Accepted Manuscript

Possibilistic and fuzzy clustering methods for robust analysis of non-precise data

Maria Brigida Ferraro, Paolo Giordani

Please cite this article in press as: M.B. Ferraro, P. Giordani, Possibilistic and fuzzy clustering methods for robust analysis of non-precise data, *Int. J. Approx. Reason.* (2017), http://dx.doi.org/10.1016/j.ijar.2017.05.002
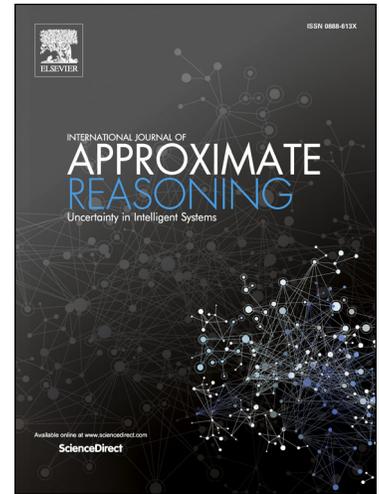
Highlights

- A robust clustering method for imprecise data is proposed
- The clustering process is based on fuzzy and possibilistic approaches
- Imprecision is managed in terms on fuzzy sets
- A new cluster validity index is suggested

Possibilistic and fuzzy clustering methods for robust analysis of non-precise data

Maria Brigida Ferraro, Paolo Giordani

Dipartimento di Scienze Statistiche, Sapienza Università di Roma,
P.le Aldo Moro, 5 - 00185, Rome, Italy

Abstract

This work focuses on robust clustering of data affected by imprecision. The imprecision is managed in terms of fuzzy sets. The clustering process is based on the fuzzy and possibilistic approaches. In both approaches the observations are assigned to the clusters by means of membership degrees. In fuzzy clustering the membership degrees express the degrees of sharing of the observations to the clusters. In contrast, in possibilistic clustering the membership degrees are degrees of typicality. These two sources of information are complementary because the former helps to discover the best fuzzy partition of the observations while the latter reflects how well the observations are described by the centroids and, therefore, is helpful to identify outliers. First, a fully possibilistic k-means clustering procedure is suggested. Then, in order to exploit the benefits of both the approaches, a joint possibilistic and fuzzy clustering method for fuzzy data is proposed. A selection procedure for choosing the parameters of the new clustering method is introduced. The effectiveness of the proposal is investigated by means of simulated and real-life data.

Keywords: Imprecise information, Robustness, Fuzzy clustering, Possibilistic clustering, Cluster validity.

1. Introduction

In most practical applications the results of the statistical analysis may be poor due to some outliers or other departures from the ideal conditions on which the statistical methods are based. In the cluster analysis framework, the presence of contaminated data is usually deleterious: a limited number

of outliers may lead to a completely wrong and inaccurate partition of the observations. In this work, following the fuzzy approach and the closely related possibilistic one, some robust clustering procedures will be proposed. In doing so, we assume to deal with a special kind of data, i.e., non-precise data. A fruitful way to handle imprecision is by means of fuzzy sets [1, 2, 3]. In this connection, it is important to distinguish between the epistemic and ontic nature of the fuzzy data. In the epistemic approach fuzzy data are seen as imprecise measurements of precise data. Thus, the available information on a precise quantity is ill-known and the lack of precision is managed through fuzzy sets. In the ontic approach fuzzy data are seen as whole entities, hence the quantity under investigation is assumed to be intrinsically imprecise. In practice, the distinction between the epistemic and ontic fuzzy sets has a relevant impact on the statistical tools to apply. See, for more details, [4, 5]. In this work we assume to deal with ontic fuzzy sets.

A lot of standard clustering procedures have been generalized to the fuzzy data case. The use of belief functions in the clustering process is considered in [6]. Clustering fuzzy data by means of mixtures of distributions is suggested in [7, 8]. The large majority of the proposals are based on the fuzzy k-means algorithm and consist mainly in introducing suitable dissimilarity measures for fuzzy data [9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19]. Robust clustering methods for fuzzy data can be found in [20, 21, 22, 23, 24, 25]. These are robust versions of the fuzzy k-means algorithm for such a kind of data and can be distinguished with respect to the approach adopted for handling the outliers. In the precise data case, these can be roughly summarized as follows (we refer to the review in [26] for a deeper insight). An approach consists in the use of *medoids* (see, e.g., [27]). This is a a timid kind of robustification because it does not explicitly manage contaminated data reducing their influence in the clustering process [28]. An alternative approach is represented by *trimming* (see, e.g., [29]). The key idea is to simultaneously discard a proportion of observations and to apply the clustering procedure on the clean data. Thus, in the trimming approach the observations are considered either outliers or not. A softer approach allowing the existence of "outliers to a certain extent" consists in adding a *noise cluster* to the k "good" clusters [30]. The role of the noise cluster is that the outliers will be assigned to it with high membership degrees and, therefore, will have small membership degrees to the "good" clusters. A distinct approach is represented by the use of *metrics* able to mitigate the influence of outliers (see, e.g., [31, 32]). A different strategy is offered by the *possibilistic* approach [33]. Its peculiarity

2

is that the membership degree is only based on the distance between the observation and the involved centroid. Hence, the outliers, far from the bulk of the data, will have low membership degrees to all the clusters (see, for a deeper insight, [33]).

In this work, following the possibilistic approach, two new robust fuzzy clustering methods for fuzzy data will be proposed. The first method is fully possibilistic. However, as we will see, it may suffer from the risk of obtaining coincident clusters, i.e., clusters characterized by the same centroids. To overcome this problem, a second robust method is introduced preventing the occurrence of coincident clusters. The outline of the paper is as follows. In the next section we recall the theory of fuzzy sets describing the general family of LR fuzzy data and a dissimilarity measure for LR fuzzy data. Then, we discuss the concept of fuzzy data outliers. In Section 3 we recall the fuzzy k-means algorithm for LR fuzzy data [22] and propose a possibilistic clustering method for LR fuzzy data. Since it is not guaranteed that coincident clusters do not occur, the so-called possibilistic fuzzy clustering method for LR fuzzy data (PFkM-F) is suggested in Section 4. A selection procedure for choosing the parameters to be used in PFkM-F is discussed in Section 5. The effectiveness of the proposal is illustrated in Section 6 by means of a simulation study and some applications to real data. Finally, some concluding remarks are made in Section 7.

2. Fuzzy data

A fuzzy set $\widetilde{X}$ is identified by a membership function $\mu_{\widetilde{X}}(z)$, i.e. a mapping $\mu_{\widetilde{X}}(z) : \mathbb{R} \to [0,1]$ (see [1]). Let $K_c(\mathbb{R})$ be the class of non-empty compact convex subsets of $\mathbb{R}$, the class of fuzzy numbers is $F_c(\mathbb{R}) = \{\mu_{\widetilde{X}}(z) : \mathbb{R} \to [0,1] : \widetilde{X}_\alpha \in K_c(\mathbb{R})\}$, where $\widetilde{X}_\alpha$ is the α-level set of $\widetilde{X}$. For $0 < \alpha \leq 1$, it can be defined as the non-empty compact convex subset of $\mathbb{R}$ such that $\widetilde{X}_\alpha = \{z : \mu_{\widetilde{X}}(z) \geq \alpha\}$. For $\alpha = 0$, $\widetilde{X}_0 = cl(\{z : \mu_{\widetilde{X}}(z) > 0\})$ ($cl()$ indicates the closure of a set).

The most common class of fuzzy numbers is the LR one. In this case, the generic fuzzy datum $\widetilde{X}$ can be defined by four parameters, namely the left center (c_1), the right center (c_2), the left spread $(l > 0)$ and the right spread $(r > 0)$, and the following membership function:

$$\mu_{\widetilde{X}}(z) = \begin{cases} L\left(\frac{c_1-z}{l}\right) & z \leq c_1, \\ 1 & c_1 \leq z \leq c_2, \\ R\left(\frac{z-c_2}{r}\right) & z \geq c_2, \end{cases} \quad (1)$$

3
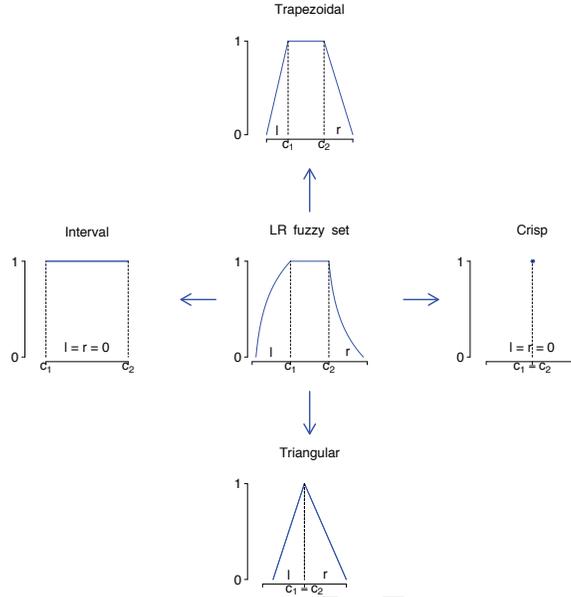
Figure 1: An LR fuzzy number and its specific cases. From the top in clockwise direction, a trapezoidal fuzzy number, a crisp number, a triangular fuzzy number and an interval are reported.

where the function $L : \mathbb{R} \rightarrow [0, 1]$ (and R) is a convex upper semi-continuous function so that $L(0) = 1$ and $L(z) = 0$, for all $z \in \mathbb{R} \setminus [0, 1]$. The centers provide information about the location of the fuzzy datum, whilst the spreads inform us about the associated imprecision (the size). If $L(z) = 1 - z$ and $R(z) = 1 - z$ for $0 \leq z \leq 1$, then $\widetilde{X}$ is a trapezoidal fuzzy number when $c_1 \neq c_2$ and a triangular fuzzy number when $c_1 = c_2 = c$. If $l = r = s \neq 0$, then $\widetilde{X}$ is a symmetric LR fuzzy number. If $c_1 \neq c_2$ and $l = r = 0$ we get an interval. Finally, a crisp number (non-fuzzy datum) is obtained when $c_1 = c_2 = c$ and $l = r = 0$. All the above specific cases are represented in Figure 1.

