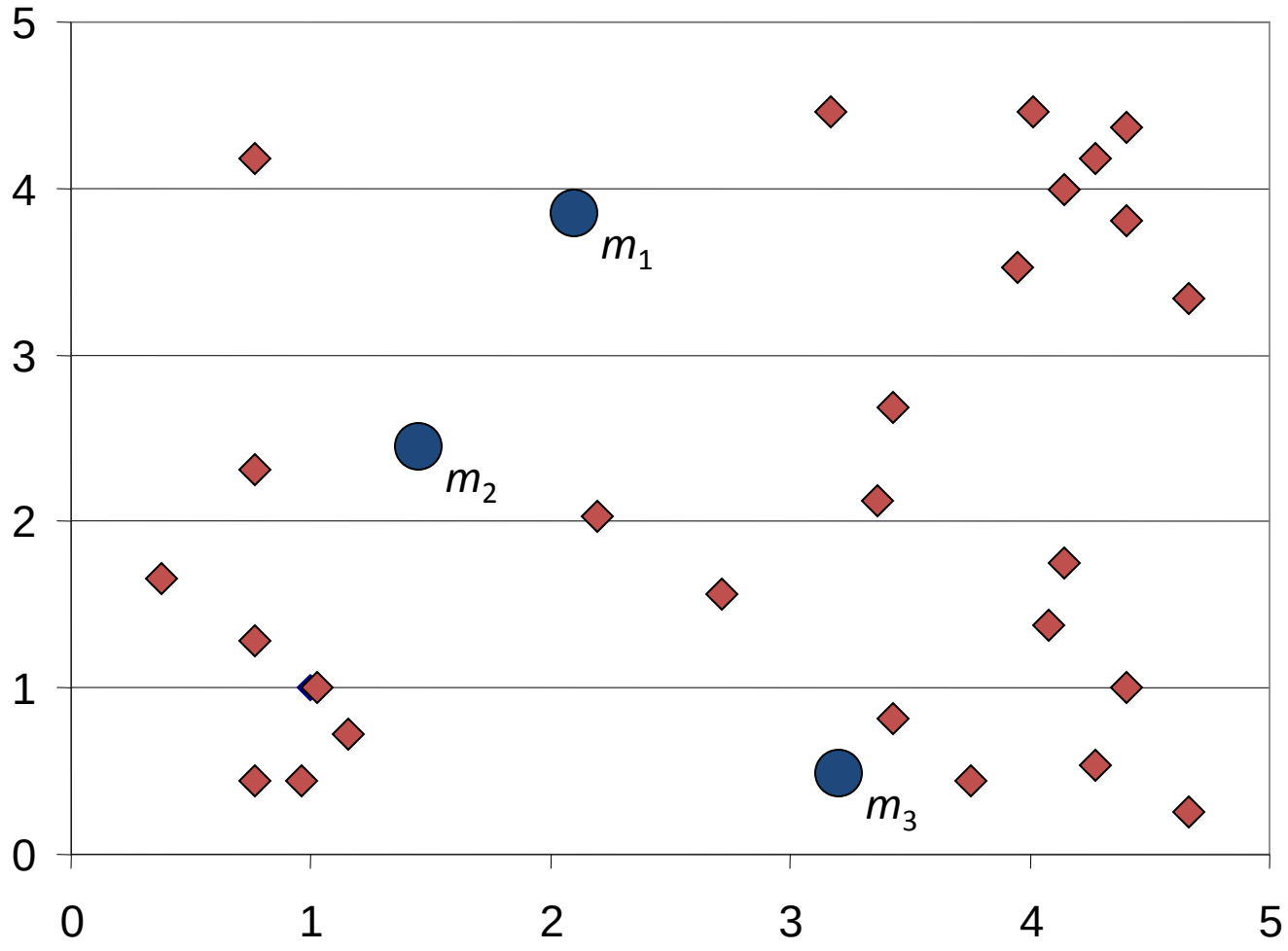
K-means

- **Partition $\{x_1,\ldots,x_n\}$ into K clusters**
  - K is predefined
- **Initialization**
  - Specify the initial cluster centers (centroids)
- **Iteration until no change**
  - For each data x_i
    - Calculate the distances between x_i and the K centroids
    - (Re)assign x_i to the cluster whose centroid is the closest to x_i
  - Update the cluster centroids based on current assignment

