Multiple Kernel Fuzzy Clustering

Hsin-Chien Huang, Yung-Yu Chuang and Chu-Song Chen

***Abstract*—While fuzzy c-means is a popular soft clustering method, its effectiveness is largely limited to spherical clusters. By applying kernel tricks, the kernel fuzzy c-means algorithm attempts to address this problem by mapping data with non-linear relationships to appropriate feature spaces. Kernel combination, or selection, is crucial for effective kernel clustering. Unfortunately, for most applications, it is not easy to find the right combination. We propose a multiple kernel fuzzy c-means (MKFC) algorithm which extends the fuzzy c-means algorithm with a multiple kernel learning setting. By incorporating multiple kernels and automatically adjusting the kernel weights, MKFC is more immune to ineffective kernels and irrelevant features. This makes the choice of kernels less crucial. In addition, we show multiple kernel k-means (MKKM) to be a special case of MKFC. Experiments on both synthetic and real-world data demonstrate the effectiveness of the proposed MKFC algorithm.**

***Index Terms*—Clustering, soft clustering, fuzzy c-means, multiple kernel learning.**

I. Introduction

CLUSTERING is an unsupervised method for dividing data into disjoint subsets with high intra-cluster similarity and low inter-cluster similarity. Over the past decades, many clustering algorithms have been proposed, including k-means clustering [1], mixture models [1], spectral clustering [2], locality-sensitive hashing [3], and maximum margin clustering [4], [5]. Most of these approaches perform hard clustering, that is, they assign each item to a single cluster. This works well when clustering compact and well-separated groups of data, but in many real-world situations, clusters overlap. Thus, for items that belong to two or more clusters, it may be more appropriate to assign them with gradual memberships to avoid coarse-grained assignments of data [6]. This class of clustering methods is called soft – or fuzzy – clustering.

Fuzzy c-means (FCM) [7], [8] is one of the most promising fuzzy clustering methods. In most cases, it is more flexible than the corresponding hard clustering algorithms. Unfortunately, as with other clustering methods that are based on the L_2-norm distance in the observation space, it has been shown while it is effective for spherical clusters it does not perform well for more general clusters [9]. Thus kernel-based clustering has been proposed to perform clustering in a typically higher-dimensional feature space spanned by embedding maps and corrsponding kernel functions [10]. The fuzzy c-means algorithm has also been extended to the kernel fuzzy c-means algorithm [11] which yields better performance. However, for such kernel-based methods, a crucial step is the combination or selection of the best kernels among an extensive range of possibilities. This step is often heavily influenced by prior knowledge about the data and by the patterns we expect to discover [12]. Unfortunately, it is unclear which kernels are more suitable for a particular task [13], [14].

The problem is aggravated for many real-world clustering applications, in which there are multiple potentially useful cues. For such applications, to apply kernel-based clustering, it is often necessary to aggregate features from different sources into a single aggregated feature. However, these features are often not equally relevant to clustering; some are irrelevant, and some are less important than others [9]. As most clustering methods do not embed a feature selection capability, such feature imbalances often necessitate an additional process of feature selection, or feature fusion, before clustering.

Instead of a single fixed kernel, multiple kernels may be used. Recent developments in multiple kernel learning have shown that the construction of a kernel from a number of basis kernels allows for more flexible encoding of domain knowledge from different sources or cues. However, as observed by Zhao *et al.*, previous multiple kernel learning approaches have focused on supervised and semi-supervised learning [13]. A notable exception is their work on multiple kernel maximum margin clustering [13] which is designed for hard clustering.

We here extend the multiple kernel learning paradigm to fuzzy clustering. The proposed multiple kernel fuzzy c-means (MKFC) algorithm simultaneously finds the the best degrees of membership and the optimal kernel weights for a non-negative combination of a set of kernels. We also embed the feature weight computation into the clustering procedure. The incorporation of multiple kernels and the automatic adjustment of kernel weights renders MKFC more immune to unreliable features or kernels. It also makes combining kernels more practical since appropriate weights are assigned automatically. Effective kernels or features tend to contribute more to the clustering and therefore improve results. Compared to Zhao *et al.*'s work [13], our approach provides the following advantages. First, our method does not require explicit evaluation in the feature space but conducts only kernel-based evaluations. Thus our method is more suitable for relational data than their method. Second, MKFC is easy to implement. As mentioned by Zhao *et al.* [13], their formulation leads to a non-convex integer optimization problem which is much more difficult to solve. Finally, MKFC yields fuzzy (soft) clustering results which are more appropriate when clusters have significant overlap.

Manuscript received September 16, 2010; revised February 20, 2011 and June 16, 2011. This work was supported in part by the National Science Council of Taiwan, R.O.C., under Grants NSC 98-2221-E-001-012-MY3 and NSC100-2622-E-002-016-CC2.

Hsin-Chien Huang is with the Department of Computer Science and Information Engineering, National Taiwan University and Institute of Information Science, Academia Sinica, Taipei, Taiwan. e-mail: sean@cmlab.csie.ntu.edu.tw.

Yung-Yu Chuang is with the Department of Computer Science and Information Engineering, National Taiwan University, Taipei, Taiwan. e-mail: cyy@csie.ntu.edu.tw.

Chu-Song Chen is with Research Center for Information Technology Innovation and Institute of Information Science, Academia Sinica, Taipei, Taiwan. e-mail: song@iis.sinica.edu.tw.

The rest of the paper is organized as follows. In Section II we discuss related work, and in Section III we review the fuzzy c-means algorithm. We derive the MKFC method in Section IV, and we present in Section V experiments on both synthetic and real data. We conclude in Section VI.

II. Related work

In the fuzzy c-means algorithm, a data item may belong to more than one cluster with different degrees of membership. The algorithm was first developed by Dunn in 1973 [7] and was later improved by Bezdek in 1981 [8]. Dave and Krishnapuram [15] analyzed several popular robust clustering methods and established the connection between fuzzy set theory and robust statistics. Hathaway and Bezdek [16] extended the RFCM algorithm to arbitrary (non-Euclidean) dissimilarity data. Dave and Sen [17] proposed the fuzzy relational data clustering algorithm which can handle data sets containing outliers and can deal with all kinds of relational data. Parameters such as the fuzzification degree greatly affect the performance of FCM. While Pal and Bezdek [18] suggest that a good setting for this degree for some applications is 2, this choice was based on empirical studies and may not be appropriate for some real data sets. Yu and Yang [19] presented the generalized FCM algorithm, proposing an approach for setting algorithm parameters. Krishnapuram *et al.* [20] presented the fuzzy c-medoid relational clustering algorithm, which can efficiently cluster large data sets.

The use of kernels has received considerable attention because kernels make it possible to map data onto a high dimensional feature space in order to increase the representation capability of linear machines. Genton [21] presented classes of kernels for machine learning from a statistical perspective. As FCM is similar to the k-means algorithm in that it uses the squared Euclidean distance to measure similarity between prototypes and data points, it is more effective when clustering spherical clusters [11]. Girolami generalized the approach for a wider variety of clusters when he proposed kernel-based clustering [10]. Camastra and Verri [22] presented a kernel-based clustering algorithm inspired by the k-means algorithm that iteratively refines results using a one-class support vector machine. Tzortzis *et al.* [23] proposed a deterministic and incremental algorithm to overcome the cluster initialization problem: their algorithm maps data points from the input space to a higher dimensional feature space through the use of a kernel function and optimizes the clustering error. Later, Zhang and Chen proposed the kernel-based fuzzy c-means (KFC) algorithm [11] which also allows for incomplete data. Shen *et al.* addressed the same problem using weighted KFC for better feature selection [9]. Leski extended the fuzzy c-means algorithm with insensitivity control so that the resulting method is more robust to noise and outliers [24]. Filippone *et al.* [25] contributed a survey of kernel and spectral clustering methods. Kernel clustering methods are the kernel versions of many classical clustering algorithms such as k-means and SOM. Hathaway *et al.* [26] extended kernelization to relational data clustering by proposing a kernelized form of the non-Euclidean relational fuzzy c-means algorithm. Chiang and Hao [27] proposed a multiple spheres support vector clustering algorithm based on the adaptive cell growing model which maps data points to a high dimensional feature space using the desired kernel function. As mentioned by Graves and Pedrycz [14], KFC is divided into two categories. In the first category, prototypes reside in the feature space and are implicitly mapped to the kernel space through the use of a kernel function, whereas in the second category, prototypes are directly constructed in the kernel space, which allows more freedom for prototypes in the feature space.

Our method is related to multiple kernel learning. For kernel methods, the key to success is the formation of a suitable kernel function [13]. However, a single kernel selected from a pre-defined group is sometimes insufficient to represent the data. Different features chosen for data can result in different similarity measures corresponding to distinct kernels. The combination of multiple kernels from a set of basis kernels has therefore gained acceptance as a way to refine the results of single kernel learning. Multiple kernel learning originates from Lanckriet *et al.*'s work [28] which results in a convex optimization problem for support vector machines. Bach *et al.* suggested an alternative algorithm based on sequential minimization optimization [29]. Efficiency issues of multiple kernel learning were later addressed by Sonnenburg *et al.* using semi-infinite linear programming [30] and by Rakotomamonjy *et al.* using a two-step alternation optimization scheme [31]. Varma and Babu studied superlinear combinations of kernels [32] and Gonen *et al.* studied local combinations of kernels [33]. Frigui *et al.* [34] proposed a semi-supervised algorithm that clusters and aggregates relational data (SS-CARD): this algorithm not only partitions the data into meaningful clusters, but also aggregates pairwise distances from multiple relational matrices and learns a relevance weight for each matrix in each cluster. However, most effort along this direction has been spent on supervised learning, in particular, support vector classification and regression. An exception to extend multiple kernels to unsupervised learning, hard clustering in particular, is Zhao *et al.*'s work [13] which is based on maximum margin clustering. Our work is the first to extend multiple kernels to soft clustering.

