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Global Fuzzy C-Means with Kernels

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***Abstract*—Fuzzy c-means (FCM) is a simple but powerful clustering method using the concept of fuzzy sets that have been proved to be useful in many areas. There are, however, several well-known problems with FCM, such as sensitivity to initialization, sensitivity to outliers, and limitation to convex clusters. In this paper, a new clustering method, which is an extension of global fuzzy c-means (G-FCM) and kernel fuzzy c-means (K-FCM), is proposed to resolve the shortcomings mentioned above. G-FCM is a variant of FCM that uses an incremental seed selection method and is effective in alleviating the sensitivity to initialization. There are several approaches to reduce the influence of noise and properly partition non-convex clusters and K-FCM is one of them. K-FCM is used in this paper because it can easily be extended with different kernels, which provide sufficient flexibility to allow for resolution of the shortcomings of FCM. By combining G-FCM and K-FCM, the proposed method, kernelized global FCM (KG-FCM), can resolve the shortcomings mentioned above. The usefulness of KG-FCM is demonstrated by experiments using artificial and real world data sets.**

Keywords— Fuzzy C-Means; Global Initialization; Kernel Method; Non-Convex Cluster; Noise Robustness

I. INTRODUCTION

Clustering, also known as cluster analysis, assigns an unlabeled data set $X = \{x_1; \ldots, x_N\}$ into $K(1 < K < N)$ homogeneous clusters based on a similarity measure [1] and has formed an important area in pattern recognition, image processing, and, most recently, data mining. A variety of clustering algorithms has been proposed, including fuzzy c-means (FCM), which is the main concern of this paper. Although FCM is an efficient algorithm, there are several difficulties with it: (1) choosing the initial cluster seeds; (2) suppressing noise; (3) accommodating non-convex clusters; and (4) determining the optimal number of clusters. In this paper, we try to solve the problems all but the last problem assuming the number of clusters is known. To address the remaining problems, global fuzzy c-means (G-FCM), which is an extension of global k-means (GKM), is further extended using kernelized fuzzy clustering. G-FCM uses a deterministic approach to select a set of initial seeds to resolve the initialization problem. Kernelized fuzzy clustering is a non-linear counterpart of fuzzy clustering and can accommodate non-convex clusters. Some kernelized clustering methods also has noise robustness according to the kernel used. Although there have been attempts to solve the shortcomings in FCM, they tried to solve one problem at a time. By combining global and kernelized clustering, however, the proposed method can resolve the shortcomings simultaneously.

It has long been known that FCM is only guaranteed to converge on a locally optimal solution, which is sensitive to initial state. Since the problem of obtaining a globally optimal initial state and a globally optimal solution has been shown to be NP-hard, the initialization method for a sub-optimal solution is more practical and of great value. There exist various initialization methods for clustering, which can be categorized into three groups [2]: random sampling methods, distance optimization methods, and density estimation methods. In random sampling methods, probably the most widely adopted ones, multiple runs of clustering with random initial seeds are conducted, and the best or aggregated one is selected as the final clustering result [3]. Although they are simple and statistically sound, they depend heavily on the number of runs, and the computational cost is very high.

Distance optimization methods are used to maximize the distance among the seeds. As many clustering methods, including FCM, try to minimize the intra-cluster variance without optimizing the inter-cluster separation, it is natural to maximize the inter-cluster distance beforehand. The MaxMin procedure [4] and its variants, in which a data point having the largest distance to the existing set of seeds is iteratively added, are the most widely used ones. Although they are simple and efficient, some of them also require multiple runs and the resulting set of seeds tends to be placed on the boundary of data.

Density estimation methods select a set of seeds based on local density, the estimation of which is crucial in these methods. The k-nearest neighbor or ε-radius ball is generally used to decide neighboring points [5], and each requires one additional parameter. G-FCM [6] also belongs to this group, which iteratively adds a data point optimizing the original objective function for clustering as a seed. Due to its deterministic property, it does not require multiple runs and does not need any extra parameter, i.e. does not have the shortcomings in other methods, and demonstrated better results than other methods.

The global clustering method was first formulated for hard clustering [7,8] and extended to soft clustering [6]. These global methods, however, are still affected by noise and cannot accommodate non-convex clusters. The sensitivity to noise can be alleviated in several ways and adopting kernel methods is one of them. Kernel methods were originally proposed to convert linear methods into non-linear ones [9], but it is also well known that some kernels have outlier robustness together with their non-linear properties [10]. Another reason for adopting kernel methods is that they can be extended in several ways using different kernels. There exist other ways to accommodate non-convex clusters and clustering with non-Euclidean distance [11] and spectral clustering [12,13] are well-known and widely adopted ones

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together with kernelized clustering [14]. However, non-Euclidean distance is sensitive to noise, which is also demonstrated in the experiments, and spectral clustering has been proved to be equivalent to kernel clustering [15,16].

In this paper, G-FCM is extended to a kernel-based method, called kernelized global fuzzy c-means (KG-FCM), and realized using two different kernels. First, KG-FCM is implemented using the Cauchy kernel to improve noise robustness, called KG-FCM with Cauchy kernel (KG-FCM-C). KG-FCM-C can be used to determine initial seeds efficiently and treat outliers in a robust way. KG-FCM is also implemented in another way using the random walk kernel [17,18] to accommodate non-convex clusters effectively, called KG-FCM with random walk kernel (KG-FCM-RW). KG-FCM-C is more noise resistant than existing methods and KG-FCM-RW is the most efficient one for clustering non-convex clusters.

