

FCMdd-type Linear Fuzzy Clustering for Incomplete Non-Euclidean Relational Data

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Abstract—A linear fuzzy clustering model based on Fuzzy c -Medoids (FCMdd) was proposed for extracting intrinsic local linear substructures from relational data. In the same way with Non-Euclidean Relational Fuzzy (NERF) c -Means, β -spread transformation was also proved to be useful for handling non-Euclidean relational data in FCMdd-type linear clustering. In this paper, the FCMdd-type linear clustering model is further modified in order to handle incomplete data including missing values. In several numerical experiments, it is demonstrated that some pre-imputation strategies contribute to properly selecting representative medoids of each cluster.

Keywords—relational clustering, linear fuzzy clustering, missing value.

I. INTRODUCTION

Relational data analysis is an important technique for revealing intrinsic structure of relational data composed of mutual relations among objects. Besides the basic fuzzy clustering models for object-type data such as Fuzzy c -Means (FCM) [1], which is a fuzzy extension of k -Means [2], several relational fuzzy clustering models have been proposed for extracting cluster substructures from relational data. Relational Fuzzy c -Means (RFCM) [3] is the basic FCM-type relational clustering model, which can be identified with FCM when mutual relations are given by Euclidean distances. k -Medoids approach [5] is an alternative of FCM-type clustering where cluster prototypes are not given by mean vectors but are chosen from object sets. Krishnapuram *et al.* [4] extended (hard) k -Medoids to Fuzzy c -Medoids (FCMdd), in which the chosen object called “medoid” is the representative object of a cluster. FCMdd-type clustering models can easily be applied to relational data matrices without calculating cluster centroids in a intrinsic data space.

FCM-type linear fuzzy clustering models such as Fuzzy c -Lines (FCL) [6] and its variants [7] use linear-shape prototypes like lines, planes and linear varieties. Fitting lines or linear varieties to data sets, the linear clustering models perform fuzzy principal component analysis (fuzzy PCA) [8] in each cluster [9]. Haga *et al.* [10] proposed an FCMdd-type linear clustering model where each linear prototype is spanned by several representative “medoids”.

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When relational data are not Euclidean, FCM-type and FCMdd-type clustering models cannot be directly applied because their algorithms are essentially designed for Euclidean data space. Hathaway and Bezdek [11] proposed non-Euclidean-type Relational Fuzzy (NERF) c -Means, in which a spreading transformation called β -spread transformation is performed in order to decrease the influences of non-Euclidean relations. Yamamoto *et al.* [12] applied the β -spread transformation to FCMdd-type linear clustering and demonstrated that a suitable data transformation is achieved by selecting proper parameter values automatically.

In [13], Hathaway and Bezdek demonstrated that the β -spread transformation is also useful for handling missing elements in relational data matrices, in which the bad influences of imputation errors are decreased by β -spread transformation. This paper demonstrates that the performance of FCMdd-type linear fuzzy clustering for incomplete relational data can also be improved by β -spread transformation through several experiments.

II. FCMDD-TYPE LINEAR CLUSTERING FOR RELATIONAL DATA

A. FCM-type Linear Clustering

Assume that we have m dimensional observations of n samples $\mathbf{x}_i = (x_{i1}, \dots, x_{im})^T, i = 1, \dots, n$ and that the goal is to partition the n samples into C clusters. The objective function for FCM-type clustering is defined as:

$$L_{fcm} = \sum_{c=1}^C \sum_{i=1}^n u_{ci}^\theta D_{ci} \quad (1)$$

where u_{ci} is the fuzzy membership degree of sample i to cluster c , and θ is the fuzzification parameter. The larger the θ , the fuzzier the membership assignment. The clustering criterion D_{ci} is the distance between sample i and the prototype of cluster c . Besides point-type prototypes in FCM, FCL used linear prototypes defined as:

$$Line_c(\mathbf{b}_c, \mathbf{a}_c) = \{\mathbf{x} | \mathbf{x} = \mathbf{b}_c + t\mathbf{a}_c; t \in R\}, \quad (2)$$

where $\mathbf{a}_c$ is the basis vector of the principal sub-space. The clustering criterion is calculated as:

$$D_{ci} = \|\mathbf{x}_i - \mathbf{b}_c\|^2 - |\mathbf{a}_c^T(\mathbf{x}_i - \mathbf{b}_c)|^2. \quad (3)$$