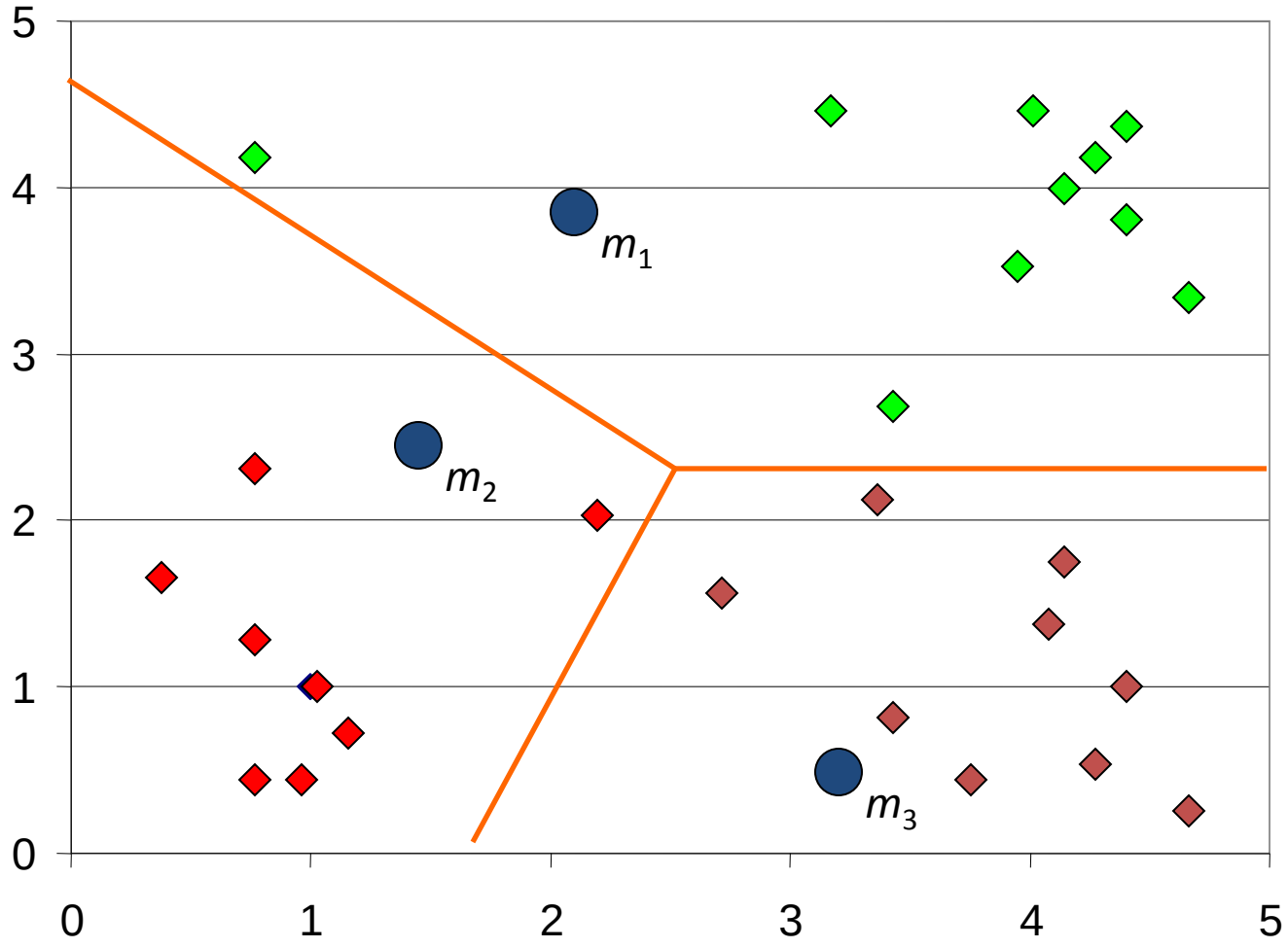
K-means: Initialization

Initialization: Determine the three cluster centers



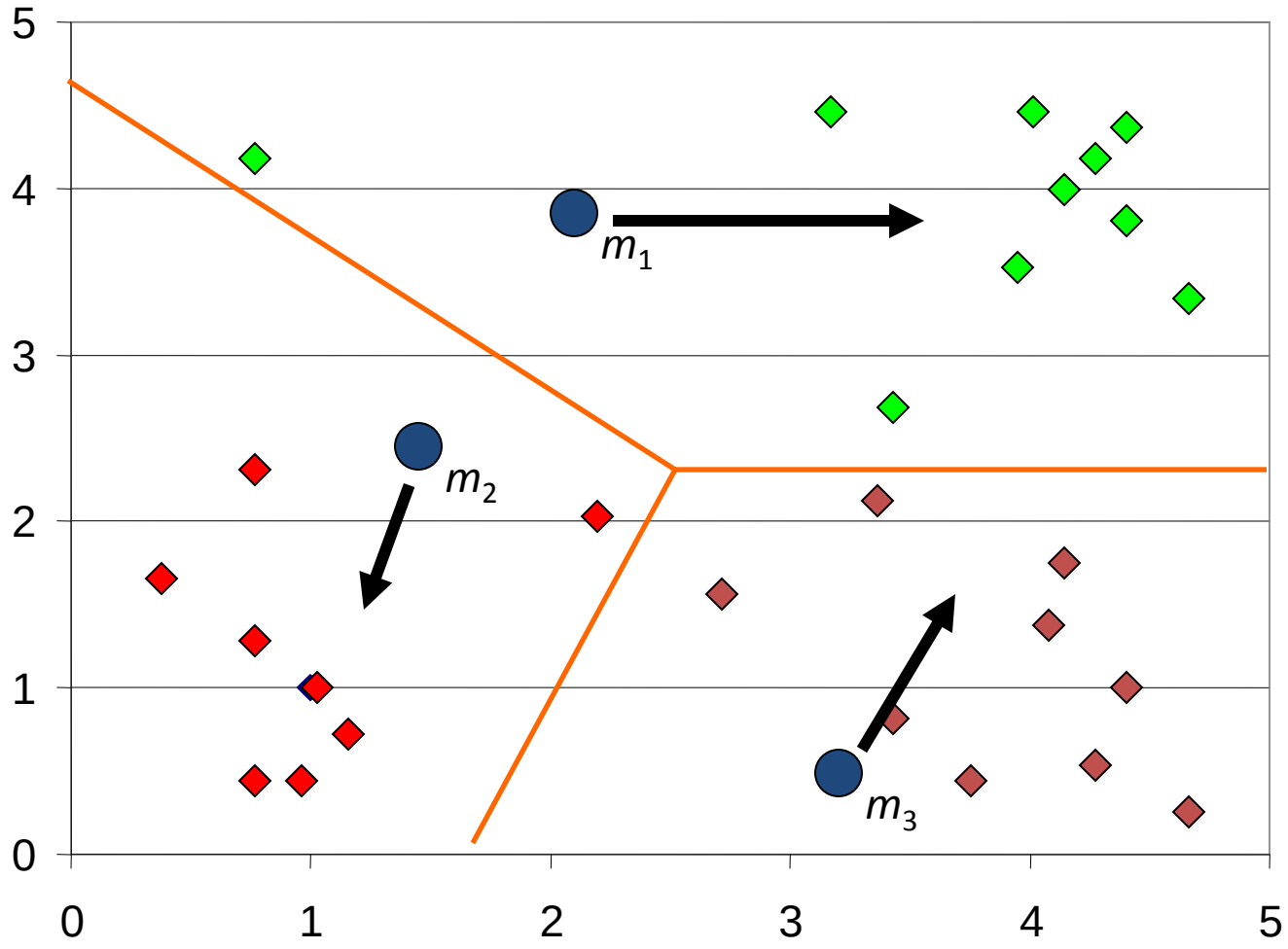
K-means Clustering: Cluster Assignment

Assign each data point to the cluster which has the closet