When p LR fuzzy variables are collected on a set of n observations, we have the fuzzy data matrix

$$\widetilde{\mathbf{X}} = \left\{ \widetilde{X}_{ij} \equiv (c_{1ij}, c_{2ij}, l_{ij}, r_{ij})_{LR}, i = 1, ..., n, j = 1, ..., p \right\}, \qquad (2)$$

where $\widetilde{X}_{ij} \equiv (c_{1ij}, c_{2ij}, l_{ij}, r_{ij})_{LR}$ represents the j-th LR fuzzy variable collected on the i-th observation with left center c_{1ij}, right center c_{2ij}, left spread

4

l_{ij} and right spread r_{ij}. We can define the matrices of the left centers ($\mathbf{C}_1$), of the right centers ($\mathbf{C}_2$), of the left spreads ($\mathbf{L}$) and of the right spreads ($\mathbf{R}$) of order ($n \times p$) with generic elements c_{1ij}, c_{2ij}, l_{ij} and r_{ij}, respectively. Hence, $\tilde{\mathbf{x}}_i \equiv (\mathbf{c}_{1i}, \mathbf{c}_{2i}, \mathbf{l}_i, \mathbf{r}_i)_{LR}$ is the fuzzy vector of length p for observation i, where $\tilde{\mathbf{x}}_i$, $\mathbf{c}_{1i}$, $\mathbf{c}_{2i}$, $\mathbf{l}_i$ and $\mathbf{r}_i$ are the i-th rows of $\widetilde{\mathbf{X}}$, $\mathbf{C}_1$, $\mathbf{C}_2$, $\mathbf{L}$ and $\mathbf{R}$, respectively.

2.1. Dissimilarity measures for fuzzy data

In order to develop clustering methods for LR fuzzy data we need a suitable dissimilarity measure. We adopt the one introduced in [22]. It is defined as a weighted sum of the (squared) Euclidean distances between centers and spreads. In detail, given two LR fuzzy observations, $\tilde{\mathbf{x}}_i$ and $\tilde{\mathbf{x}}_{i'}$ we have

$$d_w^2(\tilde{\mathbf{x}}_i, \tilde{\mathbf{x}}_{i'}) = w^2[d^2(\mathbf{c}_{1i}, \mathbf{c}_{1i'}) + d^2(\mathbf{c}_{2i}, \mathbf{c}_{2i'})] + (1-w)^2[d^2(\mathbf{l}_i, \mathbf{l}_{i'}) + d^2(\mathbf{r}_i, \mathbf{r}_{i'})], \ (3)$$

where $d(\cdot, \cdot)$ is the standard Euclidean distance (for non-fuzzy data), w and $1-w$ are weights for the center component and the spread component, respectively. By means of $d_w^2(\tilde{\mathbf{x}}_i, \tilde{\mathbf{x}}_{i'})$ we compute the dissimilarity between two LR fuzzy observations as the weighted sum of the squared Euclidean distances for the (left and right) centers and the (left and right) spreads. The weights w and $1-w$ must be non-negative. Moreover, taking into account that the membership function takes the maximum value in the centers, they must be such that the distances for the centers play a more relevant role than those for the spreads, hence, $w \geq 1 - w \geq 0$. It follows that w must belong to $[0.5, 1]$ (and $1 - w$ to $[0, 0.5]$). As we shall see, w will be estimated within the clustering problem. It must be underlined that (3) is utilized for evaluating the existing differences among observations belonging to a given data set and, therefore, the estimated weight is optimal only for the involved data set.

Remark 1. *The squared dissimilarity in (3) is valid for the general class of LR fuzzy numbers. Some particular cases are worth mentioning. For instance, in the case of triangular fuzzy data, (3) can still be applied. When we have symmetric triangular fuzzy data (3) reduces to the squared dissimilarity proposed in [19]. Finally, in case of non-fuzzy data, (3) coincides with the squared Euclidean distance.*

2.2. Fuzzy data and outliers

There exist different kinds of contamination. Fuzzy data can be considered outliers with respect to their centers (see top of Figure 2). In this case the contamination is due to the location. Another kind of contamination is
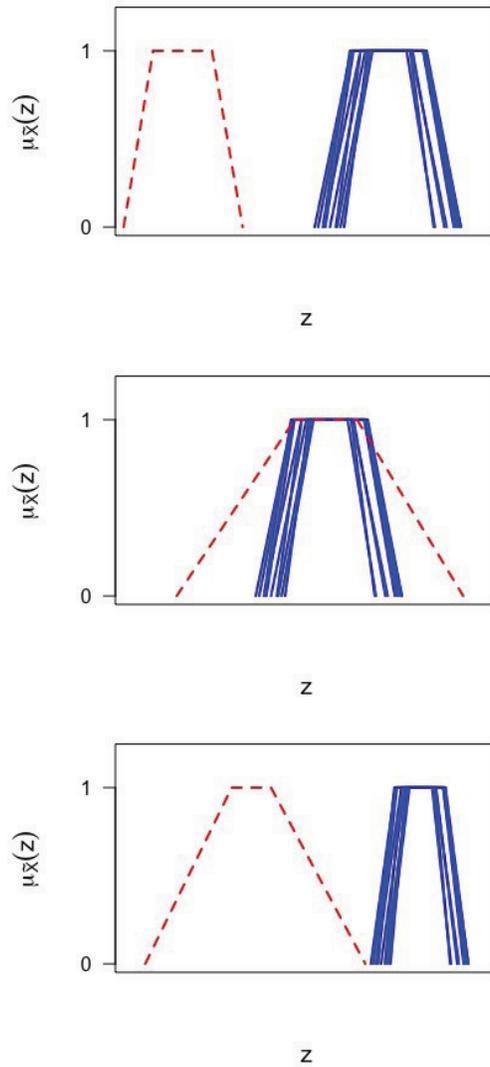
Figure 2: From top to bottom: outlier w.r.t. center, outlier w.r.t. spread, outlier w.r.t. center and spread (red dashed line).

due to the size (see middle of Figure 2), i.e., outliers with respect to their

6

spreads. Finally, there are outliers with respect to both centers and spreads (see bottom of Figure 2), that are outliers due to both the location and the size. When clustering fuzzy data we should apply methods able to mitigate the distortion produced by all these kinds of contamination.

3. Fuzzy and possibilistic k-means algorithms for fuzzy data

In order to cluster n observations described by p LR fuzzy variables, the fuzzy k-means clustering method for LR fuzzy data (FkM-F) proposed by Coppi et al. [22] can be applied. The FkM-F optimization problem can be written as

$$\min_{\mathbf{U},\widetilde{\mathbf{H}},w} J_{FkM-F} \quad = \quad \sum_{i=1}^{n}\sum_{g=1}^{k} u_{ig}^{m} d_{w}^{2}\left(\widetilde{\mathbf{x}}_{i}, \widetilde{\mathbf{h}}_{g}\right), \tag{4}$$

$$\text{s.t.} \quad u_{ig} \geq 0, \quad i = 1,\ldots,n, \quad g = 1,\ldots,k, \tag{5}$$

$$\sum_{g=1}^{k} u_{ig} = 1, \quad i = 1,\ldots,n, \tag{6}$$

$$w \in [0.5, 1], \tag{7}$$

where u_{ig} is the membership degree of observation i to cluster g, stored in the matrix $\mathbf{U}$ of order $(n \times k)$, and

$$\widetilde{\mathbf{H}} = \left\{ \widetilde{H}_{gj} \equiv \left(h_{gj}^{C_1}, h_{gj}^{C_2}, h_{gj}^{L}, h_{gj}^{R}\right)_{LR}, g = 1, ..., k, j = 1, ..., p \right\}. \tag{8}$$

In (8) $\widetilde{H}_{gj} \equiv \left(h_{gj}^{C_1}, h_{gj}^{C_2}, h_{gj}^{L}, h_{gj}^{R}\right)_{LR}$ represents the j-th LR fuzzy variable for the g-th centroid with left center $h_{gj}^{C_1}$, right center $h_{gj}^{C_2}$, left spread h_{gj}^{L} and right spread h_{gj}^{R}. We can define the centroid matrices of the left centers ($\mathbf{H}^{C_1}$), of the right centers ($\mathbf{H}^{C_2}$), of the left spreads ($\mathbf{H}^{L}$) and of the right spreads ($\mathbf{H}^{R}$) of order $(k \times p)$ with generic elements $h_{gj}^{C_1}$, $h_{gj}^{C_2}$, h_{gj}^{L} and h_{gj}^{R}, respectively. Therefore, $\widetilde{\mathbf{h}}_{g} \equiv (\mathbf{h}_{g}^{C_1}, \mathbf{h}_{g}^{C_2}, \mathbf{h}_{g}^{L}, \mathbf{h}_{g}^{R})_{LR}$ is the fuzzy vector of length p for centroid g, where $\widetilde{\mathbf{h}}_{g}$, $\mathbf{h}_{g}^{C_1}$, $\mathbf{h}_{g}^{C_2}$, $\mathbf{h}_{g}^{L}$ and $\mathbf{h}_{g}^{R}$ are the g-th rows of $\widetilde{\mathbf{H}}$, $\mathbf{H}^{C_1}$, $\mathbf{H}^{C_2}$, $\mathbf{H}^{L}$ and $\mathbf{H}^{R}$, respectively. Thus, the centroids are assumed to have a complex structure inherited from the observed data. In other words, the imprecision of the observed data is propagated to the centroids that are of fuzzy nature. The squared dissimilarity $d_{w}^{2}\left(\widetilde{\mathbf{x}}_{i}, \widetilde{\mathbf{h}}_{g}\right)$ recalled in (3) is used for comparing observation i with centroid g. Finally, $m > 1$ is the fuzziness

7

parameter. The membership degrees of the observations to the clusters are such that they are inversely related to the *relative* dissimilarities between the observations and the centroids. For this reason, the membership degrees can be interpreted as degrees of sharing (of the observations to the clusters).

