K-means & *K*-medoids

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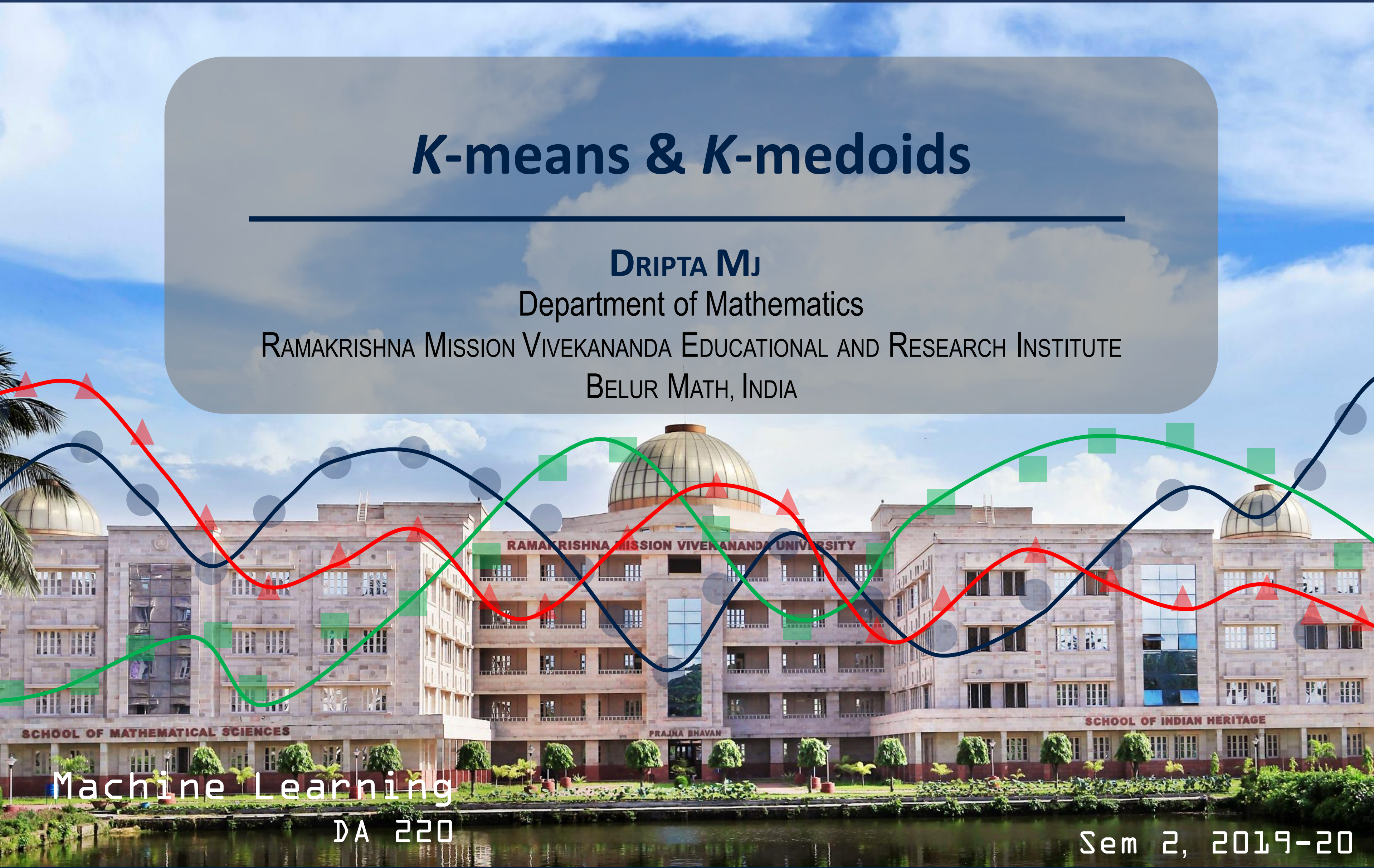
RAMAKRISHNA MISSION VIVEKANANDA UNIVERSITY
SCHOOL OF MATHEMATICAL SCIENCES
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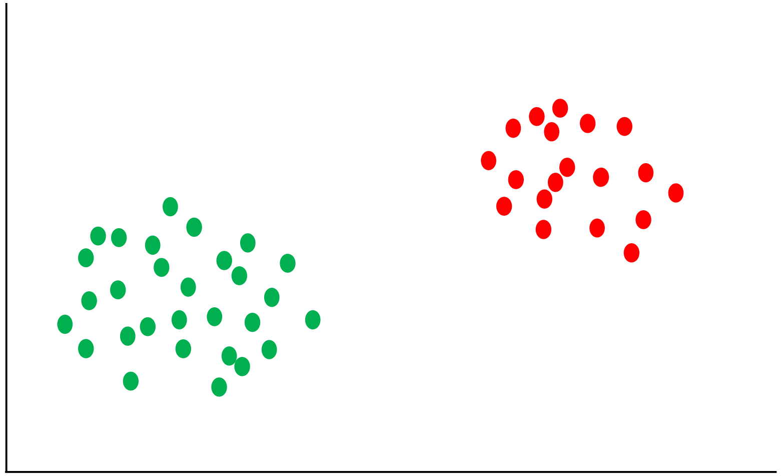
Machine Learning
DA 220

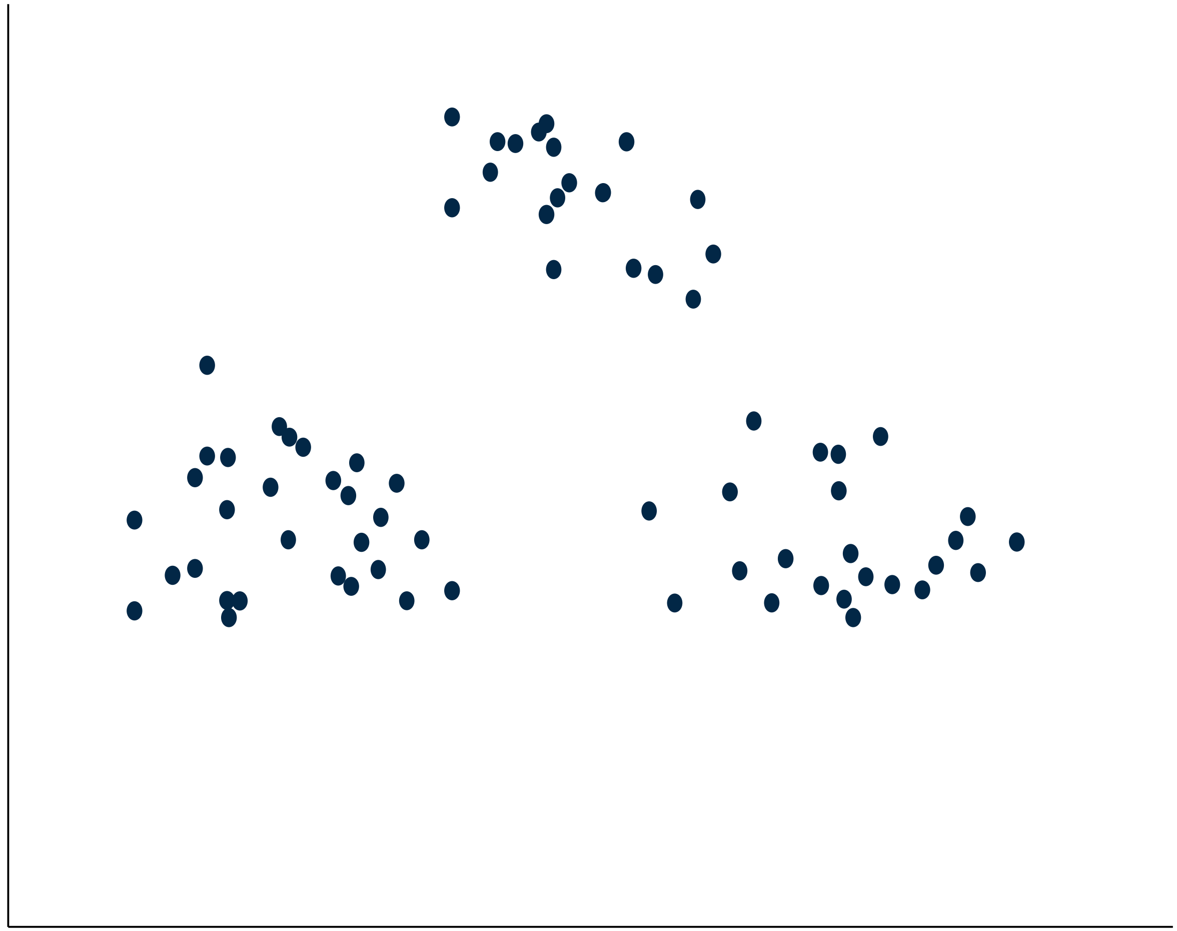
Sem 2, 2019-20

Clustering

- Unsupervised learning: Learn structures in the data as defined by the model.
- Unlabelled data is organized into groups called clusters.
- A cluster contains data items which are "similar". These data items are dissimilar to data items in other clusters.



