EE2211 Pre-Tutorial 11

Dr Feng LIN

feng_lin@nus.edu.sg

Agenda

- Recap
- Self-learning
- Tutorial 11

Today’s Attendance

Recap

- Introduction of unsupervised learning
- K-means Clustering
  - The most popular clustering technique
- Fuzzy Clustering

Unsupervised Learning

Introduction

Motivation: we do not always have labeled data.

In **unsupervised learning**, the dataset is a collection of **unlabeled examples** $\{\mathbf{x}_i\}_{i=1}^{M}$.

Evaluation of unsupervised learning is hard:

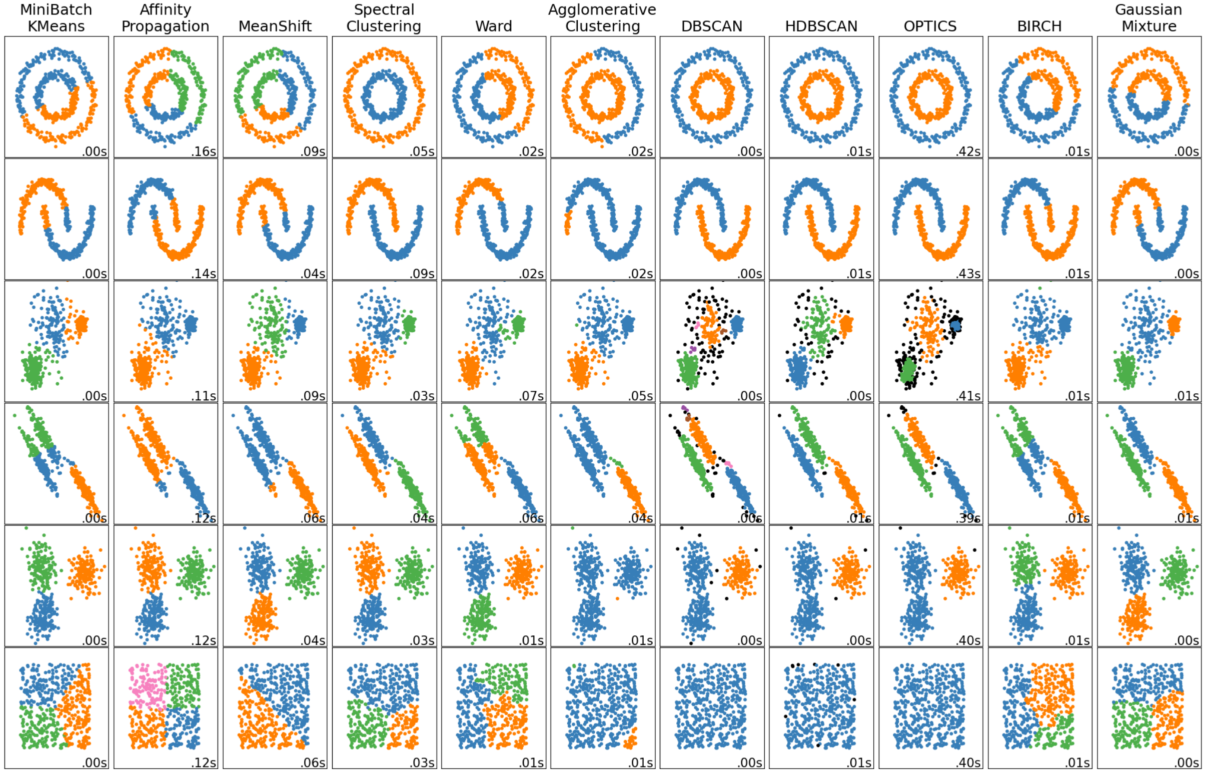
- The absence of labels representing the desired behavior for your model means the absence of a solid reference point to judge the quality of your model.