In case of outliers, the fuzzy approach fails due to the unit-sum constraints of the membership degrees. By relaxing these constraints we move from the fuzzy to the possibilistic approach [33]. The so-called possibilistic k-means clustering method for LR fuzzy data (PkM-F) can be formalized as

$$\min_{\mathbf{T},\widetilde{\mathbf{H}},w} J_{PkM-F} = \sum_{i=1}^{n}\sum_{g=1}^{k} t_{ig}^{\eta} d_{w}^{2}\left(\widetilde{\mathbf{x}}_{i},\widetilde{\mathbf{h}}_{g}\right) + \sum_{g=1}^{k}\gamma_{g}\sum_{i=1}^{n}(1-t_{ig})^{\eta}, \quad (9)$$

$$\text{s.t.} \quad t_{ig} \in [0,1], \quad i=1,\ldots,n, \quad g=1,\ldots,k, \quad (10)$$

$$w \in [0.5,1], \quad (11)$$

where t_{ig} is the membership degree of observation i to cluster g, stored in the matrix $\mathbf{T}$ of order $(n \times k)$. As for the standard possibilistic k-means clustering method for non-fuzzy data [33], the membership degrees are possibility values and are usually referred to as the degrees of typicality (of the observations to the clusters), although, as an anonymous reviewer noted, t_{ig} is not a possibility value in a strict sense because, for the generic i-th observation, t_{ig}'s should be normalized so that $\max_{g} t_{ig} = 1$. γ_{g} is a cluster-specific parameter tuning the importance of the clusters and η (> 1) is the fuzzifier. The parameter γ_{g} can be defined as

$$\gamma_{g} = \gamma \frac{\sum_{i=1}^{n} u_{ig}^{m} d_{w}^{2}\left(\widetilde{\mathbf{x}}_{i},\widetilde{\mathbf{h}}_{g}\right)}{\sum_{i=1}^{n} u_{ig}^{m}}, \quad g=1,\ldots,k, \quad (12)$$

where, usually, $\gamma = 1$ and $\mathbf{h}_{g}$'s and u_{ig}'s are obtained from FkM-F. (12) can be motivated by noting that the γ_{g}'s give the relative weight of the second term of the loss compared to the first one. The second term avoids the trivial solution with $\mathbf{T} = \mathbf{0}$. When the γ_{g}'s have approximately the same order of the $d_{w}^{2}\left(\widetilde{\mathbf{x}}_{i},\widetilde{\mathbf{h}}_{g}\right)$'s, then the two terms of the loss are weighted roughly equally. The values of the γ_{g}'s differ among clusters and depend on their overall sizes and shapes. The choice of the γ_{g}'s determines the zones of influence of the clusters. In particular, γ_{g} gives the dissimilarity at which the degree of

8

typicality of an observation to cluster g becomes 0.5. When γ_g is low or high, we expect degrees of typicality t_{ig}'s low or high, respectively.

The solution of PkM-F can be derived by using the iterative algorithm proposed in the next section. In PkM-F the degrees of typicality are inversely related to the *absolute* dissimilarities between the observations and the centroids. In fact, a common property of clustering methods based on the possibilistic approach is that the membership degrees are computed by considering only the dissimilarity between the observation and the involved centroid, regardless of the centroids of the remaining clusters. Intuitively, this clarifies how the possibilistic approach well manages contaminated data. Outliers are far from the bulk of the data and, thus, far from all the centroids. Therefore, they usually have degrees of typicality close to 0 to all the clusters (see, for an deeper discussion, [33]).

The PkM-F problem is a novel clustering method and represents an extension to the fuzzy data case of the algorithm introduced in [33]. Note, however, that PkM-F is not the first possibilistic clustering method for LR fuzzy data proposed in the literature. In fact, taking inspiration from [39], Coppi et al. [22] propose a different possibilistic clustering method for fuzzy data (hereinafter, C-PkM-F). The PkM-F and C-PkM-F methods can be formulated in the same way except for the second term of the cost function. Such a second term (not reported here for C-PkM-F) avoids solutions with $\mathbf{T} = \mathbf{0}$.

Although the possibilistic approach to clustering works well, it suffers from a well-known limitation, i.e., the risk of obtaining a trivial solution with coincident clusters [34]. Since the sum of the degrees of typicality for every observation to all the clusters is no longer required to be equal to one, it may occur that the centroids of the clusters are the same. This can be explained by noting that the loss functions of the possibilistic procedures can usually be decomposed into the sum of k terms (one for every cluster) that can be minimized independently of each other. It is easy to show that such a comment holds for PkM-F and C-PkM-F. A heuristic remedy to the coincident cluster problem is the use of a rational starting point. For instance, the iterative algorithm of PkM-F can be run starting from the FkM-F solution. This strategy has also been adopted for C-PkM-F. Although very common, this remedy does not always exclude the occurrence of trivial solutions with coincident clusters.

It should be clear that in practical applications PkM-F will be rarely used. Nonetheless, it is useful to derive the here-proposed clustering method.

9

More specifically, in order to solve the coincident clustering problem, at least two strategies can be followed. The first one consists in adding a repulsion term among centroids in the loss function. Such a repulsion term forces the centroids to be far from each other. In [23] a possibilistic clustering method with repulsion constraints for symmetric triangular fuzzy data is developed. Its extension to the general family of LR fuzzy data is not straightforward. A different strategy for preventing coincident clusters is the hybridization of the fuzzy and possibilistic approaches, namely of FkM-F and PkM-F, exploiting their potentialities and overcoming their drawbacks. This is pursued in this work.

4. Possibilistic fuzzy k-means algorithm for fuzzy data

The possibilistic fuzzy k-means clustering method for LR fuzzy data (PFkM-F) can be formalized as

$$\min_{\mathbf{U},\mathbf{T},\widetilde{\mathbf{H}},w} J_{PFkM-F} = \sum_{i=1}^{n}\sum_{g=1}^{k}\left(au_{ig}^{m}+bt_{ig}^{\eta}\right)d_{w}^{2}\left(\widetilde{\mathbf{x}}_{i},\widetilde{\mathbf{h}}_{g}\right)+\sum_{g=1}^{k}\gamma_{g}\sum_{i=1}^{n}\left(1-t_{ig}\right)^{m} \quad (13)$$

$$\text{s.t.} \quad u_{ig}\geq 0, \quad i=1,\ldots,n, \quad g=1,\ldots,k, \quad (14)$$

$$\sum_{g=1}^{k}u_{ig}=1, \quad i=1,\ldots,n, \quad (15)$$

$$t_{ig}\in[0,1], \quad i=1,\ldots,n, \quad g=1,\ldots,k, \quad (16)$$

$$w\in[0.5,1], \quad (17)$$

where $m>1$ denotes the parameter of fuzziness and η and γ_g have the same meanings discussed in PkM-F. The idea underlying PFkM-F is to exploit the potentialities of FkM-F and PkM-F. This goal is achieved by minimizing a cost function which is a linear combination of those of FkM-F and PkM-F, respectively, with weights given by a and b, respectively. The non-negative quantities a and b tune the relative importance of the degrees of sharing (in $\mathbf{U}$) and of the degrees of typicality (in $\mathbf{T}$) in the objective function. These two sources of information are not exclusive because they jointly allow for a thorough analysis of the cluster structure. The matrix $\mathbf{T}$ helps to detect outliers. Generally speaking, an observation can be considered an outlier when all its degrees of typicality are low. In addition, the fuzzy partition of the observations can be assessed by looking at $\mathbf{U}$. The non-negative parameters a and b tune the importance of the degrees of sharing

10

and typicality in the clustering process. The higher a (b) is, the more relevant is the emphasis of the fuzzy (possibilistic) approach. In fact, if a is high, then the centroids (in $\widetilde{\mathbf{H}}$) mainly depend on the degrees in $\mathbf{U}$. Similarly, if b is high, the degrees in $\mathbf{T}$ remarkably influence the centroids. Therefore, in order to reduce the effect of outliers, a larger value of b can be set. Coincident clusters could occur for large values of b, but the problem can easily be solved by increasing a. In other words, the simultaneous use of FkM-F and PkM-F allows to eliminate the drawbacks of the two methods. On the one hand, the FkM-F part of the cost function avoids (for sufficiently large values of a) that the centroids are coincident and therefore the degrees of typicality have a practical meaning. On the other hand, the PkM-F part mitigates the influence of the outliers in the obtained partition. In case of particularly large values of a and b, it might be convenient to select a high value for γ in (12) to avoid that the second term of (13) plays a negligible role in the clustering process. For a deeper insight into the properties of clustering methods jointly based on the fuzzy and possibilistic approaches the interested reader may refer to [35, 36].

Remark 2. *A lot of existing clustering methods can be obtained as special cases of PFkM-F. If $b = 0$ and $\gamma_g = 0$, $g = 1, \ldots, k$, then we obtain FkM-F [22], while for $a = 0$ the problem coincides with PkM-F. When PFkM-F is run using non-fuzzy data (i.e., $\widetilde{\mathbf{X}} \equiv \mathbf{X}$ with $\mathbf{C}_1 = \mathbf{C}_2 = \mathbf{X}$ and $\mathbf{L} = \mathbf{R} = \mathbf{0}$ being $\mathbf{0}$ the matrix of order $(n \times p)$ with zero elements), then the PFkM-F reduces to the procedure proposed in [36]. If $\widetilde{\mathbf{X}} \equiv \mathbf{X}$, then the PFkM-F coincides with the standard fuzzy k-means (FkM) algorithm [37] when $b = 0$ and $\gamma_g = 0$, $g = 1, \ldots, k$, and with the standard possibilistic k-means (PkM) algorithm [33] when $a = 0$.*

In PFkM-F the number of clusters k and the parameters (m, η, a, b) must be chosen. In Section 5 we focus on this problem by proposing a heuristic procedure for providing good values for these quantities.

4.1. Iterative algorithm

The optimal solution of PFkM-F can be found by minimizing the constrained optimization problem in (13)-(17) with respect to every group of parameters. In order to obtain the optimal fuzzy membership degree matrix

11

U, we consider the Lagrangian function

$$L(\mathbf{U}, \mathbf{T}, \widetilde{\mathbf{H}}, w, \lambda) \;=\; \sum_{i=1}^{n}\sum_{g=1}^{k}\left(au_{ig}^{m} + bt_{ig}^{\eta}\right)d_{w}^{2}\left(\widetilde{\mathbf{x}}_{i}, \widetilde{\mathbf{h}}_{g}\right) \tag{18}$$
$$+ \sum_{g=1}^{k}\gamma_{g}\sum_{i=1}^{n}\left(1 - t_{ig}\right)^{\eta} - \lambda\left(\sum_{g=1}^{k}u_{ig} - 1\right).$$

We compute the partial derivatives of (18) with respect to u_{ig} and λ and we set them equal to 0:

$$\frac{\vartheta L(\mathbf{U}, \mathbf{T}, \widetilde{\mathbf{H}}, w, \lambda)}{\vartheta u_{ig}} = 0 \Leftrightarrow mu_{ig}^{m-1}ad_{w}^{2}\left(\widetilde{\mathbf{x}}_{i}, \widetilde{\mathbf{h}}_{g}\right) - \lambda = 0, \tag{19}$$

$$\frac{\vartheta L(\mathbf{U}, \mathbf{T}, \widetilde{\mathbf{H}}, w, \lambda)}{\vartheta \lambda} = 0 \Leftrightarrow \sum_{g=1}^{k}u_{ig} - 1 = 0. \tag{20}$$