Unlabelled data



Notations

- Training dataset comprise N data points:

$$\mathbf{X} = \{\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, ..., \mathbf{x}^{(N)}\}$$

- Partition data into K clusters:

$$\left\{\mathcal{C}_1, \mathcal{C}_2, ..., \mathcal{C}_K\right\}$$

- Cluster prediction for the nth data point:
  - Label encoding: $z^{(n)} \in \{1, 2, ..., K\}$.
  - One-hot encoding: $\mathbf{z}^{(n)}$ is a K-dimensional vector with

$$\mathbf{z}_k^{(n)} = \begin{cases} 1 & \text{if } \mathbf{x}^{(n)} \text{ is assigned } \mathcal{C}_k \\ 0 & \text{otherwise} \end{cases}$$

Procedure

- Step 1: Initialize (randomly) the centroids (means) of the K clusters:

$$\{\mu_1, \mu_2, ..., \mu_K\}.$$

- Step 2: For $n = 1, 2, ..., N$:
  - Compute the distance of the nth data point to all the K centroids, and assign $\mathbf{x}^{(n)}$ to the cluster to which it is the closest:

$$z^{(n)} = \arg\min_k ||\mathbf{x}^{(n)} - \mu_k||^2$$

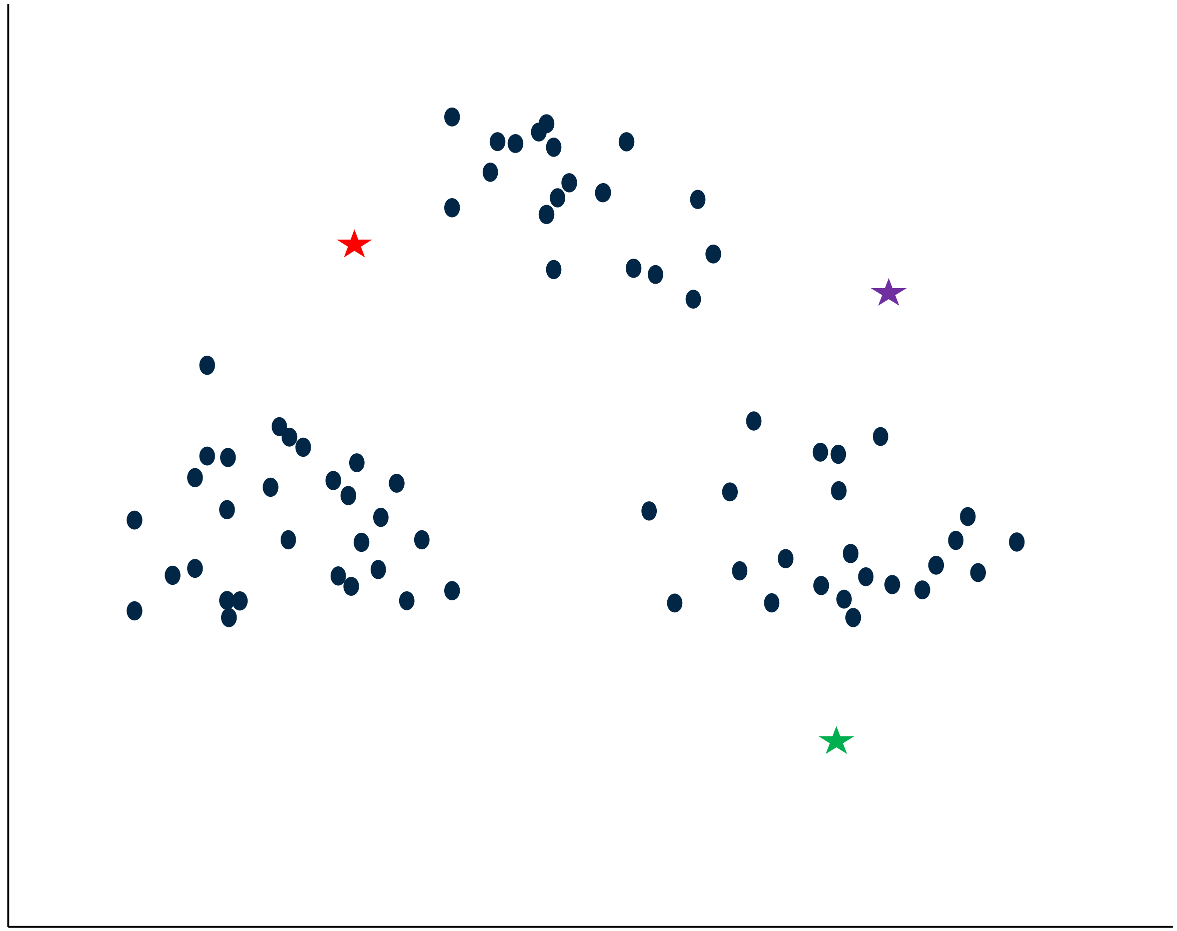
- Step 3: Recompute the cluster centroids with the most recently assigned memberships:

$$\mu_k = \frac{1}{n_k} \sum_{j:\mathrm{x}^{(j)} \in \mathcal{C}_k} \mathbf{x}^{(j)}$$