In the next two sections, the hard and soft global clustering algorithms – global k-means and global fuzzy c-means, respectively – are briefly described. In Section 4, global fuzzy c-means is extended to kernelized global fuzzy c-means. Experimental results are given in Section 5 and discussions and further research are given in Section 6.

II. GLOBAL K-MEANS (GKM)

The k-means algorithm [19] is an iterative algorithm that finds K crisp and hyper-spherical clusters in the data such that an objective function defined in Eq. (1) is minimized:

$$E(V|X) = \sum_{i=1}^{N} \sum_{k=1}^{K} I(x_i \in C_k) ||x_i - v_k||^2 , \quad (1)$$

where $I(x_i \in C_k)$ is an indicator function having a value of one if data point x_i belongs to the kth cluster (C_k) and zero otherwise. Commonly, the K cluster centers, $V = \{v_1, \dots, v_K\}$, are initialized randomly with data points. Although k-means is one of the simplest learning algorithms and is still in use, one of its major problems is its sensitivity to initialization. To resolve this problem, several methods for initialization have been proposed and global k-means is one of them. Global k-means [7,8] is an incremental approach to clustering that dynamically adds one cluster at a time through a deterministic search procedure. The assumption on which the method is based is that an optimal clustering solution to the k clustering problem can be obtained through N local searches using k-means starting from an initial state with

1. the (k - 1) seeds placed at the centers from the (k - 1) clustering problem and

2. the remaining kth seed placed at a data point x_i($1 < i < N$).

The original version of GKM requires O(N) executions of k-means for one new seed, which results in O(KN) executions of k-means and is not feasible with a large N. Thus a fast GKM algorithm was proposed, in which only one data point maximizing an objective function is considered as a new seed [7]. The objective function is defined as

$$J_k^l = \sum_{j=1}^{N} max\left(\left(d_{k-1}^j\right)^2 - ||x_l - x_j||^2, 0\right) , \quad (2)$$

where d^j_{k-1} is the distance between x_j and the center closest to x_j among the (k-1) cluster centers obtained so far. The quantity J^l_k measures the guaranteed reduction in the objective function obtained by inserting a new cluster center at x_l. The modified algorithm significantly reduces the number of k-means executions from O(KN) to O(K). The fast GKM algorithm is summarized in Fig. 1, where d is the dimensionality of data.

Require: K : number of clusters, X : data set ($N \times d$)
1: $V_1 = \frac{1}{N}\sum_{i=1}^{N} x_i$
2: for k = 2 to K do
3: for l = 1 to N do
4: $J_k^l = \sum_{j=1}^{N} max\left(\left(d_{k-1}^j\right)^2 - ||x_l - x_j||^2, 0\right)$
5: end for
6: $\alpha = argmax_{1 \le l \le N} J_k^l$
7: $V_k = V_{k-1} \cup \{x_\alpha\}$
8: $[V_k] \leftarrow$ k-means(X, V_k)
9: end for
10: return V_K

Fig. 1. GKM: Fast global k-means

III. GLOBAL FUZZY C-MEANS (G-FCM)

With the introduction of fuzzy memberships, global fuzzy c-means (G-FCM) is a direct extension of global k-means (GKM) as FCM is a direct extension of k-means. k-means tries to minimize the sum of squared distances in Eq. (1), which can be extended to FCM by relaxing the indicator function to have continuous values with appropriate constraints. The objective function of FCM can be written as

$$E(U, V|X) = \sum_{i=1}^{N} \sum_{k=1}^{K} u_{ki}^m ||x_i - v_k||^2 , \quad (3)$$

where m is a fuzzifier constant and u_{ki} is the membership of the ith point to the kth cluster satisfying

$$0 \le u_{ki} \le 1 , \quad (4a)$$

$$\sum_{k=1}^{K} u_{ki} = 1 , \quad (4b)$$

$$0 \le \sum_{i=1}^{N} u_{ki} \le N . \quad (4c)$$

G-FCM uses the same algorithm as GKM, except for two things. First, FCM is used instead of k-means. Equations (5) and (6) show the update equations for FCM [20]:

$$u_{ki} = \frac{||x_i - v_k||^{-\frac{2}{m-1}}}{\sum_{j=1}^{K} ||x_i - v_j||^{-\frac{2}{m-1}}} , \quad (5)$$

$$v_k = \frac{\sum_{i=1}^{N} u_{ki}^m x_i}{\sum_{i=1}^{N} u_{ki}^m} , \quad (6)$$

Another difference lies in the objective function for seed selection. Using Eq. (2), GKM tries to find a data point minimizing Eq. (1). Likewise, in G-FCM, one should find a data point minimizing Eq. (3). Equation (3) can be re-formulated using Eq. (5) as [21]

$$E'_{FCM}(V|X) = \sum_{i=1}^{N} \left(\sum_{k=1}^{K} ||x_i - v_k||^{\frac{2}{1-m}}\right)^{1-m} . \quad (7)$$

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The objective function for seed selection then becomes

$$J_k^l = E'_{FCM}(V_{k-1} \cup \{x_l\}|X) . \quad (8)$$

Therefore, Equation (8) should be divided in two according to the type of a center: one from the previous (k-1) clustering problem and the other from a data point.

$$J_k^l = \sum_{i=1}^{N} \left(\sum_{j=1}^{k-1} ||x_i - v_j||^{\frac{2}{1-m}} + ||x_i - x_l||^{\frac{2}{1-m}} \right)^{1-m} . \quad (9)$$

The data point x_α minimizing Eq. (9) is selected as the initial position of a new cluster center. The G-FCM algorithm is summarized in Fig. 2. One thing that should be noted is that memberships do not appear in the algorithm explicitly. However, all the algorithms proposed satisfy the constraints in Eq. (4) due to the re-formulation using Eq. (5).

Require: K : number of clusters, X : data set ($N \times d$)
1: $V_1 = \frac{1}{N}\sum_{i=1}^{N} x_i$
2: for k = 2 to K do
3: for l = 1 to N do
4: $J_k^l = \sum_{i=1}^{N} \left(\sum_{j=1}^{k-1} ||x_i - v_j||^{\frac{2}{1-m}} + ||x_i - x_l||^{\frac{2}{1-m}} \right)^{1-m}$
5: end for
6: $\alpha = argmax_{1 \le l \le N} J_k^l$
7: $V_k = V_{k-1} \cup \{x_\alpha\}$
8: $[V_k] \leftarrow$ FCM(X, V_k)
9: end for
10: return V_K

Fig. 2. G-FCM: Global fuzzy c-means

IV. KERNELIZED GLOBAL FUZZY C-MEANS (KG-FCM)

Although global fuzzy c-means can be used to efficiently decide initial seeds, it still has drawbacks in that it is sensitive to outliers and it is limited to convex clusters. Several approaches have been proposed to alleviate these problems and kernel-based clustering was used in this paper.

Kernel methods were first introduced to clustering by Girolami [14], who proposed kernel k-means. Other kernel-based clustering algorithms were proposed after that [15]. The direct extension of FCM using kernels, kernel FCM (K-FCM), tries to minimize the following objective function:

$$E(U, V|X) = \sum_{i=1}^{N}\sum_{k=1}^{K} u_{ki}^m ||\phi(x_i) - \phi(v_k)||^2 , \quad (10)$$

where $\phi(\cdot)$ is a mapping function. The update equations for K-FCM can be written as

$$u_{ki} = \frac{||\phi(x_i) - \phi(v_k)||^{-\frac{2}{m-1}}}{\sum_{j=1}^{K} ||\phi(x_i) - \phi(v_j)||^{-\frac{2}{m-1}}} , \quad (11)$$

$$\phi(v_k) = \frac{\sum_{i=1}^{N} u_{ki}^m \phi(x_i)}{\sum_{i=1}^{N} u_{ki}^m} . \quad (12)$$

Due to the dimensionality of the mapped data, however, Eqs. (11) and (12) cannot be evaluated directly and one has to use a kernel trick to evaluate the values indirectly using kernels. To make KG-FCM noise-robust, instead of the commonly used Gaussian kernel, the Cauchy kernel was used, which results in kernel FCM with Cauchy kernel (K-FCM-C). The Cauchy kernel has been shown to be outlier-robust and able to effectively accommodate clusters with different densities compared to the Gaussian kernel [10]. The Cauchy kernel can be defined as

$$\kappa_C(x, y) = \frac{1}{1+\beta||x-y||^2} , \quad (13)$$

where β is a kernel parameter. Using Eq. (13), the update equations can be written as [10]

$$u_{ki} = \frac{(1-\kappa_C(x_i, v_k))^{-\frac{1}{m-1}}}{\sum_{j=1}^{K}(1-\kappa_C(x_i, v_j))^{-\frac{1}{m-1}}} , \quad (14)$$

$$v_k = \frac{\sum_{i=1}^{N} u_{ki}^m \kappa_C(x_i, v_k)^2 x_i}{\sum_{i=1}^{N} u_{ki}^m \kappa_C(x_i, v_k)^2} . \quad (15)$$

Although the coordinates of cluster centers in the feature space (Eq. (12)) cannot be evaluated due to dimensionality, the corresponding ones in the input space (Eq. (15)) can be calculated when the Cauchy kernel is used. In Eq. (15), the kernel function $\kappa(x_i, v_k)$ works as a weighting function. The function $\kappa(x_i, v_k)$ weights a data point based on the similarity between x_i and v_j, which results in noise robustness. To do a global search, Eq. (9) also should be kernelized as

$$J_k^l = \sum_{i=1}^{N} \left(\begin{matrix} \sum_{j=1}^{k-1} ||\phi(x_i) - \phi(v_j)||^{\frac{2}{1-m}} \\ +||\phi(x_i) - \phi(v_l)||^{\frac{2}{1-m}} \end{matrix} \right)^2 , \quad (16)$$

which can be simplified as

$$J_k^l = \sum_{i=1}^{N} \left(\begin{matrix} \sum_{j=1}^{k-1} (2 - 2\kappa_C(x_i, v_j)^{\frac{2}{1-m}} \\ +(2 - 2\kappa_C(x_i, x_l)^{\frac{2}{1-m}} \end{matrix} \right)^2 . \quad (17)$$

The final consideration is the evaluation order of the update equations. At the beginning of a k clustering problem, the membership in Eq. (14) must be calculated first to incorporate the current problem into the prior information – the optimal clustering result from the (k-1) clustering problem and the data point minimizing Eq. (17). Figure 3 summarizes K-FCM-C. Kernelized global FCM with Cauchy kernel (KG-FCM-C) is summarized in Fig. 4. Together with its non-linear property, the proposed algorithm can be used to decide initial seeds efficiently and is more robust to outliers than existing methods. However, it still cannot efficiently accommodate non-convex clusters due to its noise suppressing property. This problem can be tackled by the introduction of a random walk kernel.

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Require: K : number of clusters, X : data set ($N \times d$), V_{K-1} : initial centers (($K-1$) × d), α : data point index
1: $V_k = V_{k-1} \cup \{x_\alpha\}$
2: repeat
3: for k = 1 to K do
4: for i = 1 to N do
5: $u_{ki} = \frac{(1-\kappa_C(x_i,v_k))^{-\frac{1}{m-1}}}{\sum_{j=1}^{K}(1-\kappa_C(x_i,v_j))^{-\frac{1}{m-1}}}$
6: end for
7: $v_k = \frac{\sum_{i=1}^{N} u_{ki}^m \kappa_C(x_i,v_k)^2 x_i}{\sum_{i=1}^{N} u_{ki}^m \kappa_C(x_i,v_k)^2}$
8: end for
9: until U satisfies the convergence criterion
10: return V_K, U_K

Fig. 3.K-FCM-C: Kernel FCM with the Cauchy kernel

Require: K : number of clusters, X : data set ($N \times d$)
1: $V_1 = \frac{1}{N}\sum_{i=1}^{N} x_i$
2: for k = 2 to K do
3: for l = 1 to N do
4: $J_k^l = \sum_{i=1}^{N}\left(\sum_{j=1}^{k-1}(2-2\kappa_C(x_i,v_j)^{\frac{2}{1-m}} + (2-2\kappa_C(x_i,x_l)^{\frac{2}{1-m}}\right)^2$
5: end for
6: $\alpha = argmin_{1\le l\le N} J_k^l$
7: $V_k = V_{k-1} \cup \{x_\alpha\}$
8: $[V_k, U_k] \leftarrow$ K-FCM-C(X, V_{k-1}, σ, k)
9: end for
10: return V_K, U_K

Fig. 4. KG-FCM-C: Kernelized global FCM with the Cauchy kernel

The random walk distance is a graph theoretic distance, in which each data point is considered as a node and the distance between two points is defined using Markov property. The random walk distance was formally established by Klein and Randic [17] and is also known as resistance distance following the electronic circuit analogy. Of the two distance measures that can be computed following the property of Markov chain, the average commute time is used in this paper. The average commute time is defined as the average time that a random walker, starting at node i, will take to enter node j($\neq i$) for the first time and go back to node i [18]. The traditional shortest path distance does not consider the number of paths connecting two nodes, but the random walk distance decreases as the number of paths increases or the length of a path decreases. The average commute time can be calculated in terms of the pseudo-inverse of Laplacian matrix, L+, as in Fig. 5. In Fig. 5, σ_i denotes the distance to the ($2d$ + 1)th nearest neighbor from x_i, where d is the dimensionality of data. By deciding the parameter in this way, one can efficiently reduce the effect of noise and accommodate clusters with different densities [22]. To obtain more detailed information, refer to [18] and the references therein. Using the average commute time, the random walk kernel can be defined as

$$\kappa_{RW}(x,y) = exp\left(-\frac{D_C(x,y)}{\sigma^2}\right), \quad (18)$$

where σ is a kernel parameter. The update equation for K-FCM with random walk kernel (K-FCM-RW) can be written in a way similar to Eq. (14) as

$$u_{ki} = \frac{(1-\kappa_{RW}(x_i,v_k))^{-\frac{1}{m-1}}}{\sum_{j=1}^{K}(1-\kappa_{RW}(x_i,v_j))^{-\frac{1}{m-1}}}. \quad (19)$$

Require: K : number of clusters, X : data set ($N \times d$
1: Build an affinity matrix A,
$A_{ij} = A(x_i,x_j) = exp\left(-\frac{||x_i-x_j||^2}{\sigma_i\sigma_j}\right)$
2: Calculate a diagonal degree matrix D,
$D_{ij} = \begin{cases}\sum_{k=1}^{N} A_{ik}, & if\ i=j,\\ 0, & otherwise.\end{cases}$
3: Calculate a Laplacian matrix $L = D - A$ and its pseudo-inverse L^+.
4: Build an average commute time matrix D_C,
$D_{C,ij} = V_G(L_{ii}^+ + L_{jj}^+ - 2L_{ij}^+)$, where $V_G = \sum_{k=1}^{N} D_{kk}$.
5: return D_C

Fig. 5. Average commute time

The cluster center cannot be evaluated in the feature space nor in the input space when the random walk kernel is used, however, $\kappa_{RW}(x_i, v_k)$ can be evaluated as a weighted sum of dot-products between data points,

$$\kappa_{RW}(x_i,v_j) = \frac{\sum_{a=1}^{N} u_{ja}^m \kappa_{RW}(x_a,x_i)}{\sum_{a=1}^{N} u_{ja}^m}. \quad (20)$$

Equation (20) can be used to update membership values in Eq. (19) and to calculate the objective function for seed selection in Eq. (16). The algorithm in Fig. 3 also should be modified, because the coordinates of centers cannot be evaluated in K-FCM-RW and the membership values describe the centers indirectly. Thus, the set of centers, V, in Fig. 3 should be replaced with the membership matrix U, whose kth column represents the membership vector to the kth cluster. The initial value U_1 in kernelized global FCM with random walk kernel (KG-FCM-RW) can be initialized with an ($N \times 1$) vector of ones. Figure 6 summarizes K-FCM-RW and Fig. 7 does KG-FCM-RW.

