Fuzzy Possibility C-Mean Based on Mahalanobis Distance and Separable Criterion

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Abstract: The well known fuzzy partition clustering algorithms are most based on Euclidean distance function, which can only be used to detect spherical structural clusters. Gustafson-Kessel (GK) clustering algorithm and Gath-Geva (GG) clustering algorithm, were developed to detect non-spherical structural clusters, but both of them based on semi-supervised Mahalanobis distance needed additional prior information. An improved Fuzzy C-Mean algorithm based on unsupervised Mahalanobis distance, FCM-M, was proposed by our previous work, but it didn’t consider the relationships between cluster centers in the objective function. In this paper, we proposed an improved Fuzzy C-Mean algorithm, FPCM-MS, which is not only based on unsupervised Mahalanobis distance, but also considering the relationships between cluster centers, and the relationships between the center of all points and the cluster centers in the objective function, the singular and the initial values problems were also solved. A real data set was applied to prove that the performance of the FPCM-MS algorithm gave more accurate clustering results than the FCM and FCM-M methods, and the ratio method which is proposed by us is the better of the two methods for selecting the initial values.

Key-Words: FPCM-MS; FPCM-M; FCM-M; GK algorithms; GG algorithms; Mahalanobis distance

1 Introduction
Fuzzy partition clustering is a branch in cluster analysis, it is widely used in pattern recognition field. The well known ones, such as, C. Bezdek’s “Fuzzy C-Mean (FCM)” [1], are all based on Euclidean distance function, which can only be used to detect the data classes with same super spherical shapes.

Extending Euclidean distance to Mahalanobis distance, the well known fuzzy partition clustering algorithms, Gustafson-Kessel (GK) clustering
algorithm [2] and Gath-Geva (GG) clustering algorithm [3] were developed to detect non-spherical structural clusters, but these two algorithms fail to consider the relationships between cluster centers in the objective function, GK algorithm must have prior information of shape volume in each data class, otherwise, it can only be considered to detect the data classes with same volume. GG algorithm must have prior probabilities of the clusters. An improved algorithm, based on Mahalanobis distance, “Fuzzy Possibility C-Mean Based on Mahalanobis Distance and Separable Criterion (FPCM-MS)” is proposed by our previous work [4, 5, 6, 7, 8].

Yin et al. [9] described an extended objective function consisting of a fuzzy within-cluster scatter matrix and a new between-cluster centers scattering matrix. The corresponding fuzzy clustering algorithm assures the compactness between data points and cluster centers and also strengthens the separation between cluster centers based on the separation criterion. Then clustering algorithm solved the relationships between cluster centers question, but they did not consider the distance between the center of all points and the center of each cluster. This problem was also solved and presented in this paper. Moreover, In this paper, an improved fuzzy clustering algorithm, denoted FPCM-MS, was developed based on FCM-M to obtain better quality clustering results with new separable criterion and better initial value. The improved equations for the membership and the cluster center were derived from the alternating optimization algorithm. The distance between the center of all points and the center of each cluster was considered by the authors of this paper, the singular problem was also solved. A real data set was applied to prove that the performance of the FPCM-MS algorithm gave more accurate clustering results than the FCM-M and FCM methods, and the ratio method which is proposed by us is the better of the two methods for selecting the initial values.

2 Some Exist Algorithms

2.1 Fuzzy c-Mean Algorithm
Fuzzy C-Mean Algorithm (FCM) is the most popular objective function based fuzzy clustering algorithm, it is first developed by Dunn [10] and improved by Bezdek [1].The objective function used in FCM is given by Equation (1).

\[ J_{FCM} (U, A, X) = \sum_{i=1}^{c} \sum_{j=1}^{n} \mu_{ij}^{m} ||x_i - a_j|| \]  

\( \mu_{ij} \in [0,1] \) is the membership degree of data object \( x_i \) in cluster \( C_j \), and it satisfies the following constraint given by Equation (2).

\[ \sum_{j=1}^{n} \mu_{ij} = 1, \forall j = 1,2,\ldots,n \]  

C is the number of clusters, \( m > 1 \), which controls the fuzziness of the method. They are both parameters and need to be specified before running the algorithm. \( d_{ij}^2 = ||x_i - a||^2 \) is the square Euclidean distance between data object \( x_i \) to center \( a_j \).