Unsupervised Learning

Main Tasks/Approaches

- **Clustering**
  - ✓ Groups a set of objects in such a way that objects in the same group (called a **cluster**) are **more similar** (in some sense) to each other than to those in other groups (clusters).
- **Density Estimation**
  - ✓ Models the probability density function (pdf) of the unknown probability distribution from which the dataset has been drawn.
- **Component Analysis**
  - ✓ Breaks down the data from the perspective of signal analysis.
- **Unsupervised Neural Networks**
  - ✓ Autoencoder

Overview of Clustering Methods



https://scikit-learn.org/stable/modules/clustering.html

K-Means Clustering

Distance based grouping method

- Feature vectors that are closed to each other

K-means

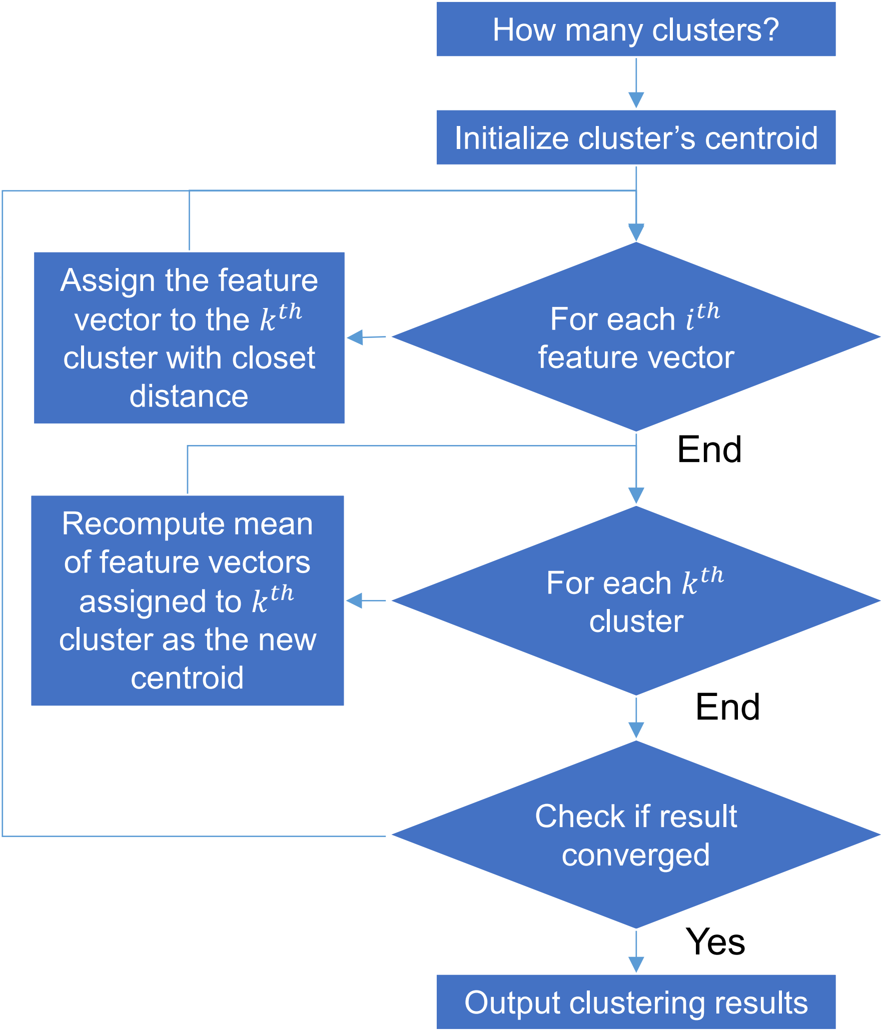
- K = number of clusters
- Means = average or centroid is the average of feature vectors

K-means Clustering

Basic/Naïve K-means Clustering

Looping between
Assignment and Centroid Update

1. First, we choose K — the number of clusters. Then we randomly select K feature vectors, called **centroids**, to the feature space.
2. Next, compute the distance from each example **x** to each centroid **c** using some metric, like the Euclidean distance. Then we assign the closest centroid to each example (like if we labeled each example with a centroid id as the label).
3. For each centroid, we calculate the average feature vector of the examples labeled with it. These average feature vectors become the new locations of the centroids.
4. We recompute the distance from each example to each centroid, modify the assignment and repeat the procedure until **the assignments don't change after the centroid locations are recomputed.**
5. Finally, we conclude the clustering with a list of assignments of centroids IDs to the examples.



