

On Mahalanobis Distance Based Fuzzy c -Means Clustering for Uncertain Data Using Penalty Vector Regularization

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Abstract—This paper presents Mahalanobis distance based fuzzy c -means clustering for uncertain data using penalty vector regularization. When we handle a set of data, data contains inherent uncertainty e.g., errors, ranges or some missing value of attributes. In order to handle such uncertain data as a point in a pattern space the concept of penalty vector has been proposed. Some significant clustering algorithms based on it have been also proposed. In conventional clustering algorithms, Mahalanobis distance have been used as dissimilarity as well as squared L_2 and L_1 -norm. From the viewpoint of the guideline of dissimilarity, Mahalanobis distance based fuzzy c -means clustering for uncertain data should be considered. In this paper, we introduce fuzzy c -means clustering for uncertain data using penalty vector regularization as our conventional works. Next, we propose Mahalanobis distance based one. Moreover, we show the effectiveness of proposed method through numerical examples.

Index Terms—fuzzy c -means clustering, penalty vector regularization, uncertain data, Mahalanobis distance.

I. INTRODUCTION

Advanced data analysis methods are required in order to discover important properties from massive and complex databases. Data analysis method consists of supervised learning and unsupervised one. Data clustering simply called clustering is the most well-known unsupervised learning method. Clustering is a method which divides a set of objects into some groups which are referred to as clusters. Objects in same cluster are considered similar, while objects in different cluster are considered dissimilar. The method of K -means which referred to as hard c -means clustering (HCM) is the most popular clustering method [1]. Fuzzy c -means clustering (FCM) [2], [3] is an extension of HCM. In fuzzy c -means clustering, squared Euclidean distance [1]–[3], L_1 -norm [4], [5] and Mahalanobis distance [6], [7] are used as dissimilarity.

By the way, each data is conventionally handled as a point in a pattern space and analyzed in clustering procedures. However, there are many cases that data contains inherent uncertainty such as errors, ranges or missing value of attributes. Typical examples of uncertain data are as follows:

- **Errors being introduced when the object is mapped from the real space to pattern space:**

This kind of error is one of the most typical examples. A round-off error, a truncation error, and a reading error margin are introduced when we map a data from the real space to the pattern space.

- **Missing value of attributes:**

When we handle data from the questionnaires, there are several questions which are not answered. This causes the missing value of attributes.

These uncertain data are represented by other form instead of a point [8], [9]. Even now, handling uncertain data have been actively studied in many researches [8]–[10]. This means handling uncertain data is one of the significant problems in the field of data mining.

From the viewpoint of handling uncertain data, a concept of tolerance has been proposed and formulated into clustering procedures as the constraint [11]. Moreover, clustering algorithms for data with tolerance have been also proposed [12]–[14]. In these clustering methods for data with tolerance, uncertain data is handled as data with tolerance.

In addition, the concept of penalty vector have been proposed to remove the constraint for tolerance [15], [16]. This concept is formulated on the basis of the concept of regularization such as L_2 or L_1 regularization terms. By introducing regularization terms, some fuzzy c -means clustering algorithms have been proposed [17], [18]. In these clustering algorithms, the L_1 -norm [17] and the squared L_2 -norm [18] are used as dissimilarity. However, Mahalanobis distance based fuzzy c -means clustering using penalty vector concept has not been discussed. From that sense, we propose Mahalanobis distance based fuzzy c -means clustering for uncertain data using penalty vector regularization.

The contents of this paper are the followings. In the second section, we denote some symbols, fuzzy c -means clustering (FCM). In the third section, we introduce the concept of penalty vector regularization. In the forth section, Mahalanobis distance based fuzzy c -means clustering for uncertain data using penalty vector regularization (FCMQS). In the fifth section, we show the effectiveness of proposed method through

numerical examples. In the last section, we conclude this paper.