Minimizing objective function (1) with constraint (2) is a non-trivial constraint nonlinear optimization problem with continuous parameters \( a_j \) and discrete parameters \( \mu_{ij} \). So there is no obvious analytical solution. Therefore an alternating optimization scheme, alternatively optimizing one set of parameters while the other set of parameters are considered as fixed, is used here. Then the updating function for \( a_j \) and \( \mu_{ij} \) is obtained as Eq. (3) to Eq. (5).

Step 1: Determining the number of cluster; \( c \) and \( m \)-value (let \( m=2 \)), given converging error, \( \varepsilon > 0 \) (such as \( \varepsilon = 0.001 \)), randomly choose the initial membership matrix, such that the memberships are not all equal;

\[ U^{(0)} = \begin{bmatrix} \mu^{(0)}_{11} & \cdots & \mu^{(0)}_{1c} \\ \vdots & \ddots & \vdots \\ \mu^{(0)}_{n1} & \cdots & \mu^{(0)}_{nc} \end{bmatrix} = \begin{bmatrix} \mu^{(0)}_{11} & \cdots & \mu^{(0)}_{1n} \\ \vdots & \ddots & \vdots \\ \mu^{(0)}_{n1} & \cdots & \mu^{(0)}_{nn} \end{bmatrix} \]  

(3)

Step 2: Find

\[ a_j^{(k)} = \frac{\sum_{i=1}^{n} \left[ \frac{\mu^{(k-1)}_{ij}}{m} \right]^m x_i}{\sum_{i=1}^{n} \left[ \frac{\mu^{(k-1)}_{ij}}{m} \right]^m} \quad i = 1,2,\ldots,c \]  

(4)

\[ \mu_{ij}^{(k)} = \frac{1}{\left[ \sum_{j=1}^{c} \left( \frac{x_i - a_j^{(k)}}{x_i - a_j^{(k)}} \right)^2 \right]^{1/2}} \]  

(5)

Step 3: Increment k; until \( \max_{i,j} \left[ ||a_j^{(k)} - a_j^{(k-1)}|| \right] < \varepsilon \).
2.2 FCM-M Algorithm

For improving the above two problems, our previous work [4, 5, 6, 7, 8] proposed the improved algorithm FCM-M which added a regulating factor of covariance matrix, \(-\ln \left| \Sigma_j^{-1} \right|\), to each class in objective function, and deleted the constraint of the determinant of covariance matrices, \(|\Sigma_j| = \rho_j\), in GK Algorithm as the objective function (6).

Using the Lagrange multiplier method, to minimize the objective function (6) with respect to parameters \(\mu_i, \Sigma_i\), we can obtain the solutions as (10), (11), and (13).

To avoid the singular problem and to select the better initial membership matrix, the updating functions for \(\mu_i, \Sigma_i\), and \(\Sigma\) are obtained as Eq. (8) to (13).

Note that:
(1). Both of FCM and FCM-M can not exploit all of the memberships with the same value.
(2). FCM is a special case of FCM-M, when \(\lambda = 0\).

Determining the number of cluster; \(c\) and \(m\)-value (let \(m=2\), given converging error, \(\varepsilon > 0\) (such as \(\varepsilon = 0.001\)).

Method 1: choose the result membership matrix of FCM algorithm as the initial one.

Method 2: \(d^{(0)}_{ij}, i=1,2,...,c\) let be the result centers of k-mean algorithm, and \(d_{ij} = \|x_i - \omega_{(0)}^j\|\) be distances between data object \(x_i\) to center \(\omega_{(0)}^j\).

\[
d^{(0)}_i = \max_{j=1}^{c} \|x_i - \omega_{(0)}^j\|, \quad d^{(0)}_j = \min_{i=1}^{n} \|x_i - \omega_{(0)}^j\|, \quad \omega_{(0)}^j = \frac{1}{c} \sum_{i=1}^{n} \mu_{ij}^0 x_i
\]

Step 2: Find

\[
\Sigma_j^{(k)} = \frac{\sum_{i=1}^{n} \mu_{ij}^{(k)} (x_i - \omega_{(k)}^j)^2}{\sum_{i=1}^{n} \mu_{ij}^{(k)}}
\]

Step 3: Increment \(k\); until \(\max_{1 \leq i \leq n} \|\omega_{(k)}^i - \omega_{(k-1)}^{(k)}\| < \varepsilon\).