The updating rules for membership u_{ci} and the cluster center $\mathbf{b}_c$ are derived as:

$$u_{ci} = \left[\sum_{l=1}^C \left(\frac{D_{ci}}{D_{li}} \right)^{\frac{1}{\theta-1}} \right]^{-1}, \quad (4)$$

$$\mathbf{b}_c = \frac{\sum_{i=1}^n u_{ci}^\theta \mathbf{x}_i}{\sum_{i=1}^n u_{ci}^\theta}. \quad (5)$$

The basis vectors $\mathbf{a}_c$ are the principal eigenvectors of the generalized fuzzy scatter matrix:

$$S_{fc} = \sum_{i=1}^n u_{ci}^\theta (\mathbf{x}_i - \mathbf{b}_c)(\mathbf{x}_i - \mathbf{b}_c)^\top. \quad (6)$$

B. FCM-type Relational Clustering

When we have relational data composed of mutual relations among samples $D = \{d_{ij}\}$, the FCM-type objective function is redefined as [3]:

$$L_{rfcm} = \sum_{c=1}^C \sum_{i=1}^n \sum_{j=1}^n \frac{u_{ci}^\theta u_{cj}^\theta d_{ij}^2}{2 \sum_{t=1}^n u_{ct}^\theta}. \quad (7)$$

If the mutual relation d_{ij} is given by the Euclidean distance among samples i and j , the relational clustering model is equivalent to FCM with object-type data. However, the clustering model can derive only poor results if the relational information is not Euclidean.

In order to transform a non-Euclidean matrix to one of Euclidean form, Hathaway and Bezdek [11] considered the following β -spread transformation:

$$D_\beta = D + \beta \times (M - I), \quad (8)$$

where I is a unit matrix and β is a suitably chosen scalar. M is a matrix whose elements are all 1. It was shown that D_β is Euclidean if $PD_\beta P$ with $P = I - (1/n)M$ is negative semi-definite, i.e., β is greater than or equal to the largest eigenvalue of PDP . In NERF, β is gradually increased from 0 to a certain value by considering the negative elements of clustering criteria because negative values of the clustering criterion signal the non-existence of Euclidean space and indicate that the current value of β should be increased so that the basic RFCM iteration can be continued.

C. FCMdd-type Linear Clustering

Assume that d_{ij} is the mutual Euclidean distance such that

$$d_{ii} = 0, d_{ij} \geq 0, d_{ij} = d_{ji}, i, j = 0, \dots, n. \quad (9)$$

FCMdd [4] is a fuzzy extension of k -Medoids, which performs an FCM-like clustering by selecting $\mathbf{b}_c$ from objects $\mathbf{x}_i$, $i = 1, \dots, n$. The representative objects are called ‘medoids’.

Haga et al. [10] applied the idea to linear fuzzy clustering, in which two representative medoids are selected in each cluster and the prototypical line is defined as:

$$Line_c(\mathbf{x}_{c1}, \mathbf{x}_{c2}) = \{\mathbf{x} | \mathbf{x} = \mathbf{x}_{c1} + t(\mathbf{x}_{c2} - \mathbf{x}_{c1}); t \in R\}. \quad (10)$$

The squared Euclidean distance between object i and the prototypical line $Line_c$ is given as:

$$D_{ci} = d_{i,c1}^2 - \frac{(d_{i,c1}^2 - d_{i,c2}^2 + d_{c1,c2}^2)^2}{4d_{c1,c2}^2}. \quad (11)$$

