Clustering Data with the K-means Algorithm

Objectives-

- Introduce the K-means algorithm
- Illustrate K-means with an example
- Identify considerations

Clustering: Organizing data in groups

given $\underline{a}_i \in \mathbb{R}^N$, $i = 1, 2, \cdots, M$, find centroids $\underline{\mu}_j$, $j = 1, \cdots K$ and clusters $S_j = \{ i \mid \underline{a}_i \text{ belongs to cluster } j \}$

Example:

$$\underline{A} = [\underline{a}_1\ \underline{a}_2\ \underline{a}_3\ \underline{a}_4\ \underline{a}_5] = \begin{bmatrix} 1 & 3 & 4 & 2 & 5 \\ 2 & 4 & 5 & 1 & 3 \end{bmatrix}$$

$S_1 = \{2, 3, 5\}$, $\underline{\mu}_1 = \begin{bmatrix} 4 \\ 4 \end{bmatrix}$; $S_2 = \{1, 4\}$, $\underline{\mu}_2 = \begin{bmatrix} 1.5 \\ 1.5 \end{bmatrix}$

Unsupervised learning: data w/o labels, # clusters unknown

Matrix factorization: $\underline{A} \approx \underline{T}\,\underline{W}^T$, $\underline{T} = [\underline{\mu}_1\ \underline{\mu}_2 \cdots \underline{\mu}_K]$

$$\underline{T} = [\underline{\mu}_1\ \underline{\mu}_2], \quad \underline{W}^T = \begin{bmatrix} 0 & 1 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \end{bmatrix}$$

$$[\underline{W}^T]_{\ell m} = \begin{cases} 1, & m \in S_\ell \\ 0, & m \notin S_\ell \end{cases}$$

The K-Means Algorithm (k clusters)

Clusters: $S_j = \{ i \mid \underline{a}_i \in \text{cluster } j \}$, $|S_j| = \#\,\underline{a}_i \text{ in } S_j$

centroids: $\underline{\mu}_j = \frac{1}{|S_j|} \sum_{i \in S_j} \underline{a}_i$ coherence: $c_j = \sum_{i \in S_j} \|\underline{a}_i - \underline{\mu}_j\|_2^2$

Overall coherence $C = \sum_{j=1}^{k} c_j = \sum_{j=1}^{k} \sum_{i \in S_j} \|\underline{a}_i - \underline{\mu}_j\|_2^2 = \|\underline{A} - \underline{T}\,\underline{W}^T\|_F^2$

1) Initialize: choose $\underline{\mu}_j^0$, $j = 1, 2, \ldots, K$ randomly from $\underline{a}_i$; set $\ell = 0$

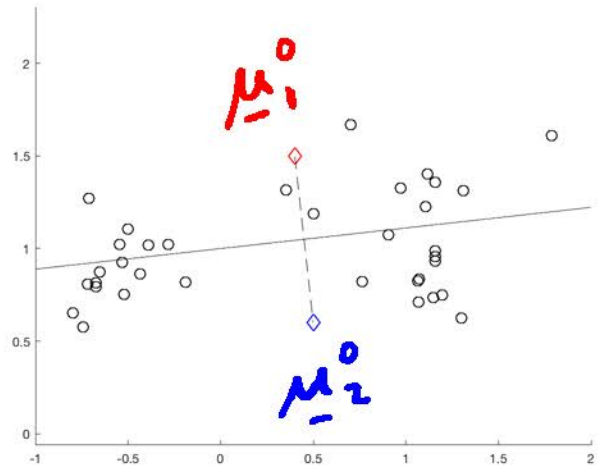
2) Assignment: put $\underline{a}_i \in S_j^\ell$ if $\underline{a}_i$ is closest to $\underline{\mu}_j^\ell$

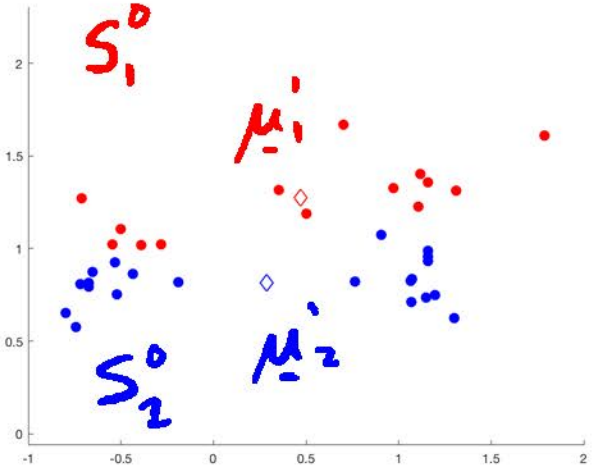
3) Update Centroids: $\underline{\mu}_j^{\ell+1} = \frac{1}{|S_j^\ell|} \sum_{i \in S_j^\ell} \underline{a}_i$