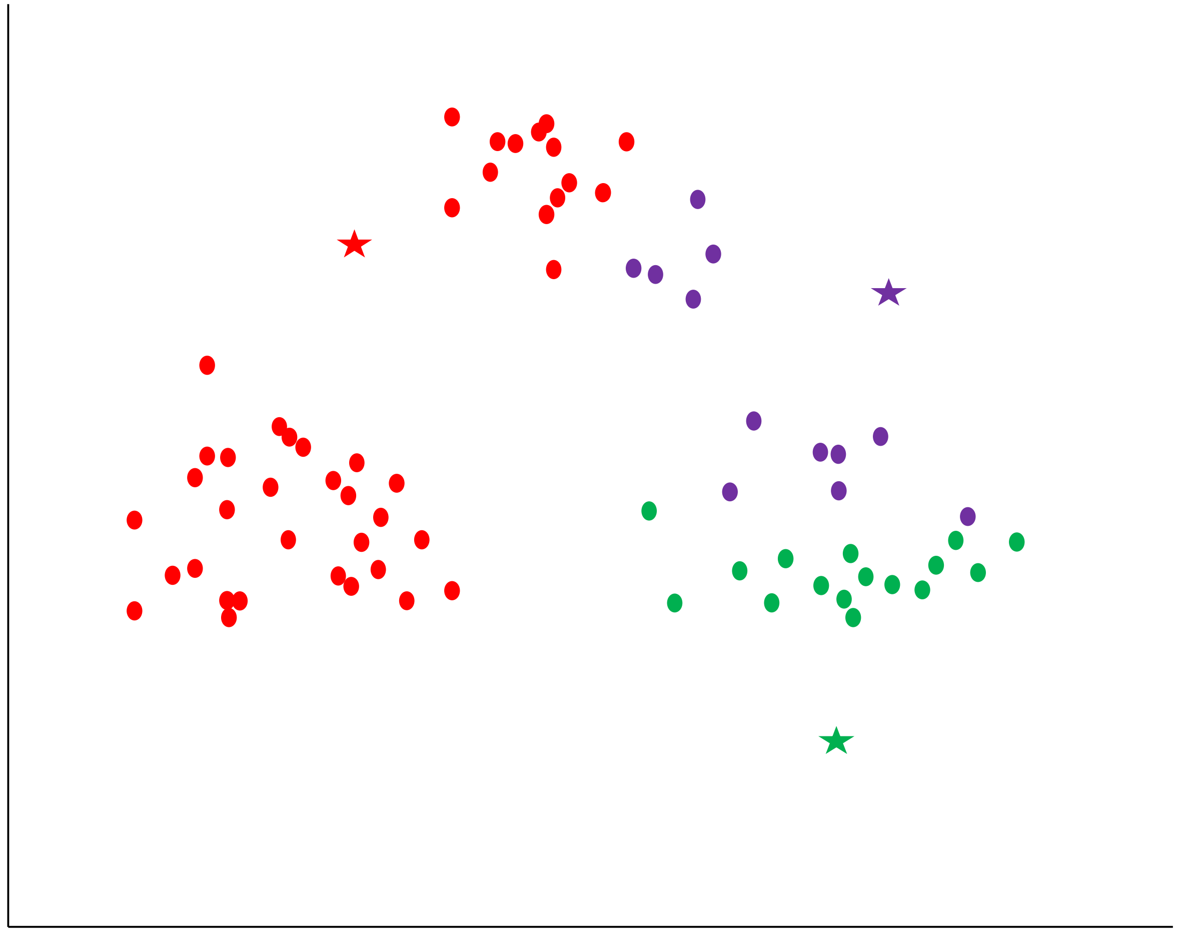
  where n_k is the number of points in cluster $\mathcal{C}_k$.

- If none of the cluster assignments have changed, STOP. Else, REPEAT from Step 2.