How many clusters?
Initialize cluster's centroid
For each i^{th} feature vector
Assign the feature vector to the k^{th} cluster with closet distance
End
For each k^{th} cluster
Recompute mean of feature vectors assigned to k^{th} cluster as the new centroid
End
Check if result converged
Yes
Output clustering results

K-means Clustering

Optimization Objective Function (within-cluster variance)

Minimize J

m: # of samples; i: index of samples
K: # of clusters; k: index of clusters

$$J = \sum_{i=1}^{m} \sum_{k=1}^{K} w_{ik} \|\mathbf{x}_i - \mathbf{c}_k\|^2 \quad (1)$$

$$w_{ik} = \begin{cases} 1 & if\ x_i\ is\ assigned\ to\ clasl\ k \\ 0 & else \end{cases}$$

$$
w \quad
\begin{array}{c|ccc}
 & & K & \\
\hline
 & 0 & 0 & 1 \\
 & 1 & 0 & 0 \\
 & 0 & 1 & 0 \\
m & \dots & \dots & \dots \\
 & \dots & w_{ik} & \dots \\
 & \dots & \dots & \dots
\end{array}
$$

1st sample is in cluster 3

2nd sample is in cluster 1

The term w_{ik} is equal to 1 for data point $\mathbf{x}_i$ if the data point belongs to cluster S_k, else $w_{ik} = 0$.

> Note: The optimization objective function was called $C(\mathbf{w})$ in Lecture 8. Here, we use J (with parameters w_{ik} and $\mathbf{c}_k$) so that it is differentiated from the centroids $\mathbf{c}_k$.

Ref: https://towardsdatascience.com/k-means-clustering-algorithm-applications-evaluation-methods-and-drawbacks-aa03e644b48a
https://en.wikipedia.org/wiki/K-means_clustering

K-means Clustering

Naïve K-means Algorithm

Computing distances to all centroids

1. **Assignment Step (fix $\mathbf{c}$ and update w):**

$$\mathbf{x}_i \in S_k \ (w_{ik} = 1) \text{ if } \|\mathbf{x}_i - \mathbf{c}_k\|^2 < \left\|\mathbf{x}_i - \mathbf{c}_j\right\|^2 \ (\text{else } w_{ik} = 0),$$
$$i = 1, \cdots, m; \ \ j, k = 1, \ldots, K.$$

2. **Update Step (fix w and update $\mathbf{c}$):**

$$\frac{\partial J}{\partial \mathbf{c}_k} = -2 \textstyle\sum_{i=1}^{m} w_{ik}(\mathbf{x}_i - \mathbf{c}_k) = 0 \quad \Rightarrow \quad \mathbf{c}_k = \frac{\Sigma_{i=1}^{m} w_{ik}\mathbf{x}_i}{\Sigma_{i=1}^{m} w_{ik}}$$

Solving an optimization, i.e., setting derivative to 0

Note: $\|\mathbf{x} - \mathbf{c}\| = \sqrt{\Sigma_{d=1}^{D}(x_d - c_d)^2}$ is called the Euclidean distance.

where $\mathbf{x} = (x_1, x_2, \ldots, x_\mathrm{D}), \mathbf{c} = (c_1, c_2, \ldots, c_\mathrm{D})$

K-means Clustering

1. **Assignment Step (fix c and update w):**

$$\mathbf{x}_i \in S_k \ (w_{ik} = 1) \text{ if } \|\mathbf{x}_i - \mathbf{c}_k\|^2 < \left\|\mathbf{x}_i - \mathbf{c}_j\right\|^2 \ (\text{else } w_{ik} = 0), \quad i = 1, \cdots, m; \ \ j, k = 1, \ldots, K.$$

2. **Update Step (fix w and update c):**

$$\frac{\partial J}{\partial \mathbf{c}_k} = -2\sum_{i=1}^{m} w_{ik}(\mathbf{x}_i - \mathbf{c}_k) = 0 \ \Rightarrow \ \mathbf{c}_k = \frac{\Sigma_{i=1}^{m} w_{ik}\mathbf{x}_i}{\Sigma_{i=1}^{m} w_{ik}}$$