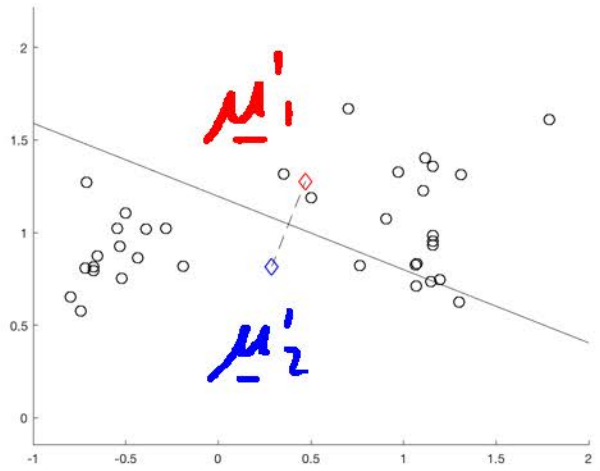
4) If converged $\longrightarrow$ stop

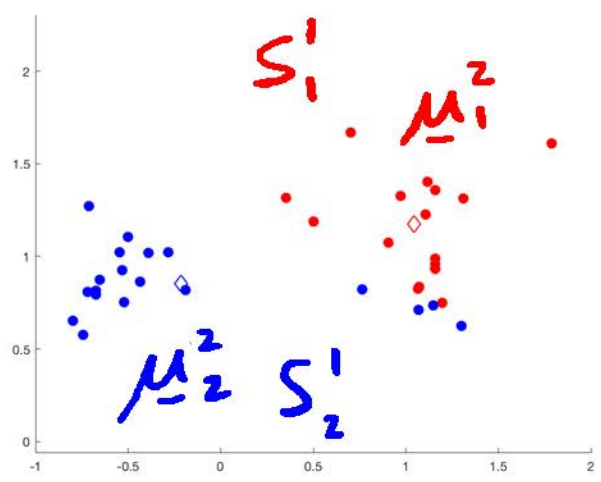
else $\longrightarrow$ $\ell = \ell + 1$, go to 2)

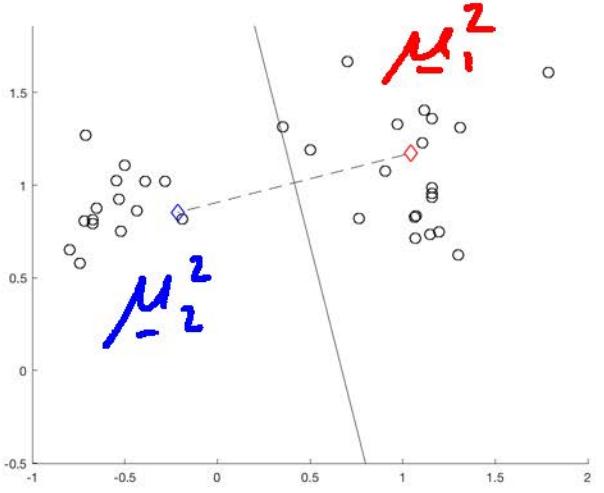
K-Means Algorithm Example

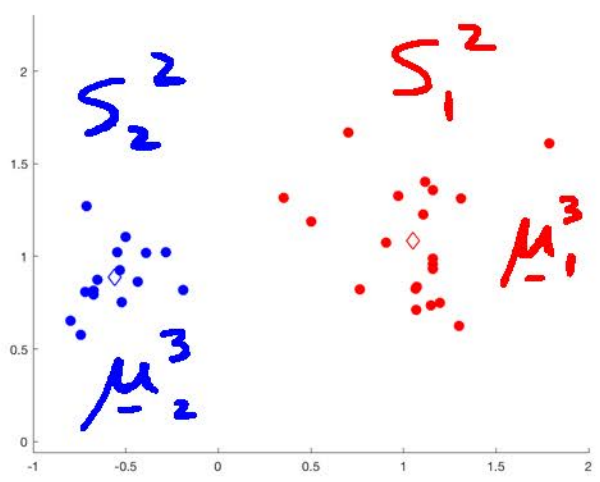












K-Means Algorithm Options

- Initialization: many variations
- Termination: change in clusters or overall coherence or fix iterations
- Use different norms to assign clusters

Challenges

- Convergence to local minima
  repeat for multiple initializations
- Unknown K
  try multiple values