II. PRELIMINARIES

Let a data, a cluster and its cluster center be $x = (x_{k1}, \dots, x_{kp})^T \in \mathbb{R}^p$, ($k = 1, \dots, n$), C_i ($i = 1, \dots, c$) and $v_i = (v_{i1}, \dots, v_{ip})^T \in \mathbb{R}^p$, respectively. Moreover, u_{ki} is the membership grade of x_k belonging to C_i and we denote a partition matrix $U = (u_{ki})_{1 \leq k \leq n, 1 \leq i \leq c}$. Here, a set of data and a set of cluster center be $X = \{x_1, \dots, x_n\}$, $V = \{v_1, \dots, v_c\}$, respectively.

A. Fuzzy c -Means Clustering

Fuzzy c -means clustering is based on optimizing an objective function under the constraint for membership grade.

We consider following two objective functions J_s and J_e .

$$J_s(U, V) = \sum_{k=1}^n \sum_{i=1}^c (u_{ki})^m d_{ki},$$

$$J_e(U, V) = \sum_{k=1}^n \sum_{i=1}^c \{u_{ki} d_{ki} + \lambda^{-1} u_{ki} \log u_{ki}\}.$$

here, m and λ is fuzzified parameters.

J_s is a well-known objective function as standard fuzzy c -means clustering (sFCM) proposed by Bezdek [2] and J_e is an entropy based fuzzy c -means clustering (eFCM) [3].

The constraint for u_{ki} is as follows:

$$\mathcal{U}_f = \left\{ (u_{ki}) : u_{ki} \in [0, 1], \sum_{i=1}^c u_{ki} = 1, \forall k \right\}. \quad (1)$$

The dissimilarity for clustering is generally the squared L_2 -norm between each data and a cluster center:

$$d_{ki} = \|x_k - v_i\|^2 = \sum_{j=1}^p (x_{kj} - v_{ij})^2.$$

In addition, the L_1 -norm based FCM [4], [5] Mahalanobis distance based one [6], [7] are also considered. In Mahalanobis distance based FCM, the dissimilarity is as follows:

$$d_{ki} = (x_k - v_i)^T S_i (x_k - v_i).$$

where $S_i = (S_{ijl})_{1 \leq i \leq c, 1 \leq j, l \leq p}$ is a positive definite matrix having p^2 elements. In Mahalanobis distance based FCM, S_i is handled as a variable for optimization. The set of S_i is denoted by $S = \{S_1, \dots, S_c\}$. The constraint for S_i is as follows:

$$|S_i| = \rho_i, (\rho_i > 0), \forall i. \quad (2)$$

where ρ_i is a constant and $|S_i|$ is the determinant of S_i .

B. Concept of Tolerance

In general, each data is regarded as one point and classified into clusters. However, the uncertain data should be often represented in other form, instead of a point. In the concept of tolerance, data is handled as data with tolerance $x_k + \varepsilon_k$ [11]. A tolerance vector $\varepsilon_k = (\varepsilon_{k1}, \dots, \varepsilon_{kp})^T \in \mathbb{R}^p$ is within the tolerance κ_k . A set of tolerance vector is denoted as $E = \{\varepsilon_1, \dots, \varepsilon_n\}$. By introducing this concept, clustering

algorithms for data with tolerance have been proposed [12]–[14]. A constraint for tolerance vector is as follows:

$$(\varepsilon_{kj})^2 \leq (\kappa_{kj})^2, (\kappa_{kj} \geq 0), \forall k, j. \quad (3)$$

III. CONCEPT OF PENALTY VECTOR REGULARIZATION

Next, we introduce a concept of penalty vector. In the above-mentioned clustering algorithms for data with tolerance, the upper bound of ε_k is constrained by (3). Therefore, those clustering algorithms can not handle the data with unknown range. Thus, we have to consider another way to handle uncertain data with unknown range. From the viewpoint of handling uncertain data with unknown range, the concept of penalty vector has been proposed [15], [16]. A penalty vector is denoted as $\delta_k = (\delta_{k1}, \dots, \delta_{kp})^T \in \mathbb{R}^p$ and a set of δ_k is $\Delta = \{\delta_1, \dots, \delta_n\}$. In clustering algorithms by using the concept of penalty vector, the data is represented as $x_k + \delta_k$ [17], [18]. The regularization terms for penalty vector are as follows:

$$\sum_{k=1}^n \sum_{j=1}^p \omega_{kj} (\delta_{kj})^2, \quad (4)$$

$$\sum_{k=1}^n \sum_{j=1}^p \omega_{kj} |\delta_{kj}|. \quad (5)$$

where, $\omega_{kj} > 0$ is a regularization parameter.