3 New Algorithm - FPCM-MS

The clustering optimization was based on objective function, the choice of an appropriate objective function is the point to the success of the cluster analysis. In FCM-M algorithm, it didn’t consider the relationships between cluster centers in the objective function, now, we proposed an improved Fuzzy C-Mean algorithm, FPCM-MS, which is not only based on unsupervised Mahalanobis distance, but also considering the relationships between cluster centers, and the relationships between the center of all points and the cluster centers in the objective function, the singular and the initial values problems were also solved. Let \(\{x_1, x_2, x_3, ..., x_n\}\) be a set of \(n\) data points represented by \(p\)-dimensional feature vectors \(x_j=(x_{j1}, x_{j2}, ..., x_{jp})^T \in \mathbb{R}^p\). The \(p \times n\) data matrix \(Z\) has the cluster center matrix \(A=[a_{ij}], 1 < c < n\) and the membership matrix \(U=[\mu_{ij}]\), where \(\mu_{ij}\) is the membership value of \(x_i\) belonging to \(a_i\).

\[V = [v_{ik}]\] express the weighting matrix, and \(v_{ik}\) is the weighting value between \(v_i\) and \(v_k\). The fuzzy exponent \(m\) is greater than 1 [11]. Thus, we can
obtained the objective function of Fuzzy Possibility c-Mean based on Mahalanobis distance (FPCM-M) as following

\[ J_{FPCM-M}(U, A, T, \Sigma, X) = \sum_{i=1}^{n} \sum_{j=1}^{n} \left( \mu_{ij}^{m} + t_{ij}^{m} \right) \left( (x_{i} - \bar{x}_{j}) \Sigma^{-1} (x_{i} - \bar{x}_{j}) - \ln |\Sigma| \right) \]

\[ - \frac{1}{c(\varepsilon - 1)} \sum_{i=1}^{n} \sum_{j=1}^{n} v_{ij} \left( \bar{x}_{i} - \bar{x}_{j} \right) \left( \bar{x}_{i} - \bar{x}_{j} \right) \]  

constraints: membership \[ \sum_{j=1}^{n} \mu_{ij} = 1, \quad \forall j = 1, 2, \ldots, n \]

typicality \[ \sum_{i=1}^{n} t_{ij} = 1, \quad \forall i = 1, 2, \ldots, c \]

\[ v(k)_{il} = \frac{w_{il}^{k-1} - \min_{1 \leq r, s \leq c} w_{rs}^{k-1}}{\max_{1 \leq r, s \leq c} w_{rs}^{k-1} - \min_{1 \leq r, s \leq c} w_{rs}^{k-1}}, \quad (15) \]

where \[ w_{rs}^{k-1} = \left\| \bar{x}_{r} - \bar{x}_{s}(k-1) \right\|^2 + \left\| \bar{x}_{r} - \bar{x}_{s}(k-1) \right\|^2 \]

The new fuzzy clustering algorithm can be summarized in the following steps:

Step 1: Determining the number of cluster; c and m-value (let m=2), given converging error, \( \varepsilon > 0 \) (such as \( \varepsilon = 0.001 \)).

Method 1: choose the result membership matrix of FCM algorithm as the initial one.

Method 2: let \( a_{i}^{(n)}, i = 1, 2, \ldots, c \) be the result centers of k-mean algorithm, and be distances between data object \( x \) to center \( a_{i}^{(n)} \).

\[ z_{i}^{(n)} = \begin{cases} \frac{d_{i} - d_{j}}{d_{j} - d_{i}}, & \text{if } d_{i} > d_{j} \\ \frac{d_{j} - d_{i}}{d_{j} - d_{i}}, & \text{if } d_{j} > d_{i} \end{cases}, \quad i = 1, 2, \ldots, c; \quad j = 1, 2, \ldots, n \]

\[ z_{i}^{(n)} = \sum_{j=1}^{n} \frac{t_{ij}^{(n)}}{\sum_{j=1}^{n} t_{ij}^{(n)}}, \quad i = 1, 2, \ldots, c; \quad j = 1, 2, \ldots, n \]