With fixed fuzzy memberships u_{ci} , the optimal representative medoids $\mathbf{x}_{c1}$ and $\mathbf{x}_{c2}$ in cluster c are derived by $\mathbf{x}_{q1}$ and $\mathbf{x}_{q2}$ as follows:

$$(q1, q2) = \arg \min_{\substack{(k1, k2) \\ 1 \leq k1, k2 \leq n \\ k1 \neq k2}} \sum_{i=1}^n u_{ci}^\theta D_{ci}. \quad (12)$$

In order to reduce the computational cost of the combinatorial optimization problem, a simplified medoid search process was also proposed such that medoids are selected from a subset X_c of objects having large memberships as follows:

$$(q1, q2) = \arg \min_{\substack{(k1, k2) \\ \mathbf{x}_{k1}, \mathbf{x}_{k2} \in X_c \\ k1 \neq k2}} \sum_{i=1}^n u_{ci}^\theta D_{ci}, \quad (13)$$

where $X_c = \{\mathbf{x}_i : u_{ci} > M_{min}\}$.

This linear fuzzy clustering model was also extended to the 2-D prototype case by spanning 2-D prototypical planes using three medoids [10].

When $D = d_{ij}$ is Non-Euclidean, the clustering criterion of Eq.(11) can be negative. From the practical view point, we have no trouble in operating the conventional FCMdd-type linear clustering algorithm if all clustering criteria are not negative. Yamamoto *et al.* [12] proposed a method for automatically transforming non-Euclidean relational data with β -spread transformation when clustering criteria have negative value in FCMdd-type linear clustering. If all relational data elements satisfy triangle inequality, clustering criteria are non-negative, i.e., if triangle inequality ($d_{c1,c2} \leq d_{i,c1} + d_{i,c2}$) is satisfied, the clustering criterion D_{ci} is positive. For all objects, the following triangle inequality transformed by β -spread transformation should be satisfied.

$$d_{c1,c2} + \beta \leq d_{i,c1} + \beta + d_{i,c2} + \beta. \quad (14)$$

Then, the β should satisfy the following relation:

$$\beta \geq d_{c1,c2} - d_{i,c1} - d_{i,c2}. \quad (15)$$

and, a plausible value of $\Delta\beta$ in a iteration step is obtained as:

$$\Delta\beta = \max\{d_{c1,c2} - d_{i,c1} - d_{i,c2} - \beta\}, \quad (16)$$

where $\Delta\beta = 0$ if $\Delta\beta < 0$. Then, β is monotonically increasing.

A sample procedure including the automated β -spread transformation can be summarized as follows:

- Step.1 Set $\beta = 0$. Randomly initialize the prototypical medoids (two representative objects) of each cluster.
- Step.2 Calculate the clustering criteria D_{ci} .
- Step.3 If there are at least one object that has $D_{ci} < 0$, update $\beta = \beta + \Delta\beta$ by Eq.(16).
- Step.4 Update fuzzy memberships.

Step.5 Search medoids in each cluster.

Step.6 Repeat Steps 2-5 until a certain stopping criterion is satisfied.

III. APPLICATION TO INCOMPLETE RELATIONAL DATA INCLUDING MISSING ELEMENTS

In real applications, relational data matrices may have missing elements. In such cases, the FCMdd-type linear clustering algorithm should be applied after imputing the missing elements. Hathaway and Bezdek [13] demonstrated that the β -spread transformation is also useful for handling missing elements in relational data matrices, in which β -spread transformation is responsible for decreasing the bad influences of imputation errors. This paper considers the applicability of several imputation techniques used in [13] in FCMdd-type linear clustering.

Hathaway and Bezdek [13] used three imputation technique based on triangle inequality-based approximation(TIBA).