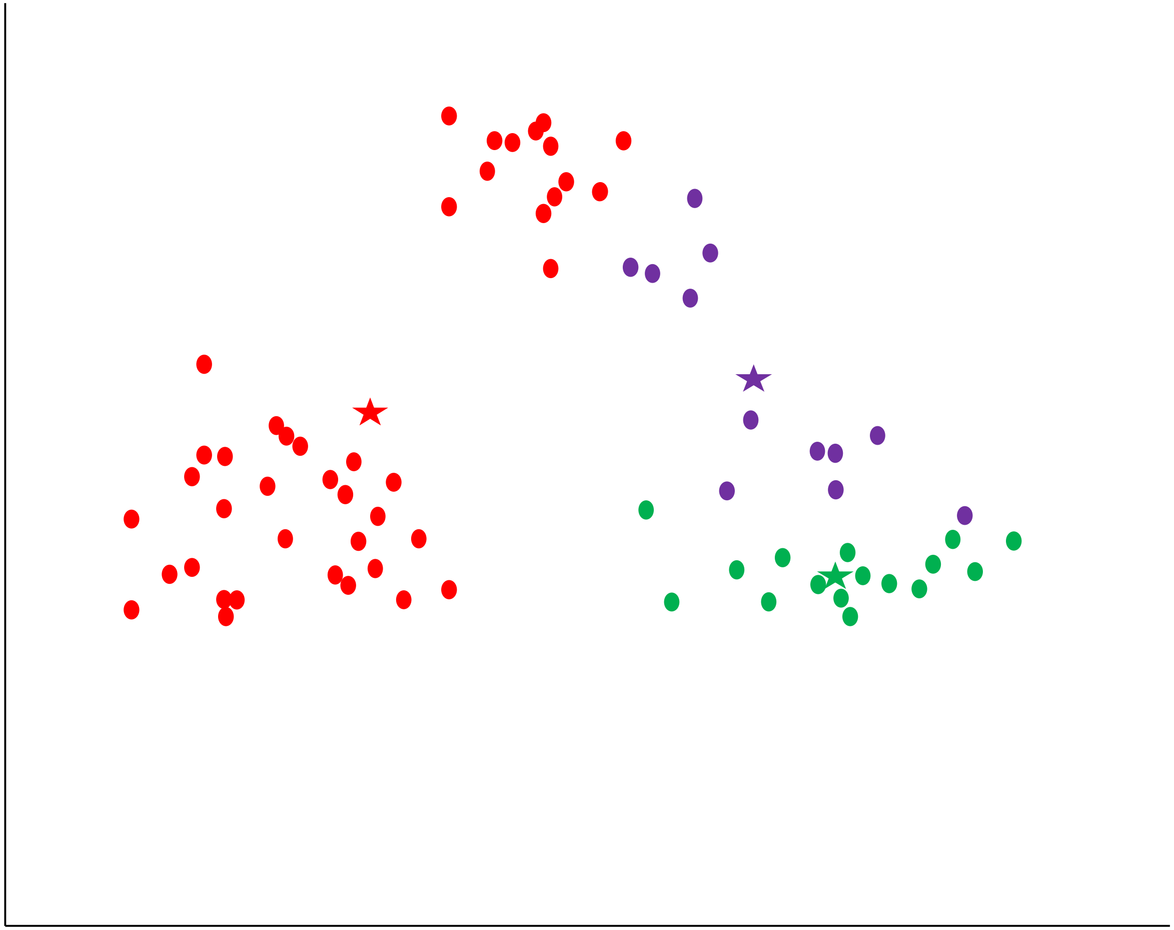
K-means



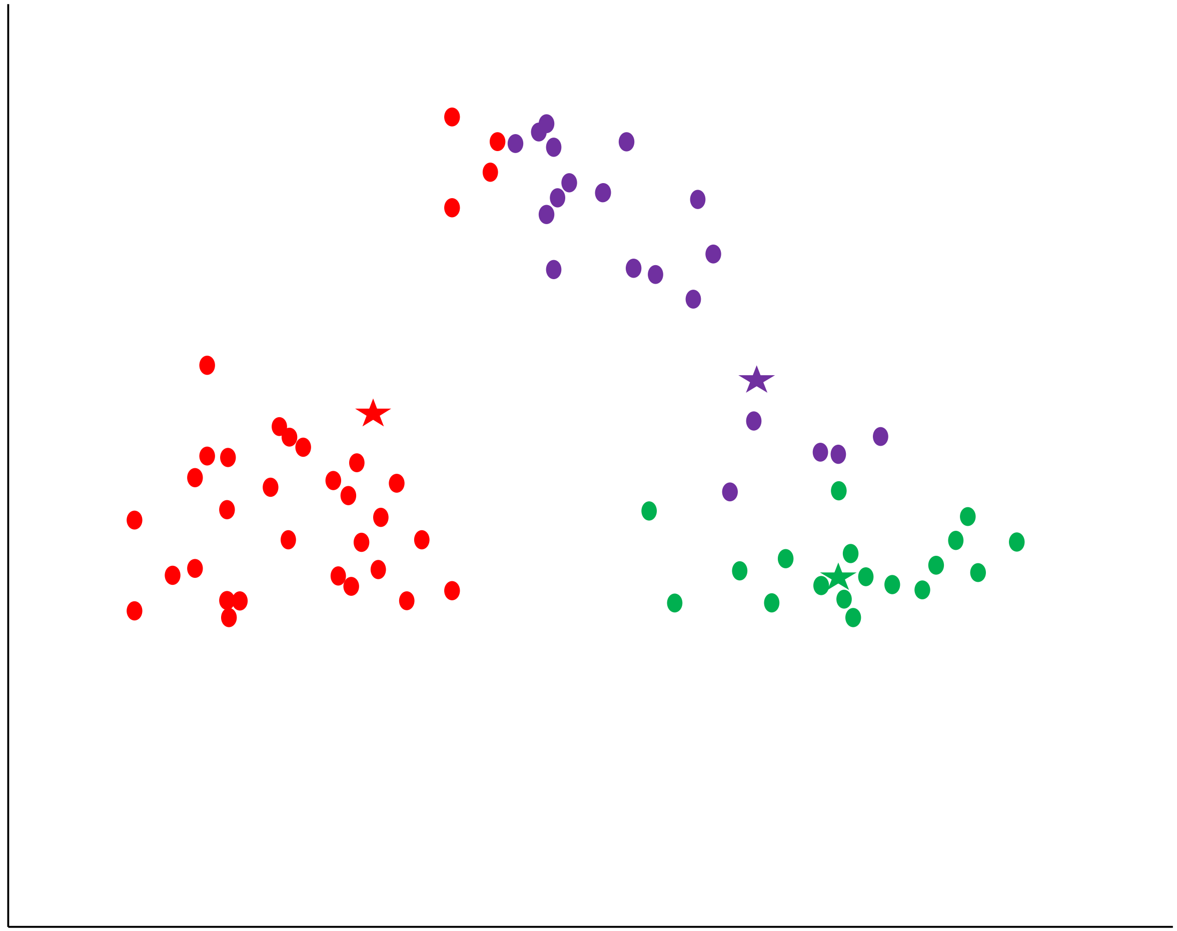
K-means



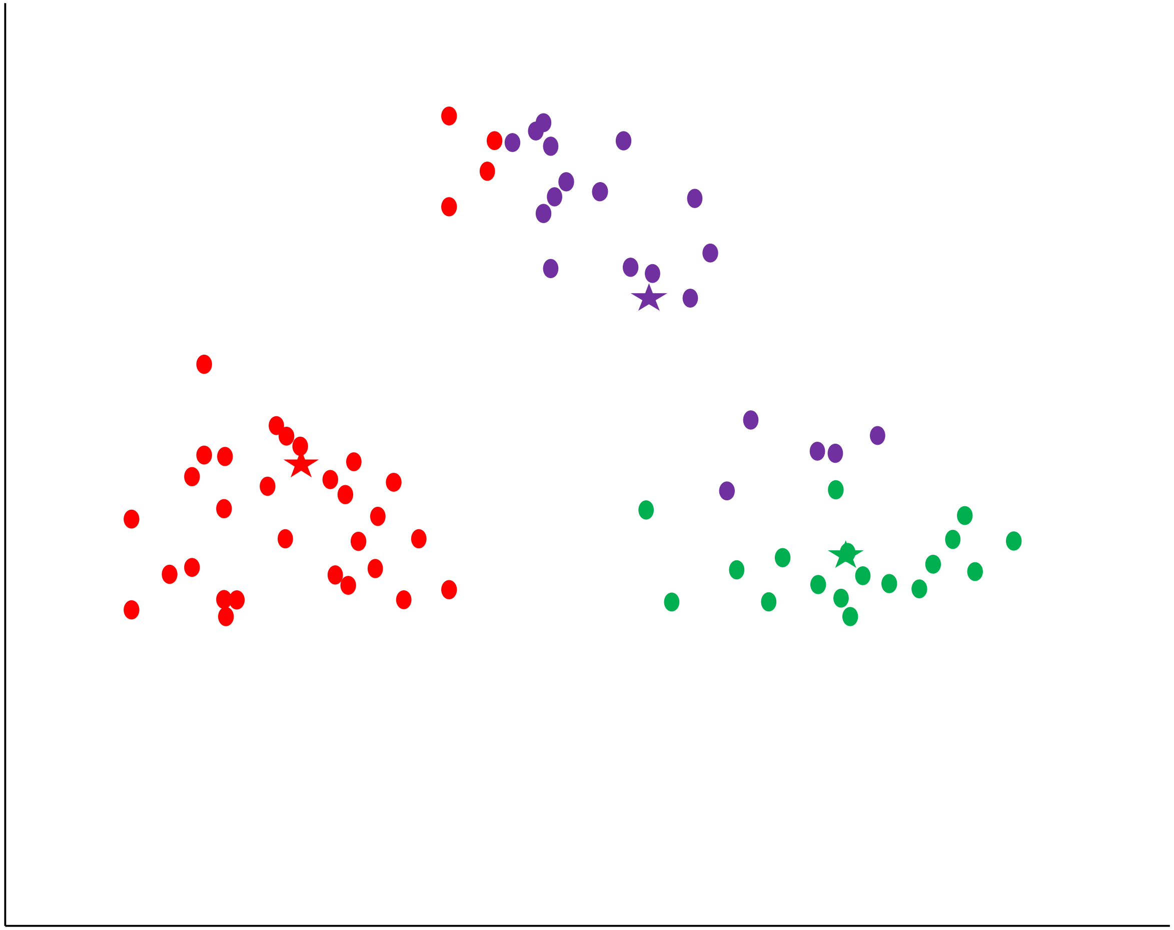
K-means



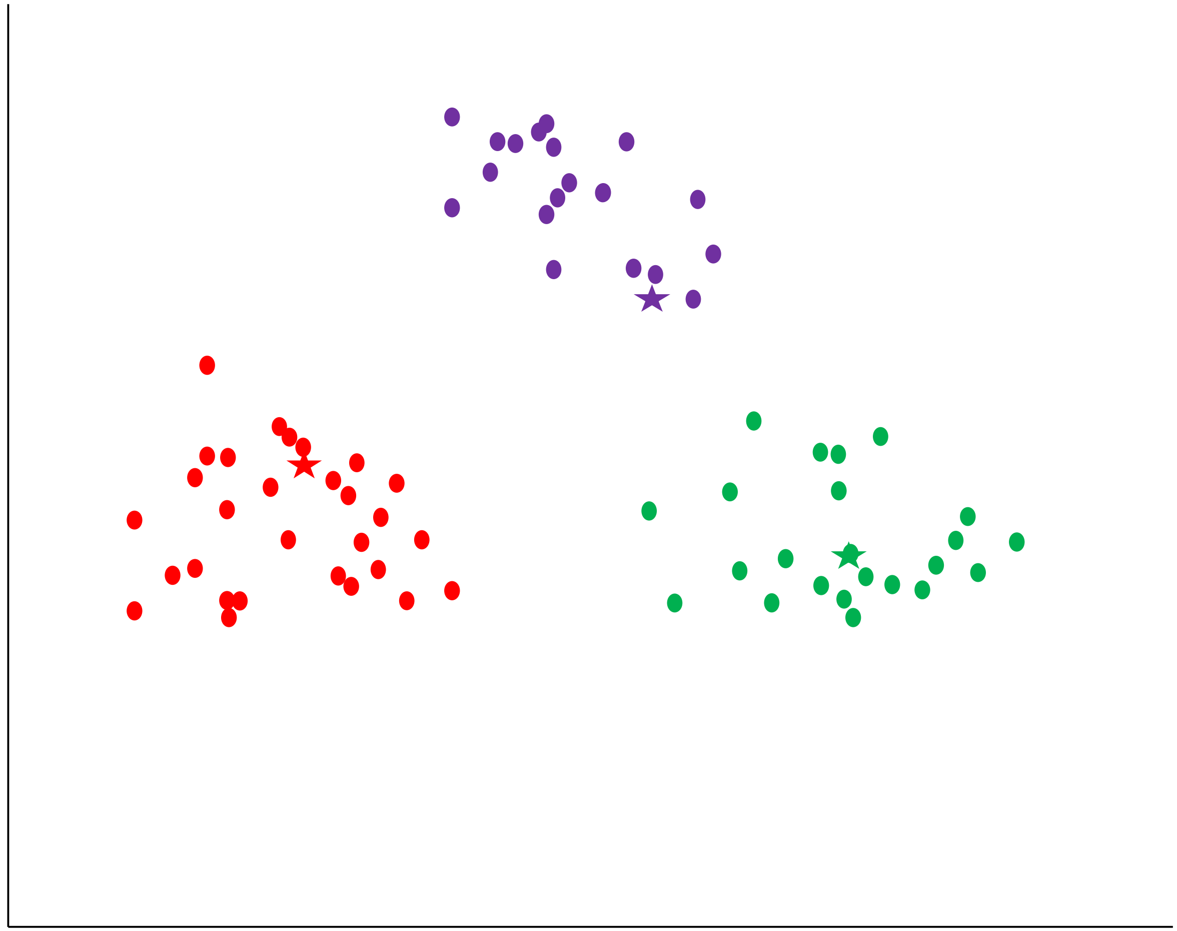
K-means



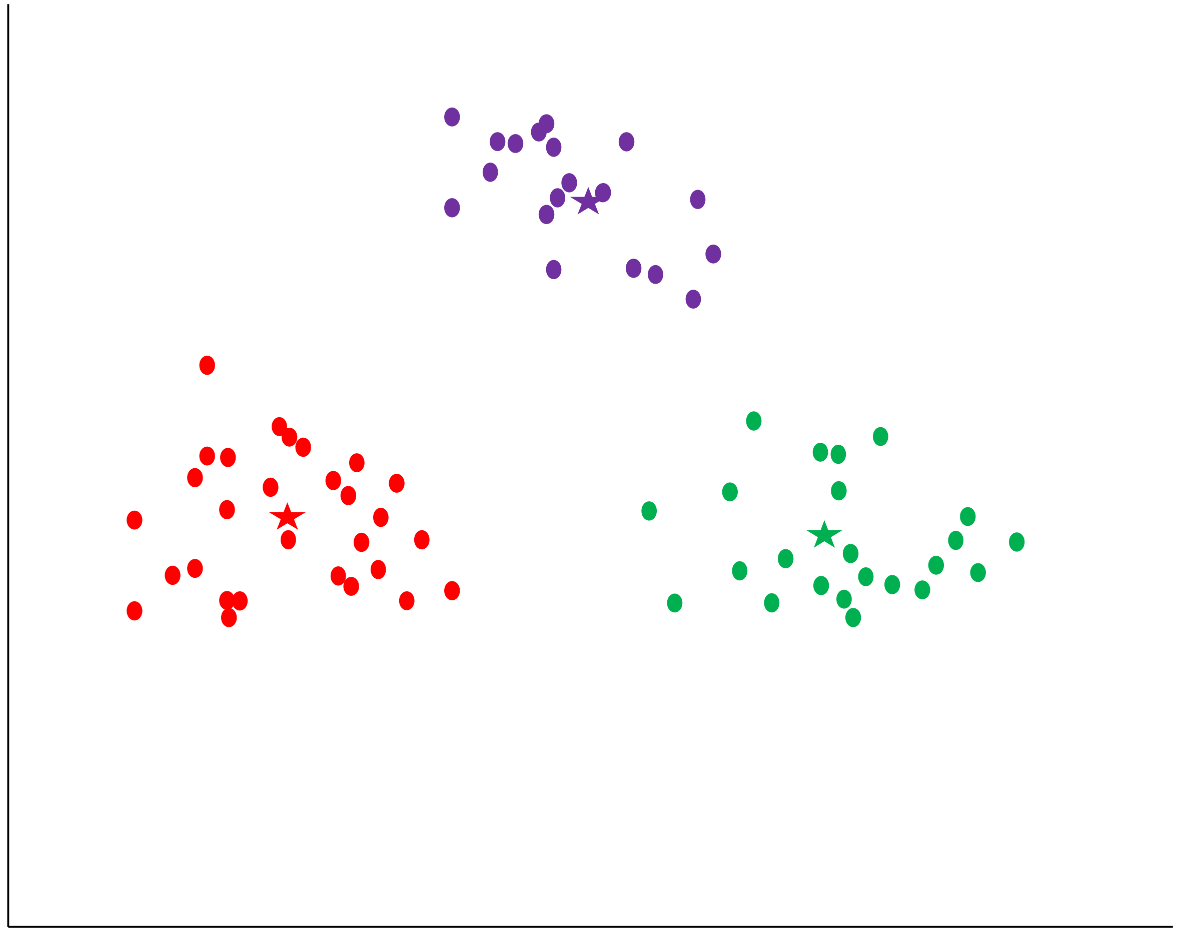
K-means



K-means



K-means



Matrix notation

- Inputs:

$$\mathbf{X} = \begin{bmatrix} \left(\mathbf{x}^{(1)}\right)^{\mathrm{T}} \\ \left(\mathbf{x}^{(2)}\right)^{\mathrm{T}} \\ . \\ . \\ \left(\mathbf{x}^{(N)}\right)^{\mathrm{T}} \end{bmatrix} = \begin{bmatrix} x_1^{(1)} & x_2^{(1)} & . & . & x_D^{(1)} \\ x_1^{(2)} & x_2^{(2)} & . & . & x_D^{(2)} \\ . & . & . & . & . \\ . & . & . & . & . \\ x_1^{(N)} & . & . & . & x_D^{(N)} \end{bmatrix}$$

- Cluster assignments:

$$\mathbf{Z} = \begin{bmatrix} \left(\mathbf{z}^{(1)}\right)^{\mathrm{T}} \\ \left(\mathbf{z}^{(2)}\right)^{\mathrm{T}} \\ . \\ . \\ \left(\mathbf{z}^{(N)}\right)^{\mathrm{T}} \end{bmatrix} = \begin{bmatrix} z_1^{(1)} & z_2^{(1)} & . & . & z_K^{(1)} \\ z_1^{(2)} & z_2^{(2)} & . & . & z_K^{(2)} \\ . & . & . & . & . \\ . & . & . & . & . \\ z_1^{(N)} & . & . & . & z_K^{(N)} \end{bmatrix}$$

Mathematics

- Loss function:

$$L(\mathbf{X}, \mathbf{Z}, \boldsymbol{\mu}) = \sum_{n=1}^{N} \sum_{k=1}^{K} z_k^{(n)} ||\mathbf{x}^{(n)} - \mu_k||^2$$

$$= ||\mathbf{X} - \mathbf{Z}\boldsymbol{\mu}||_F^2$$

- Minimize the loss function $L(\mathbf{X}, \mathbf{Z}, \boldsymbol{\mu})$.