\[ \mu_{ij}^{(0)} = \frac{z_{i}^{(n)}}, \quad i = 1, 2, \ldots, c; \quad j = 1, 2, \ldots, n \]

\[ t_{ij}^{(0)} = \frac{z_{j}^{(n)}}, \quad i = 1, 2, \ldots, c; \quad j = 1, 2, \ldots, n \]

\[ v(k)_{il} = \frac{w_{il}^{k-1} - \min_{1 \leq r, s \leq c} w_{rs}^{k-1}}{\max_{1 \leq r, s \leq c} w_{rs}^{k-1} - \min_{1 \leq r, s \leq c} w_{rs}^{k-1}} \]

\[ U^{(0)} = \left[ \begin{array}{c} \mu_{11}^{(0)} \mu_{12}^{(0)} \ldots \mu_{1c}^{(0)} \\ \mu_{21}^{(0)} \mu_{22}^{(0)} \ldots \mu_{2c}^{(0)} \\ \vdots \vdots \vdots \\ \mu_{c1}^{(0)} \mu_{c2}^{(0)} \ldots \mu_{cc}^{(0)} \end{array} \right] \]

\[ A^{(0)} = \left[ \begin{array}{c} a_{1}^{(0)} a_{2}^{(0)} \ldots a_{c}^{(0)} \end{array} \right] \]

\[ \Sigma^{(0)} = \left[ \begin{array}{cccc} \Sigma_{11}^{(0)} & \Sigma_{12}^{(0)} & \ldots & \Sigma_{1c}^{(0)} \\ \Sigma_{21}^{(0)} & \Sigma_{22}^{(0)} & \ldots & \Sigma_{2c}^{(0)} \\ \vdots & \vdots & \ddots & \vdots \\ \Sigma_{c1}^{(0)} & \Sigma_{c2}^{(0)} & \ldots & \Sigma_{cc}^{(0)} \end{array} \right] \]

Step 2: Find
where
\[ w_r (k-1) = \left\| u_r - a_r (k-1) \right\|^2 + \left\| u_r - d_a (k-1) \right\|^2 \]

\[ a_r = \left[ F_r \right]^{\top} \left\{ \sum_{i=1}^n \left[ \mu_i (k) \right] a_i ^{\top} + \left[ \nu_i (k) \right] b_i ^{\top} \right\} x_r - d_i \]

\[ F_r = \left[ \sum_{i=1}^n \left[ \mu_i (k) \right] a_i ^{\top} + \left[ \nu_i (k) \right] b_i ^{\top} \right] \left[ \Sigma_i ^{\top} \right]^{-1} + d_i \]

\[ \mu_i (k) = \left[ \sum_{j=1}^c \left[ F_j \right]^{\top} \left[ \mu_j (k) \right] a_j ^{\top} + \left[ \nu_j (k) \right] b_j ^{\top} \right] \left[ \Sigma_i ^{\top} \right]^{-1} \]

\[ \nu_i (k) = \left[ \sum_{j=1}^c \left[ F_j \right]^{\top} \left[ \mu_j (k) \right] a_j ^{\top} + \left[ \nu_j (k) \right] b_j ^{\top} \right] \left[ \Sigma_i ^{\top} \right]^{-1} \]

\[ \Sigma_i ^{i(i)} = \sum_{i=1}^n \left[ \mu_i (k) \right] a_i ^{\top} + \left[ \nu_i (k) \right] b_i ^{\top} \]

Step 3: Increment k; until \( \max_{i=1,2,...,c} \left\| u_i (k) - a_r (k-1) \right\| < \varepsilon \).

4 Experiment
A real data set of students with sample size 493 from elementary schools was selected. These data included the independent variables, test scores of four mathematics concepts (division, ordering, multiplication, and place value) and 10 questions.

At first, the main factors of the data were calculated by using factor analysis. Next, according to the main factors, the samples were assigned to 4 clusters based on the clustering analysis using the k-mean clustering of SPSS for Windows 10.0. The results were shown in Table 1.