A. minimax TIBA

The triangle inequality, which Euclidean relational data always satisfy, is represented as follows:

$$d_{ij} \leq d_{ik} + d_{kj}. \quad (17)$$

Assume that an element of relational matrix $\tilde{d}_{ij}$ is missing and that it brings

$$\tilde{d}_{ij} = \tilde{d}_{ji}. \quad (18)$$

Let K_{ij} as the corresponding index set as

$$K_{ij} = \{k | d_{ik} \text{ and } d_{kj} \text{ exist}\}. \quad (19)$$

Although it is very rare that K_{ij} is empty, $\tilde{d}_{ij}$ is defined as zero value if K_{ij} is empty. For each $k \in K_{ij}$, the triangle inequality Eq.(17) is given as upper bound of $\tilde{d}_{ij}$. In minimax TIBA, missing elements are replaced with the minimum upper bound of $\tilde{d}_{ij}$:

$$\tilde{d}_{ij} = \tilde{d}_{ji} = \min_k \{d_{ik} + d_{kj}\}. \quad (20)$$

B. maximin TIBA

The triangle inequality is also represented as follows:

$$d_{ik} \leq \tilde{d}_{ij} + d_{jk} \quad (21)$$

$$d_{jk} \leq \tilde{d}_{ji} + d_{ik}. \quad (22)$$

and brings the following inequalities:

$$\tilde{d}_{ij} \geq d_{ik} - d_{jk} \quad (23)$$

$$\tilde{d}_{ji} \geq d_{jk} - d_{ik} \quad (24)$$

So, the lower bound of $\tilde{d}_{ij}$ is given as:

$$\tilde{d}_{ij} \geq |d_{ik} - d_{jk}|. \quad (25)$$

In maximin TIBA, missing elements are replaced with the maximum lower bound of $\tilde{d}_{ij}$:

$$\tilde{d}_{ij} = \tilde{d}_{ji} = \max_k \{|d_{ik} - d_{jk}|\}. \quad (26)$$

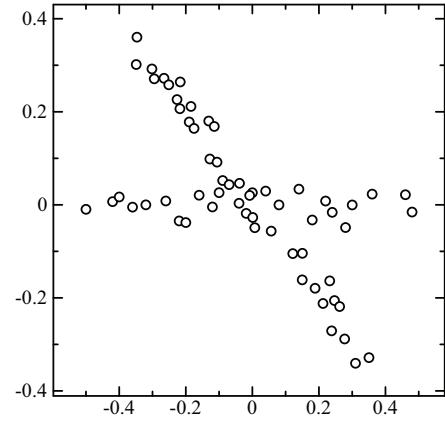


Fig. 1. 2-D plots of artificial data set

C. Average TIBA

It is also reasonable to use the complement value of the previous two imputation values. In average TIBA, the average values of minimax TIBA and maximin TIBA is used for imputing missing elements.

These imputation techniques based on triangle inequalities can be easily applied to relational clustering problems. In the next section, these three imputation approaches are compared in FCMdd-type linear clustering tasks in conjunction with β -spread transformation.

IV. NUMERICAL EXPERIMENTS

Several experimental results are shown in order to consider the applicability of the three TIBA imputation techniques in FCMdd-type linear clustering with β -spread transformation.

A. Artificial Data Set 1

First numerical experiment was performed using an artificially generated relational data set. The relational data set composed of 60 objects was generated from a 2-D data set shown in Fig. 1, in which objects form two line-shape clusters. The first relational data matrix was generated by Euclidean norm. The iterative algorithm was performed until the medoids become unchanged and the model parameters were set as $(C, \theta) = (2, 2)$. In order to demonstrate the characteristics of the algorithm, the initial memberships were given in a supervised manner, i.e., $(u_{1i}, u_{2i}) = (0.9, 0.1)$ for the first visual cluster and $(u_{1i}, u_{2i}) = (0.1, 0.9)$ for the second one.

Figure 2 shows the cluster partition (maximum membership partition) derived by FCMdd-based linear fuzzy clustering without missing elements, where objects were partitioned into two clusters of circles and times, smaller times has very fuzzy memberships, and the medoids and prototypical lines are indicated by black circles and lines, respectively. This Euclidean relational data can be successfully partitioned without β -spread transformation.

