

Paper:

Fuzzified Even-Sized Clustering Based on Optimization

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Clustering is a method of data analysis without the use of supervised data. Even-sized clustering based on optimization (ECBO) is a clustering algorithm that focuses on cluster size with the constraints that cluster sizes must be the same. However, this constraints makes ECBO inconvenient to apply in cases where a certain margin of cluster size is allowed. It is believed that this issue can be overcome by applying a fuzzy clustering method. Fuzzy clustering can represent the membership of data to clusters more flexible. In this paper, we propose a new even-sized clustering algorithm based on fuzzy clustering and verify its effectiveness through numerical examples.

Keywords: clustering, machine learning, even-sized, fuzzy

1. Introduction

Clustering is a method of machine learning for data analysis, in which a given dataset is automatically classified into clusters. K -means [1] (KM) and fuzzy c -means [2] (FCM) are established clustering methods based on optimization. In these methods, the value of the objective function [3, 4] can be used as an evaluation index of the clustering result. From this point of view, many clustering methods are modeled as optimization problems with objective functions and constraints.

K -member clustering (KMC) has been proposed as a method that focuses on cluster size. KMC classifies a dataset into clusters whose size is at least K . KMC is expected to be applied to k -anonymization and task distribution problems. Representatively, the following three algorithms can be mentioned: greedy k -member clustering (GKC) [5], one-pass k -means (OKA) [6], and clustering-based k -anonymity (CBK) [7]. These conventional methods sometimes yield unnatural classification results. This is because these methods are not based on the optimization of the objective function. In addition, as a related

study focusing on cluster size, there is a method introducing size control variables [8].

Microaggregation has been proposed as a method based on optimization [9, 10]. This method works under constraints that the size of each cluster is greater than or equal to K and less than or equal to $2K$. Microaggregation has demonstrated great results with K -anonymization.

Some authors have also proposed even-sized clustering based on optimization (ECBO) [11, 12] as a method based on optimization. The constraint considered in the ECBO is that each cluster size is K or $K + 1$. ECBO is constructed by adding cluster size constraints to KM, and the membership of each object is obtained by iteratively optimizing the objective function using the simplex method. Numerical experiments show that ECBO demonstrates suitable results.

Since the constraints considered in the ECBO are so severe, it is inconvenient if each cluster size does not need to be even. For example, when classifying 100 objects into three clusters, each cluster size set to 33 or 34 in ECBO. However, it may be sufficient to set each cluster size to approximately 30 in many cases. In such cases, ECBO is inconvenient due to severe constraints. Better clustering results are expected by relaxing severe constraints of cluster size.

There are two methods to solve the above problem. The first is to relax cluster size constraints directly. Concretely, the parameter K is given a certain width α . In this method, the degree of the cluster size constraint can be controlled by varying α . From this point of view, some authors have proposed a clustering algorithm based on ECBO. The proposed algorithm is referred to as controlled sized clustering based on optimization (COCBO) [13, 14] since each cluster size can be controlled. The second is fuzzification of the membership. In this method, the membership can be represented more flexibly, and as a result, the constraints are relaxed. This method can be considered to be fuzzification of ECBO; in other words, it is constructed by adding size constraints to FCM.

In this paper, a clustering algorithm based on the sec-

ond method is proposed, and the methods are evaluated through numerical examples.

2. Fuzzy c -Means and Even-Sized Clustering Based on Optimization

In this section, FCM and ECBO are introduced as existing methods. First, the following variables are defined. The data set $X = \{x_k \mid k = 1, \dots, n\}$ is given, $x_k = \{x_{k1}, \dots, x_{kp}\} \in \mathcal{R}^p$ is the k -th object of the dataset. C_i is the i -th cluster. A set of cluster centers is denoted by $V = \{v_i \mid i = 1, \dots, c\}$ and $v_i \in \mathcal{R}^p$ is the i -th cluster center. Moreover, let $U = (u_{ki})_{k=1, \dots, n, i=1, \dots, c}$ be a matrix of memberships. u_{ki} means the membership of x_k to c_i . $\|\cdot\|$ is the Euclidean norm and $d_{ki} = \|x_k - v_i\|^2$.

2.1. Fuzzy c -Means (FCM)

FCM is an established method of fuzzy clustering. In fuzzy clustering, the membership is defined as $u_{ki} \in [0, 1]$. FCM consists of the following objective function and constraint.

$$\text{minimize } J_{\text{FCM}}(U, V) = \sum_{k=1}^n \sum_{i=1}^c u_{ki}^m d_{ki}, \quad \dots \quad (1)$$

$$\text{s.t. } \sum_{i=1}^c u_{ki} = 1, \quad (k = 1, \dots, n) \quad \dots \quad (2)$$

Here, parameter m is the fuzzification parameter and it satisfies $m > 1$. Eq. (1) is the objective function of FCM, and it is alternately optimized for U and V . The optimal solution for U is obtained by using the following equation using the method of Lagrange multipliers.

$$u_{ki} = \frac{\left(\frac{1}{d_{ki}}\right)^{\frac{1}{m-1}}}{\sum_{j=1}^c \left(\frac{1}{d_{kj}}\right)^{\frac{1}{m-1}}}. \quad \dots \quad (3)$$

The optimal solution for V is obtained by the following equation.

$$v_i = \frac{\sum_{k=1}^n (u_{ki})^m x_k}{\sum_{k=1}^n (u_{ki})^m}. \quad \dots \quad (4)$$

The FCM algorithm finds the optimal solutions by iterative optimization as **Algorithm 1**.

FCM is known to have a the solution dependent on the initial value, since it converges to a local optimum. In many cases, many initial cluster centers are given randomly to prevent initial value dependence.

2.2. Even-Sized Clustering Based on Optimization (ECBO)

Even-sized clustering based on optimization (ECBO) [11, 12] divides datasets into clusters in

Algorithm 1 FCM

Step 1. Give the constant c .

Step 2. Choose the initial cluster centers V from X randomly.

Step 3. Update U by Eq. (3) with fixing V .

Step 4. Update V by Eq. (4) with fixing U .

Step 5. If V changes from previous V , go back to **Step 3**. Otherwise, stop.

which the cluster sizes are almost even. Here, “cluster size” means “the number of objects in the cluster.” ECBO is an algorithm adding cluster size constraints to KM; hence its solution is obtained by minimizing the objective function. The objective function and the constraints are as follows:

$$\text{minimize } J_{\text{ECBO}}(U, V) = \sum_{k=1}^n \sum_{i=1}^c u_{ki} d_{ki}, \quad \dots \quad (5)$$

$$\text{s.t. } \sum_{i=1}^c u_{ki} = 1, \quad (k = 1, \dots, n) \quad \dots \quad (6)$$

$$K \leq \sum_{k=1}^n u_{ki} \leq K + 1, \quad (i = 1, \dots, c) \quad \dots \quad (7)$$

Equations (5) and (6) are the same objective function and constraint as KM. Eq. (7) is the constraint of cluster size. Depending on the size of the dataset, it may not be possible to divide the dataset evenly; hence each cluster size is defined as K or $K + 1$.

Before starting the ECBO algorithm, a constant K or a cluster number c is needed. The relation between the dataset size n , c , and K in ECBO was considered in [12]. Here, a more precise relation is under consideration.

The relation between n , c , and K is $K = \lfloor n/c \rfloor$. If n and c are given, K exists. On the other hand, even if n and K are given, c does not always exist. Thus, it is necessary to satisfy the following relation between n and K :

$$0 < n \leq (K + 1) \frac{n - (n \bmod K)}{K}. \quad \dots \quad (8)$$

If Eq. (8) holds true,

$$c = \frac{n - (n \bmod K)}{K}. \quad \dots \quad (9)$$

The objective function and constraints are linear with respect to U ; hence, the optimal solution of U can be obtained by using the simplex method. The cluster centers V can be obtained by the following equation.

$$v_i = \frac{\sum_{k=1}^n u_{ki} x_k}{\sum_{k=1}^n u_{ki}}. \quad \dots \quad (10)$$

The ECBO algorithm is shown as **Algorithm 2**.

Algorithm 2 ECBO

Step 1. Give the constant, K or c .

Step 2. Choose the initial cluster centers V from X randomly.

Step 3. Update U by using the simplex method with fixing V .

Step 4. Update V by Eq. (10) with fixing U .

Step 5. If V changes, go back to **Step 3**. Otherwise, stop.

Suitable results can be obtained by using ECBO because ECBO classifies datasets in the framework of optimization. However, constraint (7) is very strict, making ECBO inconvenient to apply when each cluster size does not need to be even. In the following section, the clustering algorithm is proposed to solve these problems.

3. Proposed Method (FECBO)

FCM is constructed by fuzzifying KM. Concretely speaking, the objective function of the FCM is the non-linearized one of the KM by raising the membership u_{ki} to the m -th power.

ECBO could be reconstructed as above. In case of crisp clustering, the concept of “cluster size” is clear. However, the concept in this paper is different from the above. As mentioned in Section 1, there are two ways to classify a dataset into clusters with almost the same cluster size. One way is COCBO [13, 14], another way is proposed in this paper, that is, the membership degree is not crisp, but fuzzy. More suitable results can be obtained based on fuzzy membership by the proposed method than by the crisp method. The meaning of cluster size K is not the same for FECBO as for COCBO. K is allowed as not only an integer but also as a fraction. In this paper, K is calculated as follows.

$$K = \frac{n}{c} (11)$$

The objective function of the ECBO is the same as KM. Therefore, the objective function of the fuzzified ECBO (FECBO) should be the same as the FCM and the constraints are the same as the ECBO, that is,

$$\text{minimize } J_{\text{FECBO}}(U, V) = \sum_{k=1}^n \sum_{i=1}^c u_{ki}^2 d_{ki}, \quad . \quad (12)$$

$$\text{s.t.} \quad \sum_{i=1}^c u_{ki} = 1, \quad (k = 1, \dots, n) \quad \dots (13)$$

$$\sum_{k=1}^n u_{ki} = K. \quad (i = 1, \dots, c) \quad . \quad . \quad (14)$$

The objective function (12) and the constraints (13) are the same as the FCM and the constraints (14) are added to the FCM.

Algorithm 3 FECBO

Step 1. Give the constant c .

Step 2. Choose the initial cluster centers V from X randomly.

Step 3. Update U by the primal-dual path-following method with fixing V .

Step 4. Update V by Eq. (4) with fixing U .

Step 5. If V changes from previous V , go back to **Step 3**. Otherwise, stop.

Therefore, the FECBO is considered not only as an extension of the ECBO by fuzzification but also as an extension of the FCM by adding the constraint of Eq. (14).

FECBO calculates membership by alternate optimization of U and V for the objective function. The optimization for U must satisfy the above constraints. In general, it is very difficult to obtain the optimal solutions to this optimal problem. However, the problem resolves itself into a convex quadratic programming problem in case of $m = 2$, and consequently, it is solved using the primal-dual path-following method [15]. This method was selected for computational efficiency. The optimal solution for V is obtained in the same way as FCM.

The FECBO algorithm is shown as **Algorithm 3**.

4. Numerical Examples

Three datasets, a two-dimensional artificial dataset, the Breast Cancer Wisconsin Database, and a map dataset were used to verify the effectiveness of the proposed algorithm through comparing the FCM, the ECBO, and the proposed FECBO. In case of the FECBO and the FCM, each object is reclassified into a cluster that has the largest membership degree.

4.1. Adjusted Rand Index

In this paper, the Adjusted Rand Index (ARI) [16] is used to evaluate clustering results. The ARI is a measure of the similarity between two classifications, and it is often used as the performance evaluation criteria of clustering results.

Given a dataset of n objects X and suppose two different partitions of the objects in X , $G = \{g_1, \dots, g_R\}$ and $H = \{h_1, \dots, h_C\}$. Here $\bigcup_{i=1}^R g_i = \bigcup_{j=1}^C h_j = X$ and $g_i \cap g_{i'} = h_j \cap h_{j'} = \emptyset$ for $i \neq i'$ and $j \neq j'$. Let ζ_{ij} , ζ_{i*} , and ζ_{*j} are the numbers of objects which are in both clusters g_i and h_j , in the cluster g_i , and in the cluster h_j , respectively. $\zeta_{i*} = \sum_{j=1}^C \zeta_{ij}$ and $\zeta_{*j} = \sum_{i=1}^R \zeta_{ij}$. The ARI is represented

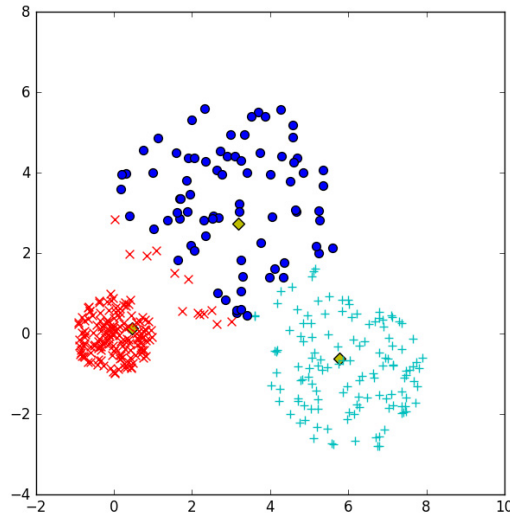


Fig. 1. The partition result by FCM.

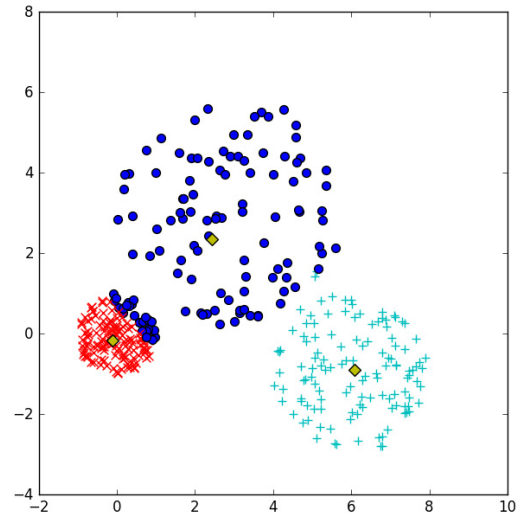


Fig. 2. The partition result by ECBO.

as follows:

$$\text{ARI} = \frac{\sum_{i,j} \binom{\zeta_{ij}}{2} - \left(\sum_i \binom{\zeta_{is}}{2} \sum_j \binom{\zeta_{sj}}{2} \right) / \binom{n}{2}}{\frac{1}{2} \left(\sum_i \binom{\zeta_{is}}{2} + \sum_j \binom{\zeta_{sj}}{2} \right) - \left(\sum_i \binom{\zeta_{is}}{2} \sum_j \binom{\zeta_{sj}}{2} \right) / \binom{n}{2}}. \quad (15)$$

The ARI takes $\text{ARI} = 1 \in [0, 1]$. If the two partitions are the same, $\text{ARI} = 1$. The more similar the two clusters are the closer to 1 the ARI is. Conversely, the more different the two clusters are, the closer to 0 the ARI is.

In order to estimate the performance of each algorithm, it is compared by ARI, with G as the correct dataset and H as the partition by each algorithm.

4.2. Artificial Dataset

This dataset consists of three clusters. Cluster A is a circle with a radius of 1, center at (0.00, 0.00), consisting of 150 objects that are randomly placed. Cluster B is a circle with a radius of 3, center at (3.00, 3.00), consisting of 100 objects that are randomly placed. Cluster C is a circle with a radius of 2, center at (6.00, -1.00), consisting of 120 objects that are randomly placed. Each algorithm classified the dataset with $c = 3$, and 100 times by changing initial values. The results of minimizing the objective function are shown as **Figs. 1–3**.

Table 1 shows the ARI scores and cluster sizes by each method.

In the partition of the artificial dataset, the value of ARI of the proposed method is almost one. It shows that a result close to the correct partition is obtained. You can see natural division in **Fig. 3**, the ECBO cannot classify the dataset naturally because constraint (7) is too strict, and the value of ARI is also the smallest among the three

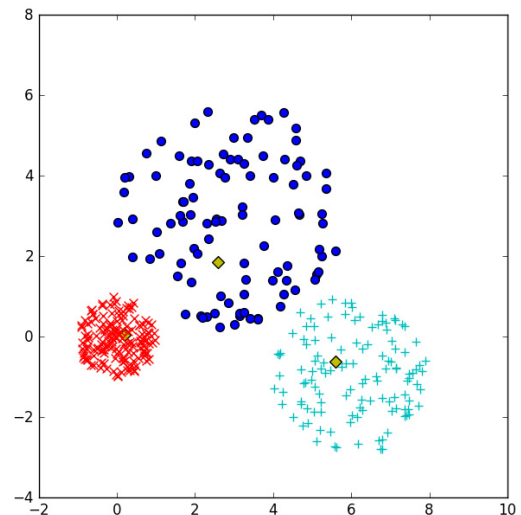


Fig. 3. The partition result by FECBO.

methods. The partition result by the FCM appears least natural.

Next, the cluster center is examined. The cluster centers of A, B, and C obtained using FCM are (0.11, 0.00), (3.07, 3.47), and (6.13, -0.88), respectively. From **Fig. 1**, it can be seen that the boundary line is approximately equidistant from both cluster centers. In contrast, the cluster centers of A, B, and C obtained using FECBO are (-0.03, -0.08), (2.72, 2.68), and (6.15, -0.92), respectively. From **Fig. 3**, it is found that partition is not performed at equidistant positions from both cluster centers. This is owed to the constraints of membership degree; furthermore, in FECBO, the membership degree to A was

Table 1. The ARI and cluster sizes by each method.

	ARI	A	B	C
FCM	0.843	163	78	129
ECBO	0.790	124	123	123
FECBO	0.993	150	99	121

Table 2. The partition results of BCWD.

	ARI	A	B
Correct partition		213	236
FECBO	0.813	217	232
ECBO	0.750	225	224
FCM	0.712	234	215

smaller than FCM.

4.3. Breast Cancer Wisconsin Database

Breast Cancer Wisconsin Database (BCWD) [17] is a dataset summarizing the screening results of patients who had tumors in the chest at the University of Wisconsin Hospital. It includes 9-dimensional indicators, such as tumor status, patient condition, and other data including diagnosis results of whether the patient's tumor is benign (A) or malignant (B). Data that excludes duplicates and treats missing values as 0 were used. Therefore, the number of objects in the experiment data will be less than the number of objects in the original data.

Each algorithm classified the dataset with $c = 2$, $K = 224.5$, and 10 times by changing initial values. The results of minimizing the objective function are shown as **Table 2**.

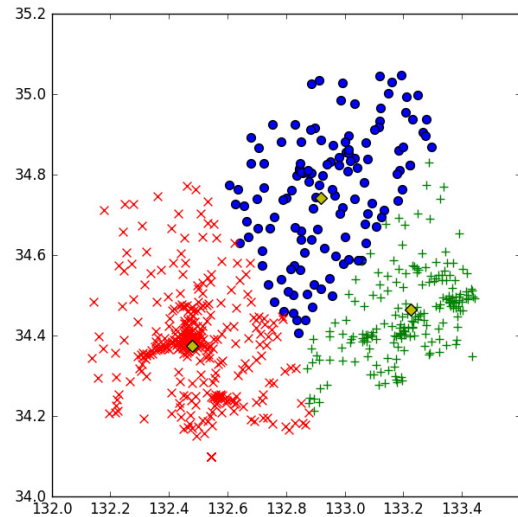
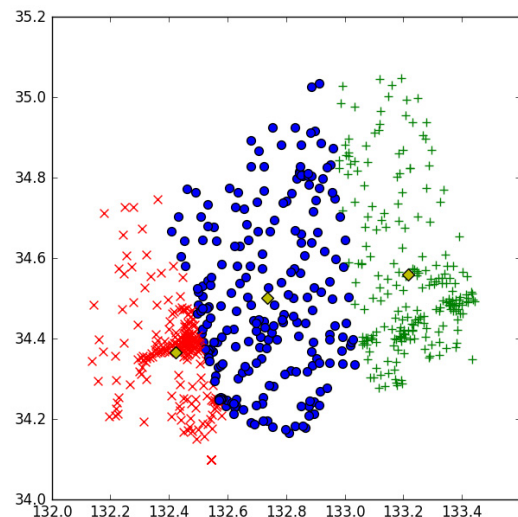
From the ARI value, it is apparent that the FECBO classified the BCWD closest to the correct partition. Moreover, the value of ARI by ECBO is higher than FCM. This is probably because there is no big difference in the cluster size of the correct partition.