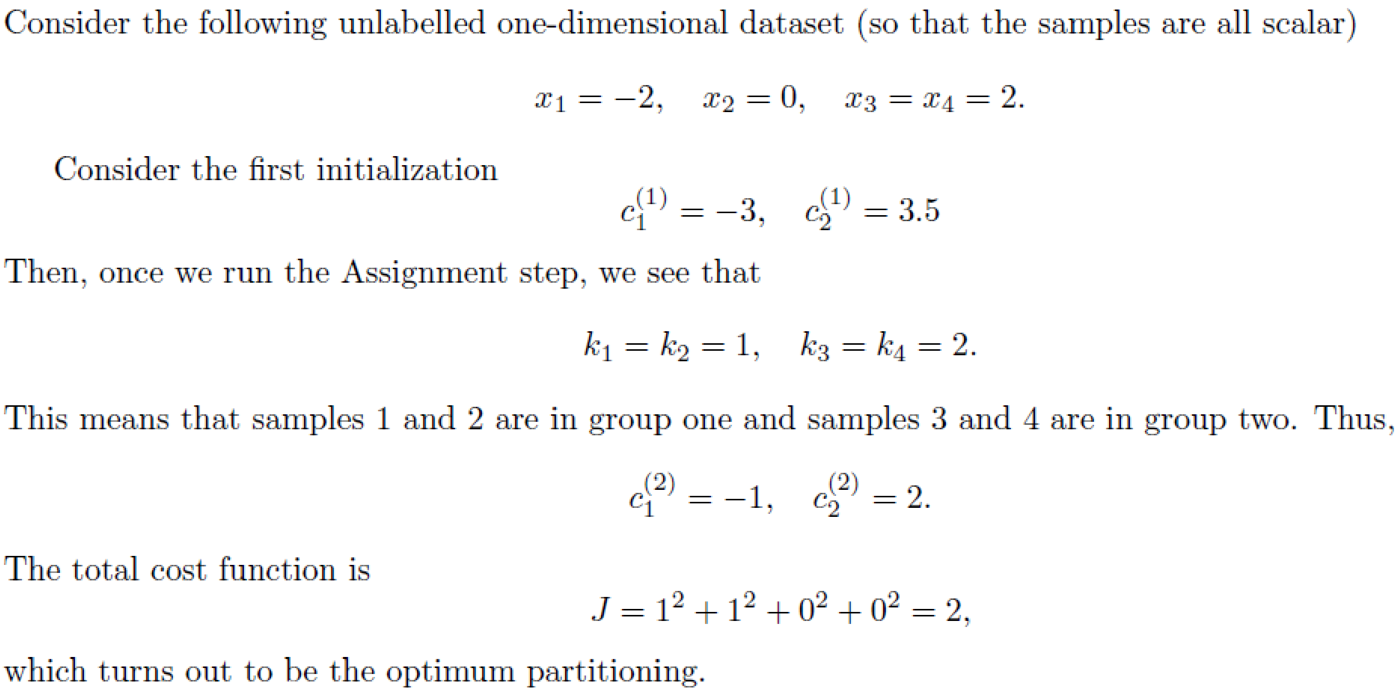
By repeating this two steps, the total loss $J = \sum_{i=1}^{m} \sum_{k=1}^{K} w_{ik}\|\mathbf{x}_i - \mathbf{c}_k\|^2$, is ***guaranteed to NOT increase (i.e., remain the same or decrease)*** until convergence.

Why?

At Step 2: we compute the new mean, by solving an optimization, i.e., compute the derivative and set to zero, and solve $\mathbf{c}_k$.
This means that, the new $\mathbf{c}_k$ is guaranteed to give a smaller J value.

At Step 1: we only change the assignment, if the distance to the new centroid is smaller! In other words, we either remain in the old group, or change to a new group that is closer (i.e., gives a smaller J)

An Example of K-means



Consider the following unlabelled one-dimensional dataset (so that the samples are all scalar)

$$x_1 = -2, \quad x_2 = 0, \quad x_3 = x_4 = 2.$$

Consider the first initialization

$$c_1^{(1)} = -3, \quad c_2^{(1)} = 3.5$$

Then, once we run the Assignment step, we see that

$$k_1 = k_2 = 1, \quad k_3 = k_4 = 2.$$

This means that samples 1 and 2 are in group one and samples 3 and 4 are in group two. Thus,