III. Fuzzy c-means

In this section we briefly review the fuzzy c-means (FCM) algorithm and its derivation. Given the number of clusters C and a set of data $\mathbf{X}$ containing N l-dimensional vectors, $\mathbf{x}_i$, the fuzzy c-means algorithm outputs the degrees of membership u_{ic}, that is, the possibility that data $\mathbf{x}_i$ belongs to the c-th cluster, by minimizing the following objective function:

$$J(\mathbf{U},\mathbf{V}) = \sum_{i=1}^{N}\sum_{c=1}^{C} u_{ic}^{m} d^2(\mathbf{x}_i,\mathbf{v}_c) \tag{1}$$

$$\text{subject to} \quad \sum_{c=1}^{C} u_{ic} = 1, \quad \forall i$$

$$\text{and} \quad u_{ic} \geq 0, \quad \forall i, c$$

$$\text{and} \quad \sum_{i=1}^{N} u_{ic} > 0, \quad \forall c,$$

Algorithm 1 Fuzzy c-means (FCM). Given a set of N data points $\mathbf{X} = \{\mathbf{x}_i\}_{i=1}^{N}$ and the desired number of clusters C, output a membership matrix $\mathbf{U} = \{u_{ic}\}_{i,c=1}^{N,C}$.

procedure FCM(Data $\mathbf{X}$, Number C)
  Initialize membership matrix $\mathbf{U}^{(0)}$
  repeat
    update $\mathbf{V}^{(t)} = [\mathbf{v}_c]$ by calculating centers $\mathbf{v}_c$ using Equation (4)
    update $\mathbf{U}^{(t)} = [u_{ic}]$ by calculating memberships u_{ic} using Equation (3)
  until $\| \mathbf{U}^{(t)} - \mathbf{U}^{(t-1)} \| < \epsilon$
  return $\mathbf{U}^{(t)}$
end procedure

where m is the fuzzification degree, which should be larger than 1; $d(\cdot,\cdot)$ is the Euclidean distance; $\mathbf{v}_c$ is the center of the c-th cluster; $\mathbf{U} = [u_{ic}]_{i=1..N,c=1..C}$ is an $N \times C$ membership matrix whose elements are the degrees of membership; and $\mathbf{V} = [\mathbf{v}_1 \mathbf{v}_2 \cdots \mathbf{v}_C]$ is a $l \times C$ matrix whose columns correspond to cluster centers. In the fuzzy c-means algorithm we solve the above constrained optimization problem using Lagrange multipliers:

$$J_\lambda(\mathbf{U},\mathbf{V}) = \sum_{i=1}^{N}\sum_{c=1}^{C} u_{ic}^m d^2(\mathbf{x}_i,\mathbf{v}_c) + \lambda\left(\sum_{c=1}^{C} u_{ic} - 1\right). \quad (2)$$

The problem is solved by iteratively updating degrees of membership with fixed centers and updating centers with fixed degrees of membership. The closed-form formulas for updates are derived by taking the partial derivatives with respect to both and setting them to zero.

$$u_{ic} = \frac{1}{\sum_{c'=1}^{C}\left(\frac{d(\mathbf{x}_i,\mathbf{v}_c)}{d(\mathbf{x}_i,\mathbf{v}_{c'})}\right)^{\frac{2}{m-1}}} \quad (3)$$

and

$$\mathbf{v}_c = \frac{\sum_{i=1}^{N} u_{ic}^m \mathbf{x}_i}{\sum_{i=1}^{N} u_{ic}^m} \quad (4)$$

One thing to note is that although we do not add any Lagrange multiplier for the non-negative constraints in Equation (1), it can be verified that the above formula implicitly satisfies constraints such as $u_{ic} \geq 0, \ \forall i, c$. In addition, when m is very close to 1, the fuzzy c-means algorithm degenerates to the k-means algorithm. Algorithm 1 summarizes the fuzzy c-means algorithm.

IV. Multiple kernel fuzzy c-means

A. Objective function

To discover nonlinear relationships among data, kernel methods use embedding mappings that map features of the data to new feature spaces [12]. Consider a set of M such mappings, $\Phi = \{\phi_1, \phi_2, \cdots, \phi_M\}$. Each mapping ϕ_k recodes the l-d data $\mathbf{x}$ as a vector $\phi_k(\mathbf{x})$ in its feature space whose dimensionality is L_k. Let $\{\kappa_1, \kappa_2, \cdots, \kappa_M\}$ be the Mercer kernels corresponding to these implicit mappings respectively,

$$\kappa_k(\mathbf{x}_i,\mathbf{x}_j) = \phi_k(\mathbf{x}_i)^T \phi_k(\mathbf{x}_j).$$

To combine these kernels and also ensure that the resulted kernel still satisfies Mercer's condition, we consider a non-negative combination of these feature maps, ϕ', that is,

$$\phi'(\mathbf{x}) = \sum_{k=1}^{M} \omega_k \phi_k(\mathbf{x}) \quad \text{with } \omega_k \geq 0.$$

Unfortunately, as these implicit mappings do not necessarily have the same dimensionality, such a linear combination may be impossible. Hence, we construct a new set of independent mappings, $\Psi = \{\psi_1, \psi_2, \cdots, \psi_M\}$, from the original mappings Φ as

$$\psi_1(\mathbf{x}) = \begin{bmatrix} \phi_1(\mathbf{x}) \\ \mathbf{0} \\ \vdots \\ \mathbf{0} \end{bmatrix}, \psi_2(\mathbf{x}) = \begin{bmatrix} \mathbf{0} \\ \phi_2(\mathbf{x}) \\ \vdots \\ \mathbf{0} \end{bmatrix}, \cdots, \psi_M(\mathbf{x}) = \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \\ \vdots \\ \phi_M(\mathbf{x}) \end{bmatrix}.$$

Each of these constructed mappings converts $\mathbf{x}$ into a L-d vector, where $L = \sum_{k=1}^{M} L_k$. Note that it is possible that some feature spaces have infinite dimensionalities. In such cases, we can always interlace the dimensions of these features so that they still form a set of orthogonal bases. However, as we later eliminate evaluation in the feature space, this will not matter. Constructing new mappings in this way ensures that the feature spaces of these mappings have the same dimensionality and their linear combination can be well defined. In addition, these mappings form a new set of orthogonal bases since

$$\begin{aligned} &\psi_k(\mathbf{x}_i)^T \psi_k(\mathbf{x}_j) = \kappa_k(\mathbf{x}_i,\mathbf{x}_j) \\ &\psi_k(\mathbf{x}_i)^T \psi_{k'}(\mathbf{x}_j) = 0 \qquad \text{if } k \neq k'. \end{aligned}$$

As such orthogonal bases prevent cross terms between different implicit mappings, we can focus on the inner product of data of the same mapping that can be well evaluated by the original kernel functions. We seek to find $\psi(\mathbf{x}) = \sum_{k=1}^{M} \omega_k \psi_k(\mathbf{x})$, a non-negative linear expansion of the bases in Ψ, which maps data to an implicit feature space. Thus, the objective function becomes

$$J(\mathbf{w},\mathbf{U},\mathbf{V}) = \sum_{i=1}^{N}\sum_{c=1}^{C} u_{ic}^m \left(\psi(\mathbf{x}_i) - \mathbf{v}_c\right)^T \left(\psi(\mathbf{x}_i) - \mathbf{v}_c\right) \quad (5)$$

$$\psi(\mathbf{x}) = \omega_1\psi_1(\mathbf{x}) + \omega_2\psi_2(\mathbf{x}) + \cdots + \omega_M\psi_M(\mathbf{x})$$

$$\text{subject to } \ \omega_1 + \omega_2 + \cdots + \omega_M = 1 \quad (6)$$

$$\text{and } \ \omega_k \geq 0, \ \ \forall k \quad (7)$$

$$\text{and } \ \sum_{c=1}^{C} u_{ic} = 1, \ \ \forall i \quad (8)$$

$$\text{and } \ u_{ic} \geq 0, \ \ \forall i, c \quad (9)$$

$$\text{and } \ \sum_{i=1}^{N} u_{ic} > 0, \ \ \forall c,$$

where $\mathbf{v}_c$ is the center of the c-th cluster in the implicit feature space, $\mathbf{w} = (\omega_1, \omega_2, \cdots, \omega_M)^T$ is a vector consisting

of weights, $\mathbf{U}$ is a $N \times C$ membership matrix whose elements are the memberships u_{ic}, and $\mathbf{V}$ is a $L \times C$ matrix whose columns correspond to cluster centers.

B. Optimizing memberships

The goal of multiple kernel fuzzy c-means (MKFC) is to simultaneously find combination weights $\mathbf{w}$, memberships $\mathbf{U}$, and cluster centers $\mathbf{V}$ which minimize the objective function in Equation (5). However, directly evaluating the cluster centers may not be possible because they are in the implicit feature space; we show later that their associated computation can be replaced by the kernel trick. Similar to fuzzy c-means, we first fix the weights and cluster centers to find the optimal memberships. For brevity, we use D_{ic} to denote the distance between data $\mathbf{x}_i$ and cluster center $\mathbf{v}_c$, i.e., $D_{ic}^2 = (\psi(\mathbf{x}_i) - \mathbf{v}_c)^T (\psi(\mathbf{x}_i) - \mathbf{v}_c)$. Thus, Equation (5) can be written as

$$J(\mathbf{w}, \mathbf{U}, \mathbf{V}) = \sum_{i=1}^{N} \sum_{c=1}^{C} u_{ic}^m D_{ic}^2. \tag{10}$$

When the weights and cluster centers are fixed, the distances are constants. Similar to fuzzy c-means (Equation (2)), by forming an energy function with Lagrange multiplier λ for the constraint $\sum_{c=1}^{C} u_{ic} = 1$, we have the following equation:

$$J_\lambda(\mathbf{U}, \mathbf{V}) = \sum_{i=1}^{N} \sum_{c=1}^{C} u_{ic}^m D_{ic}^2 + \lambda \left(\sum_{c=1}^{C} u_{ic} - 1 \right).$$

Next, we take its derivatives with respect to the memberships and set them to zero; for each membership u_{ic}, we have

$$\frac{\partial J_\lambda}{\partial u_{ic}} = m D_{ic}^2 u_{ic}^{m-1} + \lambda = 0.$$

The solution for u_{ic} is

$$u_{ic} = \left(\frac{-\lambda}{m} \right)^{\frac{1}{m-1}} \frac{1}{D_{ic}^{2/(m-1)}}.$$

Because of the constraint $\sum_{c=1}^{C} u_{ic} = 1$, we can eliminate λ and obtain the closed-form solution for the optimal memberships as

$$u_{ic} = \frac{1}{\sum\limits_{c'=1}^{C} \left(\frac{D_{ic}^2}{D_{ic'}^2} \right)^{\frac{1}{m-1}}}. \tag{11}$$