By the usual calculations, we then get

$$u_{ig} = \frac{1}{\sum\limits_{g'=1}^{k}\left(\frac{d_{w}^{2}\left(\widetilde{\mathbf{x}}_{i}, \widetilde{\mathbf{h}}_{g}\right)}{d_{w}^{2}\left(\widetilde{\mathbf{x}}_{i}, \widetilde{\mathbf{h}}_{g'}\right)}\right)^{\frac{1}{m-1}}}, \quad i = 1, \dots, n, \quad g = 1, \dots, k. \tag{21}$$

The possibilistic degree matrix $\mathbf{T}$ is obtained by considering the partial derivative of (13) with respect to t_{ig}

$$\frac{\vartheta L(\mathbf{U}, \mathbf{T}, \widetilde{\mathbf{H}}, w, \lambda)}{\vartheta t_{ig}} = 0 \Leftrightarrow \eta t_{ig}^{\eta-1}bd_{w}^{2}\left(\widetilde{\mathbf{x}}_{i}, \widetilde{\mathbf{h}}_{g}\right) - \eta\gamma_{g}\left(1 - t_{ig}\right)^{\eta-1} = 0. \tag{22}$$

Hence, after a little algebra, we obtain

$$t_{ig} = \frac{1}{1 + \left(\frac{d_{w}^{2}\left(\widetilde{\mathbf{x}}_{i}, \widetilde{\mathbf{h}}_{g}\right)}{\gamma_{g}}\right)^{1/(\eta-1)}}, \quad i = 1, \dots, n, \quad g = 1, \dots, k. \tag{23}$$

By considering the partial derivatives of (13) with respect to $\mathbf{h}_{g}^{C_{1}}$, $\mathbf{h}_{g}^{C_{2}}$, $\mathbf{h}_{g}^{L}$ and $\mathbf{h}_{g}^{R}$ and setting them to 0, the centroid matrix is given by

$$\mathbf{h}_{g}^{C_{1}} = \frac{\sum\limits_{i=1}^{n}\left(au_{ig}^{m} + bt_{ig}^{\eta}\right)\mathbf{c}_{1i}}{\sum\limits_{i=1}^{n}\left(au_{ig}^{m} + bt_{ig}^{\eta}\right)}, \quad g = 1, \dots, k, \tag{24}$$

12

$$\mathbf{h}_g^{C_2} = \frac{\sum\limits_{i=1}^{n} \left(au_{ig}^m + bt_{ig}^\eta\right) \mathbf{c}_{2i}}{\sum\limits_{i=1}^{n} \left(au_{ig}^m + bt_{ig}^\eta\right)}, \quad g = 1, \dots, k, \tag{25}$$

$$\mathbf{h}_g^{L} = \frac{\sum\limits_{i=1}^{n} \left(au_{ig}^m + bt_{ig}^\eta\right) \mathbf{l}_{i}}{\sum\limits_{i=1}^{n} \left(au_{ig}^m + bt_{ig}^\eta\right)}, \quad g = 1, \dots, k, \tag{26}$$

$$\mathbf{h}_g^{R} = \frac{\sum\limits_{i=1}^{n} \left(au_{ig}^m + bt_{ig}^\eta\right) \mathbf{r}_{i}}{\sum\limits_{i=1}^{n} \left(au_{ig}^m + bt_{ig}^\eta\right)}, \quad g = 1, \dots, k. \tag{27}$$

Finally, to update the weight, first we note that the second term of (13) does not depend on w and, thus, can be ignored. Moreover, the loss function can be rewritten as

$$w^2 \sum_{i=1}^{n} \sum_{g=1}^{k} \left(au_{ig}^m + bt_{ig}^\eta\right) [d^2 \left(\mathbf{c}_{1i}, \mathbf{h}_g^{C_1}\right) + d^2 \left(\mathbf{c}_{2i}, \mathbf{h}_g^{C_2}\right) + d^2 \left(\mathbf{l}_i, \mathbf{h}_g^{L}\right) + d^2 \left(\mathbf{r}_i, \mathbf{h}_g^{R}\right)]$$

$$-2w \sum_{i=1}^{n} \sum_{g=1}^{k} \left(au_{ig}^m + bt_{ig}^\eta\right) [d^2 \left(\mathbf{l}_i, \mathbf{h}_g^{L}\right) + d^2 \left(\mathbf{r}_i, \mathbf{h}_g^{R}\right)]$$

$$+ \sum_{i=1}^{n} \sum_{g=1}^{k} \left(au_{ig}^m + bt_{ig}^\eta\right) [d^2 \left(\mathbf{l}_i, \mathbf{h}_g^{L}\right) + d^2 \left(\mathbf{r}_i, \mathbf{h}_g^{R}\right)]. \tag{28}$$

(28) is a parabola with respect to w. Since the parabola opens up, the minimizer is given by its vertex and, hence, we obtain

$$w = \frac{\sum\limits_{i=1}^{n} \sum\limits_{g=1}^{k} \left(au_{ig}^m + bt_{ig}^\eta\right) [d^2 \left(\mathbf{l}_i, \mathbf{h}_g^{L}\right) + d^2 \left(\mathbf{r}_i, \mathbf{h}_g^{R}\right)]}{\sum\limits_{i=1}^{n} \sum\limits_{g=1}^{k} \left(au_{ig}^m + bt_{ig}^\eta\right) [d^2 \left(\mathbf{c}_{1i}, \mathbf{h}_g^{C_1}\right) + d^2 \left(\mathbf{c}_{2i}, \mathbf{h}_g^{C_2}\right) + d^2 \left(\mathbf{l}_i, \mathbf{h}_g^{L}\right) + d^2 \left(\mathbf{r}_i, \mathbf{h}_g^{R}\right)]}. \tag{29}$$

If $w < 0.5$, then we set $w = 0.5$. This can be explained by noting that, for values of $w \geq 0.5$, the parabola is a monotonically increasing function of w.

13

At every update the loss function to minimize decreases. These updates are repeated upon, after updating all the parameter entities, the value of the loss function decreases less than a specified threshold (e.g. 10^{-5}) from the previous function value. The algorithm is summarized below.

Algorithm PFkM-F ($\widetilde{\mathbf{X}}$, a, b, m, η, k)

Step 0a. Generate randomly a feasible membership degree matrix $\mathbf{U}$.

Step 0b. Generate randomly a feasible possibilistic degree matrix $\mathbf{T}$.

Step 0c. Compute the centroid matrix $\widetilde{\mathbf{H}}$ according to (24)-(27).

Step 1. Update the weight w according to (29). If $w < 0.5$, then $w = 0.5$.

Step 2. Update the centroid matrix $\widetilde{\mathbf{H}}$ according to (24)-(27).

Step 3. Update the fuzzy membership degree matrix $\mathbf{U}$ according to (21).

Step 4. Update the possibilistic membership degree matrix $\mathbf{T}$ according to (23).

Step 5. Check convergence. If the convergence condition is not satisfied, go to *Step 1*.

Remark 3. *When the variables have different units of measurement, it is convenient to run PFkM-F on preprocessed data. Following [22] we suggest to standardize the left and right centers using the mean and the standard deviation of the (left and right) centers of each variable. Then the left and right spreads are divided by the standard deviation of the corresponding centers.*

5. Selection of PFkM-F parameters

In this section we propose a selection procedure for choosing the number of clusters k and the values of the parameters m, η, a and b.

14

5.1. Generalized Xie and Beni index

In order to determine good choices for the PFkM-F parameters, a new cluster validity index for the fuzzy and possibilistic framework is introduced. The starting point is the well-known XB index [38] defined as

$$XB = \frac{\sum_{i=1}^{n}\sum_{g=1}^{k} u_{ig}^2 d^2\left(\mathbf{x}_i, \mathbf{h}_g\right)}{n \min_{g,g'(g \neq g')} d^2\left(\mathbf{h}_g, \mathbf{h}_{g'}\right)}. \tag{30}$$

The optimal number of clusters k is the value that minimizes XB.

In the possibilistic framework, XB could be derived in a straightforward way by substituting u_{ig} with t_{ig}. Nonetheless, XB loses its validity because the row-wise sum of the t_{ig}'s is no longer constrained to be equal to one. In order to solve this problem, Yang and Wu [39] normalize the degrees of typicality as $t_{ig}^N = \frac{t_{ig}}{\sum_{g'=1}^{k} t_{ig'}}, i = 1,\ldots,n, g = 1,\ldots,k$. Rescaling the degrees of typicality is justified by the attempt to discard solutions with a large number of small degrees of typicality. In these cases, the XB index may take a low value because the numerator is close to zero, but the corresponding solution may have no practical meaning. Starting from (30), we develop a generalized version of XB for PFkM-F. The new index, called XB_{PF-F}, is

$$XB_{PF-F} = \frac{\sum_{i=1}^{n}\sum_{g=1}^{k}(u_{ig}^2 + t_{ig}^{N2})d_w^2\left(\widetilde{\mathbf{x}}_i, \widetilde{\mathbf{h}}_g\right)}{n \min_{g,g'(g \neq g')} d_w^2\left(\widetilde{\mathbf{h}}_g, \widetilde{\mathbf{h}}_{g'}\right)}. \tag{31}$$

The idea of (31) is similar to the one of XB. The numerator measures the deviation of the observations from the centroids. Such a deviation is weighted by the squared degrees of sharing and (normalized) typicality. The denominator gives the level of separation of the partition expressed in terms of the minimum dissimilarity among the centroids. It is clear that a partition is good when the XB_{PF-F} index takes a low value.

Remark 4. *In the XB_{PF-F} index the powers of the degrees of sharing and typicality are set equal to two, although in PFkM-F their exponents are m and η, respectively. This choice is also made in [38] and can be justified by a practical reason. Given $\mathbf{U}$, $\mathbf{T}$ and $\widetilde{\mathbf{H}}$, we are interested in an index that*

15

does not vary for different values of m and η. For the same practical reason we do not weigh $\boldsymbol{U}$ and $\boldsymbol{T}$ by a and b, respectively.

Remark 5. *In the literature, a large number of cluster validity indexes in the fuzzy and/or possibilistic approach have been proposed and, of course, these could be applied in PFkM-F. For instance, another widely used index is the Fuzzy Silhouette [40], which is a generalization of the standard Silhouette index [41] in the fuzzy framework. The reason why we decided to use XB_{PF-F} is that its denominator is proportional to the minimum dissimilarity between centroids. If coincident cluster occurs, then $XB_{PF-F} \longrightarrow +\infty$ and, therefore, the solution is automatically discarded. This property does not necessarily hold for other indexes, such as the Fuzzy Silhouette.*

5.2. Choice of k, m, η, a and b

We suggest to select (k, m, η, a, b) in such a way to minimize XB_{PF-F}. In doing so, we should ignore two kinds of solutions having no practical meaning. The first one is when coincident clusters occur. However, we saw in Remark 5 that this goal is always achieved. The latter situation is when a lot of degrees of typicality are low. This is the case in which the possibilistic clustering struggles to determine the cluster structure because a high percentage of observations is considered as outliers. On the basis of our preliminary analyses, we observed that valuable solutions are usually found when the values of a and b are not "too far". In fact, if a is much bigger than b then the results may be poor because the centroids are strongly affected by the outliers. Conversely, if b is much bigger than a, then the performance of PFkM-F can be unsatisfactory because the degrees of sharing have limited importance. We are going to clarify all of these points in the next section where the results of a simulation experiment are discussed.

6. Applications

In Section 6.1 the results of a simulation study carried out in order to study the behavior of PFkM-F also in comparison with its more closely related competitors, i.e., those based on the fuzzy and/or possibilistic approach, are discussed. In particular, we studied how well PFkM-F recovered the cluster structure of the data and estimated the centroids. The performance of PFkM-F was compared with FkM-F, PkM-F and C-PkM-F. Moreover, we evaluated the performance of the selection procedure proposed in Section 5.2. In Section 6.2, PFkM-F was applied to two real-case studies.

6.1. Simulated data

Simulated LR fuzzy data sets were randomly generated with a structure of $k = 2$ and 3 clusters of equal size and $p = 2$ and 8 fuzzy variables as described below. The number of observations was set equal to $n = 60$, 120, 180 and 240. The clusters had equal sizes and were distinguished with respect to either the centers (case *cen*) or the spreads (case *spr*). In the *cen* case, the observations belonging to the first cluster had left and right centers randomly generated from Unif[0, 1] and Unif[1, 2], respectively, whereas both the left and the right spreads from Unif[0, 1]. The observations belonging to the second cluster were such that their spreads were randomly generated from Unif[0, 1], whereas the left and right centers from Unif[0, 1] + *sep* and Unif[1, 2] + *sep*, respectively. When $k = 3$, the third cluster was characterized by observations with left and right centers randomly generated from Unif[0, 1] + 2*sep* and Unif[1, 2] + 2*sep*, respectively, and left and right spreads from Unif[0, 1]. Hence, in the *cen* case, the data generation process for the spreads was the same for all the clusters. The opposite comment holds for the *spr* case. In fact, the left and right centers of the clusters were randomly generated from Unif[0, 1] and Unif[1, 2], respectively. To distinguish the clusters, the spreads of the first cluster were randomly drawn from Unif[0, 1], those of the second clusters from Unif[0, 1] + *sep* and, when $k = 3$, those of the third one from Unif[0, 1] + 2*sep*. The parameter *sep* took two values tuning the level of separation of the clusters. We had partially separated clusters when *sep* = 1 (case *part*) and well separated clusters when *sep* = 2 (case *well*). The data sets were contaminated by the presence of some outliers. We considered two cases (*low* and *high*) corresponding to a percentage of outliers equal to 10% and 30%, respectively. The outliers had anomalous centers and/or spreads. In particular, for each data set, 1/3 when $k = 2$ or 1/6 when $k = 3$ of the outliers had the left and right centers randomly generated from Unif[0, 1] + *sep*/2 and Unif[1, 2] + *sep*/2, respectively, and the spreads from Unif[0, 1] + *sep*/2. Such outliers were equally far from Clusters 1 and 2. When $k = 3$, 1/6 of the outliers were equally far from Clusters 2 and 3. They had the left and right centers randomly generated from Unif[0, 1] + 3*sep*/2 and Unif[1, 2] + 3*sep*/2, respectively, and the spreads from Unif[0, 1] + 3*sep*/2. Moreover, another 1/3 of the outliers had abnormal values for the centers, since these were randomly generated from Unif[0, 1] − 2*sep* (left centers) and Unif[1, 2] − 2*sep* (right centers) and both the spreads from Unif[0, 1]. Finally, the last 1/3 of the outliers had the left and right centers randomly generated from Unif[0, 1] and Unif[1, 2], respectively, and the left and right centers both from Unif[0, 1] +

17
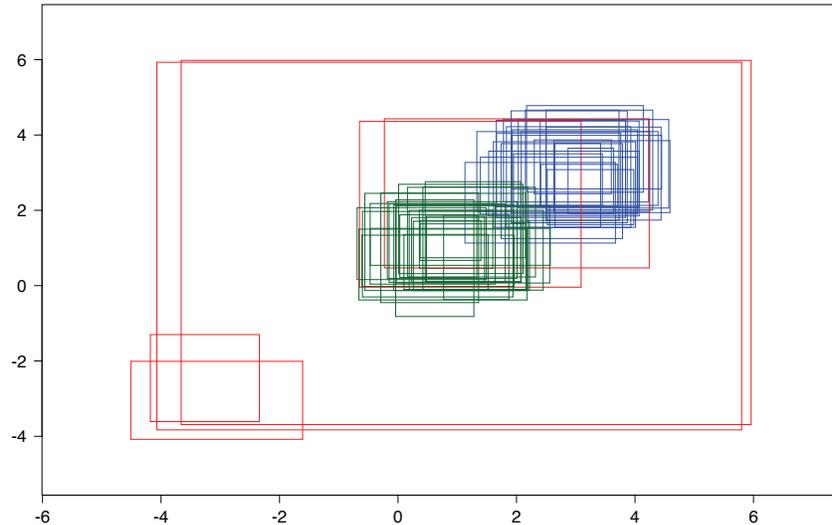
Figure 3: Example of randomly generated data set (case $sep = 2$, $n = 60$, *low*, *cen*). For each observation, reported are the supports of the two fuzzy variables. The black, red and blue rectangles refer to the outliers and to the observations belonging to Cluster 1 and 2, respectively.

$2sep$, from which it is clear that their spreads were abnormal. For every level of every design variable, 10 data sets were randomly generated. An example of randomly generated data set is reported in Figure 3. Hence, 2 (numbers of clusters, $k = 2, 3$) $\times$ 2 (numbers of variables, $p = 2, 8$) $\times$ 4 (data sizes, $n = 60, 120, 180, 240$) $\times$ 2 (cluster structures, *cen* or *spr*) $\times$ 2 (levels of separation between clusters, $sep = 1, 2$) $\times$ 2 (percentages of contamination, *low* or *high*) $\times$ 10 (replications) = 1280 LR fuzzy data sets were randomly generated during the simulation experiment. All these data sets were analyzed by PFkM-F, FkM-F, PkM-F and C-PkM-F setting $k = 2$ or $k = 3$ according to the known in advance number of clusters. Five random starts were used for PFkM-F and FkM-F. The optimal solution of FkM-F was the only one (rational) starting point for the PkM-F and C-PkM-F algorithms.

Except for k, the parameters of the PFkM-F algorithm were determined using the selection procedure proposed in Section 5.2. The possible values of

18

m and η ranged from 1.5 to 2.5 with step equal to 0.25. The parameters a and b took scores from 0.5 to 5 with step equal to 0.5. In order to guarantee that the values of a and b were not "too far", we imposed that the difference between a and b in absolute value was not higher than 2. For instance, if $a = 1.5$, then the possible values of b were $\{0.5, 1, 1.5, 2, 2.5, 3, 3.5\}$. More-over, in order to avoid solutions with a large number of observations having low degrees of typicality, i.e., observations recognized as outliers, we considered the following rule. We skipped solutions, i.e., we did not compute the XB_{PF-F} index, when the clustering method recognized at least one half of the observations as outliers. The same grid search was considered for the selection of m in FkM-F and of η in PkM-F and C-PkF-F. The optimal values of m for FkM-F and η for PkM-F were determined in such a way to minimize XB_{PF-F}. This was applied setting $a = 1$ and $b = 0$ for FkM-F and $a = 0$ and $b = 1$ for PkM-F. Note that for PkM-F and C-PkM-F we adopted the previously described rule for skipping meaningless solutions. Nonetheless, if, for a certain data set, feasible PkM-F or C-PkM-F solutions were not found, then the rule was ignored.

6.1.1. Results

First of all, the selection procedure for PFkM-F proposed in Section 5.2 gave the following average values computed using all the 1280 data sets: $m = 1.63$, $\eta = 1.72$, $a = 3.16$ and $b = 1.69$. Thus, the values of m and η were almost equal on average, whereas the selection procedure tended to choose a value of a higher than the one of b. For FkM-F the average value of m was 1.67, for C-PkM-F and PkM-F the ones of η were 1.99 and 2.32, respectively.

In order to evaluate how the clustering methods worked, we observed their ability to estimate properly the centroids and to assign the non-outliers and the outliers to the clusters with high or low degrees of sharing or typicality, respectively. To assess how well every method recovered the true centroids we computed the REC measure based on the sum of the squared dissimilarities of the centers and the spreads between all the true and estimated centroids:

$$REC = \sum_{g=1}^{k} \left[d^2 \left(\mathbf{h}_g^{C_1}, \mathbf{h}_g^{C_1\,T} \right) + d^2 \left(\mathbf{h}_g^{C_2}, \mathbf{h}_g^{C_2\,T} \right) + d^2 \left(\mathbf{h}_g^{L}, \mathbf{h}_g^{L\,T} \right) + d^2 \left(\mathbf{h}_g^{R}, \mathbf{h}_g^{R\,T} \right) \right], \quad (32)$$

where the superscript 'T' refers to the matrices of the centers and the spreads for the true centroids determined using the non-outliers, i.e., computing the average values of the observations belonging to every cluster. To analyze the

19
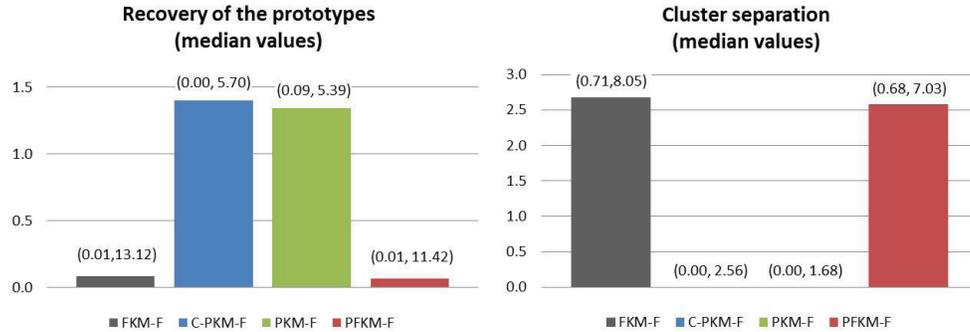
Figure 4: Median values and 10th and 90th percentiles (within parentheses) of REC and SEP.

level of separation between centroids, we computed the SEP measure, based on the minimum sum of the squared dissimilarities of the centers and the spreads between pairs of centroids:

$$SEP = \min_{g,g'(g\neq g')} \left[d^2 \left(\mathbf{h}_g^{C_1}, \mathbf{h}_{g'}^{C_1} \right) + d^2 \left(\mathbf{h}_g^{C_2}, \mathbf{h}_{g'}^{C_2} \right) + d^2 \left(\mathbf{h}_g^{L}, \mathbf{h}_{g'}^{L} \right) + d^2 \left(\mathbf{h}_g^{R}, \mathbf{h}_{g'}^{R} \right) \right] . (33)$$

Figure 4 displays the median values and the 10th and 90th percentiles of (32) and (33) for the four methods. To investigate how well the four methods assigned the observations to the clusters we studied the percentage of non-outliers assigned to the correct cluster in the hard clustering sense, i.e., with degrees of sharing or typicality higher than 0.5. With regard to the non-outliers we also checked the degrees of sharing or typicality to the correct and wrong cluster. Finally, we analyzed the maximal degree of the outliers. The median values and the 10th and 90th percentiles of the previous quantities are reported in Figure 5.