Require: K : number of clusters, X : data set ($N \times d$), U_{K-1} : initial membership matrix ($N \times (K-1)$), α : data point index
1: $V_k = V_{k-1} \cup \{x_\alpha\}$
2: repeat
3: for k = 1 to K do
4: for i = 1 to N do
5: $u_{ki} = \frac{(1-\kappa_{RW}(x_i,v_k))^{-\frac{1}{m-1}}}{\sum_{j=1}^{K}(1-\kappa_{RW}(x_i,v_j))^{-\frac{1}{m-1}}}$
6: end for
7: end for
8: until U satisfies the convergence criterion
9: return U_K

Fig. 6. K-FCM-RW: Kernel FCM with the random walk kernel

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Require: K : number of clusters, X : data set ($N \times d$)
1: $U_1 = [\,1\ 1\ \ldots\ 1\,]^T$
2: for $k = 2$ to K do
3: for $l = 1$ to N do
4: $$J_k^l = \sum_{i=1}^{N} \left(\begin{array}{c} \sum_{j=1}^{k-1} ||\phi(x_i) - \phi(v_j)||^{\frac{2}{1-m}} \\ +||\phi(x_i) - \phi(v_l)||^{\frac{2}{1-m}} \end{array} \right)^2$$
5: end for
6: $\alpha = argmin_{1 \le l \le N} J_k^l$
7: $[U_k] \leftarrow$ K-FCM-RW(X, U_{k-1}, σ, k)
8: end for
9: return U_K

Fig. 7. KG-FCM-RW: Kernelized global FCM with the random walk kernel

In this section, four kernelized algorithms were developed, two using explicit initialization (K-FCM-*) and two using global initialization (KG-FCM-*). A global method is a wrapper method of the corresponding explicit initialization method and decides initial seeds incrementally. Table 1 compares the methods described in this paper.

TABLE I. COMPARISON OF CLUSTERING METHODS

Method	Cluster boundary	Initialization	Kernel
FCM	convex	random	-
G-FCM	convex	global	-
K-FCM-C	non-convex	random	Cauchy
KG-FCM-C	non-convex	global	Cauchy
K-FCM-RW	non-convex	random	random walk
KG-FCM-RW	non-convex	global	random walk

V. EXPERIMENTAL RESULTS

To investigate the effectiveness of the proposed method, the existing and proposed methods were implemented and tested using Matlab. We tested the methods in Table 1 using artificial and UCI data sets.

A. *Experiments using artificial data sets*

In the first set of experiments, the usefulness of the global search technique is shown.

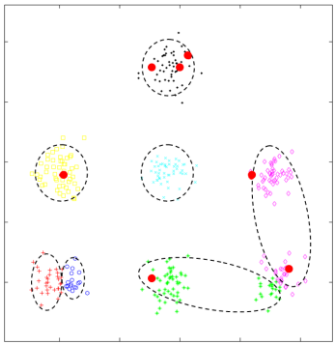

Fig. 8. A clustering result using FCM with random initial seeds represented as large dots

Figure 8 shows a clustering result using FCM. The test data (D_7) consists of seven well-separated clusters generated from Gaussian distributions with means μ = [0 0 7 7 7 14 14; 0 7 0 7 14 0 7] and equal covariance matrix $\Sigma = I$. The large dots represent the random initial seeds used in FCM. Although FCM usually finds the correct structure, it sometimes fails due to the convergence to a local optimum even in a data set with well-separated clusters. For example, only three clusters out of seven are correctly identified in Fig. 8. Figure 9 shows the initial seeds in G-FCM, which are decided in a deterministic way. Conceptually, KG-FCM works exactly the same way as in Fig. 9, but is difficult to visualize due to the dimensionality of the mapped data.

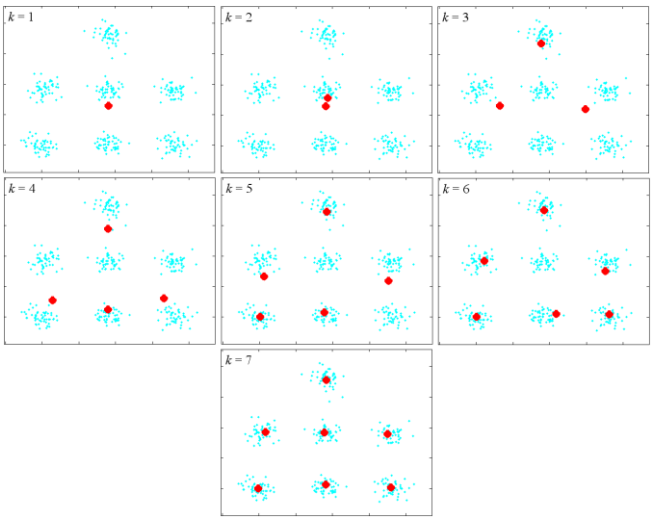

Fig. 9. Incremental seed selection in G-FCM

Table 2 summarizes the clustering results using D_7. The numbers are averaged over 100 runs. FCM occasionally falls into a local optimum. K-FCM-C is a little better than FCM, but sometimes it also falls into a local optimum. K-FCM-RW is the least satisfactory because the random walk distance is based on the path connectivity between points, which is sensitive to outliers. The large variance for K-FCM-RW also corroborates this. The two global methods, G-FCM and KG-FCM-C, always find the correct structure of D_7. KG-FCM-RW is much better than K-FCM-RW, but not as good as other global methods.