C. Optimizing weights

From Equation (11), it can be seen that when the weights $\mathbf{w}$ and cluster centers $\mathbf{V}$ are fixed, the optimal memberships $\mathbf{U}$ can be obtained. Now, let us assume the memberships are fixed. We seek to derive the optimal centers and weights to combine the kernels. By taking the derivative of $J(\mathbf{w}, \mathbf{U}, \mathbf{V})$ in Equation (5) with respect to $\mathbf{v}_c$ and setting it to zero, we have

$$\frac{\partial J(\mathbf{w}, \mathbf{U}, \mathbf{V})}{\partial \mathbf{v}_c} = -2 \sum_{i=1}^{N} u_{ic}^m (\psi(\mathbf{x}_i) - \mathbf{v}_c) = 0.$$

Hence, when $\mathbf{U}$ are given, the optimal $\mathbf{v}_c$ is the following closed-form solution represented by the combination weights:

$$\mathbf{v}_c = \frac{\sum\limits_{i=1}^{N} u_{ic}^m \psi(\mathbf{x}_i)}{\sum\limits_{i=1}^{N} u_{ic}^m} = \sum_{i=1}^{N} \hat{u}_{ic} \psi(\mathbf{x}_i), \tag{12}$$

where $\hat{u}_{ic} = \frac{u_{ic}^m}{\sum_{i=1}^{N} u_{ic}^m}$ is the normalized membership. However, these cluster centers are in the kernel-defined feature space which might be implicit or even have an infinite dimensionality. Therefore, it may be impossible to evaluate these centers directly. Fortunately, for clustering, it is often sufficient to just obtain the memberships; we later show that it is possible to obtain memberships and weights without implicitly evaluating cluster centers. Thus, we focus on finding optimal weights for fixed memberships when the cluster centers are the closed-form optimal solution (Equation (12)).

$$\begin{aligned} D_{ic}^2 =& (\psi(\mathbf{x}_i) - \mathbf{v}_c)^T (\psi(\mathbf{x}_i) - \mathbf{v}_c) \\ =& \psi(\mathbf{x}_i)^T \psi(\mathbf{x}_i) - 2\psi(\mathbf{x}_i)^T \left(\sum_{j=1}^{N} \hat{u}_{jc} \psi(\mathbf{x}_j) \right) \\ &+ \left(\sum_{j=1}^{N} \hat{u}_{jc} \psi(\mathbf{x}_j) \right)^T \left(\sum_{j'=1}^{N} \hat{u}_{j'c} \psi(\mathbf{x}_{j'}) \right) \\ =& \sum_{k=1}^{M} \omega_k^2 \kappa_k(\mathbf{x}_i, \mathbf{x}_i) - 2 \sum_{j=1}^{N} \sum_{k=1}^{M} \hat{u}_{jc} \omega_k^2 \kappa_k(\mathbf{x}_i, \mathbf{x}_j) \\ &+ \sum_{j=1}^{N} \sum_{j'=1}^{N} \sum_{k=1}^{M} \hat{u}_{jc} \hat{u}_{j'c} \omega_k^2 \kappa_k(\mathbf{x}_j, \mathbf{x}_{j'}) \end{aligned} \tag{13}$$

Since memberships are fixed and kernel functions can be evaluated, Equation (13) can be re-arranged as

$$D_{ic}^2 = \sum_{k=1}^{M} \alpha_{ick} \omega_k^2, \tag{14}$$

where the coefficient α_{ick} can be written as

$$\begin{aligned} \alpha_{ick} =& \kappa_k(\mathbf{x}_i, \mathbf{x}_i) - 2 \sum_{j=1}^{N} \hat{u}_{jc} \kappa_k(\mathbf{x}_i, \mathbf{x}_j) \\ &+ \sum_{j=1}^{N} \sum_{j'=1}^{N} \hat{u}_{jc} \hat{u}_{j'c} \kappa_k(\mathbf{x}_j, \mathbf{x}_{j'}). \end{aligned} \tag{15}$$

Note that we have eliminated cluster centers from the evaluation. Thus, the objective function in Equation (10) becomes

$$\begin{aligned} J(\mathbf{w}, \mathbf{U}) = & \sum_{i=1}^{N} \sum_{c=1}^{C} u_{ic}^m \sum_{k=1}^{M} \alpha_{ick} \omega_k^2 \\ \text{suject to } & \omega_1 + \omega_2 + \cdots + \omega_M = 1 \\ \text{and } & \omega_k \geq 0, \quad \forall k \\ \text{and } & \sum_{c=1}^{C} u_{ic} = 1, \quad \forall i \\ \text{and } & u_{ic} \geq 0, \quad \forall i, c. \end{aligned} \tag{16}$$

When memberships are fixed, we have

$$J(\mathbf{w}) = \sum_{k=1}^{M} \beta_k \omega_k^2 \quad (17)$$
$$\text{subject to } \omega_1 + \omega_2 + \cdots + \omega_M = 1$$
$$\text{and } \omega_k \geq 0, \ \forall k,$$

where the coefficient β_k is

$$\beta_k = \sum_{i=1}^{N} \sum_{c=1}^{C} u_{ic}^m \alpha_{ick}. \quad (18)$$

This is a constrained optimization problem. By introducing a Lagrange multiplier, we have

$$J_\lambda(\mathbf{w}, \lambda) = \sum_{k=1}^{M} \beta_k \omega_k^2 - 2\lambda \left(\sum_{k=1}^{M} \omega_k - 1 \right).$$

Note that for now, we ignore the constraint that weights must be non-negative. Later we show that it is satisfied in our solution. By taking the partial derivatives and setting them to zero, we have

$$\frac{\partial J_\lambda}{\partial \omega_k} = 2\beta_k \omega_k - 2\lambda = 0.$$

The solution for the above equation is $\omega_k = \frac{\lambda}{\beta_k}$. In addition, we know that

$$\sum_{k=1}^{M} \omega_k = \left(\frac{1}{\beta_1} + \frac{1}{\beta_2} + \cdots + \frac{1}{\beta_M} \right) \lambda = 1.$$

Thus, we have

$$\lambda = \frac{1}{\frac{1}{\beta_1} + \frac{1}{\beta_2} + \cdots + \frac{1}{\beta_M}},$$

and the weight is the harmonic mean

$$\omega_k = \frac{\frac{1}{\beta_k}}{\frac{1}{\beta_1} + \frac{1}{\beta_2} + \cdots + \frac{1}{\beta_M}}. \quad (19)$$

Above, we have derived the alternative optimizations of memberships and kernel combination weights. However, the derivations are based only on the equality constraints (Equations (6) and (8)) and do not take into account the inequality constraint, that is, that the memberships and weights should not be negative (Equations (7) and (9)). Since it is easy to verify that the derived memberships (Equation (11)) always satisfy $u_{ic} \geq 0$ and $\sum_{i=1}^{N} u_{ic} > 0, \ \forall c$, we show that the solution of the combination weights also satisfies the non-negative constraint, i.e., $\omega_k \geq 0$. We first show that $\beta_k \geq 0$ for all k. By definition, D_{ic}^2 should always be non-negative for all weights, that is, $\forall \omega_k, D_{ic}^2 = \sum_{k=1}^{M} \alpha_{ick} \omega_k^2 \geq 0$. Thus, we can conclude that $\forall \omega_k, \alpha_{ick} \geq 0$. Otherwise, if $\alpha_{ick'} < 0$ for some k', we can let $\omega_{k'} = 1$ and $\omega_k = 0$ if $k \neq k'$. But this set of weight assignments means that $D_{ic}^2 < 0$, which contradicts its non-negative property. Therefore, since both α_{ick} and u_{ic} are non-negative, from Equation (18), we conclude that $\beta_k \geq 0$. Finally, since ω_k's are harmonic means of non-negative β_k's as shown in Equation (19), they are also non-negative. Thus, even though we do not initially take into account the non-negative constraint, the solution we obtain automatically satisfies this constraint.

Algorithm 2 Multiple kernel fuzzy c-means (MKFC). Given a set of N data points $\mathbf{X} = \{\mathbf{x}_i\}_{i=1}^N$, a set of kernel functions $\{\kappa_k\}_{k=1}^M$, and the desired number of clusters C, output a membership matrix $\mathbf{U} = \{u_{ic}\}_{i,c=1}^{N,C}$ and weights $\{\omega_k\}_{k=1}^M$ for the kernels.

procedure MKFC(Data $\mathbf{X}$, Number C, Kernels $\{\kappa_k\}_{k=1}^M$)
  Initialize membership matrix $\mathbf{U}^{(0)}$
  repeat
    $\hat{u}_{ic}^{(t)} = \frac{{u_{ic}^{(t)}}^m}{\sum_{i=1}^N {u_{ic}^{(t)}}^m}$ ▷ calculate normalized memberships
    ▷ calculate coefficients by Equation (15)
    for $(i = 1..N; c = 1..C; k = 1..M)$ **do**
      $\alpha_{ick} \leftarrow \kappa_k(\mathbf{x}_i, \mathbf{x}_i) - 2 \sum_{j=1}^{N} \hat{u}_{jc}^{(t)} \kappa_k(\mathbf{x}_i, \mathbf{x}_j) + \sum_{j=1}^{N} \sum_{j'=1}^{N} \hat{u}_{jc}^{(t)} \hat{u}_{j'c}^{(t)} \kappa_k(\mathbf{x}_j, \mathbf{x}_{j'})$
    end for
    ▷ calculate coefficients by Equation (18)
    for $(k = 1..M)$ **do**
      $\beta_k \leftarrow \sum_{i=1}^N \sum_{c=1}^C \left(u_{ic}^{(t)} \right)^m \alpha_{ick}$
    end for
    ▷ update weights by Equation (19)
    for $(k = 1..M)$ **do**
      $\omega_k^{(t)} \leftarrow \frac{\frac{1}{\beta_k}}{\frac{1}{\beta_1} + \frac{1}{\beta_2} + \cdots + \frac{1}{\beta_M}}$
    end for
    ▷ calculate distances by Equation (14)
    for $(i = 1..N; c = 1..C)$ **do**
      $D_{ic}^2 \leftarrow \sum_{k=1}^{M} \alpha_{ick} \left(\omega_k^{(t)} \right)^2$
    end for
    ▷ update memberships by Equation (11)
    for $(i = 1..N; c = 1..C)$ **do**
      $u_{ic}^{(t)} \leftarrow \frac{1}{\sum_{c'=1}^{C} \left(\frac{D_{ic}^2}{D_{ic'}^2} \right)^{\frac{1}{m-1}}}$
    end for
  until $\| \mathbf{U}^{(t)} - \mathbf{U}^{(t-1)} \| < \epsilon$
  return $\mathbf{U}^{(t)}, \{\omega_k^{(t)}\}_{k=1}^M$
end procedure

D. Algorithm

We start from the objective function involving cluster centers, memberships, and kernel weights. We show that the cluster centers can be eliminated from the objective function so that we do not need to implicitly evaluate cluster centers, which are potentially not computable. Algorithm 2 summarizes the MKFC algorithm, which starts by initializing a random membership matrix satisfying non-negative and unity constraints. Optimal weights are calculated by fixing the memberships, and optimal memberships are updated assuming fixed weights. The process is repeated until the amount of change per iteration in the membership matrix falls below a given threshold. The computational complexity of MKFC is $O(N^2CM)$ per iteration, excluding construction of the kernel matrices.