By inspecting Figure 4 some comparative assessments about how the methods recovered the prototypes can be given. The methods based on the fuzzy approach performed better than those based on the possibilistic one (REC values reported in the left side of Figure 4). This can be motivated by observing the median SEP values (right side of Figure 4) from which we can see the tendency of the possibilistic methods to produce coincident clusters. Note that the percentage of occurrences of trivial solutions was 72.27% and 79.61% for C-PkM-F and PkM-F, respectively. A good compromise was achieved by PFkM-F that worked well by exploiting the potentialities of

20

Percentage of the non-outlier objects assigned to the correct cluster in the hard clustering sense (median values)

Degree of the non-outlier objects to the correct cluster (median values)

Degree of the non-outlier objects to the wrong cluster (median values)

Maximal degree of the outliers (median values)
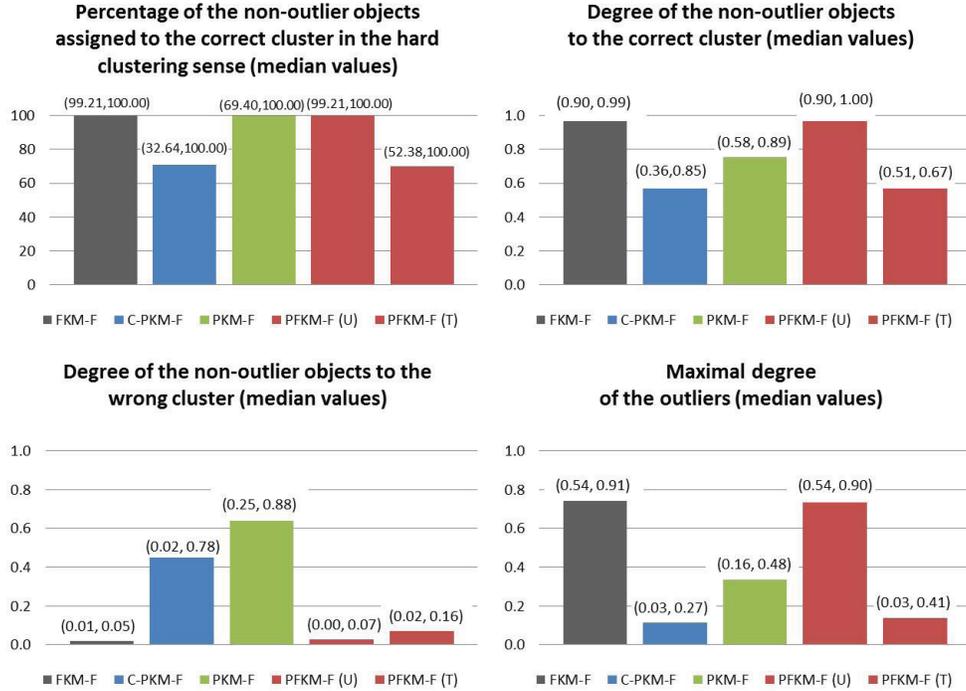
Figure 5: Median values and 10th and 90th percentiles (within parentheses) of percentages of non-outliers assigned (hard clustering sense) to the correct cluster, degrees of non-outliers assigned to the correct and wrong cluster and maximal degrees of outliers.

the possibilistic and fuzzy approaches, namely, it estimated the prototypes reasonably well and avoided coincident clusters (no trivial PFkM-F solutions were registered during the entire simulation study).

By inspecting Figure 5, we can see that the fuzzy membership degree information (the matrices **U** from FkM-F and PFkM-F) was more insightful than the possibilistic membership degree information (the matrices **T** from C-PkM-F, PkM-F and PFkM-F) with respect to the non-outliers, but was not helpful when dealing with contaminated data. In fact, non-outliers were almost always assigned to the correct cluster (top left side of Figure 5) with high (median equal to 0.97) fuzzy membership degrees (top right side of Figure 5) by applying FkM-F and PFkM-F (considering **U**). A good performance was also observed for PkM-F. However, by looking at the low and left side of the figure, we can observe that PkM-F also tended to give high

degrees of typicality to the wrong cluster. This occurred because PkM-F frequently produced coincident clusters and, hence, high degrees of typicality to all the clusters. The fuzzy membership degrees were not informative to recognize the outliers (bottom right side of Figure 5). In fact, by considering the fuzzy membership degree matrix $\mathbf{U}$ from FkM-F, we could not assess whether outliers were present in the data. This was not the case when we considered the possibilistic membership degrees. In fact, C-PkM-F and PkM-F assigned the outliers to the clusters with median degrees of typicality lower than 0.5. The above comments on fuzzy and possibilistic membership degrees jointly hold for PFkM-F. This allows us to highlight the complementary information provided by $\mathbf{U}$ and $\mathbf{T}$. More specifically, on the one hand, the degrees of typicality (in $\mathbf{T}$) allowed us to properly discover the presence of outliers. On the other hand, the degrees of sharing (in $\mathbf{U}$) allowed us to properly discover the fuzzy cluster structure.

6.1.2. Computational issues

We investigated some computational issues related to the PFkM-F algorithm for fixed values of k, a, b, m and η (without taking into account the computational time of the parameter selection procedure proposed in Section 5.2). The computational complexity of PFkM-F has the same order of magnitude as FkM and, in particular, it is linear with respect to the number of observations, $\mathcal{O}(n)$. We studied it in practice together with the tendency of the algorithm to hit local optima. The former point was analyzed by observing the computation time in seconds. Note that the simulation study was carried out on a personal computer with 2.80 GHz processor and 16.00 GB RAM and the convergence criterion was 10^{-5}. The risk of local optima was assessed by recording, for each data set, the percentage of times in which the function value was less than 0.1% bigger than that of the purported global optimum (PGO). The PGO was defined as the best estimate of the global optimum, i.e., for each data set, the best solution out of five runs of the PFkM-F. The results concerning computation time and risk of local optima referred to the runs of PFkM-F setting the parameters according to the selection procedure of Section 5.2. The average computation time of the PFkM-F algorithm was 0.39s. It mainly depended on the number of observations (the average computation times were equal to 0.14s and 0.62s when $n = 60$ and $n = 240$, respectively), the number of clusters (0.24s when $k = 2$ and 0.54s when $k = 3$), the number of variables (0.26s when $p = 2$ and 0.51s when $p = 8$) and the percentage of outliers (0.26s for the *low* level of contami-

nation and 0.51s for the *high* one). The registered computation times were almost always lower than 1.00s (93.84% of times) and the maximum one was lower than 10.00s.

The average percentage of times in which the PGO was attained was 59.97%. We observed that the PFkM-F algorithm was more prone to hit the PGO when $k = 2$, when the clusters were distinguished by the spreads (*spr* case) and when the level of contamination was low (*low* case): in such cases the percentages of attaining the PGO were 70.28%, 72.06% and 73.19%, respectively. Therefore, more than one random start is suggested to reduce the risk of local optima. In particular, the use of five random starts appears to be appropriate.

6.2. Real data

6.2.1. Sensory profiling Gamonedo cheese data

The first application to real data was an example in sensory analysis. The quality of a specific kind of cheese from Asturias (Spain), named Gamonedo blue cheese, has been investigated by the LILA institute for obtaining the Protected Designation of Origin (PDO) [42]. This was done by taking into account the subjective perceptions of experts about $n = 42$ Gamonedo cheeses made by different producers with respect to $p = 11$ characteristics: shape, rind, texture aspect, smell intensity, smell quality, texture hardness, crispness, flavour intensity, flavour quality, aftertaste, global quality. In particular, for each cheese the expert was invited to express her/his perception using a graduate scale ranging from 0% (lowest quality) to 100% (highest quality). We believed that these perceptions did not allow a precise representation. Hence, according to the ontic treatment, they were managed by fuzzy data seen as whole entities. Specifically, the perception of each characteristic was represented by means of a trapezoidal fuzzy number whose 0-level was the set of values that were compatible with the opinion of the taster at some extent and the 1-level was the set of values that were fully compatible with her/his opinion. Finally, the trapezoidal fuzzy number was obtained by linearly interpolating these two levels. The assessments made by one of the experts were analyzed by PFkM-F [1]. The optimal parameters were found in connection with the minimum of XB_{PF-F} (see, Figure 6). We got $k = 2$, $m = 1.5$, $\eta = 2$, $a = 3$ and $b = 1$.

---

[1]The data are available upon request.
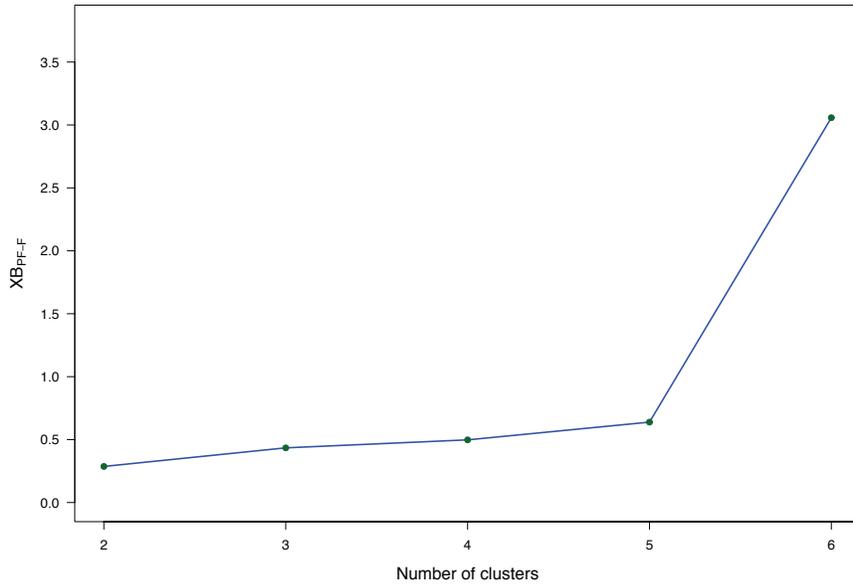
Figure 6: Values of XB_{PF-F} for number of cluster k from 2 to 6, related to the sensory profiling Gamonedo cheese data.