  - Two sets of unknown variables – $\mathbf{Z}$ and $\boldsymbol{\mu}$.
  - Cannot optimize for $\mathbf{Z}$ and $\boldsymbol{\mu}$ at the same time.

- Idea: Perform alternate optimization
  - Fixing $\boldsymbol{\mu} = \overline{\boldsymbol{\mu}}$ optimize for $\mathbf{Z}$, i.e.

$$\overline{\mathbf{Z}} = \arg\min_{\mathbf{Z}} L(\mathbf{X}, \mathbf{Z}, \overline{\boldsymbol{\mu}})$$

  - Fixing $\mathbf{Z} = \overline{\mathbf{Z}}$ optimize for $\boldsymbol{\mu}$, i.e.

$$\overline{\boldsymbol{\mu}} = \arg\min_{\boldsymbol{\mu}} L(\mathbf{X}, \overline{\mathbf{Z}}, \boldsymbol{\mu})$$

Alternate optimization – Step 1

- Minimize $L(\mathbf{X}, \mathbf{Z}, \overline{\boldsymbol{\mu}})$ with respect to $\mathbf{Z}$.

$$\begin{aligned} L(\mathbf{X}, \mathbf{Z}, \overline{\boldsymbol{\mu}}) &= \sum_{n=1}^{N} \sum_{k=1}^{K} z_k^{(n)} ||\mathbf{x}^{(n)} - \mu_k||^2 \\ &= \sum_{k=1}^{K} z_k^{(1)} ||\mathbf{x}^{(1)} - \mu_k||^2 + \ldots\ldots + \sum_{k=1}^{K} z_k^{(N)} ||\mathbf{x}^{(N)} - \mu_k||^2 \end{aligned}$$

- Approach: Minimize $L(\mathbf{X}, \mathbf{Z}, \overline{\boldsymbol{\mu}})$ with respect to each $\mathbf{z}^{(n)}$, i.e. minimize each of the above terms separately:

$$\overline{\mathbf{z}}^{(n)} = \arg\min_{\mathbf{z}^{(n)}} \sum_{k=1}^{K} z_k^{(n)} ||\mathbf{x}^{(n)} - \mu_k||^2$$

- The above is equivalent to assigning $\mathbf{x}^{(n)}$ to its nearest centroid.