distance from the centroid to the data point



K-means Clustering: Update Cluster Centroid

Compute cluster centroid as the center of the points in the cluster



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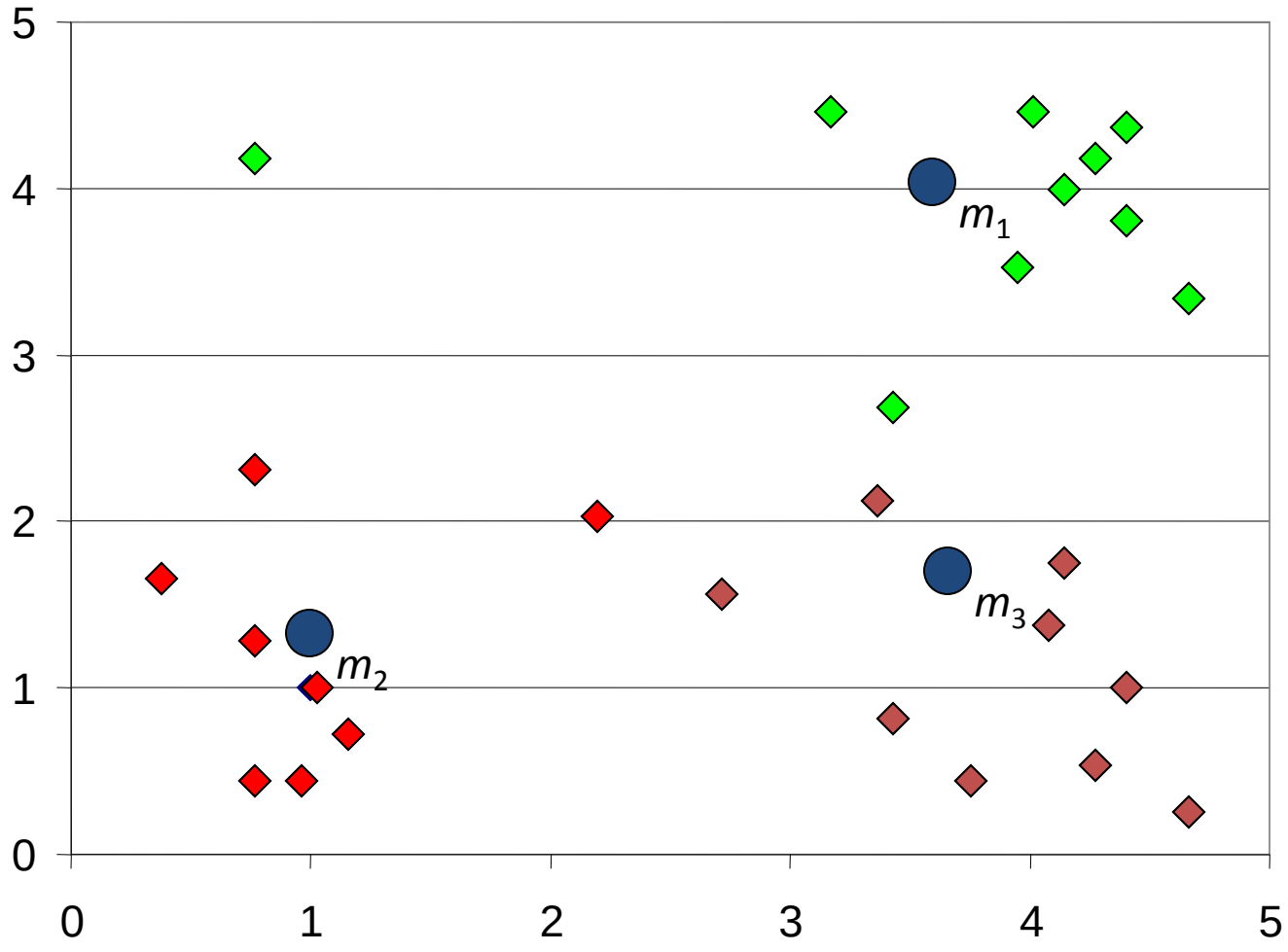