In order to visualize the results, in Figure 7 we displayed the cheeses and the centroids onto the plane found by applying Principal Component Analysis for fuzzy data [43]. First of all it was interesting to discover that the first component (x-axis) was mainly related to smell intensity, smell quality, flavour intensity, flavour quality, aftertaste and global quality, hence this component reflected the smell and taste likings, closely related to the global quality. Component 2 (y-axis) depended on shape, rind and texture aspect and, thus, was interpreted as the sight liking. By observing the centroids, the two clusters distinguished 'high quality Gamonedo cheeses' (Cluster 1) and 'low quality Gamonedo cheeses' (Cluster 2). In the hard clustering sense, the fuzzy partition was composed by clusters of size 23 (Cluster 1) and 19 (Cluster 2). Some cheeses (denoted by dashed line rectangles) shared their fuzzy membership degrees between the two clusters. In fact, they were assigned to Cluster 1 with membership degrees lower than 0.70. Hence, they had intermediate values between the two clusters. To assess how far these cheeses were from the centroids, the degrees of typicality in the matrix **T** were stud-

24
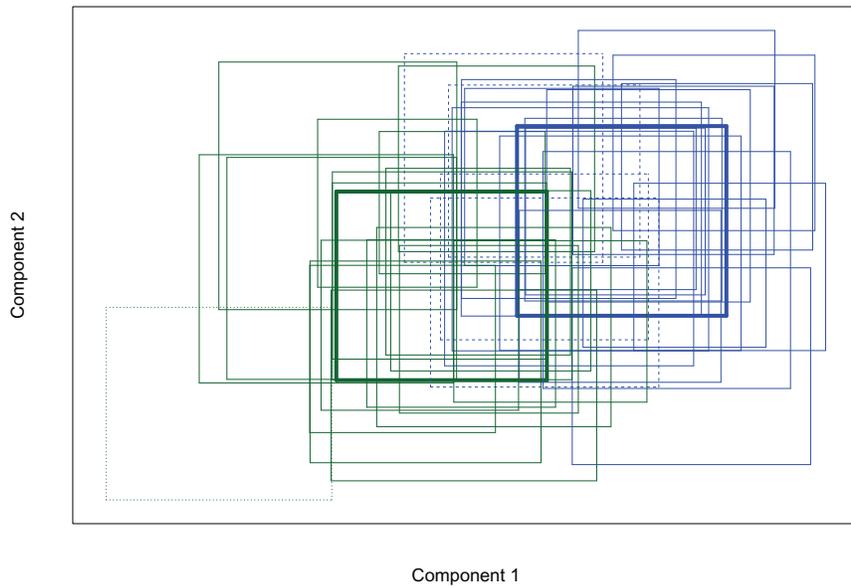
Figure 7: Plot of the first two components of the sensory profiling Gamonedo cheese data. The blue rectangles refer to cheeses assigned to Cluster 1 and the green ones to those assigned to Cluster 2; the solid or dashed lines denote cheeses assigned to the clusters with membership degree ≥ 0.70 or in the interval in the interval $(0.50, 0.70)$, respectively; the dotted line denotes the anomalous cheeses characterized by low maximal degrees of typicality; the bold solid line denotes the centroids.

ied. Among others, an interesting finding concerned the cheese represented by a dot line rectangle. It was clearly assigned to Cluster 2 (with degree of sharing equal to 0.88), but the corresponding degree of typicality was very low (0.16). This showed that the involved cheese was very far from both the clusters. It was assigned to Cluster 2 because it was extremely far from the centroid of Cluster 1. On the basis of the cluster interpretation, we concluded that such a cheese was an outlier because it was definitely not appreciated by the expert, i.e. its scores were noticeably lower than those pertaining to the other cheeses.

6.2.2. Temperature data

The data referred to the monthly temperatures in Celsius degrees of a set of geographical units in Italy. We assumed that the temperature of a

25
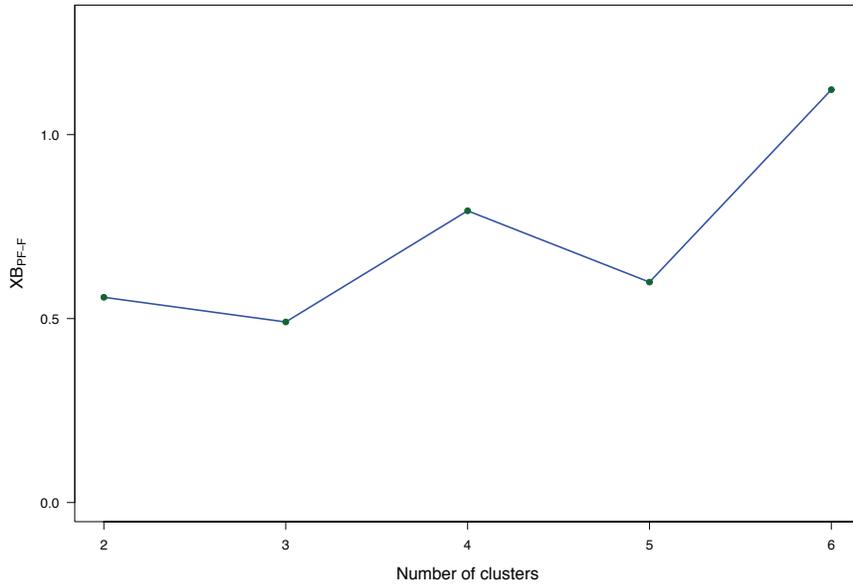
Figure 8: Values of XB_{PF-F} for number of cluster k from 2 to 6, related to the monthly temperature data.

certain geographical unit is an intrinsically fuzzy datum due to size of the area. Thus, the imprecision of the data was considered in the ontic sense. For every geographical unit ($n = 162$) and every month ($p = 12$ the information was represented by a triangular fuzzy number[2].

The use of the PFkM-F clustering algorithm aimed at discovering some common patterns among the geographical units and the existence of anomalous geographical units. The optimal parameters were found according to XB_{PF-F} (Figure 8). We got $k = 3$, $m = 1.75$, $\eta = 2$, $a = 4.5$ and $b = 2.5$.

The three clusters highlighted the presence of three levels of temperature: hot, warm and cold. In the hard clustering sense, according to the degrees of sharing in $\mathbf{U}$, such a fuzzy partition was composed by clusters of size 71, 76 and 13, respectively. A summary of the PFkM-F results is displayed in Figure 9 where we plotted the geographical units and the centroids onto the planes spanned by the first two principal components [43].

---

[2]The data are available upon request.
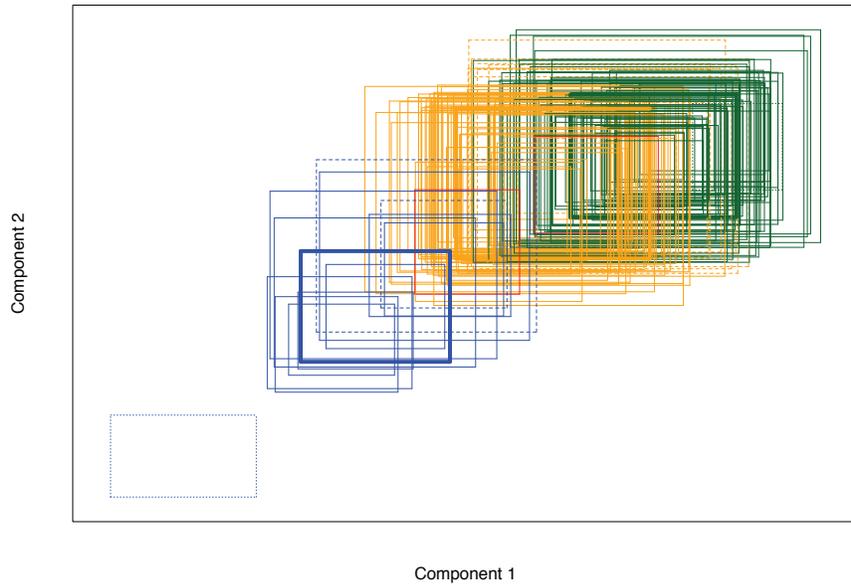
Figure 9: Plot of the first two components of the temperature data. The green rectangles refer to geographical units assigned to Cluster 1, the orange ones to those assigned to Cluster 2 and the blue ones to those assigned to Cluster 3; the solid or dashed lines denote geographical units assigned to the clusters with membership degrees ≥ 0.70 or in the interval $(0.50, 0.70)$, respectively; the red dotted rectangles denote geographical units not assigned to the clusters in the hard clustering sense (degrees of sharing < 0.50); the green or blue dotted lines denote anomalous geographical units assigned to the clusters (degrees of sharing ≥ 0.50) and characterized by low maximal degrees of typicality; the bold solid line denotes the centroids.

The locations of the centroids was consistent with the cluster interpretation taking into account that Components 1 and 2 reflected the wintertime and summertime temperatures, respectively. From the top right side to the bottom left side the centroids of Clusters 1 (green solid line rectangle), 2 (orange solid line rectangle) and 3 (blue solid line rectangle) are ordered. Apart from some exceptions, the first two clusters discriminated the geographical units with respect to their positions. In detail, Clusters 1 and 2 were composed by geographical units from Southern and Northern-Central and Italy, respectively. Instead, mountain geographical units belonged to Cluster 3. Therefore, this cluster of smaller size had the merit of highlighting the unique features of the geographical units characterized by high altitude.

27

The majority of the geographical units were assigned to the clusters with high (≥ 0.70) degrees of sharing (solid line rectangles of different colors according to the cluster memberships). A small percentage (about 13%), denoted by dashed line rectangles, was assigned to the clusters with membership degrees lower than 0.70 (and higher than 0.50). Only two geographical units, Firenzuola and Monte Calamita from Tuscany (represented by black solid line rectangles), were not assigned to the clusters with membership degrees greater than 0.50. This occurred because these units had intermediate values between two clusters. In particular, Firenzuola shared the features of Clusters 1 and 2 and Monte Calamita those of Clusters 2 and 3.