TABLE II. EXPERIMENTAL RESULTS USING D_7 (M = # OF CLUSTERS CORRECTLY IDENTIFIED)

Method	M	var(M)
FCM	6.82	0.4925
G-FCM	7.00	0.0000
K-FCM-C	6.92	0.3168
KG-FCM-C	7.00	0.0000
K-FCM-RW	6.42	3.1164
KG-FCM-RW	6.96	0.0788

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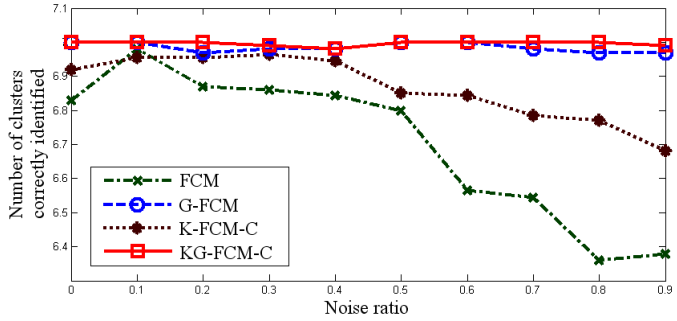
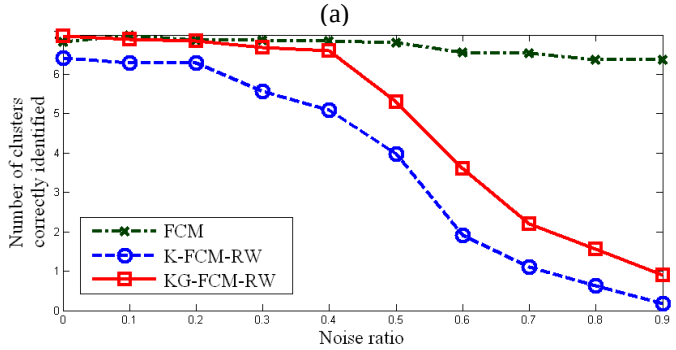
To test noise robustness, some noise points were added to D_7 and the previous experiments were repeated. Noise points were sampled from a uniform distribution and the noise ratio is given as the ratio of the number of noise points to the number of data points. Figure 10 shows the number of correctly identified clusters with respect to noise ratio. For a clear comparison, two subsets out of six methods are plotted on different scales and the numbers are averaged over 100 runs. From Fig. 10(a), we can conclude that the global methods are more robust to noise than the random initialization methods, and KG-FCM-C is best. As the noise ratio increases, the random initialization methods tend to fall into a local optimum, while the global methods do not suffer noise problems and find the right structure. In Fig. 10(b), we can see that K-FCM-RW collapses as the noise ratio increases. Although the global initialization helps, KG-FCM-RW also fails to find the right structure in noisy conditions.



(a)

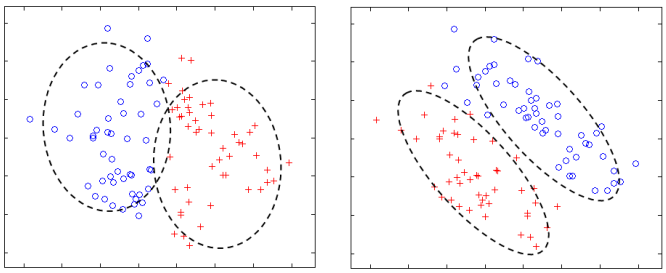


(b)

Fig. 10. Number of clusters correctly identified with respect to noise ratio using D_7

Another merit of kernel clustering methods is that they can cluster irregularly shaped clusters, including non-convex clusters. Figure 11 shows clustering results using a data set consisting of two elongated clusters ($D_{parallel}$). The data consists of two clusters generated from Gaussian distributions with means μ = [0 3; 0 3] and equal covariance matrix Σ = [5 -4; -4 5]. For $D_{parallel}$, by the introduction of another distance measure, for example, Mahalanobis distance instead of Euclidean distance, FCM can also cluster the elongated clusters correctly. Kernel-based clustering methods have another merit, however, outlier robustness. Figure 12 summarizes error rates for $D_{parallel}$ with respect to the distance between two cluster centers ($d_{between}$) and Fig. 13 does the same for the variances of error rates. The error rate is defined as the number of mis-clustered points divided by the number of data points. As there are only two clusters in $D_{parallel}$, the number of correctly identified clusters does not show clear comparison among the methods. Therefore, we used error rate in this experiment.

In this experiment, the methods using global initialization showed almost the same result as the corresponding methods with random initialization, so the results of the global methods are not plotted. As is clear from Fig. 12, FCM with Mahalanobis distance achieves the best result when $d_{between}$ is small because the distance is specialized for Gaussian distributions. However, it sometimes fails to separate the two clusters even when the $d_{between}$ is sufficiently large, because the number of data points in $D_{parallel}$ is not large enough to estimate parameters, including the covariance matrix. The overall large variance also supports that. Another interesting point in Fig. 13 is that the variance for K-FCM-C decreases as $d_{between}$ increases. On the other hand, FCM and K-FCM-RW have peaks, which can be considered as a threshold that determines marginal performance. FCM with Mahalanobis distance shows relatively large variances for all values of $d_{between}$ and does not show a clear relationship between $d_{between}$ and the variance of error rate.



(a) (b)

Fig. 11. Clustering results using (a) FCM and (b) K-FCM-C with random initialization

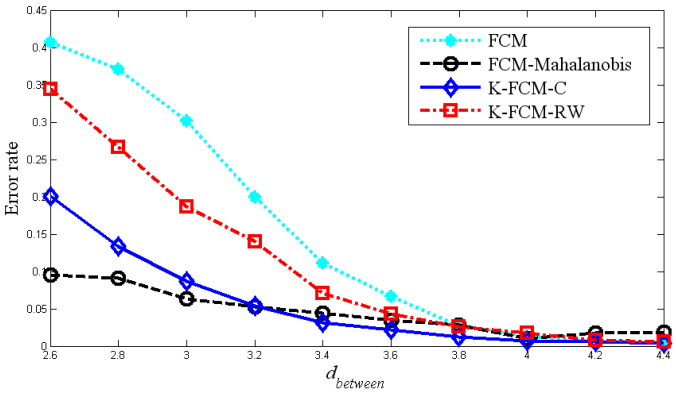


Fig. 12. Error rate with respect to the distance between two cluster centers in $D_{parallel}$

