

Computational Intelligence Lecture 18: Classification

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Classification

Hard c-Means How to choose the optimal partitions?

Fuzzy C-Means Fuzzy c-Means Algorithm

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Classification

- The data can be classified according to similar patterns, attributes, features, and other characteristics.
- Classification, also termed clustering.
- Why fuzzy clustering?
 - The regularities may not be precisely defined for clustering.
 - Using fuzzy models to formulated problem may be easier to solve computationally.
 - In fuzzy models the variables are continuous → their derivatives can be used to find the direction of search. But in crisp model they only can have 0/1 mem values.
- ► In this lecture we are introducing one of the most famous classification alg.: c-means clustering [1]

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► Consider:

- $X = \{x_1, x_2, ..., x_n\}$ set of data
- c: # of clusters (1 < c < n)
 - c = n classes \rightsquigarrow each data sample into its own class
 - c = 1 places all data samples into the same class
 - Neither case requires any effort in classification
- A family of sets $\{A_i, i = 1, 2, ..., c\}$ is a hard c-partition of X if

$$\blacktriangleright \bigcup_{i=1}^{c} A_i = X$$

- $A_i \cap A_j = \emptyset$ $1 \le i \ne j \le c$
- $0 \subset A_i \subset X$

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- ► c-partition can be reformulated by mem. fcn $(\mu_{A_i}(x_k) = \mu_{ik})$.
 - $\mu_{ik} = \begin{cases} 1 & x_k \in A_i \\ 0 & x_k \neq A_i \end{cases}$ $k = 1, ..., n, i = 1, ..., c, A_i \subset X, x_k \in X$
 - Given the value of μ_{ik} , hard c-partitions X uniquely, and vice versa.
- The μ_{ik} 's should satisfy the following three conditions
 - $\mu_{ik} \in \{0,1\}, \ 1 \le i \le c, 1 \le k \le n$
 - $\sum_{i=1}^{c} \mu_{ik} = 1, \ \forall k \in \{1, ..., k\}$
 - $0 < \sum_{k=1}^{n} \mu_{ik} < n, \forall i \in \{1, ..., c\}$

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Hard c-Means

- $\sum_{i=1}^{c} \mu_{ik} = 1, \forall k \in \{1, ..., k\}$
- $0 < \sum_{k=1}^{n} \mu_{ik} < n, \forall i \in \{1, ..., c\}$
- ► The first two conditions → each x_k ∈ X should belong to one and only one cluster.
- ► The last condition → each cluster A_i must contain at least one and at most n − 1 data points.
- μ_{ik} can be shown in a $U_{c \times n}$ matrix

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- Example: Let $X = \{x_1 = orange, x_2 = apple, x_3 = cucumber\}$
- For c = 2, which of the following matrices can be hard c-partition matrix? U₁ − [1 1 0] U₂ − [1 1 0]
- ► Hard c-partition space for X (M_c) is a set of all possible hard c-partition matrices U

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How to choose the optimal partitions?

Hard c-Means

- ▶ For example, c = 10 and n = 25, there are roughly 10¹⁸ distinct 10-partitions!!
- ► There are three types of methods for finding optimal partitions:
 - 1. Hierarchical methods
 - merging and splitting to construct new clusters are based on some measure of similarity
 - The result is a hierarchy of nested clusters.
 - 2. Graph-theoretic methods
 - x_i are considered as nodes which are connected to each other through edges
 - ► The criterion for clustering is typically some measure of connectivity
 - 3. Objective function methods
 - an objective function measuring the "desirability" of clustering candidates is established
 - ► local minima of the objective function are defined as optimal clusters.