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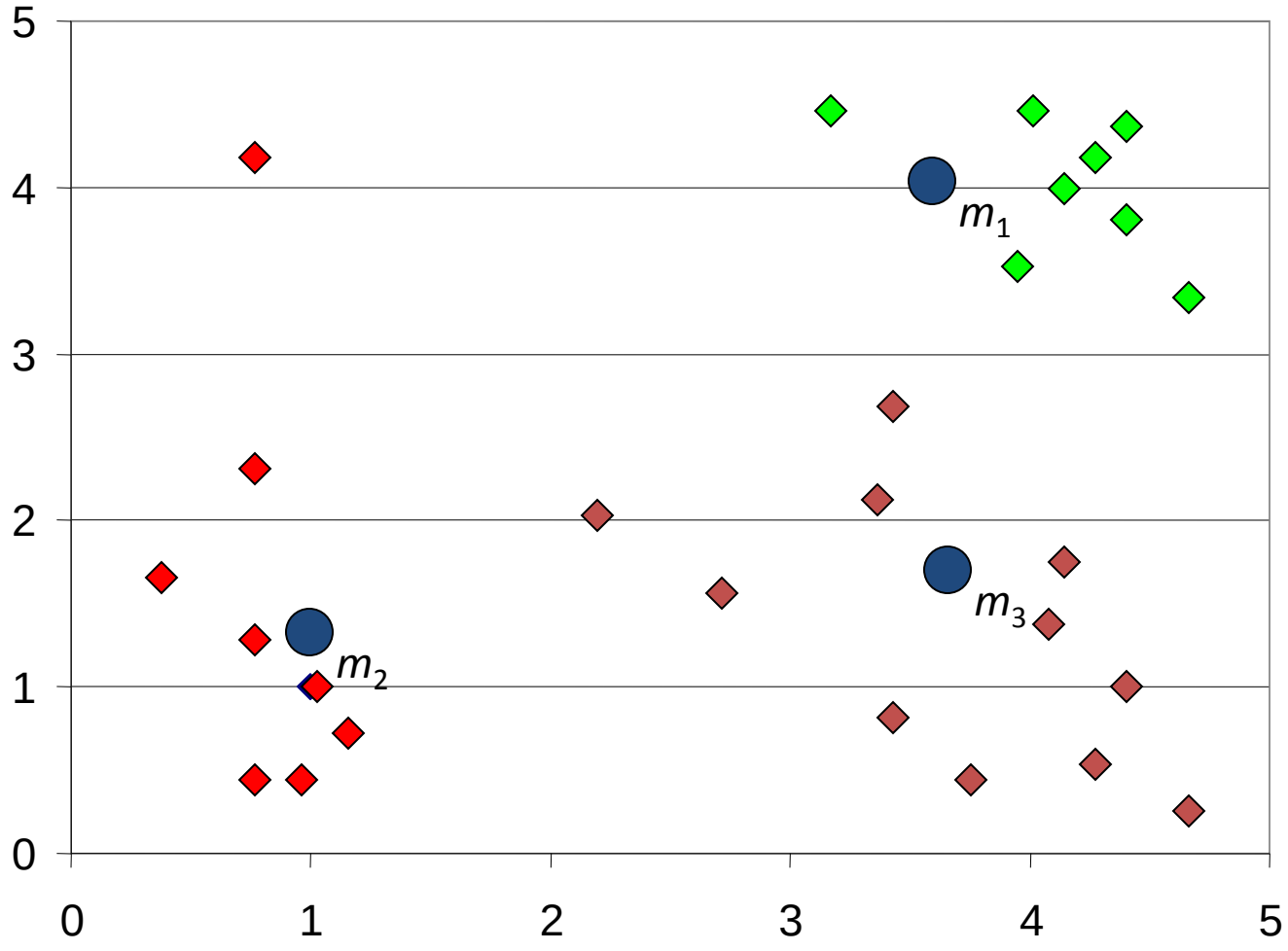