In order to detect anomalous geographical units, we inspected the typicality matrix $\mathbf{T}$. We discovered at least two outliers (Plateau Rosa and Lampedusa) displayed by dotted line rectangles. The temperatures of these geographical units were extremely far from those of all the centroids. Plateau Rosa (rectangle in the bottom left side) was assigned to Cluster 3 with degree of sharing equal to 0.76, but the corresponding degree of typicality is 0.01. It is a mountain geographical units located in front of the Matterhorn mountain with altitude higher than 3000 meters. The registered temperatures were much colder than those of the centroid of Cluster 3. The opposite comment held for Lampedusa, the southernmost part of Italy, with respect to Cluster 1 (degrees of sharing and typicality to Cluster 1 equal to 0.83 and 0.09, respectively). The associated rectangle (in the top right of the figure) had the center farthest to the right. In fact, Lampedusa had extremely hot temperatures, especially in the wintertime.

7. Concluding remarks

In this paper we have developed some robust clustering methods for nonprecise information. First we have proposed a fully possibilistic version of the k-means clustering method for LR fuzzy data (PkM-F) where, differently from the fuzzy approach, the sum of the membership degrees of an observation to all the clusters is no longer required to be equal to one. In this respect, the possibilistic membership degrees can be interpreted as degrees of typicality, rather than as degrees of sharing as is the case for the fuzzy approach. Although PkM-F should be not sensitive to outliers, it has a major limitation, namely coincident clusters may occur. To overcome this problem, a second approach has been proposed. It consists in hybridizing the fuzzy and possibilistic approaches to clustering, exploiting the benefits of both the

approaches (i.e., to extract information about the fuzzy partition and the typicality of the observations) and avoiding their limitations (i.e., disruptive effect of outliers and coincident cluster problem). We have referred to this method as possibilistic fuzzy k-means clustering method for LR fuzzy data (PFkM-F). Some parameters must be set before running the PFkM-F. A selection procedure for choosing good values for these parameters has been proposed. It is based on a novel cluster validity index for hybrid clustering methods such as PFkM-F. We have checked the adequacy of PFkM-F by means of simulation and real-case studies. This has been done by comparing the performance of PFkM-F with the ones of other related clustering methods for fuzzy data. We have found that PFkM-F worked in a satisfactory way also in comparison with its competitors.

On the basis of these good results, we indicate at least three perspectives of research: to speed up the selection procedure for the PFkM-F parameters by using, for instance, a line search strategy or a Pareto analysis; to generalize to the full LR family the possibilistic clustering method proposed in [23]; to develop biclustering methods for non-fuzzy and/or fuzzy data according to the fuzzy and possibilistic approaches.

Acknowledgements

[1] Zadeh, L.A., 1965. Fuzzy sets. Inf. Control 8, 338–353.

[2] Coppi, R., 2008, Management of uncertainty in Statistical Reasoning: The case of Regression Analysis. Int. J. Approx. Reason. 47, 284–305.

[3] Blanco-Fernández, A., Casals, M.R., Colubi, A., Corral, N., García-Bárzana, M., Gil, M.A., González-Rodríguez, G., López, M.T., Lubiano, M.A., Montenegro, M., Ramos-Guajardo, A.B., de la Rosa de Sáa, S., Sinova, B., 2014. A distance-based statistical analysis of fuzzy number-valued data. Int. J. Approx. Reason. 55, 1487–1501.

[4] Couso, I., Dubois, D., 2014. Statistical reasoning with set-valued information: ontic vs. epistemic views, Int. J. Approx. Reason. 55, 1502–1518.

[5] Colubi, A., González-Rodríguez, G., 2015. Fuzziness in data analysis: towards accuracy and robustness, Fuzzy Sets Syst. 281, 260–271.

[6] Hariz, S.B., Elouedi, Z., Mellouli, K., 2006. Clustering approach using belief function theory. In: Euzenat, J., Domingue, J. (eds.) Artificial Intelligence: Methodology, Systems, and Applications, Springer, pp.162–171.

[7] Quost, B., Denoeux, T., 2010. Clustering fuzzy data using the fuzzy EM algorithm. In: Deshpande, A., Hunter, A. (eds.) Proceedings of the 4th International Conference on Scalable Uncertainty Management, SUM'2010, Toulouse, France, Springer-Verlag, pp.333–346.

[8] Quost, B., Denoeux, T., 2016. Clustering and classification of fuzzy data using the fuzzy EM algorithm. Fuzzy Sets Syst. 286 134–156.

[9] Sato, M., Sato, Y., 1995. Fuzzy clustering model for fuzzy data. FUZZ-IEEE'95, 2123–2128.

[10] Hathaway, R.J., Bezdek, J.C., Pedrycz, W., 1996. A parametric model for fusing heterogeneous fuzzy data. IEEE Trans. Fuzzy Syst. 4, 1277–1282.

[11] Yang, M.S., Ko, C.H., 1996. On a class of fuzzy c-numbers clustering procedures for fuzzy data. Fuzzy Sets Syst. 84, 49–60.

[12] Pedrycz, W., Bezdek, J.C., Hathaway, R.J., Rogers, G.W., 1998. Two nonparametric models for fusing heterogeneous fuzzy data. IEEE Trans. Fuzzy Syst. 6, 411–425.

[13] Takata, O., Miyamoto, S., Umayahara, K., 1998. Clustering of data with uncertainties using Hausdorff distance. Proceedings of the IEEE International Conference on Intelligence Processing Systems, 67–71.

[14] Yang, M.-S., Liu, H.-H., 1999. Fuzzy clustering procedures for conical fuzzy vector data. Fuzzy Sets Syst. 106 189–200.

[15] Takata, O., Miyamoto, S., Umayahara, K., 2001. Fuzzy clustering of data with uncertainties using minimum and maximum distances based on L_1 metric. Proceedings of the Joint 9th IFSA World Congress and 20th NAFIPS International Conference, 2511–2516.

30

[16] Auephanwiriyakul, S., Keller, J.M., 2002. Analysis and efficient implementation of a linguistic fuzzy c-means. IEEE Trans. Fuzzy Syst. 10, 563–582.

[17] Coppi, R., D'Urso, P., 2003. Three-way fuzzy clustering models for LR fuzzy time trajectories. Comput. Stat. Data Anal. 43 149–177.

[18] Yang, M.-S., Hwang, P.-Y., Chen, D.-H., 2004. Fuzzy clustering algorithms for mixed feature variables, Fuzzy Sets Syst. 141, 301–317.

[19] D'Urso, P., Giordani, P., 2006. A weighted fuzzy c-means clustering model for fuzzy data. Comput. Stat. Data Anal. 50 1496–1523.

[20] Hung, W.-L., Yang, M.-S., 2005. Fuzzy clustering on LR-type fuzzy numbers with an application in Taiwanese tea evaluation fuzzy clustering on LR-type fuzzy numbers with an application in Taiwanese tea evaluation. Fuzzy Sets Syst. 150 561–577.

[21] Zarandi, M.H.F., Razaee, Z.S., 2011. A fuzzy clustering model for fuzzy data with outliers. Int. J. Fuzzy Syst. Appl. 1, 29–42.

[22] Coppi, R., D'Urso, P., Giordani, P., 2012. Fuzzy and possibilistic clustering for fuzzy data. Comput. Stat. Data Anal. 56, 915–927.

[23] Ferraro, M.B., Giordani, P., 2013. On possibilistic clustering with repulsion constraints for imprecise data. Inf. Sci. 245, 63–75.

[24] D'Urso, P., De Giovanni, L., 2014. Robust clustering of imprecise data. Chemom. Intell. Lab. Syst. 136, 58–80.

[25] Hung, W.L., Yang, M.-S., 2015. Automatic clustering algorithm for fuzzy data. J. Appl. Stat. 42, 1503–1518.

[26] Banerjee, A., Davé, R.N., 2012. Robust clustering. WIREs Data Mining Knowl. Discov. 2, 29–59.

[27] Krishnapuram, R., Joshi, A., Nasraoui, O., Yi, L., 2001. Low-complexity fuzzy relational clustering algorithms for web mining. IEEE Trans. Fuzzy Syst. 9, 595–607.

[28] García-Escudero, L., Gordaliza, A., 1999. Robustness properties of k-means and trimmed $k$means. J. Am. Stat. Assoc. 94, 956-969.

31

[29] Kim, J., Krishnapuram, R., Davé, R., 1996. Application of the least trimmed squares technique to prototype based clustering. Pattern Recogn. Lett. 17, 633–641.

[30] Davé, R.N., 1991. Characterization and detection of noise in clustering. Pattern Recogn. Lett. 12, 657–664.

[31] Jajuga, K., 2001. L_1-norm based fuzzy clustering. Fuzzy Sets Syst. 39, 43–50.

[32] Wu, K.L., Yang, M.S., 2002. Alternative c-means clustering algorithms. Pattern Recogn. 35, 2267–2278.

[33] Krishnapuram, G.L., Keller, J.M., 1993. A possibilistic approach to clustering. IEEE Trans. Fuzzy Syst. 1, 98–110.

[34] Barni, M., Cappellini, V., Mecocci, A., 1996. Comments on 'a possibilistic approach to clustering'. IEEE Trans. Fuzzy Syst. 4, 393–396.

[35] Pal, N.R., Pal, K., Bezdek, J.C., 1997. A Mixed c-Means Clustering Model. FUZZ-IEEE'97, 11–21.

[36] Pal, N.R., Pal, K., Keller, J.M., Bezdek, J.C., 2005. A possibilistic fuzzy c-means clustering algorithm. IEEE Trans. Fuzzy Syst. 13, 517–530.

[37] Bezdek, J.C., 1981. Pattern recognition with fuzzy objective function algorithm. Plenum Press, New York.

[38] Xie, X.L., Beni, G., 1991. A validity measure for fuzzy clustering. IEEE Trans. Pattern Anal. 13, 841–846.

[39] Yang, M.S., Wu, K.L., 2006. Unsupervised possibilistic clustering. Pattern Recogn. 39, 5–21.

[40] Campello, R.J.G.B., Hruschka, E.R, 2006. A fuzzy extension of the silhouette width criterion for cluster analysis. Fuzzy Sets Syst. 157, 2858–2875.

[41] Rousseeuw, P.J., 1987. Silhouettes: a graphical aid to the interpretation and validation of cluster analysis. J. Comput. Appl. Math. 20, 53–65.

[42] Ramos-Guajardo, A.B., Lubiano, M.A., 2012. K-sample tests for equality of variances of random fuzzy sets. Comput. Stat. Data Anal. 56, 956–966.

[43] Coppi, R., Giordani, P., D'Urso, P., 2006. Component models for fuzzy data. Psychometrika 71, 733-761.