- c-means method is an objective fun. method
- ► The most popular objective function: overall within-group sum of squared errors: $\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} ||x| = ||x| = ||x||^{2}$
 - $J_w(U, V) = \sum_{k=1}^{n} \sum_{i=1}^{c} \mu_{ik} ||x_k v_i||^2$
 - $U = [\mu_{ik}]$
 - $V = \{v_1, ..., v_c\}, v_i$: center of cluster A_i $v_i = \frac{\sum_{k=1}^n \mu_{ik} x_k}{\sum_{k=1}^n \mu_{ik}}$
 - ▶ v_i is the average of all the points in cluster A_i
 - ► The closer the points of each cluster to their centers (v_i), the smaller the J(U, V)

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Hard c-Means

The most popular objective function: overall within-group sum of squared errors:

$$J_w(U, V) = \sum_{k=1}^n \sum_{i=1}^c \mu_{ik} ||x_k - v_i||^2$$

- $U = [\mu_{ik}]$
- $V = \{v_1, ..., v_c\}, v_i$: center of cluster A_i $v_i = \frac{\sum_{k=1}^{n} \mu_{ik} x_k}{\sum_{k=1}^{n} \mu_{ik}}$
- ► *v_i* is the average of all the points in cluster *A_i*
- ► The closer the points of each cluster to their centers (v_i), the smaller the J(U, V)
- ▶ How to find the optimal pair (U, V) for J_w ?
- ▶ c-means alg. (ISODATA alg.) can provide an optimal method
- The objective function is developed to achieve two goals simultaneously:
 - 1. Minimize the Euclidean distance between each data point in a cluster and its cluster center
 - 2. Maximize the Euclidean distance between cluster centers.

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1. Suppose there are *n* data points, $X = \{x_1, ..., x_n\}$. Fix $c, 2 \le c < n$, and initialize $U^{(0)} \in M_c$.

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Outline Classification Hard c-Means Fuzzy C-Means Contraction And c-Means Fuzzy C-Means Contraction Co

- 1. Suppose there are *n* data points, $X = \{x_1, ..., x_n\}$. Fix $c, 2 \le c < n$, and initialize $U^{(0)} \in M_c$.
- 2. At iteration *I*, I = 0, 1, 2, ... compute the c-mean vectors $v_i^{(I)} = \frac{\sum_{k=1}^n \mu_{ik}^{(I)} x_k}{\sum_{k=1}^n \mu_{ik}^{(I)}}$ where $[\mu_{ik}^{(I)}] = U^{(I)}$, and i = 1, 2, ..., c.

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Hard c-Means

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Hard c-Means

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- 4. Compare $U^{(I)}$ with $U^{(I+1)}$: if $||U^{(I+1)} U^{(I)}|| < \epsilon$ for a small constant ϵ stop; otherwise, set I = I + 1 and go to Step 2.

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- 1. Suppose there are *n* data points, $X = \{x_1, ..., x_n\}$. Fix $c, 2 \le c < n$, and initialize $U^{(0)} \in M_c$. guess c hard clusters
- 2. At iteration *I*, *I* = 0, 1, 2, ... compute the c-mean vectors $v_i^{(I)} = \frac{\sum_{k=1}^n \mu_{ik}^{(I)} x_k}{\sum_{k=1}^n \mu_{ik}^{(I)}}$

Hard c-Means

- $\mu_{ik}^{(i)} = U^{(i)}, \text{ and } i = 1, 2, ..., c.$ 3. Update $U^{(l)}$ to $U^{(l+1)}$ using $\mu_{ik}^{(l+1)} = \begin{cases} 1 & \|x_k v_i^{(l)}\| = \min_{1 \le j \le c} (\|x_k v_j^{(l)}\|) \\ 0 & otherwise \end{cases}$
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Hard c-Means

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- 1. Suppose there are *n* data points, $X = \{x_1, ..., x_n\}$. Fix $c, 2 \le c < n$, and initialize $U^{(0)} \in M_c$. guess c hard clusters
- 2. At iteration $I_{20} I = 0, 1, 2, ...$ compute the c-mean vectors