As the generalization of (4), the quadratic term for δ_k is considered as follows [18]:

$$\sum_{k=1}^n \delta_k^T W_k \delta_k. \quad (6)$$

where, $W_k = (\omega_{kjl})_{1 \leq k \leq n, 1 \leq j, l \leq p}$ is a positive definite matrix having p^2 elements. In case that W_k is a diagonal matrix, the second term of J_s is the same as (4). In particular, the diagonal elements ω_{kjj} affect d_{ki} . The bigger ω_{kjj} is, the smaller the optimal solution δ_{kj} is. Oppositely, the smaller ω_{kjj} is, the bigger the optimal solution δ_{kj} is. Hence, we know that W_k means the uncertainty of x_k .

By using this concept, fuzzy c -means clustering for uncertain data using penalty vector regularization (FCMQ) has been constructed [18].

IV. MAHALANOBIS DISTANCE BASED FUZZY c -MEANS CLUSTERING FOR UNCERTAIN DATA USING PENALTY VECTOR REGULARIZATION

In this section, we propose Mahalanobis distance based fuzzy c -means clustering for uncertain data using penalty vector regularization (FCMQS). The dissimilarity for proposed method is Mahalanobis distance between $x_k + \delta_k$ and v_i written as follows:

$$d_{ki} = (x_k + \delta_k - v_i)^T S_i (x_k + \delta_k - v_i).$$

If we fix S_i with unit matrix, proposed method is equivalent to FCMQ.

A. Mahalanobis Distance Based Standard Fuzzy c -Means Clustering for Uncertain Data Using Penalty Vector Regularization

First of all, we propose Mahalanobis distance based standard fuzzy c -means clustering for uncertain data using penalty vector regularization (sFCMQS). The objective function of sFCMQS is as follows:

$$J_s(U, \Delta, V, S) = \sum_{k=1}^n \sum_{i=1}^c (u_{ki})^m d_{ki} + \sum_{k=1}^n \delta_k^T W_k \delta_k.$$

The constraints for u_{ki} and S_i remain the same as (1) and (2). From the convexity of objective function, the constraints (1) and (2), we introduce the following Lagrangian L_s as follows:

$$L_s = J_s(U, \Delta, V, S) + \sum_{k=1}^n \gamma_k \left(\sum_{i=1}^c u_{ki} - 1 \right) + \sum_{i=1}^c \psi_i \log \frac{|S_i|}{\rho_i}.$$

where, γ_k and ψ_i are Lagrange multiplier.

The optimal solutions for u_{ki} and v_i are derived from $\frac{\partial L_s}{\partial u_{ki}} = 0$ and $\frac{\partial J_s}{\partial v_i} = 0$ as follows:

$$u_{ki} = \frac{\left(\frac{1}{d_{ki}} \right)^{\frac{1}{m-1}}}{\sum_{l=1}^c \left(\frac{1}{d_{kl}} \right)^{\frac{1}{m-1}}}, \quad (7)$$

$$v_i = \frac{\sum_{k=1}^n (u_{ki})^m (x_k + \delta_k)}{\sum_{k=1}^n (u_{ki})^m}. \quad (8)$$

Next, we consider δ_k . From $\frac{\partial J_s}{\partial \delta_k} = 0$, we can get

$$\sum_{i=1}^c (u_{ki})^m S_i (x_k + \delta_k - v_i) + W_k \delta_k = 0. \quad (9)$$

We put two symbols A_k and B_k are as follows:

$$A_k = \sum_{i=1}^c (u_{ki})^m S_i + W_k, \\ B_k = \sum_{i=1}^c (u_{ki})^m S_i (x_k - v_i)$$

Then,

$$A_k \delta_k = B_k.$$

From above, the optimal solution for δ_k is derived as follows:

$$\delta_k = -A_k^{-1} B_k. \quad (10)$$

Last, we consider S_i . From $\frac{\partial L_s}{\partial S_i} = 0$, we can get

$$\sum_{k=1}^n (u_{ki})^m (x_k + \delta_k - v_i) (x_k + \delta_k - v_i)^T + \psi_i S_i^{-1} = 0.$$

From above,

$$S_i = -\psi_i F_i^{-1}.$$

where F_i is following:

$$F_i = \sum_{k=1}^n (u_{ki})^m (x_k + \delta_k - v_i) (x_k + \delta_k - v_i)^T$$

From the constraint $|S_i| = \rho_i$,

$$(-\psi_i)^p |F_i^{-1}| = \rho_i.$$

Hence,

$$-\psi_i = \left(\frac{\rho_i}{|F_i^{-1}|} \right)^{\frac{1}{p}}.$$

Finally, the optimal solution for S_i is derived as follows:

$$S_i = \left(\frac{\rho_i}{|F_i^{-1}|} \right)^{\frac{1}{p}} F_i^{-1}. \quad (11)$$

B. Mahalanobis Distance Based Entropy Based Fuzzy c -Means Clustering for Uncertain Data Using Penalty Vector Regularization

Next, we propose entropy based FCMQS (eFCMQS). The objective function of eFCMQS J_e is as follows:

$$J_e(U, \Delta, V) = \sum_{k=1}^n \sum_{i=1}^c \{u_{ki} d_{ki} + \lambda^{-1} u_{ki} \log u_{ki}\} + \sum_{k=1}^n \delta_k^T W_k \delta_k. \quad (12)$$

The constraints for u_{ki} and S_i remain the same as (1) and (2). By the same procedures, the optimal solutions for u_{ki} , v_i , δ_k and S_i are derived as follows:

$$u_{ki} = \frac{\exp(-\lambda d_{ki})}{\sum_{l=1}^c \exp(-\lambda d_{kl})}, \quad (13)$$

$$v_i = \frac{\sum_{k=1}^n u_{ki} (x_k + \varepsilon_k)}{\sum_{k=1}^n u_{ki}}, \quad (14)$$

$$\delta_k = -A'_k{}^{-1} B'_k, \quad (15)$$

$$S_i = \left(\frac{\rho_i}{|F_i'^{-1}|} \right)^{\frac{1}{p}} F_i'^{-1}. \quad (16)$$

where, A'_k , B'_k and F'_i are as follows:

$$A'_k = \sum_{j=1}^p u_{ki} S_i + W_k,$$

$$B'_k = \sum_{i=1}^c u_{ki} S_i (x_k - v_i),$$

$$F'_i = \sum_{k=1}^n u_{ki} (x_k + \delta_k - v_i) (x_k + \delta_k - v_i)^T$$

C. Algorithm of Proposed Method

The algorithm of FCMQS is described as Algorithm 1. Eqs. A, B, C and D used in each algorithm follow Table I.

Algorithm 1 FCMQS

- FCMQS1** Set initial values and parameters.
FCMQS2 Calculate $u_{ki} \in U$ by using Equation A.
FCMQS3 Calculate $v_i \in V$ by using Equation B.
FCMQS4 Calculate $\delta_k \in \Delta$ by using Equation C.
FCMQS5 Calculate $S_i \in S$ by using Equation D.
FCMQS6 If convergence criterion is satisfied, stop. Otherwise go back to **FCMQS2**.

TABLE I
THE OPTIMAL SOLUTIONS OF FCMQS.

Algorithm	Eq. A	Eq. B	Eq. C	Eq. D
sFCMQS	(7)	(8)	(10)	(11)
eFCMQS	(13)	(14)	(15)	(16)

V. NUMERICAL EXAMPLES

In this section, we show numerical examples of FCMQ and FCMQS with Polaris data set. This data set is the star chart of Polaris and its neighboring stars. This data set consists of 51 points which are allocated in two dimensional space and should be classified into three clusters. The fuzzified parameter $m = 2.0$ for sFCMQ and sFCMQS, while $\lambda = 1.0$ for eFCMQ and eFCMQS. Moreover, $\rho_i = 1.0$ in each algorithm.

We show classification results by sFCMQ, sFCMQS, eFCMQ and eFCMQS with some parameters W_k . In Figs. 1, 4, 7, 10, 2, 5, 8, 11 and 3, 6, 9, 12, W_k^1 , W_k^2 , and W_k^3 are used, respectively.

$$W_k^1 = \begin{pmatrix} 2.0 & 0.0 \\ 0.0 & 2.0 \end{pmatrix}, \forall k,$$

$$W_k^2 = \begin{pmatrix} 2.0 & 0.2 \\ 0.2 & 2.0 \end{pmatrix}, \forall k,$$

$$W_k^3 = \begin{pmatrix} 2.0 & 0.2 \\ 0.2 & 1.0 \end{pmatrix}, \forall k.$$

From these results, δ_k obtained by sFCMQ and eFCMQ indicate the belonging cluster center, while δ_k obtained by sFCMQS and eFCMQS indicate in the same straight line through the belonging cluster center. The reason is that A_k^{-1} and S_i work as rotation matrix for B_k .

This feature is typical difference between FCMQ and FCMQS. The effectiveness of proposed algorithm is shown from these classification results.

VI. CONCLUSIONS

In this paper, we have introduced the concept of penalty vector regularization in order to handle uncertain data. Moreover, we have proposed Mahalanobis distance based Fuzzy c -Means Clustering for uncertain data using penalty vector regularization (FCMQS). The proposed method is quite different from conventional clustering methods for uncertain data from the viewpoint of handling uncertain data as data with penalty vector. Furthermore, we have verified the effectiveness of proposed methods with numerical examples.

In future works, we will consider the relation and effect between S_i and W_k . Moreover, we will show the effectiveness

of our proposed method and consider the features of our proposed methods in detail through various kinds of data set. In particular, it is an important problem to reveal the cluster shapes obtained by proposed method

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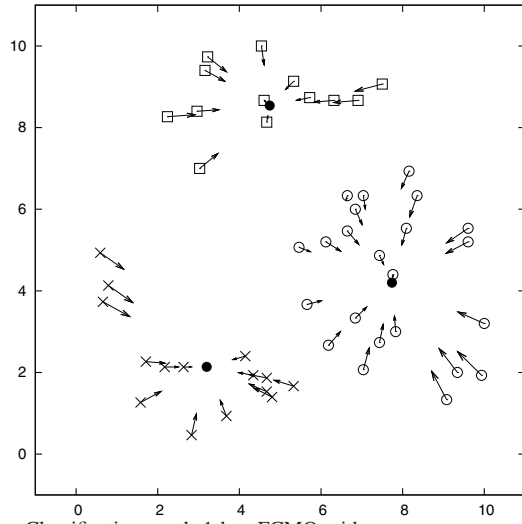


Fig. 1. Classification result 1 by sFCMQ with $\omega_{k11} = \omega_{k22} = 2.0$, $\omega_{k12} = \omega_{k21} = 0.0 \forall k$.

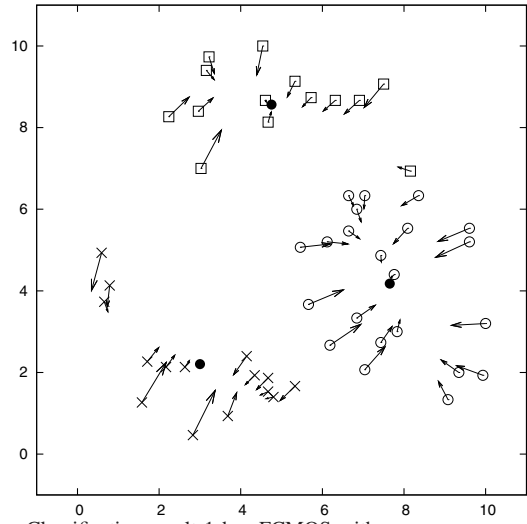


Fig. 4. Classification result 1 by sFCMQS with $\omega_{k11} = \omega_{k22} = 2.0$, $\omega_{k12} = \omega_{k21} = 0.0 \forall k$.

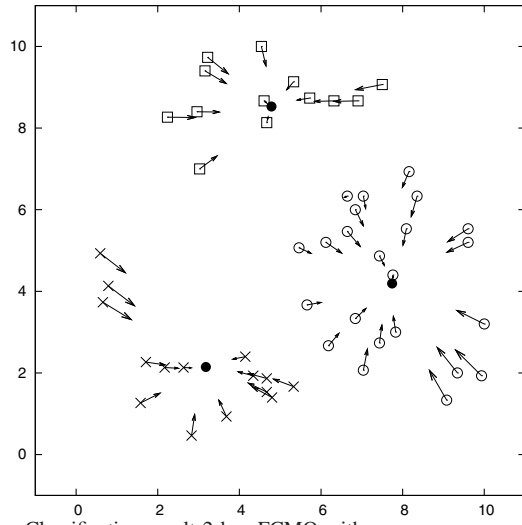


Fig. 2. Classification result 2 by sFCMQ with $\omega_{k11} = \omega_{k22} = 2.0$, $\omega_{k12} = \omega_{k21} = 0.2 \forall k$.

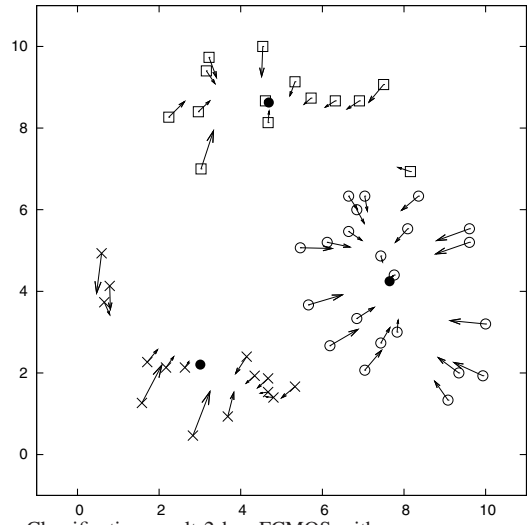


Fig. 5. Classification result 2 by sFCMQS with $\omega_{k11} = \omega_{k22} = 2.0$, $\omega_{k12} = \omega_{k21} = 0.2 \forall k$.

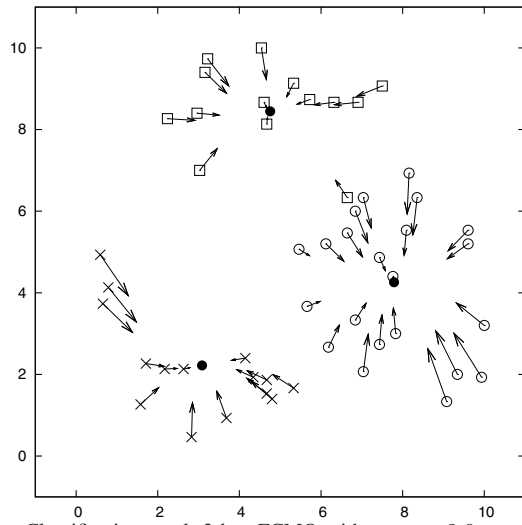


Fig. 3. Classification result 3 by sFCMQ with $\omega_{k11} = 2.0$, $\omega_{k12} = \omega_{k21} = 0.2$, $\omega_{k22} = 1.0 \forall k$.

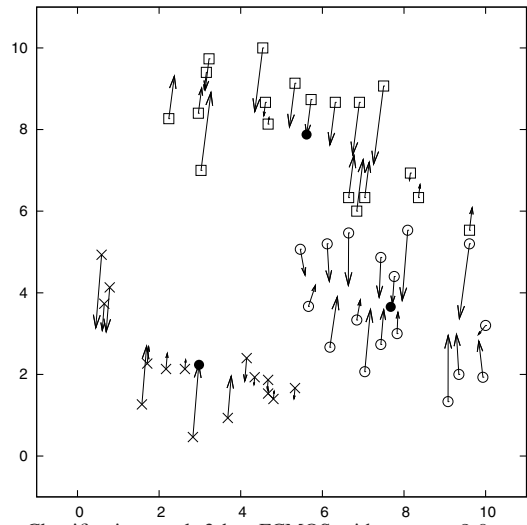


Fig. 6. Classification result 3 by sFCMQS with $\omega_{k11} = 2.0$, $\omega_{k12} = \omega_{k21} = 0.2$, $\omega_{k22} = 1.0 \forall k$.

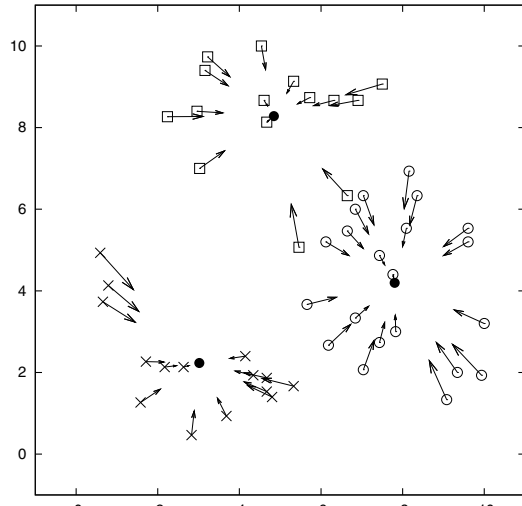


Fig. 7. Classification result 1 by eFCMQ with $\omega_{k11} = \omega_{k22} = 2.0$, $\omega_{k12} = \omega_{k21} = 0.0 \forall k$.

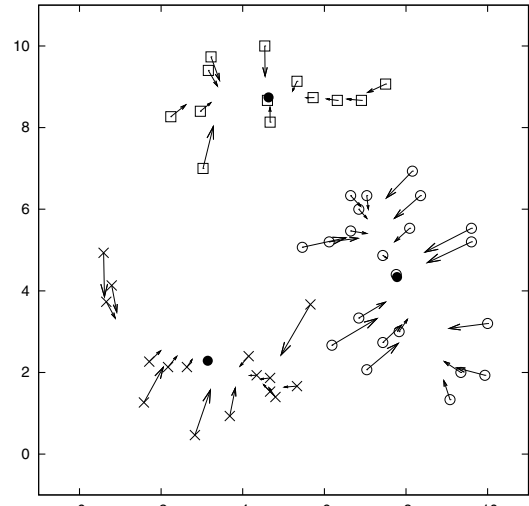


Fig. 10. Classification result 1 by eFCMQS with $\omega_{k11} = \omega_{k22} = 2.0$, $\omega_{k12} = \omega_{k21} = 0.0 \forall k$.