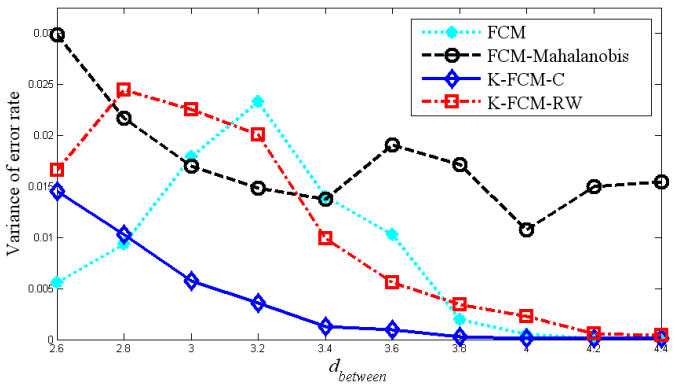


Fig. 13. Variance of error rate with respect to the distance between two cluster centers in $D_{parallel}$

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Although the random walk kernel is noise-sensitive, it is suitable for non-convex clusters. Figure 14 shows a sample data set that is not convex ($D_{non\text{-}convex}$). FCM and K-FCM-C cannot separate the two clusters in Fig. 14 for two different reasons. First, FCM fails to separate the clusters mainly due to the mean squares measure, so FCM tends to separate $D_{non\text{-}convex}$ in a vertical direction (Fig. 15(a)). Second, K-FCM-C fails to separate the clusters due to its noise suppressing property. As a result, K-FCM-C considers the points at the end of semi-circles as outliers and tends to separate $D_{non\text{-}convex}$ in a horizontal direction (Fig. 15(b)). Figure 16 shows the error rate with respect to the distance depicted in Fig. 14. As the distance decreases, the error rate of FCM increases. K-FCM-C is slightly better than FCM, but also fails to separate two clusters although the cluster boundaries in K-FCM-C are not convex. Only K-FCM-RW can correctly separate the non-convex clusters, but it also fails when two clusters are too close.

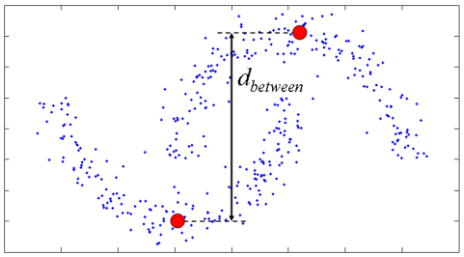
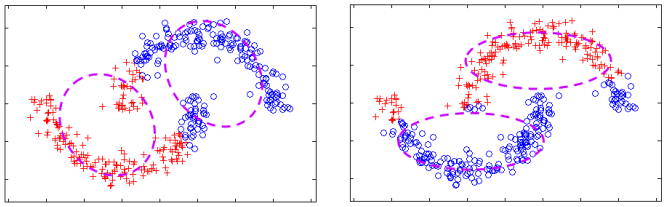


Fig. 14. Non-convex clusters and the distance between two clusters



(a) (b)

Fig. 15. Clustering results using (a) FCM and (b) K-FCM-C

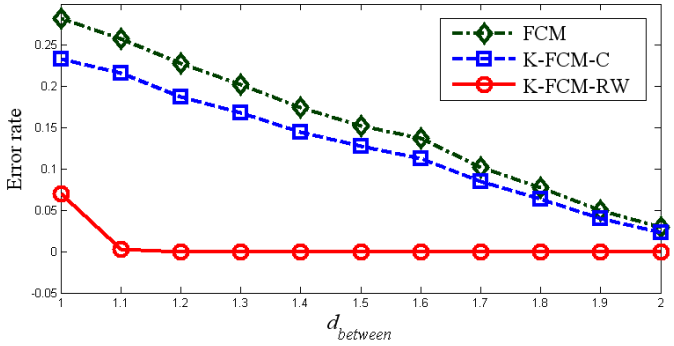


Fig. 16. Error rate with respect to the distance between two clusters $D_{non\text{-}convex}$

B. Experiments using real world data sets

The proposed methods were also applied to some UCI data sets available from the UCI Machine Learning Repository [23]. To compare the results using different clustering methods, an information-based distance, a simplified variation of information (VI) was used. As VI is a true metric on the space of clusterings and retains the comparability over different experimental conditions, it has strength over other measures. As we compared a clustering to ground truth, a modified VI was used. To obtain more detailed information about VI measure, refer to [24] and the references therein.

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TABLE III. EXPERIMENTAL RESULTS USING UCI DATA SETS

Data set	N	d	K′	Global method	D_I	Random method	D_I		
							Min.	Average	Max.
Iris	150	4	3	G-FCM	0.4041	FCM	0.4041	0.4042	0.4045
				KG-FCM-C	0.3898	K-FCM-C	0.3898	0.3898	0.3898
				KG-FCM-RW	0.2663	K-FCM-RW	0.6057	0.6164	0.6365
Wine	178	13	3	G-FCM	1.2944	FCM	1.2944	1.3088	1.3386
				KG-FCM-C	1.2284	K-FCM-C	1.2284	1.2368	1.3128
				KG-FCM-RW	1.2683	K-FCM-RW	1.1542	1.2351	1.4986
Breast cancer	569	30	2	G-FCM	0.9329	FCM	0.9329	0.9339	0.9535
				KG-FCM-C	0.8712	K-FCM-C	0.8243	0.9224	0.9535
				KG-FCM-RW	0.9381	K-FCM-RW	0.9202	0.9393	0.9535
Yeast	180	8	5	G-FCM	1.6129	FCM	1.6043	1.6139	1.7376
				KG-FCM-C	1.5855	K-FCM-C	1.8001	1.8001	1.8001
				KG-FCM-RW	1.8021	K-FCM-RW	1.6755	1.8430	1.9138