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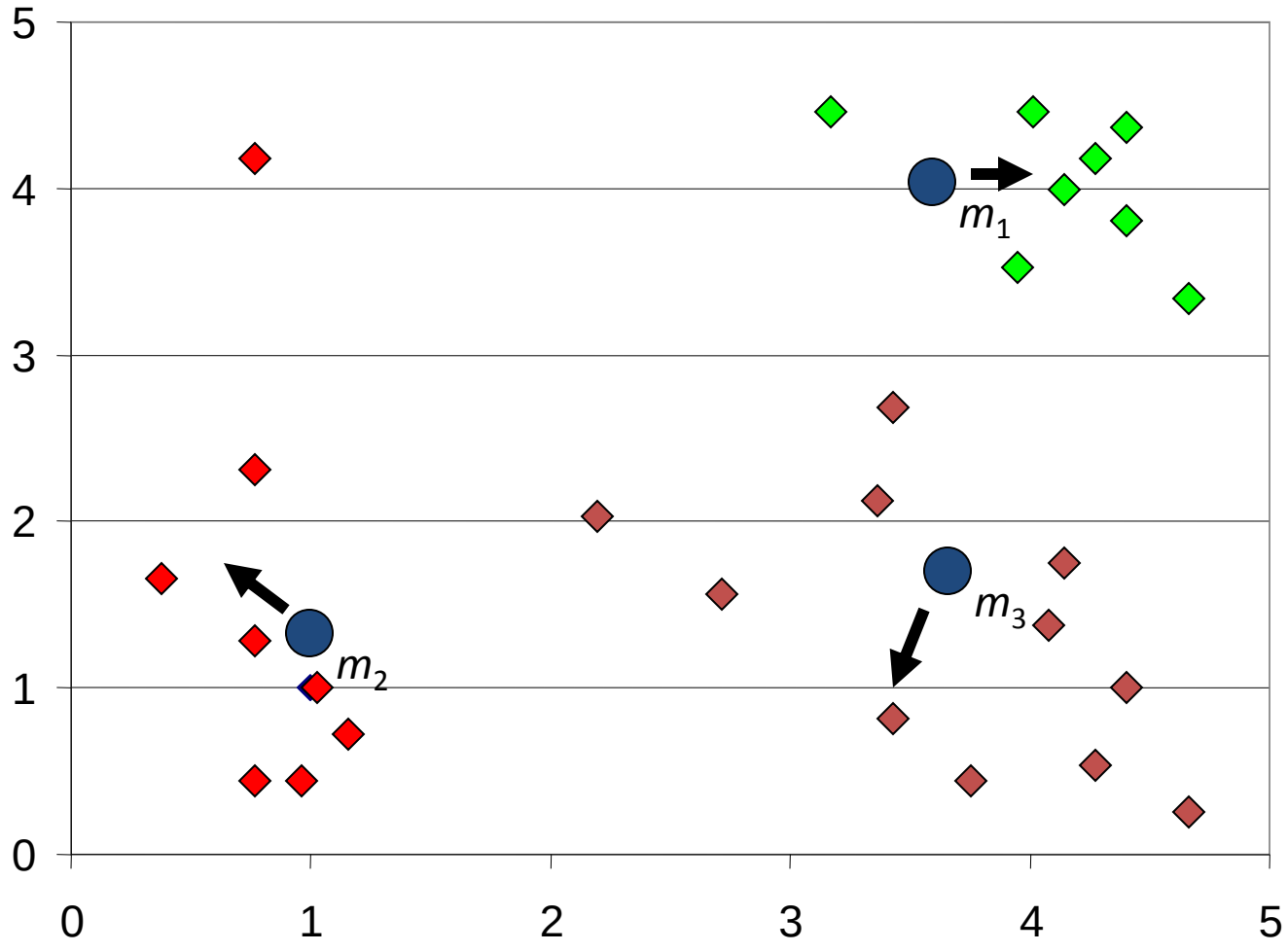