Algorithm 3 Multiple kernel k-means (MKKM). Given a set of N data points $\mathbf{X} = \{\mathbf{x}_i\}_{i=1}^N$, a set of kernel functions $\{\kappa_k\}_{k=1}^M$, and the desired number of clusters C, output a membership matrix $\mathbf{U} = \{u_{ic} \in \{0,1\}\}_{i,c=1}^{N,C}$ and weights $\{\omega_k\}_{k=1}^M$ for the kernels.

```
1: procedure MKKM(Data X, Number C, Kernels {κ_k}_{k=1}^M)
2:     Initialize membership matrix U^(0)
3:     repeat
4:         run line 4 to line 16 of Algorithm 2
5:                                          ▷ update memberships
6:         for (i = 1..N; c = 1..C) do
7:             if D_ic^2 > min{D_ic'^2}_{c'=1}^C then
8:                 u_ic^(t) ← 0
9:             else
10:
11:                u_ic^(t) ← 1
12:            end if
13:        end for
14:    until ‖ U^(t) − U^(t−1) ‖< ε
15:    return U^(t), {ω_k^(t)}_{k=1}^M
16: end procedure
```

E. Multiple Kernel K-means: a Special Case of MKFC

The proposed MKFC method can be viewed as a multiple kernel extension of k-means, the most widely used clustering algorithm. The argument is similar to that for k-means being a special case of FCM.

Consider Equation (11) when m approaches 1. If there exists any cluster c' such that $D_{ic'} < D_{ic}$, then the denominator approaches ∞. On the other hand, if D_{ic} is the smallest among all $D_{ic'}$, the denominator approaches zero. That is,

$$u_{ic} = \begin{cases} 0, & \text{if there exists } c' \text{ such that } D_{ic'} < D_{ic} \\ 1, & \text{otherwise.} \end{cases}$$

Since u_{ic} is either 1 or 0 as determined by the nearest center, MKFC reduces to hard clustering. We here refer to the resultant hard-clustering version of MKFC (when m is very close to 1) as multiple kernel k-means (MKKM). MKKM is depicted in Algorithm 3. To the best of our knowledge, there is no previous study that has extended k-means to MKKM.

V. Experiments

We begin this section by reviewing the measures we have adopted to evaluate and compare the clustering results (Section V-A), after which we discuss the issue of the base kernel selection (Section V-B). We conclude the section with a presentation of experiments on synthetic data (Section V-C), a number of real data sets from the UCI machine learning repository [35] (Section V-D), two well-known face databases from ORL [36] and CMU-PIE [37] (Section V-E), and two famous text datasets from 20 Newsgroups and Reuters-21578 (Section V-F).

For each set of experiments, we describe the data sets, the experimental settings, the choice of kernels, the experimental results, and comparisons to other methods.

These data sets are summarized in Table I. For all experiments, we set the fuzzification degree m to 1.08 and the stop threshold ϵ as 0.0001. Since the focus of this paper is not the estimation of the number of clusters, we set as the ground truth for all methods the number of clusters C. Because the performance of these clustering methods depends on the initial values, we performed 50 runs for each experiment and report the average. We compare the proposed method (MKFC) and multiple-kernel k-means (MKKM) to k-means (Kmean), fuzzy c-means (FCM), and single-kernel-based fuzzy c-means (KFC).

A. Performance measures

The fuzzy-c-means-based soft clustering algorithms (FCM, KFC, MKFC) described in this paper generate an $N \times C$ matrix $\mathbf{U} = [u_{ic}]_{i=1..N,c=1..C}$ whose elements $u_{ic} \in [0,1]$ are the membership degrees, the possibility that data $\mathbf{x}_i$ belongs to the c-th cluster. These membership degrees make it possible for us to measure the performance of these algorithms using either hard clustering measures or soft clustering measures.

Hard clustering measures. Most clustering measures are designed for the evaluation of the results of hard clustering, in which each data item is assigned to a single class. To use this kind of measure for soft clustering, one must convert the membership degrees to hard assignments. We take the conventional approach for such assignments, that is, we assign each data item to the cluster with the highest membership degree. Hard clusterings measures can be roughly categorized into pair-counting-based measures (e.g., Rand index (RI) and adjusted Rand index (ARI) [38]), set-matching-based measures (e.g., $\mathcal{H}$ criterion) and information-theoretic-based measures (e.g., mutual information and normalized mutual information (NMI) [39]).

While there are studies that evaluate these clustering measures, there is currently no definite answer as to which measure is best. Vinh *et al.* [40] reported that some popular measures do not facilitate informative clustering comparisons because they either do not have a predetermined range or do not have a constant baseline value. For these measures, a poor clustering could yield a very high performance index, especially with a large number of clusters. They suggest ARI as a faithful measure that does not have these drawbacks. However, Wu *et al.* [41] reported that, when clustering performances are hard to distinguish, we may still want to use the normalized variation of information, i.e., NMI. For fair comparisons, this paper uses both NMI and ARI as hard clustering measures.

The goal for NMI [39] is to compare two hard partitions (R and Q) of a data set $\mathbf{X}$ with N objects. Assume that R and Q have I and J clusters, respectively. The probability $P(i)$ that a randomly selected object from $\mathbf{X}$ falls into cluster R_i of partition R is

$$P(i) = \frac{|R_i|}{N}.$$

The entropy $H(R)$ associated with R is then defined as

$$H(R) = -\sum_{i=1}^{I} P(i) \log P(i).$$

TABLE I
SUMMARY OF THE DATA SETS USED IN THE EXPERIMENTS. THE FIRST TWO, *Equal* AND *Variant*, ARE SYNTHETIC DATA SETS WHOSE DIMENSIONS HAVE DIFFERENT FEATURE RELIABILITY CHARACTERISTICS. THE FOLLOWING 20 DATA SETS ARE ADOPTED FROM THE UCI MACHINE LEARNING REPOSITORY, TWO FACE DATABASES FROM ORL AND CMU-PIE, AND THE LAST TWO ARE TEXT DATASETS FROM 20 NEWSGROUPS AND REUTERS-21578

ID	Name	#instances	#features	#classes	comment
S1	*Equal*	160	10	8	
S2	*Variant*	160	10	8	
R1	*Wine*	178	13	3	
R2	*Glass Identification*	214	9	6	
R3	*SPECT Heart*	267	22	2	
R4	*Ecoli*	336	7	8	
R5	*Ionosphere*	351	34	2	
R6	*Libras Movement*	360	90	15	
R7	*Breast Cancer Wisconsin(Diagnostic)*	569	30	2	
R8	*Balance Scale*	625	4	3	
R9	*Optical Recognition of Handwritten Digits*$(1,7)$	361	64	2	digit 1 and 7 in test set
R10	*Optical Recognition of Handwritten Digits*$(2,7)$	356	64	2	digit 2 and 7 in test set
R11	*Optical Recognition of Handwritten Digits*$(0,6,8,9)$	713	64	4	digit 0,6,8 and 9 in test set
R12	*Optical Recognition of Handwritten Digits*$(1,2,7,9)$	718	64	4	digit 1,2,7 and 9 in test set
R13	*Pima Indians Diabetes*	768	8	2	
R14	*Connectionist Bench(Vowel Recognition-Deterding Data)*	990	10	11	
R15	*Yeast*	1,484	8	10	
R16	*Statlog(Landsat Satellite)*	2,236	36	2	class 1 and 2
R17	*Statlog(Landsat Satellite)*	480	36	6	randomly choose 80 instances from each class
R18	*Letter Recognition*(A,B)	1,555	16	2	letter A and B
R19	*Letter Recognition*(A,B,C,D)	3,096	16	4	letter A,B,C,D
R20	*Waveform Database Generator(Version 2)*	5,000	21	3	
F1	*ORL*	360	7744	40	
F2	*CMU-PIE*	1496	7744	68	The frontal images (Pose 27) with 22 different lightings
T1	*20 Newsgroups*	2000	25753	20	randomly choose 100 instances from each class in test set
T2	*Reuters-21578*	2189	8575	8	The test set

Let $P(i,j)$ denote the probability that an object belongs to cluster R_i in R and cluster Q_j in Q:

$$P(i,j) = \frac{|R_i \cap Q_j|}{N}.$$

The NMI between the two hard partitions R and Q can then be defined as

$$NMI(R,Q) = \frac{\sum_{i=1}^{I}\sum_{j=1}^{J} P(i,j)\log\frac{P(i,j)}{P(i)P(j)}}{\sqrt{H(R)H(Q)}}. \quad (20)$$

In describing the formula for ARI, we start with the definitions of the following quantities:

- a the number of pairs of data objects belonging to the same class in R and to the same cluster in Q
- b the number of pairs of data objects belonging to the same class in R and to different clusters in Q
- c the number of pairs of data objects belonging to different classes in R and to the same cluster in Q
- d the number of pairs of data objects belonging to different classes in R and to different clusters in Q.

The Rand index RI is then defined as

$$RI = \frac{a+d}{a+b+c+d}$$

and the adjusted Rand index (ARI) is

$$ARI = \frac{a - \frac{(a+b)(a+c)}{a+b+c+d}}{\frac{(a+b)+(a+c)}{2} - \frac{(a+b)(a+c)}{a+b+c+d}}. \quad (21)$$

By measuring the ARI between the clustering results and the ground-truth clustering, we can evaluate the clustering performance for each method.