<table>
<thead>
<tr>
<th>Clu size</th>
<th>mathematics concepts</th>
<th>average distance of the points from center of cluster</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>100 division</td>
<td>1.2879</td>
</tr>
<tr>
<td>2</td>
<td>82 ordering</td>
<td>1.7861</td>
</tr>
<tr>
<td>3</td>
<td>173 multiplication</td>
<td>1.1402</td>
</tr>
<tr>
<td>4</td>
<td>138 place value</td>
<td>1.2890</td>
</tr>
</tbody>
</table>

Each 15 sample points were randomly drawn from Cluster 1, cluster 2, and cluster 3, respectively, and 5 from cluster 4.

How to select the better initial value to improve the cluster accuracy is an important issue. In order to test the FCM-M algorithm, developed by the authors of this paper, the four .25 were selected as initial value. After calculating, the results were found that the memberships were all equal to .25 too. This evidence displayed that the FCM-M algorithm was work correctly.

There were 2 methods (Ratio, Random) to calculate the Normalized initial number which satisfied the Equation (2).

The steps of Ratio Method were as follows.
Step 1: The distance between observing value and every cluster center of every Point, say d. Compute the Average Distance of Clustering Result Marking Group.

\[ cd_i = \sum_{j=1}^c n_{ji} \]

Step 2: Compute the Difference of d and the Average Distance of Clustering Result Marking Group

\[ l_i = \left| d_i - cd_i \right|, i = 1, 2, ..., c \]

Step 3: Find the values of maximum and minimum

\[ M = \max \left\{ l_i, j = 1, 2, ..., n, i = 1, 2, ..., c \right\} \]

\[ m = \min \left\{ l_i, j = 1, 2, ..., n, i = 1, 2, ..., c \right\} \]

Step 4: Compute the initial membership Difference of every Point

\[ \mu_i = \frac{M - l_i}{(M - m)^{\top}} \]

The steps of Random Method were as follows.
Choose any 4 random numbers, r1, r2, r3, and r4.
Step 1: Choose any 4 random numbers, r1, r2, r3, and r4, such that 0 < r_i < 1, i = 1, 2, 3, 4.
Step2: Let \( S = r_1 + r_2 + r_3 + r_4 \), then \( r_1/S, r_2/S, r_3/S, r_4/S \) were calculated as one set of initial value. The classification accuracies of testing samples were shown in Table 2.

<table>
<thead>
<tr>
<th>choosing the initial membership</th>
<th>computing distance</th>
<th>Classification Accuracies (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ratio</td>
<td>FCM</td>
<td>30</td>
</tr>
<tr>
<td></td>
<td>PCM</td>
<td>32</td>
</tr>
<tr>
<td></td>
<td>FPCM</td>
<td>36</td>
</tr>
<tr>
<td></td>
<td>FPCM-M</td>
<td>44</td>
</tr>
<tr>
<td></td>
<td>FPCM-MS</td>
<td>56</td>
</tr>
<tr>
<td>Random</td>
<td>FCM</td>
<td>12</td>
</tr>
<tr>
<td></td>
<td>PCM</td>
<td>14</td>
</tr>
<tr>
<td></td>
<td>FPCM</td>
<td>30</td>
</tr>
<tr>
<td></td>
<td>FPCM-M</td>
<td>44</td>
</tr>
<tr>
<td></td>
<td>FPCM-MS</td>
<td>54</td>
</tr>
</tbody>
</table>

From the data of Table 2, we found that the FPCM-MS algorithms of **Ratio Method** could obtain the best results, up to 56%. Next, the FPCM-MS algorithms of **Random Method** could obtain the second better results, up to 54%.

5 Conclusion

An improved new fuzzy clustering algorithm, FPCM-MS, is developed to obtain better quality of fuzzy clustering results. The objective function includes a fuzzy within-cluster scatter matrix, a new between-prototypes scatter matrix, the regulating terms about the covariance matrices, and the regulating terms about the relationships between cluster centers, the relationships between the center of all points and the cluster centers. The update equations for the memberships and the cluster centers and the covariance matrices are directly derived from the Lagrange’s method, which is different from the GK and GG algorithms. The singular problem and the selecting initial values problem are improved by the Eigenvalue method and the Ratio method. Finally, a numerical example shows that the new fuzzy clustering algorithm FPCM-MS gives more accurate clustering results than the FCM and FCM-M algorithms for a real data set, the ratio method which is proposed by us is the better of the two methods for selecting the initial values.

References:


