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I. Perova, Ye. Bodyanskiy
Kharkiv National University of Radio Electronics

ADAPTIVE FUZZY CLUSTERING BASED ON MANHATTAN METRICS IN MEDICAL AND BIOLOGICAL APPLICATIONS

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Розглянуто алгоритм нечіткої кластеризації даних за наявності аномальних спостережень. Запропонований рекурсивний алгоритм нечіткої кластеризації даних ґрунтується на використанні манхеттенської метрики, що забезпечує високу швидкість обробки інформації та просту обчислювальну реалізацію. Результат апробації на даних медико-біологічних досліджень підтверджує ефективність запропонованого підходу.

Ключові слова: алгоритм нечіткої кластеризації, манхеттенська метрика, функція Лагранжа.

The problem of fuzzy clustering on the basis of the probabilistic fuzzy approach under the presence of outliers in data is considered. Recursive fuzzy clustering algorithm is proposed, which optimizes the objective function based on Manhattan metrics provides high speed of information processing and simple computational realization. The results of real data clustering confirm the effectiveness of proposed approach in medical data mining tasks.

Key words: fuzzy clustering algorithm, Manhattan metrics, Lagrange function

Introduction

Clustering and classification of datasets of different nature are now key problems of data mining, and effective solving of this tasks is important for knowledge acquisition by analysis of observations.

Generally, cluster analysis is algorithmic basis of data classification by means of separation of the available data into a number of classes (clusters) without a priori defined membership of any observation sample to one of the class (unsupervised learning). In the traditional (crisp) approach it is assumed that every observation belongs to only one class. The k -means algorithm [1] and the nearest-neighbor rule [2] are most popular examples of this approach. It is much more natural to assume that every observation may

belong to several clusters at same time with certain degrees of membership. This assumption is the basis of fuzzy cluster analysis [3, 4]. At present time many fuzzy clustering approaches are widely used, such as Bezdek's fuzzy c-means [3], the Gustafson-Kessel algorithm [5], fuzzy k-nearest neighbors [6], fuzzy shell cluster analysis by Klawonn-Kruse-Timm [7], mountain clustering by Yager and Filev [8] e.a. The approaches mentioned above are capable of efficient data clustering when the clusters are overlapping, but only with the assumption that the clusters are compact, i.e. they do not have abrupt (anomalous) outliers. Whereas real datasets usually contain up to 20% of outliers [9-11], the assumption of clusters compactness may sometimes become inadequate.

This situation often happens when processing medical and biological data sets because human subjective factor plays important role in these tasks.

The source information for all the mentioned algorithms is the data set of N n -dimensional feature vectors $X = \{x(1), x(2), \dots, x(N)\}$, $x(k) \in R^n$, $k = 1, 2, \dots, N$. The output of the algorithm is the separation of the original data into m clusters with some degree of membership $m_q(x(k))$ of the k -th vector to the q -th cluster.

In this paper, we make an attempt to derive an adaptive computationally simple stable fuzzy clustering algorithm for recursive data processing in online mode as more and more data become available, using Manhattan metrics.

Stable probabilistic fuzzy clustering algorithm

Probabilistic fuzzy-clustering approach belong to a class of objective function based algorithm [3] that are designed to solve fuzzy clustering problem via the optimization of a certain predetermined clustering criterion, and are the best-grounded from the mathematical point of view.

For pre-standardized feature vector (the standartization is performed component-wise so that all the feature vectors belong to the hypercube $[-1, 1]^n$), the objective function is

$$E^k = \sum_{k=1}^N \sum_{q=1}^m m_q^\beta(x(k)) d(x(k), c_q) \quad (1)$$

subject to constraints

$$\sum_{q=1}^m m_q(x(k)) = 1, \quad k = 1, \dots, N, \quad (2)$$

$$0 < \sum_{k=1}^N m_q(x(k)) < N, \quad q = 1, \dots, m \quad (3)$$

Here $m_q(x(k)) \in [0, 1]$ is the degree of membership of the vector $x(k)$ to the q -th cluster, c_q is the prototype (center) of the q -th cluster, β is a non-negative parameter, referred to "fuzzifier" (usually $\beta=2$), $d(x(k), c_q)$ is the distance between $x(k)$ and c_q in the adopted metrics. The result of clustering is assumed to be $N \times m$ matrix $W = \{m_q(x(k))\}$, referred to as "fuzzy partition matrix".

Note that since the elements of the matrix W can be regarded as the probabilities of the hypotheses of data vector membership to certain clusters, the procedures generated from (1) subject to constraints (2), (3) are referred to as the "probabilistic clustering algorithms".

The distance function $d(x(k), c_q)$ is usually assumed to be Minkowski L^p metrics [17]

$$d(x(k), c_q) = \left(\sum_{i=1}^n |x_i(k) - c_{qi}|^p \right)^{\frac{1}{p}}, \quad p \geq 1 \quad (4)$$

where $x_i(k)$, c_{qi} are i -th components of $(n \times 1)$ -vectors $x(k)$, c_q respectively. Assuming $\beta=p=2$ leads to the most popular, simple and quite effective Bezdek's fuzzy c-means algorithm [3]

$$\mathbf{m}_q(x(k)) = \frac{\|x(k) - c_q\|^{-2}}{\sum_{l=1}^N \|x(k) - c_l\|^{-2}}, \quad (5)$$

$$c_q = \frac{\sum_{k=1}^N \mathbf{m}_q^2(x(k))x(k)}{\sum_{k=1}^N \mathbf{m}_q^2(x(k))}. \quad (6)$$

Simplicity of (5) and (6) is determined by using of Euclidean (quadratic) metrics, those derivatives on the estimated parameters are linear forms. It allows to obtain a solution in simple analytic form.

At the same time in medical tasks it is more naturally to use Manhattan metrics ($p=1$ in (4)), i.e.

$$d(x(k), c_q) = \sum_{i=1}^n |x_i(k) - c_{qi}| = |x(k) - c_q| \quad (7)$$

whose gradient respectively c_q has the form

$$\nabla_{c_q} d(x(k), c_q) = -\text{sign}(x(k) - c_q) \quad (8)$$

where

$$\text{sign}(x(k) - c_q) = \left(\text{sign}(x_1(k) - c_{q1}), \dots, \text{sign}(x_i(k) - c_{qi}), \dots, \text{sign}(x_n(k) - c_{qn}) \right)^T.$$

By introducing the goal function of probabilistic fuzzy clustering

$$\begin{aligned} E(\mathbf{m}_q(k), c_q) &= \sum_{k=1}^N \sum_{q=1}^m \mathbf{m}_q^b(x(k)) \sum_{i=1}^n |x_i(k) - c_{qi}| = \sum_{k=1}^N \sum_{q=1}^m \mathbf{m}_q^b(x(k)) |x(k) - c_q| = \\ &= \sum_{k=1}^N \sum_{q=1}^m \mathbf{m}_q^b(x(k)) d(x(k), c_q) \end{aligned} \quad (9)$$

and taking into consideration the constraints (2) we can write the Lagrange function

$$L(\mathbf{m}_q(k), c_q, I(k)) = \sum_{k=1}^N \sum_{q=1}^m \mathbf{m}_q^b(x(k)) \sum_{i=1}^n |x_i(k) - c_{qi}| + \sum_{k=1}^N I(k) \left(\sum_{q=1}^m \mathbf{m}_q(k) - 1 \right), \quad (10)$$

where $\lambda(k)$ is an undetermined Lagrange multiplier that guarantees the fulfillment of the constraints (2), (3). The saddle point of the Lagrange function (10) could be found solving the following system of Karush-Kuhn-Tucker equations

$$\left\{ \begin{array}{l} \frac{\partial L(\mathbf{m}_q(k), c_q, I(k))}{\partial \mathbf{m}_q(k)} = 0, \\ \frac{\partial L(\mathbf{m}_q(k), c_q, I(k))}{\partial I(k)} = 0, \\ \nabla_{c_q} L(\mathbf{m}_q(k), c_q, I(k)) = \mathbf{0}. \end{array} \right. \quad (11)$$

Solving the first and the second equations of the system (11) leads to well-known result

$$\left\{ \begin{array}{l} \mathbf{m}_q(x(k)) \frac{d(x(k), c_q)^{\frac{1}{1-b}}}{\sum_{l=1}^m (d(x(k), c_l))^{\frac{1}{1-b}}} = 0, \\ I(k) = - \left(\sum_{l=1}^m (b d(x(k), c_l))^{\frac{1}{1-b}} \right)^{1-b}. \end{array} \right. \quad (12)$$

but the third one

$$\nabla_{c_q} L(\mathbf{m}(x(k)), c_q, I(k)) = \sum_{k=1}^N \mathbf{m}_q^b(x(k)) \nabla_{c_q} d(x(k), c_q) = \mathbf{r} \quad (13)$$