Next, incomplete relational data matrices were generated by removing a part of off-diagonal elements so that K_{ij} was not empty. In order to protect tridiagonal parts of relational

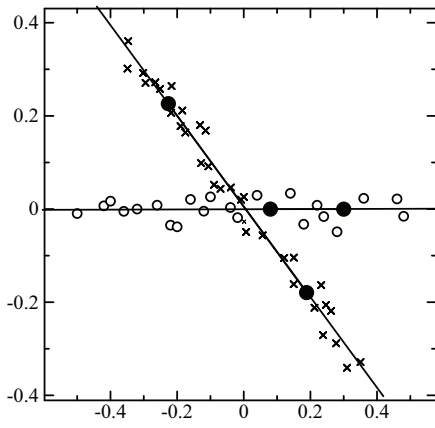


Fig. 2. Cluster partition of Euclidean data without missing elements

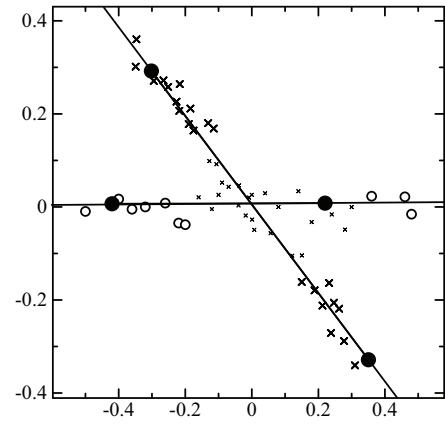
data, the maximum number of missing elements was set as $n^2 - 3n + 2$.

Clustering results are depicted in Fig. 3. Each approximation method could estimate cluster medoids for capturing the two visual linear prototypes until the numbers of missing elements are less than about 30%. Small crosses having ambiguous memberships increased more than complete relational data of Fig. 2. β -spread transformation performed on each approximation, e.g. minimax TIBA: $\beta = 0.04867$, maximin TIBA: $\beta = 0.044286$, average TIBA: $\beta = 0.051706$. The maximum eigenvalues of PDP were also calculated as minimax TIBA: 0.053808, maximin TIBA: 0.1711612, average TIBA: 0.083694. This results imply that the FCMdd-type linear clustering can successfully extract linear substructures of incomplete Euclidean relational data using β -spread transformation although the three imputation technique could regenerate non-Euclidean relational matrices only.

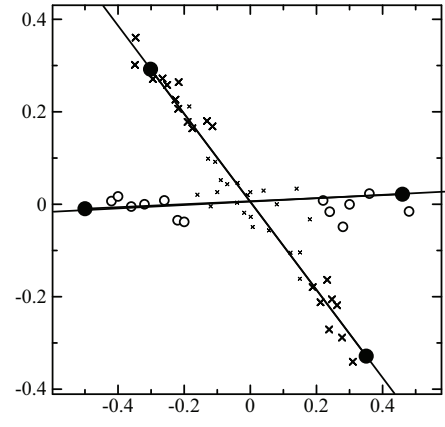
B. Artificial Data Set 2

The second relational data matrix was generated by using L1 norm from Fig. 1. Figure 4 shows the cluster partition derived without missing elements. The linear substructures were successfully estimated by using β -spread transformation with $\beta = 0.005808$, which is much smaller than the maximum eigenvalue of PDP 0.44933. In this way, β -spread transformation plays an important role for handling non-Euclidean relational data in FCMdd-type linear clustering.

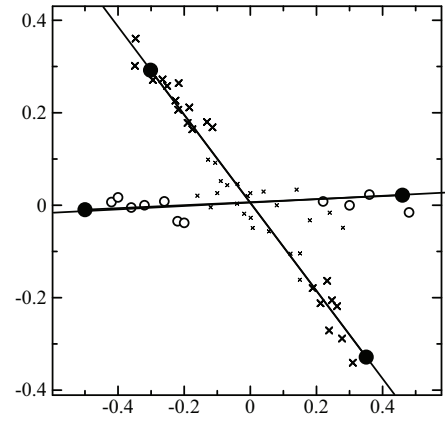
Next, incomplete relational data matrices were generated in a same manner with the Euclidean case. Clustering results were depicted in Fig. 5. Minimax TIBA and average TIBA could extract linear prototypes until the numbers of missing elements are less than about 60%, and maximin TIBA also could until about 40%. The parameters β in β -spread transformation were given as, minimax TIBA: $\beta = 0.23344$, maximin TIBA: $\beta = 0.137577$, average TIBA: $\beta = 0.165504$. The derived β values are still smaller than the maximum eigenvalues of PDP, minimax TIBA: 0.655306, maximin TIBA: 0.427750, average TIBA: 0.619776. In this way, β -spread transformation also works well in incomplete situations.



(a) minimax TIBA (# missing: 500)



(b) maximin TIBA (# missing: 400)



(c) average TIBA (# missing: 500)

Fig. 3. Comparison of cluster partitions from relational data imputed by three TIBA (Euclid norm)

C. Ekman's Color Similarities Data

Third, the proposed algorithm is applied to the Ekman's color similarities data [14]. The 14×14 data matrix is composed of mutual similarities among 14 different colors. In this experiment, mutual similarities s_{ij} are first transformed

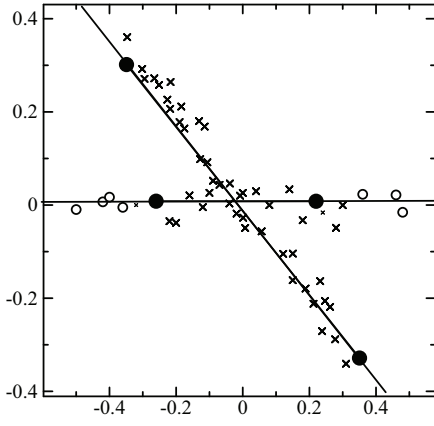


Fig. 4. Cluster partition of L1 norms without missing elements

into dis-similarity measure as follows:

$$d_{ij} = \max_{k,l} s_{kl} - s_{ij}. \quad (27)$$

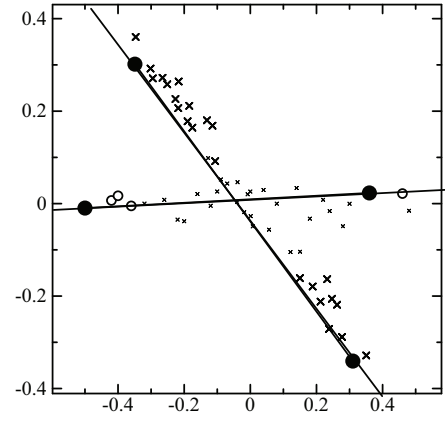
In the proposed algorithm, parameters were set as $C = 2$, $\theta = 2.0$. Figure 6 shows the derived cluster partitions on the 2-D plane constructed by multi-dimensional scaling (MDS) [15]. Minimax TIBA and average TIBA derived a same cluster partition, in which colors from purple to blue belonged to the first cluster while colors from yellow, green to red belonged to another cluster. Other colors equally belonged to both classes. This cluster partition is almost similar to the case without missing elements. Maximin TIBA also derived a similar partition to the other imputation technique, but this partition was more ambiguous. The parameters β in β -spread transformation were given as, minimax TIBA: $\beta = 275.085$, maximin TIBA: $\beta = 59.776$, average TIBA: $\beta = 134.000$. The derived β values are still smaller than the maximum eigenvalues of PDP, minimax TIBA:430.8659, maximin TIBA:150.667, average TIBA:192.596. Here, maximin TIBA gave a much smaller β value than the maximum eigenvalues of PDP. It may be the reason why it derived a very ambiguous partition.