Hard c-Means

 $\begin{aligned} v_i^{(l)} &= \frac{\sum_{k=1}^n \mu_{ik}^{(l)} x_k}{\sum_{k=1}^n \mu_{ik}^{(l)}} \\ \text{where } [\mu_{ik}^{(l)}] &= U^{(l)}, \text{ and } i = 1, 2, ..., c. \text{ find their centers} \end{aligned}$ 3. Update $U^{(l)}$ to $U^{(l+1)}$ using $\mu_{ik}^{(l+1)} &= \begin{cases} 1 & \|x_k - v_i^{(l)}\| = \min_{1 \le j \le c} (\|x_k - v_j^{(l)}\|) \\ 0 & otherwise \end{cases} \text{ reallocate} \end{aligned}$

cluster memberships to minimize squared errors between the data and the current centers

4. Compare $U^{(I)}$ with $U^{(I+1)}$: if $||U^{(I+1)} - U^{(I)}|| < \epsilon$ for a small constant ϵ stop; otherwise, set I = I + 1 and go to Step 2.

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Hard c-Means

- 1. Suppose there are *n* data points, $X = \{x_1, ..., x_n\}$. Fix $c, 2 \le c < n$, and initialize $U^{(0)} \in M_c$. guess c hard clusters
- 2. At iteration *I*, I = 0, 1, 2, ... compute the c-mean vectors $v_i^{(I)} = \frac{\sum_{k=1}^n \mu_{ik}^{(I)} x_k}{\sum_{k=1}^n \mu_{ik}^{(I)}}$ where $[\mu_{ik}^{(I)}] = U^{(I)}$, and i = 1, 2, ..., c. find their centers 3. Update $U^{(I)}$ to $U^{(I+1)}$ using $\mu_{ik}^{(I+1)} = \begin{cases} 1 & ||x_k - v_i^{(I)}|| = \min_{1 \le j \le c} (||x_k - v_j^{(I)}||) \\ 0 & otherwise \end{cases}$ reallocate cluster memberships to minimize squared errors between the data and

the current centers

Compare U^(I) with U^(I+1): if ||U^(I+1) − U^(I)|| < ε for a small constant ε stop; otherwise, set I = I + 1 and go to Step 2.stop when looping ceases to lower J_w significantly



Example

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▶ Suppose n = 15, c = 2

• The hard c-means algorithm stops at l = 3 with $U^{(3)} = U^{(4)} =$

Hard c-Means

- \blacktriangleright \therefore x_1 to x_7 are grouped into A_1
- ► x₈ to x₁₅ are grouped into A₂
- Although the fig is symmetric the clusters are unsymmetry
- x₈ cold not belong to both clusters
- A way to solve this problem is using the fuzzy c-means alg

Computational Intelligence

Lecture 18



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▶ In fuzzy c-means the mem. fcn (μ_{ik} should respect the following conditions

•
$$\mu_{ik} \in [0,1], \ 1 \le i \le c, 1 \le k \le n$$

•
$$\sum_{i=1}^{c} \mu_{ik} = 1, \ \forall k \in \{1, ..., k\}$$

- ► A_i have 1 n members (last condition of mem. fcn. for hard c-means is relaxed for fuzzy c-means)
- ► Fuzzy c-partition space for X (M_{fc}) is a set of all possible fuzzy c-partition matrices U

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Fuzzy C-Means

• In fuzzy c-means the mem. fcn (μ_{ik} should respect the following conditions

▶
$$\mu_{ik} \in [0, 1], \quad 1 \le i \le c, 1 \le k \le n$$

▶ $\sum_{i=1}^{c} \mu_{ik} = 1, \quad \forall k \in \{1, ..., k\}$

 A_i have 1 - n members (last condition of mem. fcn. for hard c-means is relaxed for fuzzy c-means)

Fuzzy C-Means

- ► Fuzzy c-partition space for X (M_{fc}) is a set of all possible fuzzy c-partition matrices U
- An example of possible U for n = 3, c = 2: $U = \begin{bmatrix} 0.9 & 0.2 & 0.9 \\ 0.1 & 0.8 & 0.1 \end{bmatrix}$
- For c-means alg. we are looking U = [µ_{ik}] ∈ M_{fc} and V = [v₁, ..., v_n] s.t.
 - $J_m(U,V) = \sum_{k=1}^n \sum_{i=1}^c (\mu_{ik})^m \|x_k v_i\|^2$ is minimized. $(m \in (1,\infty))$

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1. Suppose there are *n* data points, $X = \{x_1, ..., x_n\}$. Fix $c, 2 \le c < n$, $m \in (1, \infty)$, and initialize $U^{(0)} \in M_{fc}$.