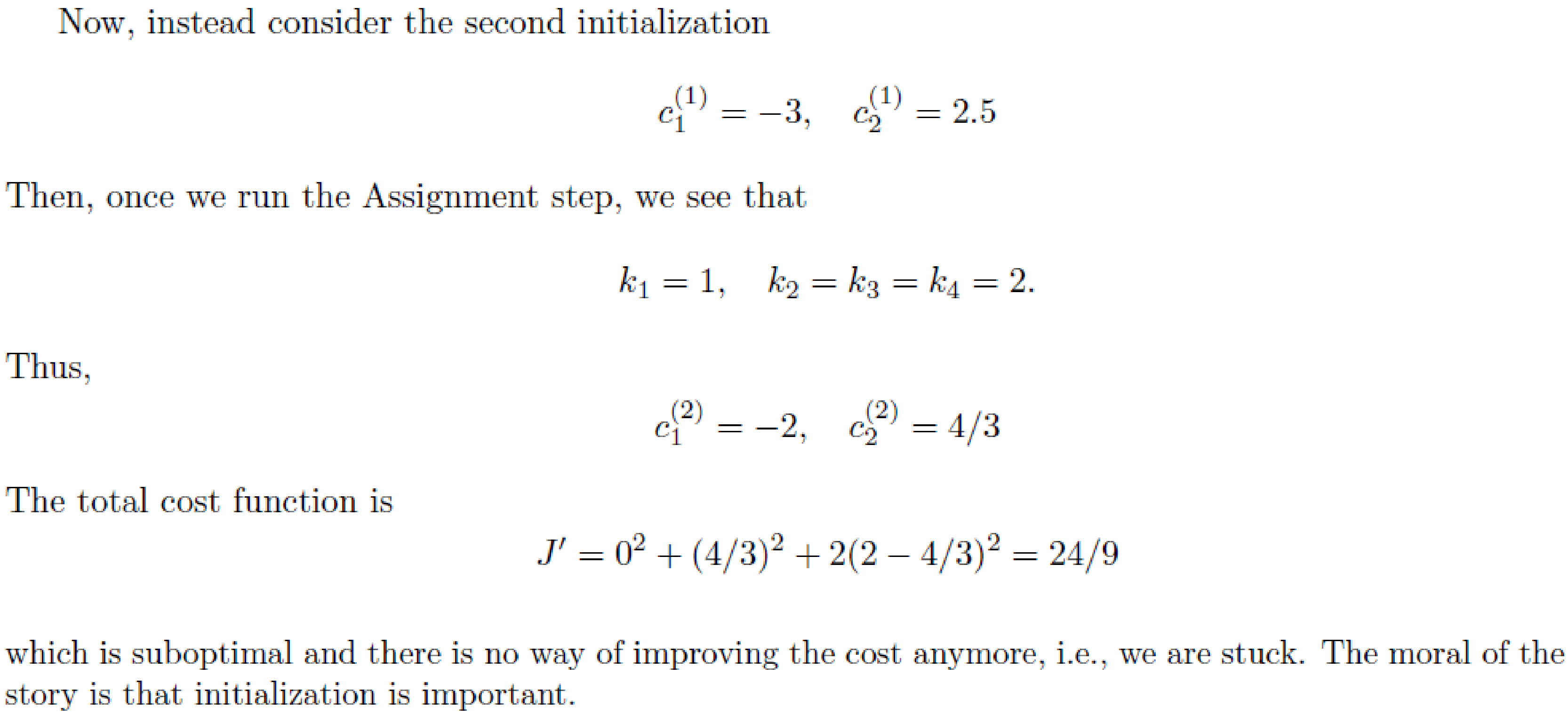
$$c_1^{(2)} = -1, \quad c_2^{(2)} = 2.$$

The total cost function is

$$J = 1^2 + 1^2 + 0^2 + 0^2 = 2,$$

which turns out to be the optimum partitioning.

An Example of K-means



Now, instead consider the second initialization

$$c_1^{(1)} = -3, \quad c_2^{(1)} = 2.5$$

Then, once we run the Assignment step, we see that

$$k_1 = 1, \quad k_2 = k_3 = k_4 = 2.$$

Thus,

$$c_1^{(2)} = -2, \quad c_2^{(2)} = 4/3$$

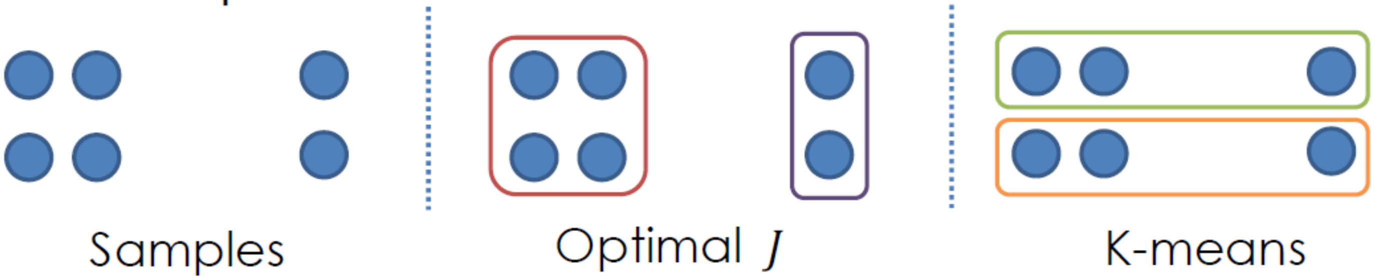
The total cost function is

$$J' = 0^2 + (4/3)^2 + 2(2 - 4/3)^2 = 24/9$$

which is suboptimal and there is no way of improving the cost anymore, i.e., we are stuck. The moral of the story is that initialization is important.