Soft clustering measures. As pointed out by Campello [42], the casting of soft clusterings to hard clusterings often fails to faithfully reflect the performance of soft clustering algorithms. For example, different fuzzy partitions (with potentially widely divergent spatial distributions) may result in the same crisp partition; accordingly, both will have the same hard clustering measure. This loss of information due to the disposal of the fuzzy membership values makes the hard clustering measures unable to discriminate between overlapped and non-overlapped clusters. As such, these hard clustering measures might not be appropriate for the assessment of fuzzy clustering algorithms. To get around these drawbacks, Campello proposed a fuzzy extension of the Rand index and other related indices [42]. The extended index is obtained by first rewriting the formulation of the Rand index in a fully equivalent form using basic concepts from set theory. Given two membership

matrices (U_1 and U_2), the quantities a, b, c, d are redefined as

$$\begin{aligned} a &= |V \cap Y| \\ b &= |V \cap Z| \\ c &= |X \cap Y| \\ d &= |X \cap Z|, \end{aligned} \tag{22}$$

where V, defined as $V(j_1, j_2) = s_{i=1}^{k} t(r_{ij_1}, r_{ij_2})$, is the set of pairs of data objects belonging to the same class in U_1; X, defined as $X(j_1, j_2) = s_{i_1,i_2 \in [1,k] | i_1 \neq i_2} t(r_{i_1 j_1}, r_{i_2 j_2})$, is the set of pairs of data objects belonging to different classes in U_1; Y, defined as $Y(j_1, j_2) = s_{l=1}^{v} t(q_{lj_1}, q_{lj_2})$, is the set of pairs of data objects belonging to the same cluster in U_2; and Z, defined as $Z(j_1, j_2) = s_{l_1,l_2 \in [1,v] | l_1 \neq l_2} t(q_{l_1 j_1}, q_{l_2 j_2})$, is the set of pairs of data objects belonging to different clusters in U_2.

Here, "t" is a t-norm used as a conjunction to implement the connective "and" of the proposition: we use the "min" operator as a t-norm. Likewise, "s" is a co-norm used as a disjunction to implement the connective "or" of the proposition: we use the "max" operator as a co-norm. Since the cardinality of a fuzzy set is given by the sum of its membership values, we rewrite Equation (22) as

$$\begin{aligned} a = |V \cap Y| &= \sum_{j_2=2}^{N} \sum_{j_1=1}^{j_2-1} t(V(j_1, j_2), Y(j_1, j_2)) \\ b = |V \cap Z| &= \sum_{j_2=2}^{N} \sum_{j_1=1}^{j_2-1} t(V(j_1, j_2), Z(j_1, j_2)) \\ c = |X \cap Y| &= \sum_{j_2=2}^{N} \sum_{j_1=1}^{j_2-1} t(X(j_1, j_2), Y(j_1, j_2)) \\ d = |X \cap Z| &= \sum_{j_2=2}^{N} \sum_{j_1=1}^{j_2-1} t(X(j_1, j_2), Z(j_1, j_2)). \end{aligned}$$

Plugging the above quantities into Equation (21) yields EARI, the fuzzy extension to ARI. As we are not aware of any soft extension for NMI, for the soft clustering measure we use only EARI. In the following experiments, we use NMI, ARI, and EARI to compare algorithms.

B. Selection of base kernels

Kernels are often used to address the problems of ineffective features and similarity measures. Features can be ineffective for two possible reasons. First, the data could exhibit non-linear relationships. For better modeling, kernel functions define the similarity of data in a more appropriate feature space. Second, the provided feature vectors may not faithfully reflect the intrinsic properties of the data, and thus the resulting similarities will not reflect the actual similarities between data items.

As kernel functions are essentially similarity measures for pairs of data, they can be used in many different ways, and sets of multiple kernels can be constructed in various ways. There are two common ways to construct kernel functions, corresponding to the two situations mentioned above. First, given a set of representative vectors for data items, one can employ a number of reproducible kernel functions in the Hilbert space for the construction of multiple kernels. For example, we could measure the similarities between data items in different nonlinear spaces by mapping data to these spaces with different Gaussian kernels. For the UCI experiment, since we did not have access to the raw data, we constructed kernels in this way. Second, given a set of raw data, different types of feature vectors can be extracted. These feature vectors often correspond to different cues and similarities can be measured in different feature spaces. For example, given a set of facial images for face clustering, one could extract different types of visual features such as colors or textures. For the face clustering experiment, we extract three types of features to define different similarity measures (kernels). For the synthetic data, to facilitate analysis, we treat each dimension as a feature. This allows for intuitive interpretation of the experimental results.

In summary, the guideline for selecting base kernels is to use kernels (features) that are known to be effective in related problems. For example, Gaussian kernels are known to be effective in many classification problems and LBP is a popular feature in face image applications. In principle, the more kernels (features) are used, the better the performance will be. We are still however limited by computational resources and the algorithm's tolerance to bad kernels.

C. Synthetic data

We first evaluate MKFC on synthetic data because we know the correct answers for this case. Our primary goal is to show that because the proposed method assigns proper weights to kernels, it is less vulnerable to irrelevant or ineffective features or kernels. For this purpose, we synthesize l-dimensional vectors and treat each dimension as a feature. Given a pair of data $\mathbf{x}_i$, $\mathbf{x}_j$ which are l-dimensional vectors, each of its dimensions $\mathbf{x}_{ir(r=1\cdots l)}$ is taken as a scalar feature, and a kernel function $\kappa(\cdot, \cdot)$ in 1-D space is used to measure the similarity between $\mathbf{x}_{ir}$ and $\mathbf{x}_{jr}$. In this way, l kernels (similarities) can be obtained for each of the data pair $\mathbf{x}_i$, $\mathbf{x}_j$. Two sets of synthetic data were generated as follows. For the first one, *Equal*, we synthesized 8 groups of 10-d data, with 20 data points in each group. We made these groups well separated by sampling 8 points whose coordinates are uniformly sampled along each dimension. These 8 points were then used as centers of Gaussians with the same width. For each Gaussian, 20 points were drawn. For this setup, it is reasonable to assume that each dimension has a roughly equal capability to separate the 8 groups. A similar procedure was used for the second set, *Variant*. The only difference lies in the widths of the Gaussians. In *Equal*, we used the same width in each dimension, but in *Variant*, the widths were increased with the dimension index. Therefore, there was more overlap in *Variant* data in the dimensions with higher indices.

Accordingly, we use a Gaussian kernel for each dimension:

$$\kappa_r(\mathbf{x}_{ir}, \mathbf{x}_{jr}) = \exp(-||\mathbf{x}_{ir} - \mathbf{x}_{jr}||^2/\sigma).$$

To choose σ, let the minimal value allowed for the Gaussian kernel over the data set be γ. We then obtain the corresponding

σ as

$$\sigma = \min_{i,j}(-||\mathbf{x}_{ir} - \mathbf{x}_{jr}||^2/log(\gamma)).$$

We set γ to 0.005. Figure 1(a) illustrates the results for the *Equal* experiment. The x-axis is for the NMI index values. Each row shows the NMI value distribution over runs for a method. From left to right, the three green points of each row are sequentially the minimal, mean, and maximal NMI values among the runs. Thirteen methods are compared: k-means (Kmean), fuzzy c-means (FCM), multiple kernel fuzzy c-means (MKFC), and 10 kernel-based fuzzy c-means (KFC) methods. In the synthetic-data experiment, k-means and FCM use 10-dimensional feature vectors, but each of the KFC methods uses only one dimension as the feature. Hence, we expect k-means and FCM to outperform each KFC since the latter method uses incomplete data. As our MKFC method uses a weighted combination of these 1-d kernels, we expect it to outperform single kernel-based methods. As can be seen, although the maximal NMI value of MKFC is the same as for Kmean and FCM, MKFC has a better mean NMI index (0.9521) than the other two (0.9486 for FCM and 0.9206 for Kmean). Note that we expect MKFC to exhibit performance similar to that of FCM, since the features are equally important in this synthetic data set. The real numbers for each KFC method are the weights discovered by MKFC. These kernel weights are all of similar magnitudes, which is appropriate, considering the artificial setting of equal weights in this synthetic data set. Note that due to the overlap between clusters and noise, the discovered weights are not perfectly equal. Figure 1(b) shows the NMI values for each MKFC iteration for the *Equal* experiment: it converges after only a few iterations.

Figure 2 shows the results for the *Variant* experiment. As in the *Equal* experiment, k-means and FCM use 10-dimensional vectors, each KFC uses only one dimension as the feature, and MKFC uses a weighted combination of these 10 dimensions. Because of the experiment settings, there is more data overlap in the dimensions of higher indices; i.e., for data in these dimensions, it is more difficult to separate the 8 groups. This is evident from Figure 2(a). We observe that the NMI value decreases as the index of KFC increases. Accordingly, MKFC assigns higher weights to the kernels corresponding to the dimensions with lower indices. For example, the weight for KFC_1 is 0.23147 while the weight for KFC_{10} is only 0.041994. Figure 3 shows the evolution of weights in a run. In the first iteration, all dimensions have roughly equal weights. With each iteration, more weight is added to the more important dimensions (those with lower indices). Overall, MKFC has a better NMI value (0.9192) than Kmean (0.9041) and FCM (0.9102). Note that in the *Variant* data set, MKFC performs noticeably better than FCM because MKFC puts more emphasis on important features.

D. UCI repository

We tested these methods on 20 data sets selected from the UCI repository. For each set, only the extracted feature vectors are available – not the raw data. Using the provided feature vectors for data items, we employ different types of kernel functions as bases for multiple kernel learning. These vectors are normalized to have zero mean and unit standard deviation. They are then substituted into the chosen kernels to calculate pairwise distances. As mentioned in Section I, optimal kernel choice is still an open research topic. Here, following the strategy of other multiple kernel learning approaches, we select a set of reasonable kernels that are frequently used by kernel methods. In our experiments, we used one polynomial kernel

$$\kappa_k(\mathbf{x}_i, \mathbf{x}_j) = (\theta + \mathbf{x}_i^T \mathbf{x}_j)^p,$$

with $\theta = 1$ and $p = 2$, and several Gaussian kernels

$$\kappa_k(\mathbf{x}_i, \mathbf{x}_j) = \exp(-(\mathbf{x}_i - \mathbf{x}_j)^T(\mathbf{x}_i - \mathbf{x}_j)/\sigma).$$

Assume that the minimal value of the Gaussian kernel over the data set is γ. We then obtain the corresponding σ as

$$\sigma = \min_{i,j}(-(\mathbf{x}_i - \mathbf{x}_j)^T(\mathbf{x}_i - \mathbf{x}_j)/log(\gamma)).$$

We vary γ over $\{0.1, 0.05, 0.01, 0.005, 0.001, 0.0005, 0.0001\}$ to obtain 7 Gaussian kernels. Finally, we normalize the value of each kernel function to the range of $[0.0001..1]$. We use $\text{KFC}_1, \cdots, \text{KFC}_8$ to denote KFC's with the above 8 kernels (1 polynomial and 7 Gaussians) respectively.