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Fuzzy c-Means Algorithm

1. Suppose there are *n* data points, $X = \{x_1, ..., x_n\}$. Fix $c, 2 \le c < n$, $m \in (1, \infty)$, and initialize $U^{(0)} \in M_{fc}$.

Fuzzy C-Means

2. At iteration *I*, I = 0, 1, 2, ... compute the c-mean vectors $v_i^{(I)} = \frac{\sum_{k=1}^n (\mu_{ik}^{(I)})^m x_k}{\sum_{k=1}^n (\mu_{ik}^{(i)})^m}$ where $[\mu_{ik}^{(I)}] = U^{(I)}$, and i = 1, 2, ..., c.

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Fuzzy c-Means Algorithm

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Fuzzy C-Means

2. At iteration I, I = 0, 1, 2, ... compute the c-mean vectors

$$v_i^{(I)} = \frac{\sum_{k=1}^{n} (\mu_{ik}^{(I)})^m x_k}{\sum_{k=1}^{n} (\mu_{ik}^{(I)})^m}$$

where $[\mu_{ik}^{(I)}] = U^{(I)}$, and $i = 1, 2, ..., c$.

3. Update
$$U^{(I)}$$
 to $U^{(I+1)}$ using

$$\mu_{ik}^{(I+1)} = \frac{1}{\sum_{j=1}^{c} \left[\frac{\|\mathbf{x}_{k} - \mathbf{v}_{j}^{(I)}\|}{\|\mathbf{x}_{k} - \mathbf{v}_{j}^{(I)}\|}\right]}, 1 \le i \le c, 1 \le k \le n$$

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Fuzzy c-Means Algorithm

1. Suppose there are *n* data points, $X = \{x_1, ..., x_n\}$. Fix $c, 2 \le c < n$, $m \in (1, \infty)$, and initialize $U^{(0)} \in M_{fc}$.

Fuzzy C-Means

- 2. At iteration I, I = 0, 1, 2, ... compute the c-mean vectors
- $v_i^{(l)} = \frac{\sum_{k=1}^n (\mu_{ik}^{(l)})^m x_k}{\sum_{k=1}^n (\mu_{ik}^{(l)})^m}$ where $[\mu_{ik}^{(l)}] = U^{(l)}$, and i = 1, 2, ..., c. 3. Update $U^{(l)}$ to $U^{(l+1)}$ using $\mu_{ik}^{(l+1)} = \frac{1}{\sum_{j=1}^c [\frac{\|x_k - v_j^{(l)}\|}{\|x_k - v_j^{(l)}\|}]}, 1 \le i \le c, 1 \le k \le n$
- 4. Compare $U^{(I)}$ with $U^{(I+1)}$: if $||U^{(I+1)} U^{(I)}|| < \epsilon$ for a small constant ϵ stop; otherwise, set I = I + 1 and go to Step 2.

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Example

- ▶ Consider previous example with $c = 2, m = 1.25, \epsilon = 0.01$
- $\blacktriangleright U^{(0)} = \begin{bmatrix} 0.854 & 0.146 & 0.854 & 0.854 & \dots & 0.854 \\ 0.146 & 0.854 & 0.146 & 0.146 & \dots & 0.146 \end{bmatrix}$
- The fuzzy c-means algorithm stops at l = 5
- ► The data in the right and left wings are well classified, while the bridge x₈ belongs to both clusters to almost the same degree



Fuzzy C-Means



J. C. Bezdek, *Patttern Recognition with Fuzzy Objective Function Algorithms*. Plenum Press, 1981.

Fuzzy C-Means



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