K-means Clustering

- Unfortunately, k-means is not guaranteed to find a global minimum, it finds only local minimum.
- Example:



- Finding the optimal J is NP-hard*
- In practice, k-means clustering usually performs well
- It can be very efficient, and its solution can be used as a starting point for other clustering algorithms

K-means Clustering

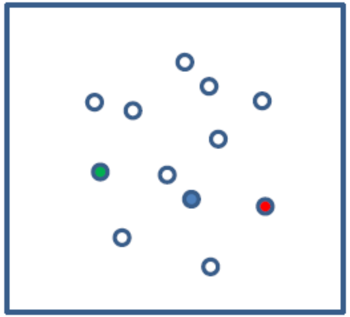
- **Initialization**

Initialization by centroid

Forgy method:

– Randomly chooses *k* observations from the dataset and uses these as the initial means.

k=3

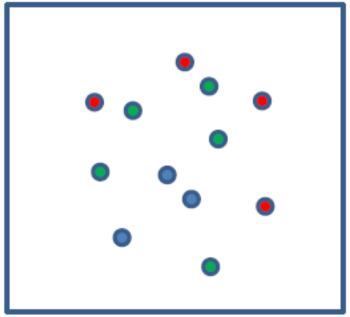


Random partition:

– First randomly assigns a cluster to each observation and then proceeds to the update step, thus computing the initial mean to be the centroid of the cluster's randomly assigned points

Initialization by grouping

k=3



Hard vs Soft Clustering

Hard clustering:

Each data point can belong only one cluster, e.g. K-means

- For example, an apple can be red OR green (hard clustering)

Soft clustering (also known as **Fuzzy clustering**):

Each data point can belong to more than one cluster.

- For example, an apple can be red AND green (fuzzy clustering)
- Here, the apple can be red to a certain degree as well as green to a certain degree.
- Instead of the apple belonging to green [green = 1] and not red [red = 0], the apple can belong to green [green = 0.3] and red [red = 0.5]. These value are normalized between 0 and 1; however, they do not represent probabilities, so the two values **do not need to add up to 1**.

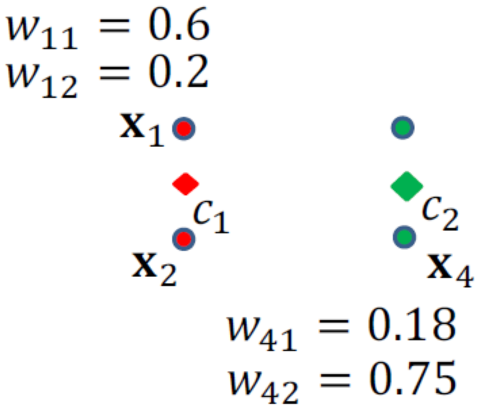
Hard vs Soft Clustering

Objective Function for Fuzzy C-means

Minimize J

$$J = \sum_{i=1}^{m} \sum_{k=1}^{C} (w_{ik})^r \|\mathbf{x}_i - \mathbf{c}_k\|^2$$

where $w_{ik} = \dfrac{1}{\sum_{j=1}^{c} \left(\frac{\|\mathbf{x}_i - \mathbf{c}_k\|}{\|\mathbf{x}_i - \mathbf{c}_j\|} \right)^{\frac{2}{r-1}}}$



Each element, $w_{ik} \in [0,1]$, tells the degree to which element, $\mathbf{x}_i$, belongs to cluster $\mathbf{c}_k$.
The fuzzifier $r > 1$ determines the level of cluster fuzziness; usually $1.25 \le r \le 2$.

- Points **closer** to a centroid c_k have **higher membership** w_{ik} in that cluster.
- Larger r leads to **softer memberships**; as r approaches 1, memberships become **sharper**, favoring the nearest cluster.

THANK YOU