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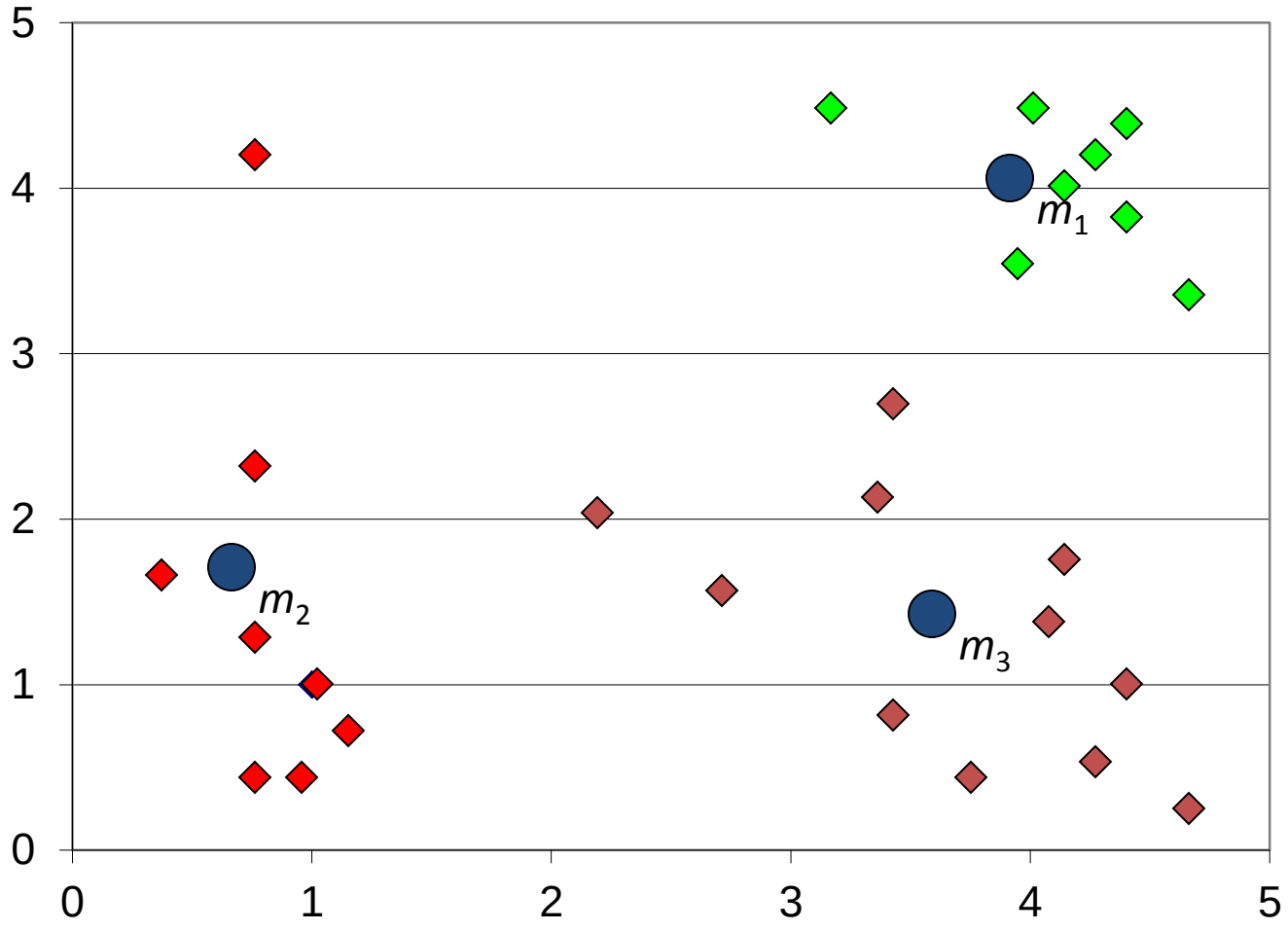
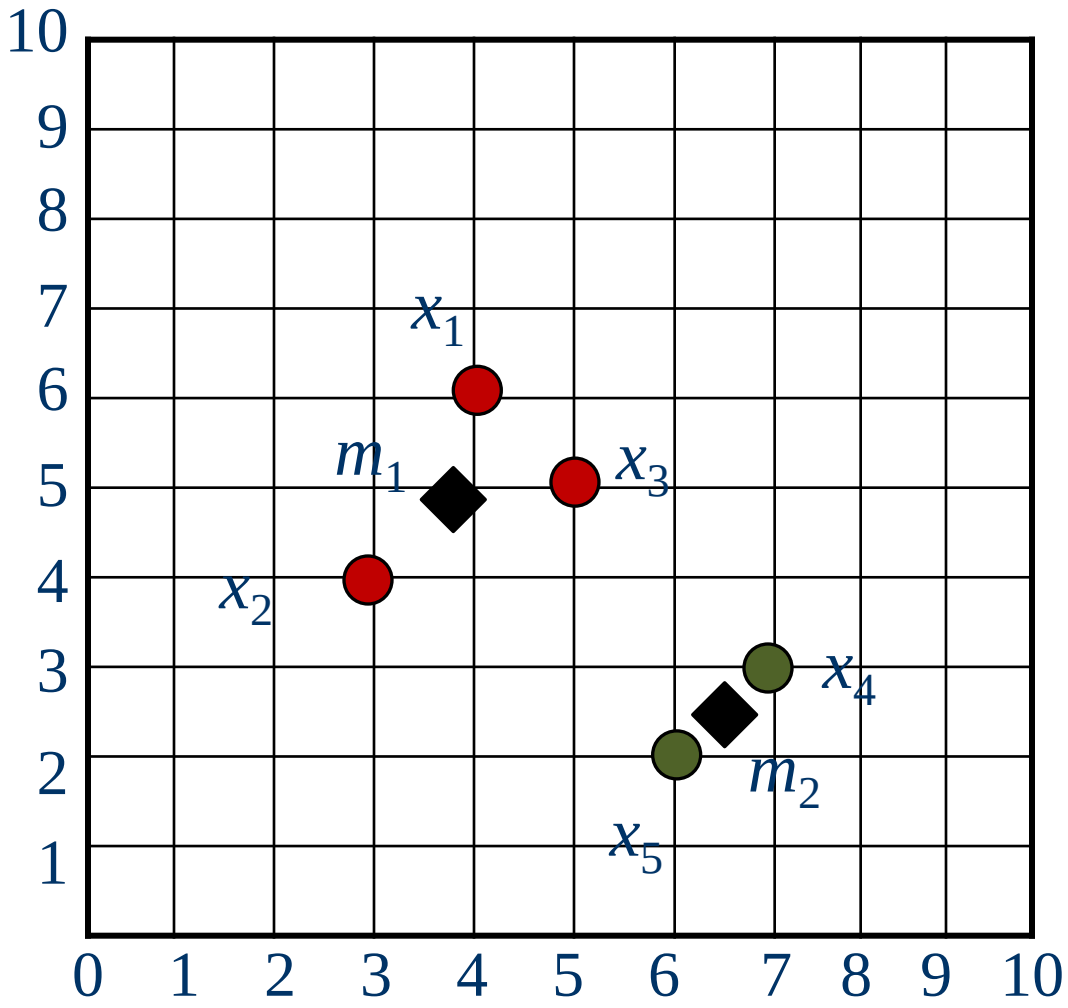


Example—Cluster Centroid Computation



Given the cluster assignment with two initial centers m1 and m2, compute the centers of the two clusters

Comments on the K-Means Method

- **Strength**
  - Efficient
  - Easy to implement
- **Issues**
  - Need to specify *K*, the number of clusters