In the FECBO and FCM, the cluster size is reversed. This is due to the constraint of membership.

4.4. Map Dataset

As an example of task division problem, we consider dividing the delivery area of a major convenience store chain in Hiroshima prefecture. In the delivery area division problem, it is necessary to minimize the distance from the center of the area to each store and to equalize the number of stores in each area. There were 667 stores in Hiroshima prefecture on December 6, 2016. The latitude and longitude data of each store was classified by each method. Let A, B, and C be the western, middle, and eastern parts of Hiroshima prefecture, respectively.

Each algorithm classifies the dataset with $c = 3$, $K = 322.33$, and 10 times by changing initial values. The results of minimizing the objective function are shown as **Figs. 4–6**.

**Fig. 4.** The partition result by FCM.**Fig. 5.** The partition result by ECBO.

The vertical and the horizontal axes show latitude and longitude, respectively. In addition, the rhombus indicates each cluster center.

Tables 3 and 4 show the cluster sizes by each method and total sum of distance between each store and the cluster center, respectively.

In the FCM result, the area of C is very small, and the area of B is extremely large. The sum of the distances of A is twice that of C. In the delivery area division problem, this result is inconvenient because the burden on each area is greatly different. In the ECBO results, the cluster sizes are almost even. However, the sum of distances is larger than other methods. On the contrary, in the pro-

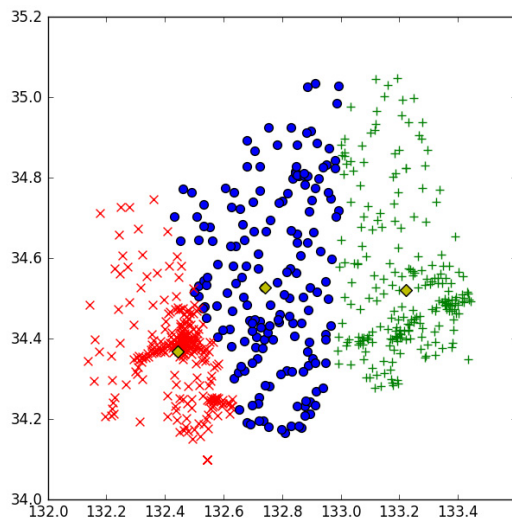


Fig. 6. The partition result by FECBO.

Table 3. Cluster sizes by each method.

Method	A	B	C
FCM	340	195	132
ECBO	223	222	222
FECBO	263	176	228

Table 4. Total sum of distance between each store and the cluster center.

Method	A	B	C	Total sum
FCM	52.8	31.3	27.4	111.5
ECBO	27.0	53.4	45.0	125.4
FECBO	32.6	41.6	44.7	118.9

posed method, the total sum of distances is kept constant while cluster size is adjusted to some extent, and a balanced result is obtained.

5. Conclusion

In this paper, we proposed an even-sized clustering based on optimization with the constraints of a fuzzified membership degree. We estimated the performance of the proposed method in comparison with two conventional methods, FCM and ECBO, using numerical examples.

In the proposed method, we relaxed the ECBO cluster size constraint. This allowed the FECBO to classify the dataset better than conventional methods when there were differences in the size of the correct cluster.

However, the results obtained using the proposed algorithm depend on the initial values as well as FCM and ECBO. Future studies include reducing the dependency on initial values and verifying robustness. With regard to

the dependence on the initial values, we believe that applying k -means++ [18] will reduce the dependency.

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- The Japan Society for Fuzzy Theory and Systems (SOFT)
- The Japanese Society for Artificial Intelligence (JSAI)
- The Institute of Electrical and Electronics Engineering (IEEE)