Alternate optimization – Step 2

- Minimize $L(\mathbf{X}, \overline{\mathbf{Z}}, \boldsymbol{\mu})$ with respect to $\boldsymbol{\mu}$.

$$L(\mathbf{X}, \overline{\mathbf{Z}}, \boldsymbol{\mu}) = \sum_{n=1}^{N} \sum_{k=1}^{K} z_k^{(n)} ||\mathbf{x}^{(n)} - \mu_k||^2$$

$$= \sum_{n=1}^{N} z_1^{(n)} ||\mathbf{x}^{(n)} - \mu_1||^2 + ... + \sum_{n=1}^{N} z_K^{(n)} ||\mathbf{x}^{(n)} - \mu_K||^2$$

- Approach: Minimize $L(\mathbf{X}, \overline{\mathbf{Z}}, \boldsymbol{\mu})$ with respect to each μ_k separately. So need to minimize each of the above terms separately.

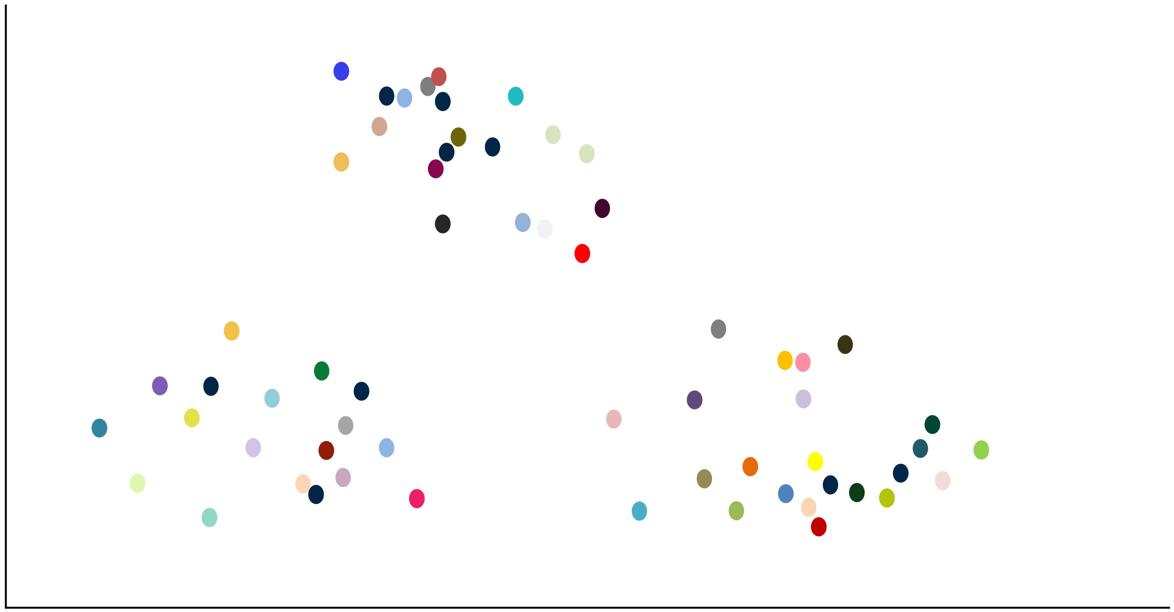
- The optimized value of μ_k is obtained as

$$\overline{\mu}_k = \arg\min_{\mu_k} \sum_{n=1}^{N} z_k^{(n)} ||\mathbf{x}^{(n)} - \mu_k||^2$$

- This is equivalent to setting $\overline{\mu}_k$ to be the mean of all the data points in the kth cluster.

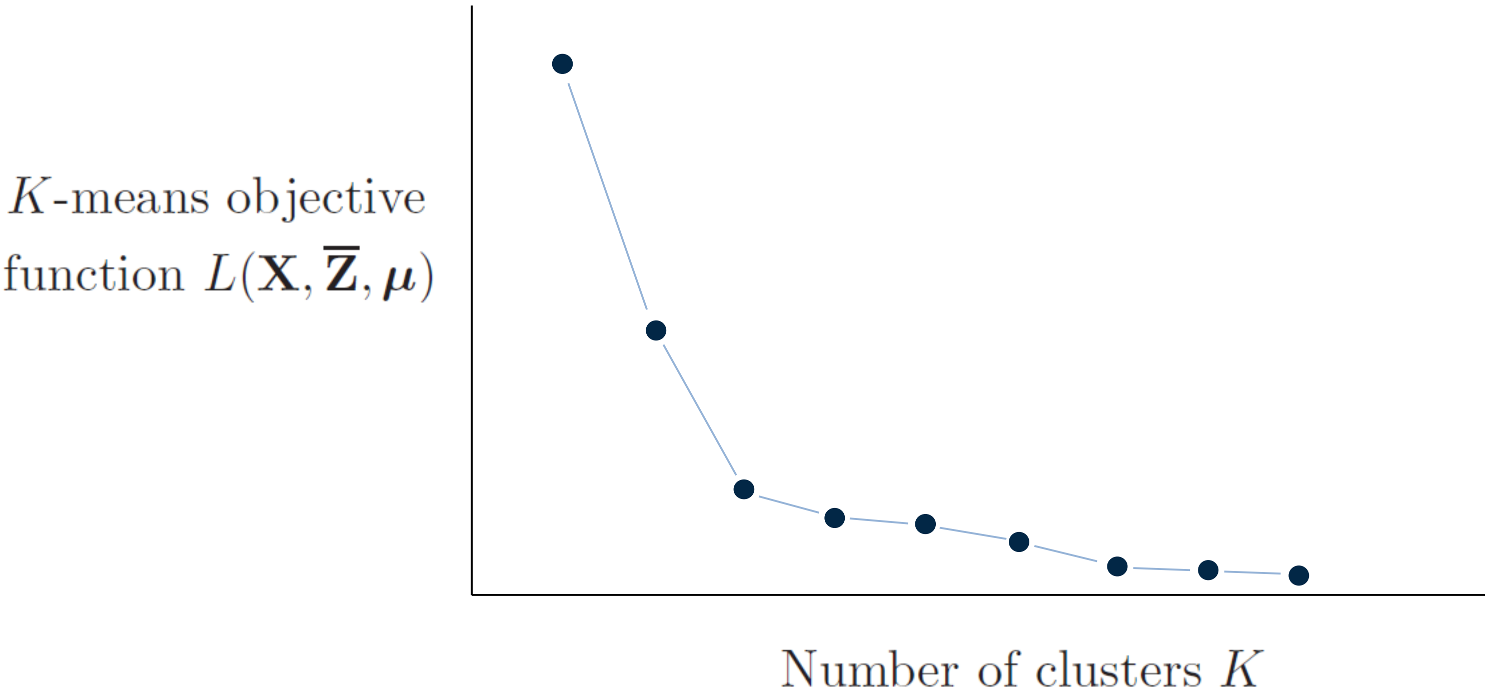
Selecting K value

- As the number of clusters K is increased, the value of the objective function $L(\mathbf{X}, \overline{\mathbf{Z}}, \boldsymbol{\mu})$ decreases.
  - For $K = N$ and $\mu_k = \mathbf{x}^{(k)}$, the value of the objective function $L(\mathbf{X}, \overline{\mathbf{Z}}, \boldsymbol{\mu})$ becomes 0.