D. Rothkopf Morse Code Confusion Data

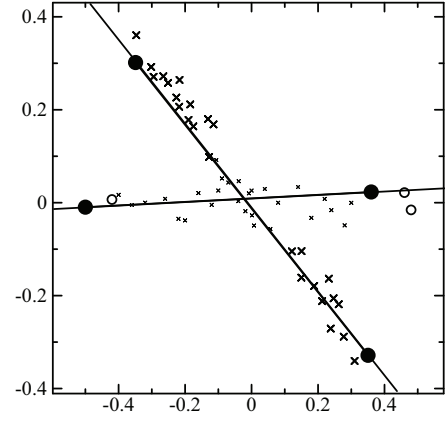
Fourth, the proposed approach is applied to the classical Rothkopf Morse code confusion data [16]. The (36×36) relational data is composed of confusion rates among 36 Morse code signals (26 letters and 10 digits). Before the experiment, the asymmetric relational data matrix, whose element s_{ij} represents the percentage of trials that i was identified as j , was transformed into a symmetric relational data matrix as follows:

$$d_{ij} = s_{ii} + s_{jj} - s_{ij} - s_{ji} \quad (28)$$

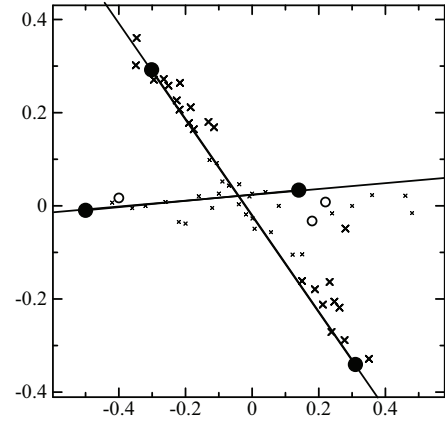
The model parameters were set as $C = 3$, $\theta = 2.0$. Clustering results are depicted in Fig. 7, which constructed on the 2-D plane by MDS. Minimax TIBA and average TIBA allowed with 30 % missing values or fewer. Maximin TIBA resulted in a good partition with 10 % missing values or



(a) minimax TIBA (# missing: 1000)



(b) maximin TIBA (# missing: 700)



(c) average TIBA (# missing: 1100)

Fig. 5. Comparison of cluster partition from relational data imputed by three TIBA (L1 norm)

fewer. The parameters β in β -spread transformation were given as, minimax TIBA: $\beta = 226.945$, maximin TIBA: $\beta = 91.523$, average TIBA: $\beta = 0.0$. The derived β values are still smaller than the maximum eigenvalues of PDP, minimax TIBA:460.808, maximin TIBA:173.284, average TIBA:132.503. In this experiment, average TIBA was the best imputation method of the three TIBA, because average

TIBA did not need β -spread transformation. However, a similar partition was derived with β -spread transformation even when missing values were imputed by other methods.

In this way, β -spread transformation also works well with incomplete real world data.

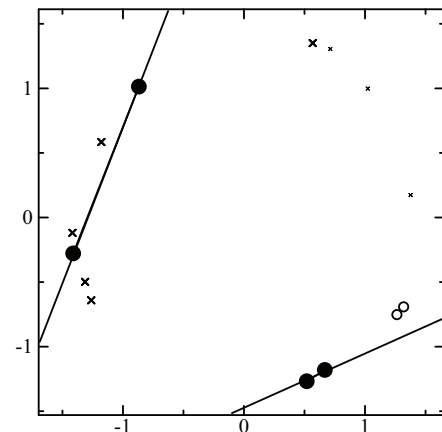
V. CONCLUSION

This paper considered the applicability of β -spread transformation for handling incomplete relational data in FCMdd-type linear clustering. In numerical experiments, three imputation techniques of minimax TIBA, maximin TIBA and average TIBA were compared using two artificially generated data sets and a real one. The experimental results indicated that β -spread transformation still works well for incomplete data while minimax TIBA and average TIBA seem to be better than maximin TIBA. It is because that relational data imputed by maximin TIBA were more non-Euclidean.

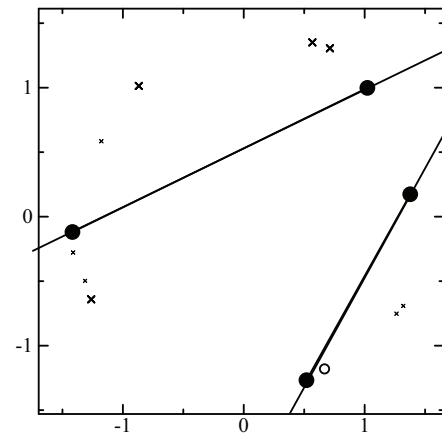
A potential future work is extension to the case of multi-dimensional prototype models.

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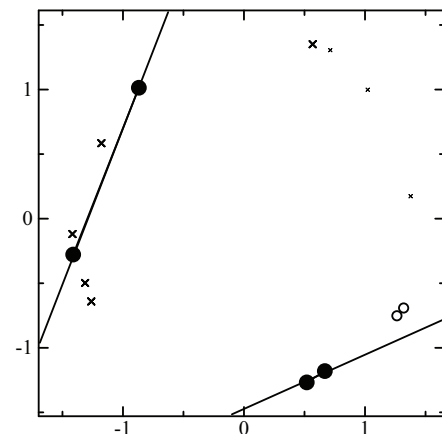
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(a) minimax TIBA (# missing: 70)

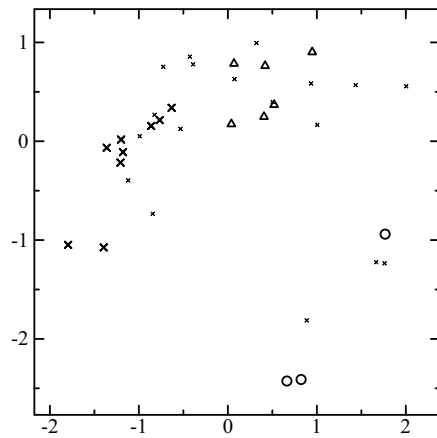


(b) maximin TIBA (# missing: 40)

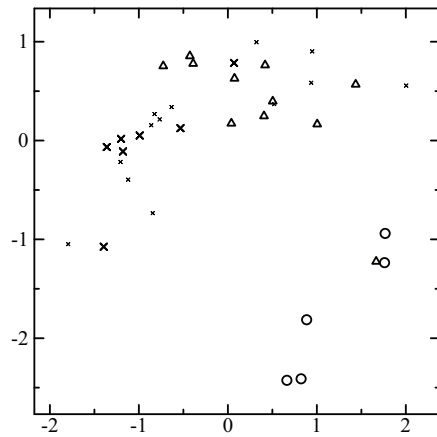


(c) average TIBA (# missing: 70)

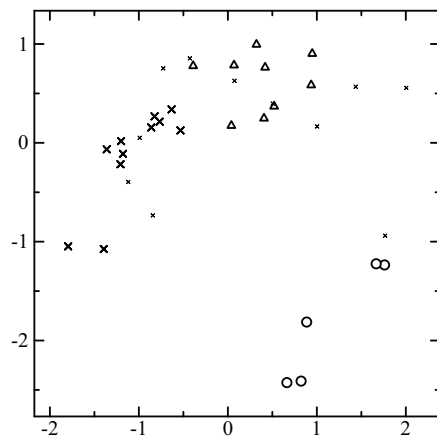
Fig. 6. Comparison of cluster partition from incomplete Ekman's color data imputed by three TIBA



(a) minimax TIBA (# missing: 300)



(b) maximin TIBA (# missing: 100)



(c) average TIBA (# missing: 300)

Fig. 7. Comparison of cluster partition from incomplete Rothkopf Morse Code Confusion Data imputed by three TIBA