We first use hard clustering measures (NMI and ARI) to compare Kmean, FCM, KFC, and MKFC. Unlike previous settings for the synthetic data, all the methods (k-means, FCM, KFC and MKFC) use data with the same dimensions (specified by the #features attribute in Table I). In Table II we present the average NMI values over 50 runs and the corresponding ranks for different algorithms on the 20 UCI data sets. The numbers in parentheses are the ranks of different methods for each data set. For example, MKFC ranks number one with an NMI of 0.909 for the data set R1 while Kmean ranks number eight with an NMI of 0.865. The last two rows (*m*NMI, *m*Rank) of Table II display the average NMI value and the average rank for each method over 20 data sets, respectively. MKFC has an average NMI 0.516 and ranks the best of all the methods in terms of average NMI (*m*NMI). In terms of average rank (*m*Rank), MKFC's average rank is 2.85, again the best of all the methods. Note that *m*NMI and *m*Rank both yield similar rankings. Table III presents the results of different algorithms in terms of ARI. Changing the measure from NMI to ARI does not change the rankings significantly. Again, MKFC is the best in terms of both *m*ARI and *m*Rank.

It is true that MKFC is not ranked number one for each

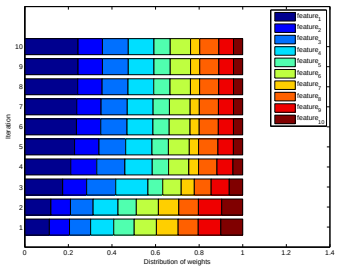
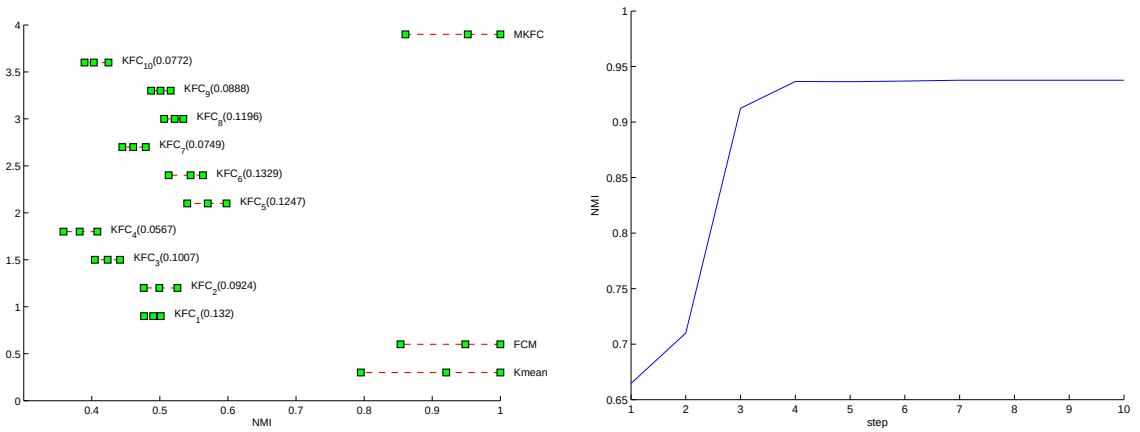
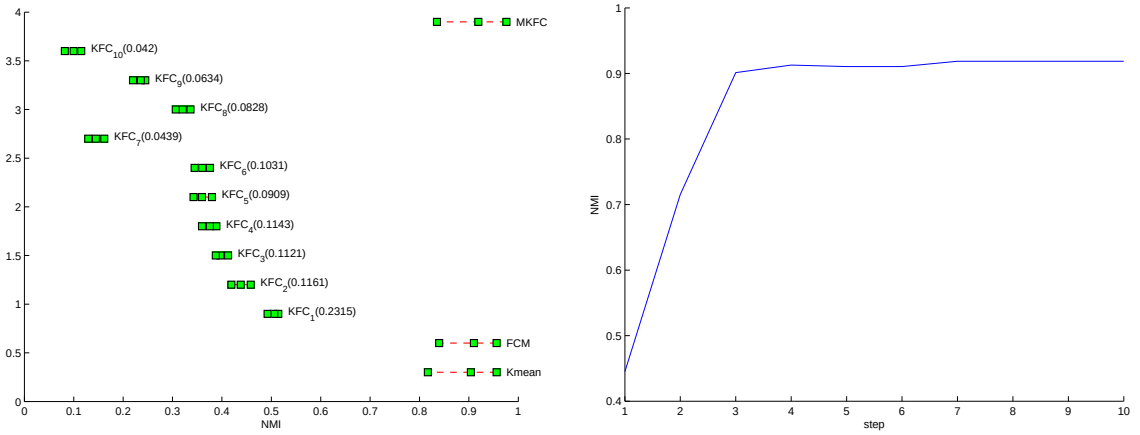


Fig. 3. The evolution of weights for the *Variant* experiment.



(a) (b)

Fig. 1. For the *Equal* experiment, (a) the results and (b) the NMI values for each step of a single run.



(a) (b)

Fig. 2. For the *Variant* experiment, (a) the results and (b) the NMI values for each step of a single run.

individual data set. However, given the data sets, we do not know in advance which kernel will perform better for each, and there is no single kernel suitable for all of them. While kernel combination does not yield the best performance in every single case, on average it yields the best overall performance. If we were to use a fixed kernel, it would have better performance for some data sets but perform worse in general. This suggests that combining kernels for clustering yields better overall performance than when using a fixed kernel. For real-world applications, we have no cues in advance as to which kernel will work best for the given problem. Despite its not always ranking the first, MKFC on average is the best and yields stable performance.

Like most fuzzy clustering algorithms, choosing the best fuzzification degree m remains an open problem. Graves and Pedrycz [14] had conducted a comparative study on fuzzy clustering and found that different applications and clustering methods may have the best performance with different m's. That is, the choice of m depends on both applications and clustering algorithms. Figure 4 shows the performance given various fuzzification degrees m. As mentioned in the experiment setting, we set m to 1.08 in all experiments. Note that

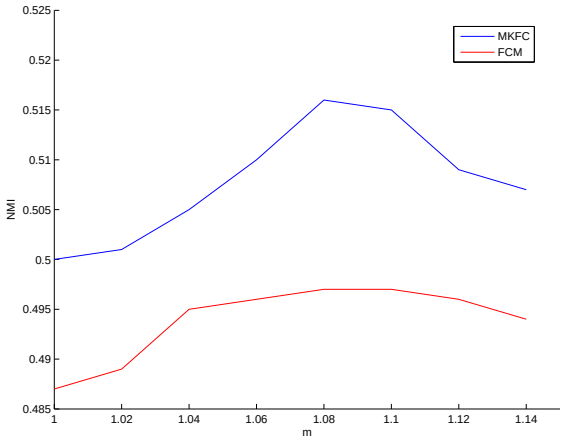


Fig. 4. The average NMI of various m for the *UCI* experiment.

both MKFC and FCM perform best around $m = 1.08$, and MKFC is consistently better than FCM for all m's. We can also see that making the clustering a little fuzzy provides better performance than hard clustering.

TABLE II
COMPARISONS OF DIFFERENT ALGORITHMS ON UCI DATA SETS IN TERMS OF NMI.

ID	Kmean	FCM	KFC_1	KFC_2	KFC_3	KFC_4	KFC_5	KFC_6	KFC_7	KFC_8	MKFC	MKKM
R1	0.865(8)	0.865(8)	0.878(6)	0.893(3)	0.893(3)	0.892(5)	0.877(7)	0.842(10)	0.842(10)	0.811(12)	0.909(1)	0.899(2)
R2	0.320(12)	0.333(11)	0.333(10)	0.335(9)	0.342(6)	0.349(5)	0.356(1)	0.356(2)	0.354(4)	0.335(8)	0.355(3)	0.338(7)
R3	0.139(11)	0.137(12)	0.153(9)	0.201(2)	0.198(3)	0.145(10)	0.167(6)	0.167(6)	0.167(6)	0.178(5)	0.226(1)	0.196(4)
R4	0.570(6)	0.574(3)	0.574(1)	0.573(5)	0.574(4)	0.568(7)	0.563(10)	0.564(9)	0.561(11)	0.556(12)	0.574(2)	0.565(8)
R5	0.125(8)	0.120(10)	0.120(10)	0.115(12)	0.122(9)	0.198(5)	0.197(6)	0.244(1)	0.231(2)	0.211(3)	0.202(4)	0.185(7)
R6	0.581(12)	0.583(11)	0.590(8)	0.596(7)	0.600(6)	0.604(3)	0.608(1)	0.606(2)	0.601(5)	0.586(10)	0.603(4)	0.590(8)
R7	0.577(5)	0.571(7)	0.584(1)	0.584(1)	0.578(3)	0.546(8)	0.527(9)	0.501(10)	0.474(11)	0.409(12)	0.578(3)	0.572(6)
R8	0.121(1)	0.118(6)	0.119(4)	0.119(3)	0.118(5)	0.112(12)	0.114(11)	0.116(7)	0.116(8)	0.116(9)	0.120(2)	0.115(10)
R9	0.980(7)	1.000(1)	1.000(1)	0.992(4)	0.990(5)	0.982(6)	0.975(8)	0.521(10)	0.483(11)	0.325(12)	1.000(1)	0.955(9)
R10	0.806(2)	0.806(2)	0.806(2)	0.806(2)	0.806(2)	0.795(8)	0.784(9)	0.743(10)	0.700(11)	0.607(12)	0.806(2)	0.808(1)
R11	0.803(5)	0.800(7)	0.801(6)	0.804(3)	0.816(1)	0.788(8)	0.755(9)	0.728(10)	0.555(12)	0.573(11)	0.812(2)	0.804(3)
R12	0.664(6)	0.707(1)	0.686(3)	0.683(5)	0.683(4)	0.653(7)	0.616(9)	0.425(10)	0.417(11)	0.403(12)	0.686(2)	0.651(8)
R13	0.102(12)	0.114(10)	0.130(8)	0.130(7)	0.127(9)	0.140(5)	0.144(3)	0.146(1)	0.145(2)	0.143(4)	0.140(6)	0.111(11)
R14	0.362(11)	0.369(9)	0.371(7)	0.371(6)	0.370(8)	0.373(4)	0.372(5)	0.377(3)	0.378(1)	0.234(12)	0.378(2)	0.366(10)
R15	0.253(3)	0.250(10)	0.253(3)	0.254(2)	0.252(8)	0.253(3)	0.253(3)	0.250(9)	0.246(11)	0.238(12)	0.253(3)	0.255(1)
R16	0.454(1)	0.411(2)	0.359(6)	0.361(5)	0.374(3)	0.350(7)	0.347(9)	0.320(11)	0.322(10)	0.302(12)	0.373(4)	0.348(8)
R17	0.722(8)	0.725(7)	0.726(6)	0.729(5)	0.732(2)	0.730(4)	0.722(9)	0.711(10)	0.703(11)	0.700(12)	0.734(1)	0.731(3)
R18	0.707(7)	0.707(7)	0.718(1)	0.718(1)	0.718(1)	0.712(6)	0.702(9)	0.677(10)	0.657(11)	0.635(12)	0.716(5)	0.718(1)
R19	0.387(11)	0.372(12)	0.389(10)	0.401(9)	0.411(8)	0.421(7)	0.441(5)	0.521(1)	0.516(2)	0.509(3)	0.493(4)	0.431(6)
R20	0.374(2)	0.374(1)	0.372(3)	0.371(4)	0.369(5)	0.352(8)	0.338(9)	0.271(10)	0.259(11)	0.243(12)	0.369(5)	0.369(5)
*m*NMI	0.497(7)	0.497(7)	0.498(5)	0.502(3)	0.504(2)	0.498(5)	0.493(9)	0.454(10)	0.436(11)	0.406(12)	0.516(1)	0.500(4)
*m*Rank	6.900(8)	6.850(7)	5.250(4)	4.750(2)	4.750(2)	6.400(6)	6.900(8)	7.100(10)	8.050(11)	9.850(12)	2.850(1)	5.900(5)