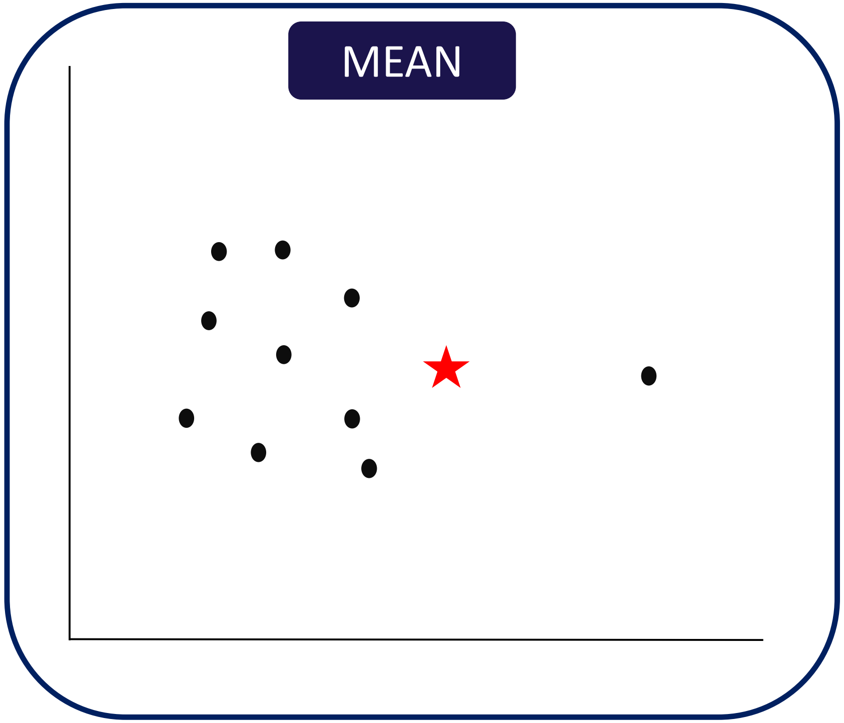
Selecting *K* value

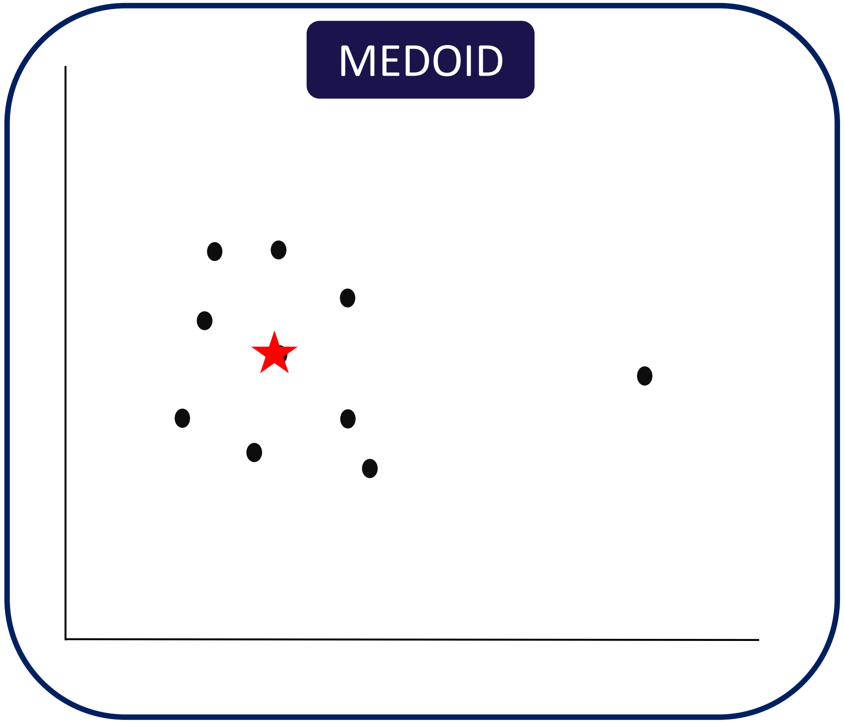
- One approach: Try K-means algorithm for different values of K, and select K to be at the "elbow point" with respect to the variation of $L(\mathbf{X}, \overline{\mathbf{Z}}, \boldsymbol{\mu})$ versus K.



K-medoids

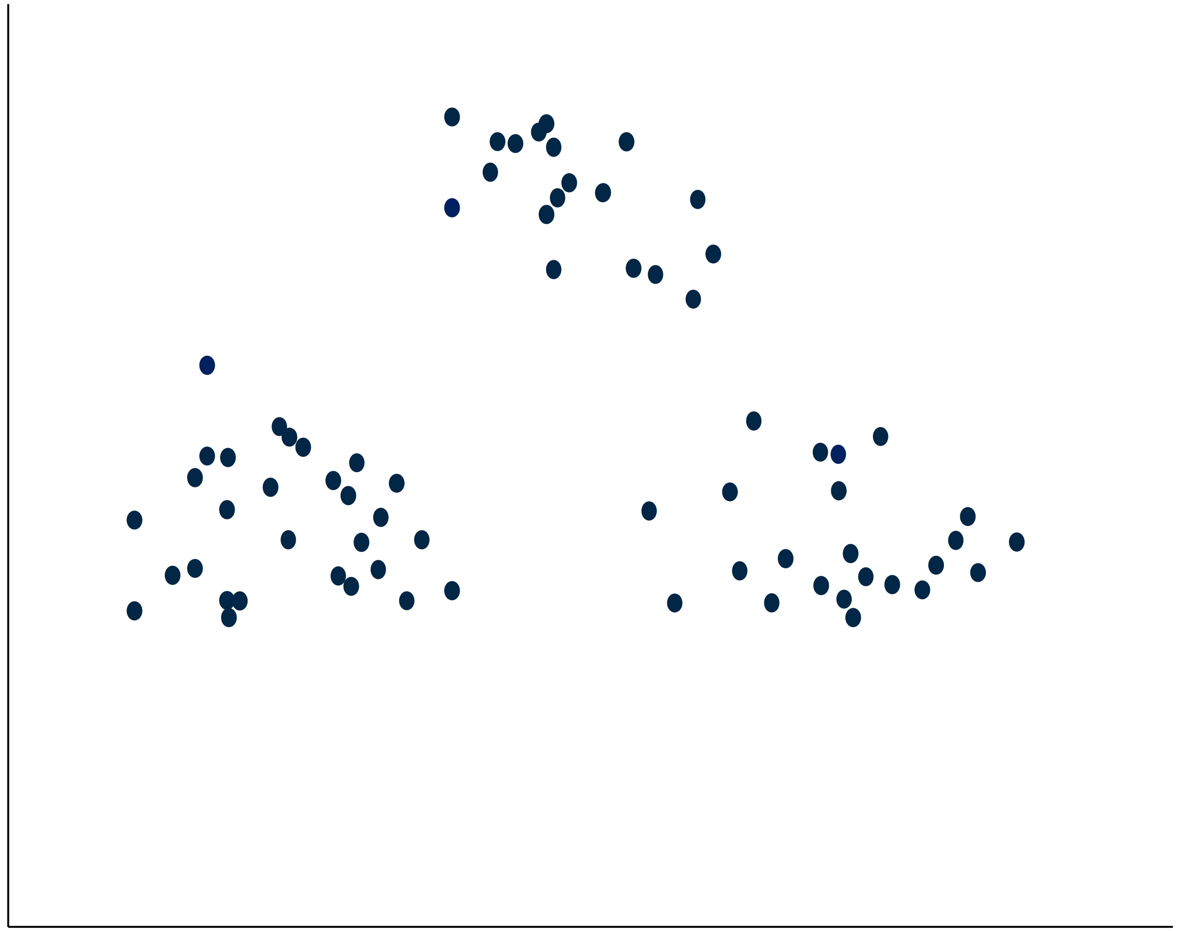
- The center of each cluster is taken to be one of the examples (data points) in the cluster.
  - In contrast, K-means take the mean of a cluster to be its center.
- K-medoids is more robust to outliers and noise.