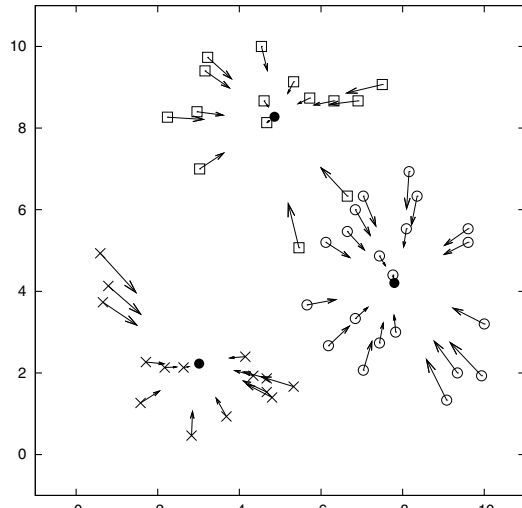


Fig. 8. Classification result 2 by eFCMQ with $\omega_{k11} = \omega_{k22} = 2.0$, $\omega_{k12} = \omega_{k21} = 0.2 \forall k$.

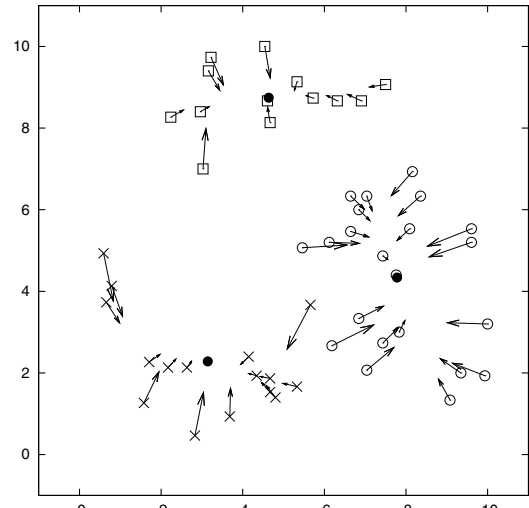


Fig. 11. Classification result 2 by eFCMQS with $\omega_{k11} = \omega_{k22} = 2.0$, $\omega_{k12} = \omega_{k21} = 0.2 \forall k$.

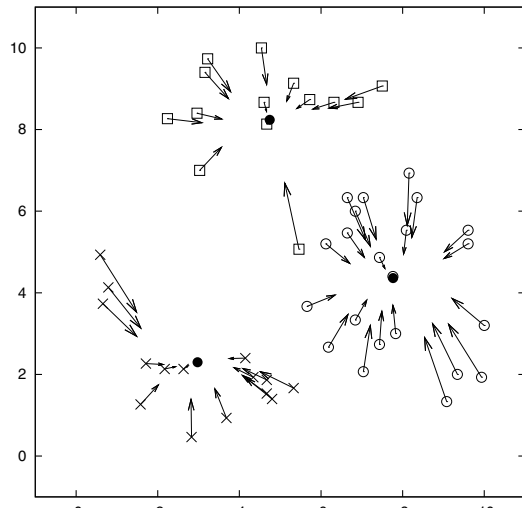


Fig. 9. Classification result 3 by eFCMQ with $\omega_{k11} = 2.0$, $\omega_{k12} = \omega_{k21} = 0.2$, $\omega_{k22} = 1.0 \forall k$.

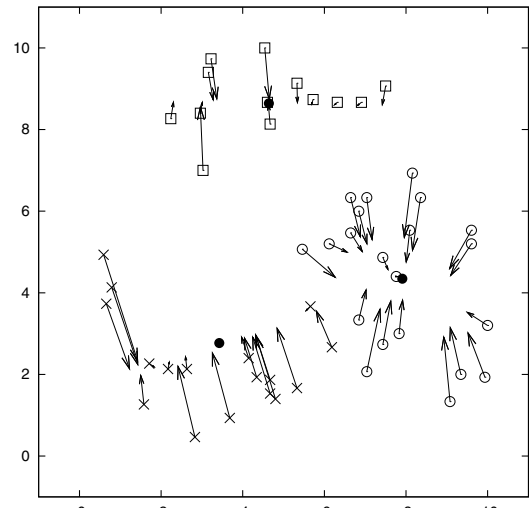


Fig. 12. Classification result 3 by eFCMQS with $\omega_{k11} = 2.0$, $\omega_{k12} = \omega_{k21} = 0.2$, $\omega_{k22} = 1.0 \forall k$.