We also implemented MKKM and compared it with the other methods. MKFC performs better than MKKM in terms of both NMI and ARI. As can be seen, the performance is still improved by when there is a slight softness in the clustering. This implies that fuzzy clustering methods may be more able to handle overlapping clusters than the corresponding hard ones, and a slightly larger fuzzification degree may help improve clustering performance.

Again, hard clustering measures do not necessarily faithfully reflect the performance of soft clustering algorithms, as they completely ignore membership degrees. As such, we also use the soft clustering measure EARI to compare FCM, KFC, and MKFC. Kmean and MKKM are omitted since they are hard clustering methods. The results in Table IV show that MKFC again ranks number one in this measure.

Table V shows the computation time results for averages over 50 runs as the number of iterations and the total time in seconds of each run for the sum of eight KFCs, MKFC, and MKKM on all real data sets respectively. Both MKFC and MKKM use all eight kernels, while a single KFC only uses one kernel. To ensure a fair comparison, we report the sum of the eight KFCs. For most cases, MKFC requires fewer iterations than the average of the KFCs. This indicates that MKFC converges more quickly. In terms of running time, MKFC took anywhere from less than a second to almost a minute for the test data, and was consistently faster than the combined running time of the eight KFCs. MKFC was a bit slower than MKKM, because MKFC uses more iterations to compute the membership of each object, which results in performance gains.

TABLE V
THE NUMBER OF ITERATIONS AND TIME PER RUN FOR THE SUM OF EIGHT KFCS, MKFC, AND MKKM ON ALL REAL DATA SETS.

ID	KFC iter.	MKFC iter.	MKKM iter.	KFC time	MKFC time	MKKM time
R1	13.6	11.3	12.1	0.066	0.046	0.050
R2	30.8	35.0	28.5	0.267	0.317	0.248
R3	22.6	27.2	20.0	0.127	0.145	0.097
R4	50.4	42.0	38.8	0.797	0.707	0.692
R5	15.2	17.4	14.5	0.127	0.132	0.125
R6	47.6	43.0	41.7	1.361	1.275	1.272
R7	21.0	14.2	11.4	0.479	0.338	0.283
R8	57.5	41.0	35.2	2.058	1.509	1.331
R9	33.8	29.6	23.9	0.329	0.317	0.280
R10	13.8	9.0	9.1	0.127	0.092	0.102
R11	33.8	20.2	16.4	1.737	1.058	0.875
R12	37.8	23.8	22.2	1.973	1.266	1.203
R13	38.2	31.2	25.0	2.012	1.675	1.367
R14	60.4	58.0	49.1	6.542	6.340	5.416
R15	78.3	70.2	61.7	16.219	14.611	12.90
R16	19.1	15.0	12.0	10.785	8.485	6.800
R17	35.7	28.6	22.7	2.423	1.970	1.586
R18	13.5	9.3	8.9	3.834	2.650	2.545
R19	50.5	38.8	33.9	70.611	54.290	47.468
R20	18.2	16.1	13.9	31.238	27.650	23.886

E. Face clustering

We also evaluated MKFC with face clustering. The face databases are from ORL and CMU-PIE. Figures 5 (a) and (b) show several sample images of a single person from the ORL and CMU-PIE databases, respectively. The face images are all nearly frontal, and those in ORL include various facial

TABLE III
COMPARISONS OF DIFFERENT ALGORITHMS ON UCI DATA SETS IN TERMS OF ARI.

ID	Kmean	FCM	$\mathbf{KFC}_1$	$\mathbf{KFC}_2$	$\mathbf{KFC}_3$	$\mathbf{KFC}_4$	$\mathbf{KFC}_5$	$\mathbf{KFC}_6$	$\mathbf{KFC}_7$	$\mathbf{KFC}_8$	MKFC	MKKM
R1	0.884(7)	0.884(7)	0.899(5)	0.915(3)	0.915(3)	0.897(6)	0.879(9)	0.862(10)	0.862(10)	0.796(12)	0.941(1)	0.931(2)
R2	0.172(10)	0.181(2)	0.182(1)	0.176(6)	0.175(8)	0.179(3)	0.177(5)	0.172(9)	0.161(11)	0.136(12)	0.179(4)	0.176(6)
R3	0.153(11)	0.153(11)	0.239(10)	0.343(2)	0.355(1)	0.306(9)	0.324(4)	0.324(4)	0.324(4)	0.324(7)	0.324(7)	0.342(2)
R4	0.384(2)	0.387(1)	0.379(6)	0.380(4)	0.380(5)	0.371(8)	0.361(9)	0.349(10)	0.342(11)	0.329(12)	0.383(3)	0.379(6)
R5	0.146(1)	0.141(2)	0.133(3)	0.124(4)	0.108(7)	0.098(8)	0.074(9)	0.056(10)	0.033(11)	0.010(12)	0.123(5)	0.109(6)
R6	0.297(12)	0.299(10)	0.307(9)	0.313(7)	0.320(3)	0.321(1)	0.317(4)	0.316(6)	0.317(5)	0.297(11)	0.321(2)	0.312(8)
R7	0.695(7)	0.690(8)	0.701(1)	0.701(1)	0.701(1)	0.695(5)	0.672(9)	0.621(10)	0.573(11)	0.379(12)	0.695(5)	0.701(1)
R8	0.129(11)	0.138(1)	0.136(2)	0.136(2)	0.132(7)	0.135(4)	0.133(6)	0.130(9)	0.127(12)	0.131(8)	0.135(5)	0.130(9)
R9	0.960(4)	1.000(1)	1.000(1)	0.956(5)	0.954(6)	0.798(8)	0.715(9)	0.579(10)	0.472(11)	0.346(12)	1.000(1)	0.954(6)
R10	0.869(1)	0.869(1)	0.869(1)	0.869(1)	0.869(1)	0.859(8)	0.859(8)	0.848(10)	0.838(11)	0.787(12)	0.869(1)	0.869(1)
R11	0.770(9)	0.779(7)	0.785(6)	0.802(3)	0.804(2)	0.794(4)	0.773(8)	0.700(10)	0.674(11)	0.644(12)	0.824(1)	0.794(4)
R12	0.634(6)	0.663(1)	0.652(3)	0.662(2)	0.639(5)	0.619(7)	0.583(9)	0.507(10)	0.480(11)	0.262(12)	0.651(4)	0.610(8)
R13	0.136(2)	0.143(1)	0.135(3)	0.116(4)	0.109(7)	0.099(8)	0.096(9)	0.086(10)	0.081(12)	0.083(11)	0.116(5)	0.112(6)
R14	0.165(12)	0.171(11)	0.173(9)	0.174(5)	0.175(3)	0.174(8)	0.174(7)	0.175(2)	0.175(1)	0.171(10)	0.175(4)	0.174(5)
R15	0.127(9)	0.130(1)	0.130(3)	0.130(4)	0.130(2)	0.129(7)	0.128(8)	0.126(10)	0.122(11)	0.111(12)	0.130(5)	0.130(5)
R16	0.456(1)	0.409(2)	0.333(3)	0.308(6)	0.307(7)	0.320(5)	0.305(8)	0.278(9)	0.245(11)	0.208(12)	0.332(4)	0.265(10)
R17	0.661(1)	0.618(10)	0.639(7)	0.641(6)	0.642(5)	0.650(2)	0.644(4)	0.638(8)	0.614(11)	0.582(12)	0.649(3)	0.637(9)
R18	0.759(6)	0.759(6)	0.761(1)	0.761(1)	0.761(1)	0.755(8)	0.752(9)	0.726(10)	0.693(11)	0.643(12)	0.761(1)	0.761(1)
R19	0.336(8)	0.324(12)	0.334(10)	0.338(7)	0.339(5)	0.345(4)	0.350(2)	0.346(3)	0.356(1)	0.335(9)	0.339(6)	0.330(11)
R20	0.258(1)	0.258(1)	0.258(3)	0.257(4)	0.256(5)	0.250(8)	0.244(9)	0.190(10)	0.169(11)	0.142(12)	0.256(6)	0.255(7)
*m*ARI	0.449(6)	0.450(5)	0.452(4)	0.455(2)	0.454(3)	0.440(8)	0.428(9)	0.402(10)	0.383(11)	0.336(12)	0.461(1)	0.449(6)
*m*Rank	6.050(7)	4.800(5)	4.350(4)	3.850(2)	4.200(3)	6.050(7)	7.250(9)	8.500(10)	9.400(11)	11.200(12)	3.650(1)	5.650(6)

expressions and those in CMU PIE include variable lighting conditions. In contrast to the UCI datasets, for this application, we have only the raw data. Thus, our first step is to extract features from the image data. All images were first normalized and cropped to 88×88 pixels. To utilize cues from different perspectives, we extracted three different features.