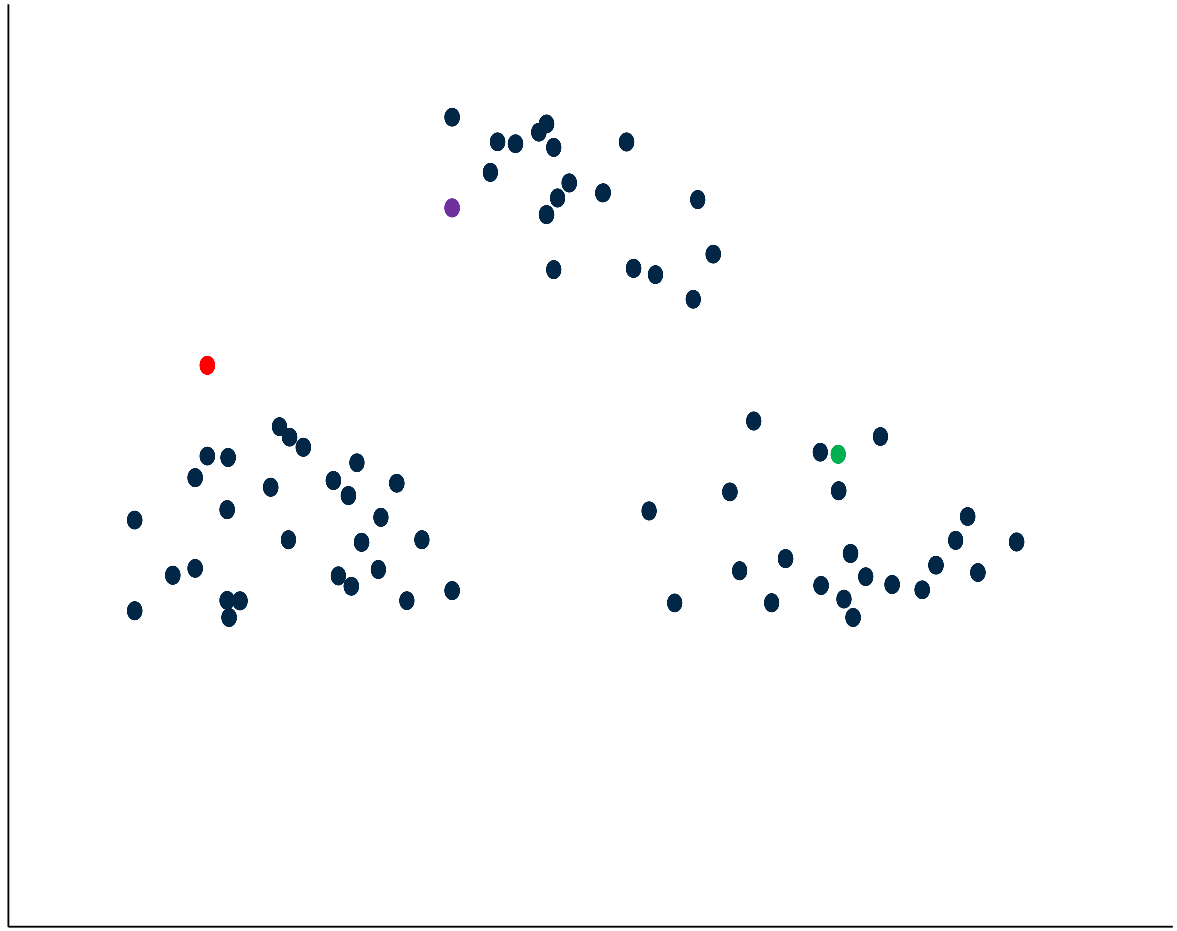


Figures for illustration only.

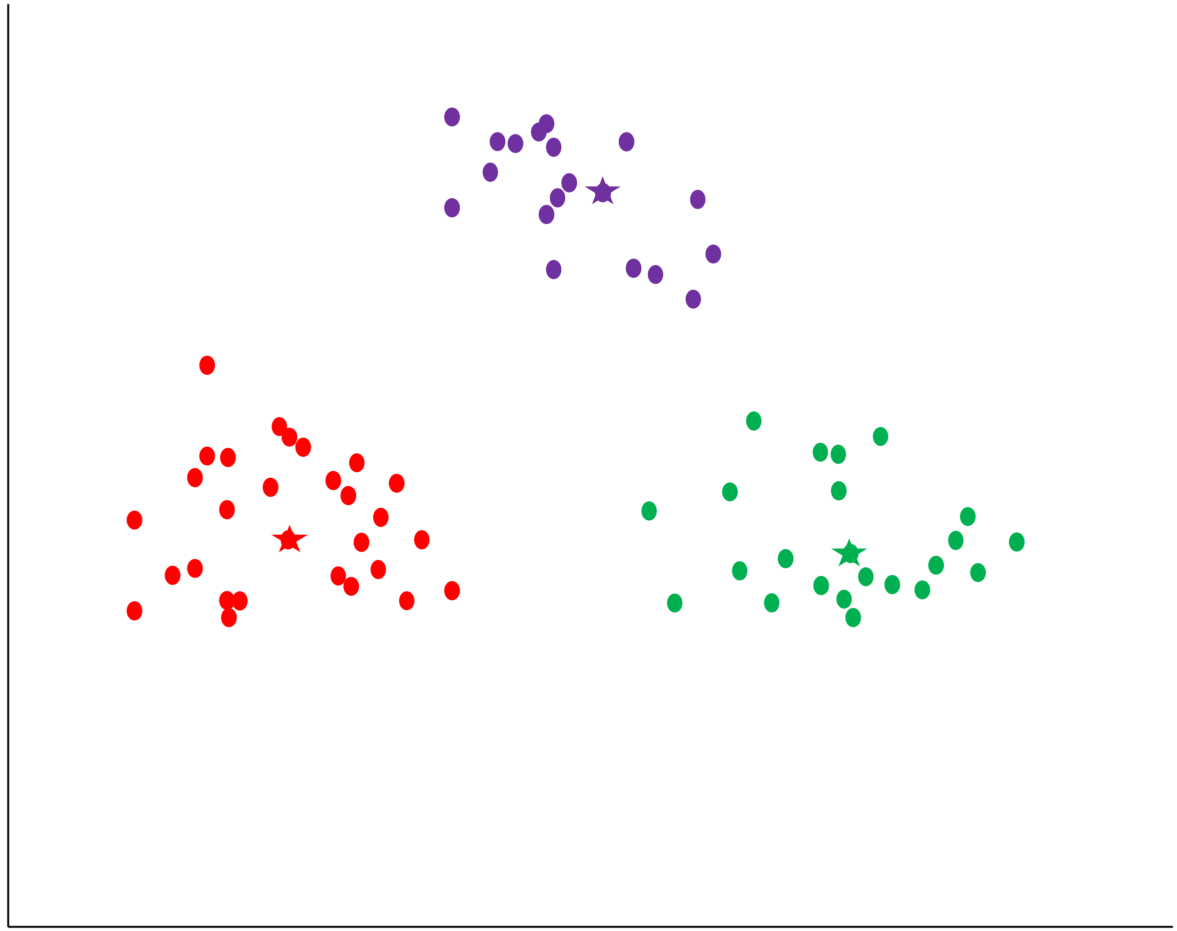
Dataset



K-medoids initialization



K-medoids



Procedure

- Step 1: Initialize the centers of K clusters – one approach is to randomly select K of the given N data points.

- Step 2: For $n = 1, 2, ..., N$:
  - Compute the distance of the nth data point to all the K centers, and assign $\mathbf{x}^{(n)}$ to the cluster to which it is the closest:

$$z^{(n)} = \arg\min_k ||\mathbf{x}^{(n)} - \mu_k||^2$$

- Step 3: Recompute the medoid of each cluster. The medoid of the kth cluster is computed as

$$\mu_k = \arg \min_{\mathrm{x}^{(i)} \in \mathcal{C}_k} \sum_{j:\mathrm{x}^{(j)} \in \mathcal{C}_k} ||\mathbf{x}^{(j)} - \mathbf{x}^{(i)}||^2$$

- If none of the cluster assignments have changed, STOP. Else, REPEAT from Step 2.