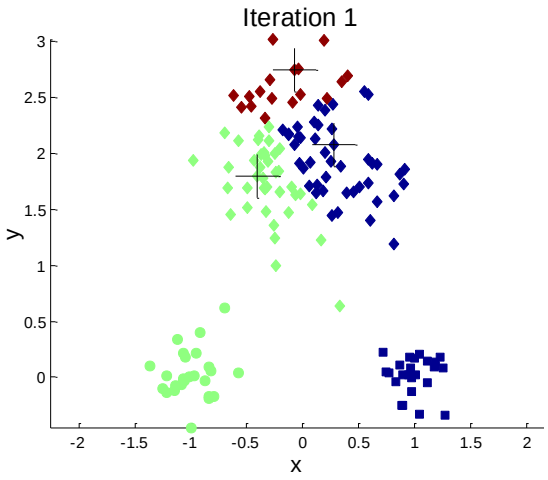
Problems with Selecting Initial Points

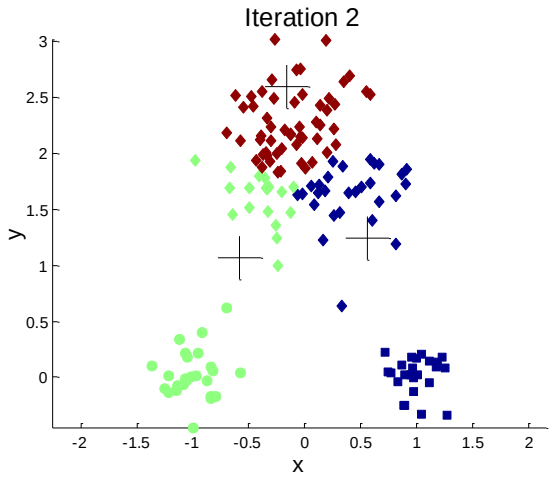
- If there are *K* 'real' clusters then the chance of selecting one centroid from each cluster is small
  - Chance is relatively small when *K* is large
  - If clusters are the same size, *n*, then

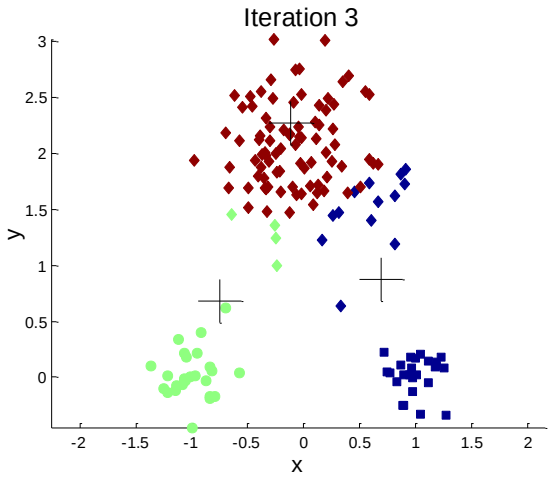
$$P = \frac{\text{number of ways to select one centroid from each cluster}}{\text{number of ways to select } K \text{ centroids}} = \frac{K!n^K}{(Kn)^K} = \frac{K!}{K^K}$$

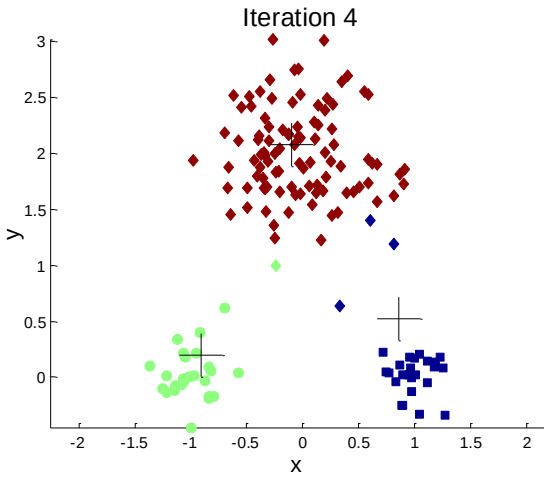
  - For example, if K = 10, then probability = $10!/10^{10}$ = 0.00036
  - Sometimes the initial centroids will readjust themselves in 'right' way, and sometimes they don't

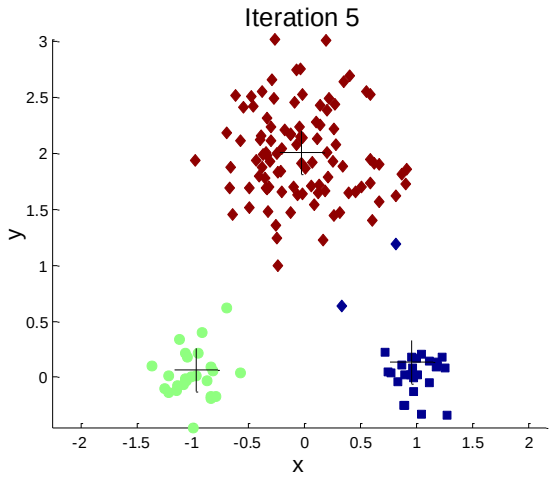
Importance of Choosing Initial Centroids