obviously has no analytical solution. The solution of (13) could be computed with use of a local modification of Lagrange function [12] and the recursive fuzzy clustering algorithms [22]. Furthermore, searching the saddle point of the local Lagrange function

$$L(\mathbf{m}_q(x(k)), c_q, I(k)) = \sum_{q=1}^m \mathbf{m}_q^b(x(k)) d(x(k), c_q) + I(k) \left(\sum_{q=1}^m \mathbf{m}_q(x(k)) - 1 \right) \quad (14)$$

using the Arrow-Hurwitz-Uzawa procedure gives the following algorithm:

$$\begin{cases} \mathbf{m}_q(x(k)) = \frac{d(x(k), c_q^{(k)})^{\frac{1}{1-b}}}{\sum_{l=1}^m (d(x(k), c_l^{(k)}))^{\frac{1}{1-b}}}, \\ c_{qi}(k+1) = c_{qi}(k) - \mathbf{h}(k) \frac{\partial L_k(\mathbf{m}_q(x(k)), c_q, I(k))}{\partial c_{qi}} = \\ = c_{qi}(k) + \mathbf{h}(k) \mathbf{m}_q^b(x(k)) \text{sign}(x_i(k) - c_{qi}(k)) \end{cases} \quad (15)$$

where $\mathbf{h}(k)$ is the learning rate parameter, $c_{qi}(k)$ is the i -th component of the q -th prototype vector calculated at the k -th step, or the same in vector form

$$\begin{cases} \mathbf{m}_q(x(k)) = \frac{d(x(k), c_q(k))^{\frac{1}{1-b}}}{\sum_{l=1}^m (d(x(k), c_l(k)))^{\frac{1}{1-b}}}, \\ c_q(k+1) = c_q(k) + \mathbf{h}(k) \mathbf{m}_q^b(x(k)) \text{sign}(x(k) - c_q(k)), \end{cases} \quad (16)$$

that from computational point of view is essentially simpler than the robust fuzzy clustering algorithm, proposed in [23].

Especially simple form this algorithm obtains when $\beta=2$

$$\begin{cases} \mathbf{m}_q(x(k)) = \frac{|x(k) - c_q(k)|^{-1}}{\sum_{l=1}^m |x(k) - c_l(k)|^{-1}}, \\ c_q(k+1) = c_q(k) + \mathbf{h}(k) \mathbf{m}_q^2(x(k)) \text{sign}(x(k) - c_q(k)). \end{cases} \quad (17)$$

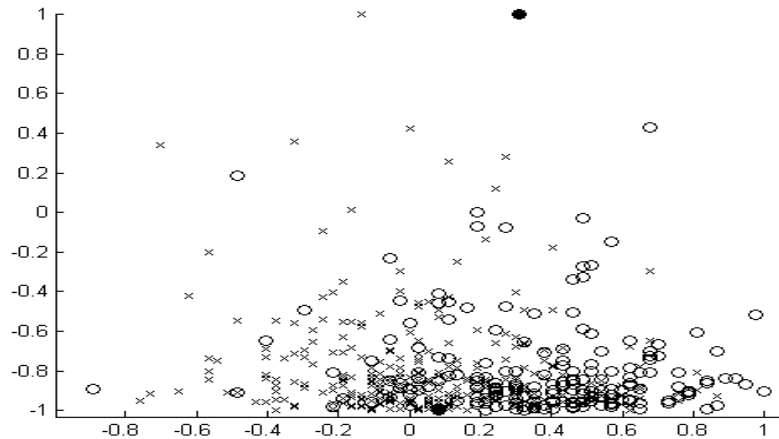


Fig. 1

Experiments

We have used the proposed algorithm in the problem of data clustering of data set from the UCI machine learning database: "heart-disease" [24]. This data set contains 2 clusters. On fig.1 the results of clustering labeled as 'o' and 'x' are shown using two-dimensional projection from nine-dimensional of 1 and 3 properties. Centers of clusters was labeled as '•'. Using adaptive fuzzy clustering based on Manhattan metrics provides satisfactory quality of clustering that is better than quality of clustering based on standard fuzzy-c-means algorithm.

Conclusion

In the paper stable adaptive probabilistic fuzzy clustering algorithm based on the objective function of a special form (Manhattan metrics), suitable for heavy-tailed data distribution with outliers, is proposed. The algorithm could be used in a wide range of applications, such as medical data mining, fault detection, pattern recognition in self-organizing mode when the size of the data set is not known a priori, and the data must be processed in sequential mode, those is typical for medical and biological research.

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