(N : # of data points, d : data dimension, K′ : # of classes)

Suppose two different clusterings, $C = \{C_1, \dots, C_K\}$ and $C' = \{C'_1, \dots, C'_{K'}\}$ (corresponds to the set of known labels), which cluster the data into K and K' clusters respectively. The probability of a point being in cluster C_k equals $p(k) = N_k / N$, where N_k is the number of points belonging to the kth cluster and N is the number of data points. The numbers satisfy

$$N = \sum_{k=1}^{K} N_k = \sum_{k=1}^{K'} N'_k \,. \tag{21}$$

The information contained in clustering C' can be represented as the entropy of the random variable $p(k')$,

$$H(C') = -\sum_{k=1}^{K'} p(k') \log p(k') \,, \tag{22}$$

and the amount of information common to both clusterings can be represented as the mutual information of the two random variables, $p(k)$ and $p(k')$,

$$I(C, C') = \sum_{k=1}^{K'} \sum_{k'=1}^{K'} p(k, k') \log \frac{p(k,k')}{p(k)p(k')} \,, \tag{23}$$

where $p(k, k') = |C_k \cap C'_{k'}| / N$ is the probability that a point belongs to C_k in clustering C and to $C'_{k'}$ in clustering C'. Then the difference between the two terms represents the amount of information that is not described by a clustering C:

$$D_I(C, C') = H(C') - I(C, C') \,. \tag{24}$$

Equation (24) is zero if and only if the two clusterings are identical when $K = K'$, and can be considered as a distance of a clustering (C) from another clustering or ground truth (C'). As the number of clusters in C increases, the mutual information increases and D_I decreases. Experimentally, clustering with large number of clusters, $K > K'$, showed a smaller D_I than that with the same number of clusters, $K = K'$, but the relative performance did not change. Therefore, the number of clusters (K) is set to be equal to the number of classes (K') in this paper. Table 3 summarizes the experimental results using UCI data sets. DI values for random methods in Table 3 are averaged over 100 runs.

- Iris: On average, the global method is better than the corresponding random method, and the kernel-based methods are better than the input space method. KG-FCM-RW is best for the iris data because the iris data is relatively noise-free and one of the three clusters is clearly separated from the others. One interesting thing is that K-FCM-RW is likely to fall into a local optimum. Conversely, FCM and K-FCM-C rarely fall into a local optimum.

- Wine: As before, the kernel-based methods show better results, and KG-FCM-C shows the best result. One thing that should be noted is that K-FCM-RW with random initialization hits the minimum and, on average, K-FCM-RW is better than KG-FCM-RW.

- Breast cancer: Although the number of classes is only two, the dimensionality is higher than those in previous data sets. Again, the global methods are better than the random methods, but K-FCM-RW performs worst. This is mostly due to the small size of the data, which distributes the data sparsely in high dimensional space and makes it difficult to estimate the connectivity information. In this experiment, KG-FCM-C also fails to achieve the minimum of K-FCM-C.

- Yeast: Only 5 of 10 classes were used in this experiment. The results are almost the same as the previous ones using the breast cancer data. As the number of clusters increases, K-FCM-RW becomes more unstable and K-FCM-RW performs worst in this experiment.

From the experiments using UCI data sets, we can conclude that:

- The global initialization is useful for deciding initial seeds, although the global methods sometimes fail to achieve the minimum of the corresponding random methods. This failure is mainly due to the different sets of possible initial values, which originates from the fact that the random methods can only have data points as their initial positions but the global methods can have non-occupied positions.

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- KG-FCM-C is more robust to outliers than other methods and shows better and more stable results on test data sets.

- KG-FCM-RW shows better result on the iris data, which is clean and has a relatively well separated cluster structure. However, as the dimensionality of data or the number of clusters increases, it is more likely to fall into a local optimum.

VI. DISCUSSION

Fuzzy c-means (FCM) is a simple and efficient method for clustering. However there are also several well-known shortcomings with FCM. In this paper, we developed kernelized global fuzzy c-means (KG-FCM) to solve the problems in FCM: sensitivity to initialization, sensitivity to noise, and inability to accommodate non-convex clusters. KG-FCM is based on global fuzzy c-means (G-FCM) then extended with the help of kernel methods. KG-FCM is implemented using two different kernels: the Cauchy kernel to suppress noise and the random walk kernel to accommodate non-convex clusters. Experimental results show that, on average, the global methods are superior to the random methods, and KG-FCM-C gave the best results for test data sets most of the time. KG-FCM-RW shows good results only when data are clean and have well-separated clusters, for example, the iris data.

Although the proposed algorithm, KG-FCM, is better than existing methods, it can still be further improved. Initially, kernel methods were adopted because of the various effects obtained using different kernels. As is clear from the experiments, the Cauchy kernel is good at suppressing outliers and the random walk kernel is efficient at separating non-convex clusters. However, each kernel has the other's strength as its weakness. Still another kernel may combine the strengths of the two; this is under investigation. Another weakness of the global methods is that they sometimes show poorer results than the corresponding random methods. A different seed selection function may solve this problem, which is left for further research.

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