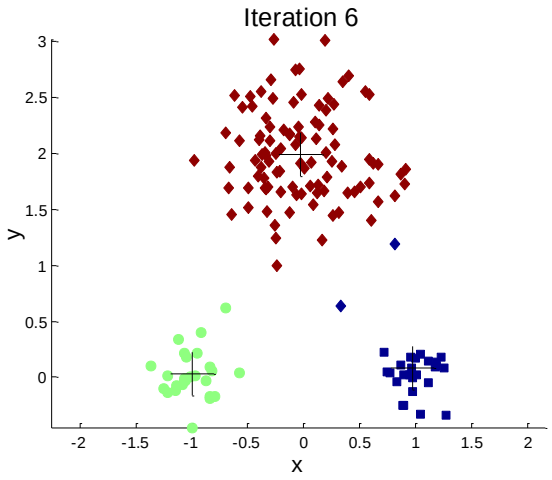












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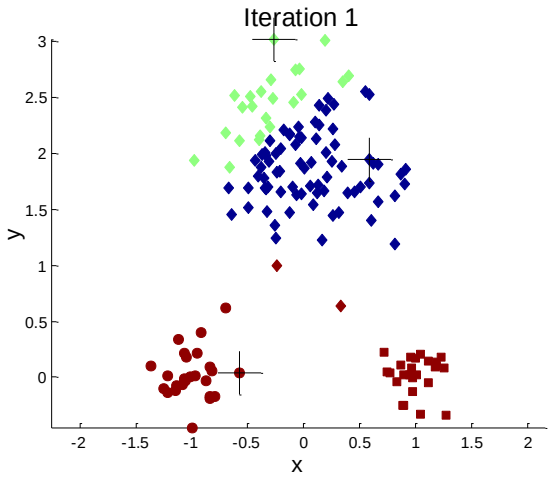

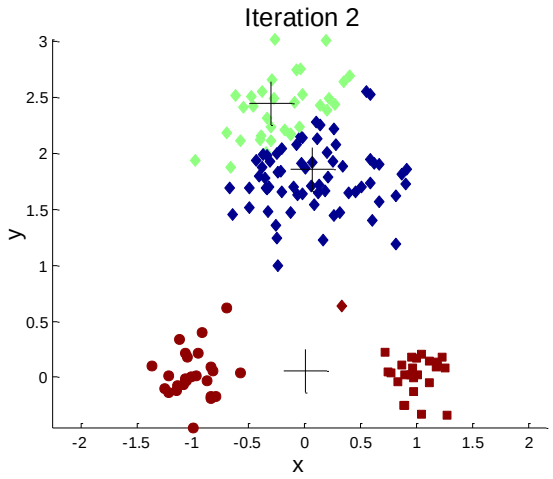

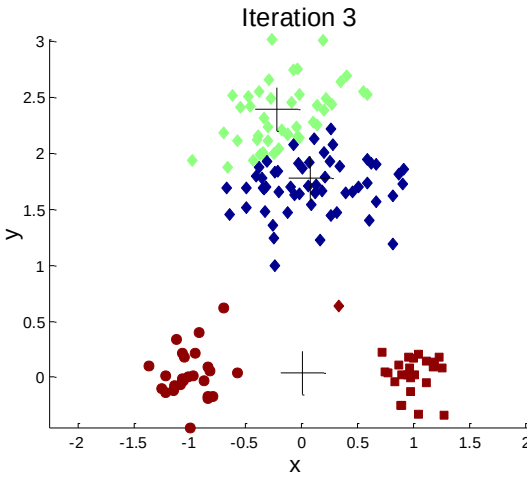

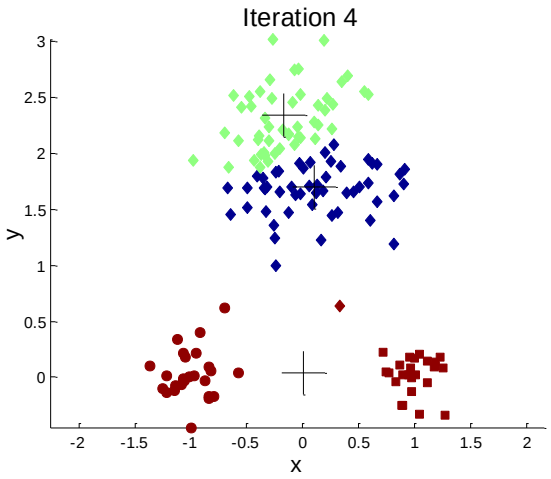

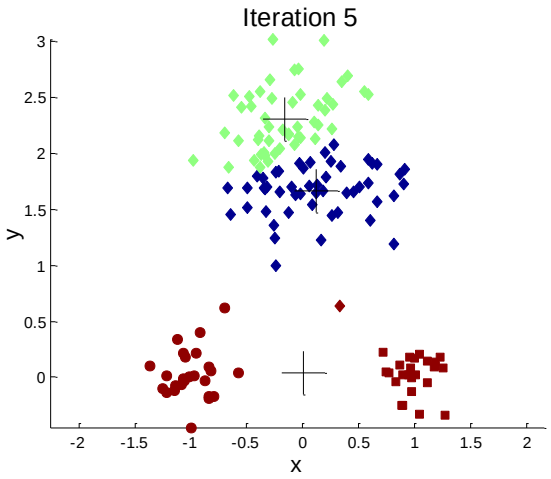

Solutions to Initial Centroids Problem

- Multiple runs
  - Average the results or choose the one that has the smallest sum of the squared errors
- 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—Use K-means' results as other algorithms' initialization
- Bisecting K-means
  - Not as susceptible to initialization issues

Pre-processing and Post-processing

- **Pre-processing**
  - Normalize the data
  - Eliminate outliers
- **Post-processing**
  - Eliminate small clusters that may represent outliers