1) Eigenface [43]. After performing principal component analysis, each face image was projected into the eigenspace which preserves 90% of the energy of the eigenvalues.
2) Gabor texture [44]. Each face image was filtered with 40 Gabor filters generated with five different scales and eight orientations.
3) Local binary pattern (LBP) [45]. We used a uniform LBP with 8 neighbors and radius 1. Thus, each face image was represented as a 256-bin histogram.

These three features are frequently used for face recognition and represent face images from different perspectives. After extracting these three features, each feature was treated as a vector; these vectors were substituted into the Gaussian kernel to calculate pairwise distances. As with the UCI data sets, we set γ to 0.005. We denote as KFC_e, KFC_g, and KFC_l the resulting three different kernels from these three features (Eigenface, Gabor texture, and LBP), respectively.

In this experiment, we compared the proposed method (MKFC) to single-kernel-based fuzzy c-means (KFC) and multiple-kernel k-means (MKKM). Tables VI and VII show the ARI, NMI, EARI, the average number of iterations, and the average total time in seconds for ORL and CMU-PIE, respectively. The eigenface, Gabor, and LBP kernel weights as determined by MKFC were 0.175, 0.164, and 0.661 for ORL and 0.626, 0.157, and 0.217 for CMU-PIE.

TABLE VI
COMPARISON OF DIFFERENT METHODS ON FACE DATABASE ORL IN TERMS OF ARI, NMI, EARI, # OF ITERATIONS, AND TIME PER RUN.

	$\mathbf{KFC}_e$	$\mathbf{KFC}_g$	$\mathbf{KFC}_l$	MKFC	MKKM
ARI	0.046	0.139	0.406	0.464	0.383
NMI	0.369	0.562	0.755	0.783	0.744
eARI	0.108	0.296	0.411	0.462	0.383
Iterations(I)	53.260	5.980	46.180	48.320	36.000
Time(T)	0.625	0.081	0.495	1.7830	1.3284

Notably, LBP was more effective for ORL (varying facial expressions) while Eigenface was the best for CMU-PIE (lighting changes). MKFC successfully combined the strengths of different features for different datasets and outperformed all other measures for both datasets. As with the UCI data sets, MKKM performed slightly worse than MKFC, showing that fuzzy methods are more able to separate overlapping data than hard methods. The combined computation times for all three KFCs are 1.201 and 14.211 seconds for ORL and CMU-PIE, respectively, while MKFC took 1.783 and 10.562 seconds. MKFC was thus comparable to the combination of the three KFCs. However, MKFC performs feature selection automatically and provides better clustering results. MKFC was slightly slower than MKKM but yielded better clustering performance.

F. Text clustering

For text clustering, we used two popular text datasets, 20 Newsgroups and Reuters-21578, downloaded from [46]. Each of them is pre-processed by four steps: **all-terms**, **no-**

TABLE IV
COMPARISON OF DIFFERENT ALGORITHMS ON UCI DATA SETS IN TERMS OF EARI.

ID	FCM	$\mathbf{KFC}_1$	$\mathbf{KFC}_2$	$\mathbf{KFC}_3$	$\mathbf{KFC}_4$	$\mathbf{KFC}_5$	$\mathbf{KFC}_6$	$\mathbf{KFC}_7$	$\mathbf{KFC}_8$	MKFC
R1	0.876(6)	0.893(4)	0.902(3)	0.908(2)	0.891(5)	0.875(7)	0.839(8)	0.818(9)	0.751(10)	0.918(1)
R2	0.266(5)	0.266(4)	0.268(2)	0.267(3)	0.265(7)	0.265(6)	0.264(8)	0.264(9)	0.262(10)	0.272(1)
R3	0.149(10)	0.238(9)	0.329(3)	0.353(1)	0.317(8)	0.321(7)	0.322(5)	0.321(6)	0.323(4)	0.350(2)
R4	0.389(1)	0.381(5)	0.382(4)	0.382(3)	0.376(6)	0.366(7)	0.354(8)	0.346(9)	0.332(10)	0.388(2)
R5	0.160(1)	0.155(2)	0.119(6)	0.137(3)	0.120(5)	0.090(7)	0.081(8)	0.052(9)	0.037(10)	0.180(4)
R6	0.327(3)	0.325(9)	0.326(4)	0.323(10)	0.330(2)	0.330(1)	0.326(7)	0.325(8)	0.326(5)	0.327(6)
R7	0.688(1)	0.687(2)	0.686(3)	0.683(4)	0.667(6)	0.655(7)	0.588(8)	0.528(9)	0.357(10)	0.683(5)
R8	0.161(10)	0.165(9)	0.174(8)	0.178(7)	0.191(5)	0.197(4)	0.198(3)	0.200(2)	0.208(1)	0.190(6)
R9	0.992(1)	0.992(1)	0.980(4)	0.977(5)	0.938(7)	0.959(6)	0.795(8)	0.730(9)	0.601(10)	0.992(1)
R10	0.902(1)	0.902(3)	0.899(4)	0.897(5)	0.887(6)	0.881(7)	0.858(8)	0.845(9)	0.802(10)	0.902(1)
R11	0.859(3)	0.868(1)	0.851(4)	0.833(5)	0.827(6)	0.820(7)	0.801(8)	0.792(9)	0.754(10)	0.860(2)
R12	0.637(5)	0.638(4)	0.649(3)	0.652(2)	0.635(6)	0.632(7)	0.616(8)	0.591(9)	0.520(10)	0.661(1)
R13	0.141(1)	0.132(3)	0.114(4)	0.109(5)	0.095(6)	0.087(7)	0.073(8)	0.069(9)	0.068(10)	0.136(2)
R14	0.181(9)	0.181(10)	0.182(7)	0.181(8)	0.183(6)	0.184(3)	0.185(2)	0.184(3)	0.186(1)	0.184(3)
R15	0.129(9)	0.133(1)	0.132(2)	0.130(4)	0.129(10)	0.129(6)	0.130(5)	0.129(8)	0.129(7)	0.132(3)
R16	0.400(1)	0.383(3)	0.337(5)	0.321(6)	0.343(4)	0.314(7)	0.285(8)	0.250(9)	0.215(10)	0.393(2)
R17	0.620(8)	0.641(6)	0.645(5)	0.650(3)	0.661(2)	0.649(4)	0.635(7)	0.618(9)	0.599(10)	0.663(1)
R18	0.722(9)	0.722(9)	0.728(8)	0.730(1)	0.730(1)	0.730(1)	0.728(6)	0.728(6)	0.728(5)	0.730(1)
R19	0.292(10)	0.294(9)	0.315(8)	0.324(7)	0.350(5)	0.355(4)	0.380(3)	0.391(2)	0.400(1)	0.350(6)
R20	0.254(1)	0.254(1)	0.254(3)	0.254(4)	0.254(6)	0.254(7)	0.254(8)	0.254(9)	0.254(10)	0.254(5)
mEARI	0.458(6)	0.463(4)	0.464(3)	0.464(2)	0.460(5)	0.455(7)	0.436(8)	0.422(9)	0.393(10)	0.478(1)
mRank	4.750(4)	4.750(4)	4.500(3)	4.400(2)	5.450(6)	5.600(7)	6.700(8)	7.600(9)	7.700(10)	2.750(1)

(a) ORL (b) CMU-PIE

Fig. 5. Sample images of a subject from (a) ORL and (b) CMU-PIE datasets. Note that ORL exhibits more variation in facial expressions while CMU-PIE exhibits various lighting conditions.

TABLE VII
COMPARISON OF DIFFERENT METHODS ON FACE DATABASE CMU-PIE IN TERMS OF ARI, NMI, EARI, # OF ITERATIONS, AND TIME PER RUN.

	$\mathbf{KFC}_e$	$\mathbf{KFC}_g$	$\mathbf{KFC}_l$	MKFC	MKKM
ARI	0.914	0.088	0.597	0.931	0.875
NMI	0.983	0.584	0.845	0.987	0.975
eARI	0.912	0.230	0.587	0.935	0.875
Iterations(I)	24.280	7.300	74.320	25.660	19.020
Time(T)	3.291	0.965	9.955	10.562	7.829

short, **no-stop** and **stemmed**. We use the datasets *20ng-test-stemmed* and *r8-test-stemmed* to evaluate MKFC. Let $D = \{d_1, \cdots, d_n\}$ be the set of documents and $T = \{t_1, \cdots, t_m\}$ the set of distinct words occurring in D. We denote the frequency of word $t \in T$ in the document $d \in D$ as $tf\,(d,t)$. tf-idf is a weighting scheme which weights the frequency of a word t in the document d with a factor that discounts its importance with its occurrences in the whole document collection, which is defined as

$$tf\text{-}idf\,(d,t) = tf\,(d,t) \times log(\frac{|D|}{df\,(t)}),$$

where $df\,(t)$ is the number of documents in which the word t appears. Thus, the feature vector representation of a document d is defined as

$$\overrightarrow{t_d} = \left(tf\text{-}idf\,(d,t_1), \cdots, tf\text{-}idf\,(d,t_m)\right).$$

After normalizing the vectors to a unit length, we used the following four kernels to calculate the pairwise distances between two documents.

1) Euclidean distance.

$$\kappa_{ed}(\overrightarrow{t_{d_i}}, \overrightarrow{t_{d_j}}) = \left(\sum_{t=1}^{m} |tf\text{-}idf\,(d_i,t) - tf\text{-}idf\,(d_j,t)|^2\right)^{\frac{1}{2}},$$

TABLE VIII
COMPARISON OF DIFFERENT METHODS ON TEXT DATASET 20 NEWSGROUPS IN TERMS OF ARI, NMI, EARI, # OF ITERATIONS, AND TIME PER RUN.

	KFC$_{ed}$	**KFC**$_{cs}$	**KFC**$_{jc}$	**KFC**$_{pcc}$	**MKFC**	**MKKM**
ARI	0.131	0.140	0.129	0.139	0.143	0.139
NMI	0.381	0.386	0.379	0.391	0.394	0.388
eARI	0.192	0.201	0.187	0.200	0.205	0.139
Iterations(I)	18.100	22.900	19.600	22.880	25.340	19.250
Time(T)	2.559	3.384	2.870	3.371	15.343	11.656

TABLE IX
COMPARISON OF DIFFERENT METHODS ON TEXT DATASET REUTERS-21578 IN TERMS OF ARI, NMI, EARI, # OF ITERATIONS, AND TIME PER RUN.

	KFC$_{ed}$	**KFC**$_{cs}$	**KFC**$_{jc}$	**KFC**$_{pcc}$	**MKFC**	**MKKM**
ARI	0.273	0.287	0.236	0.275	0.305	0.275
NMI	0.418	0.428	0.406	0.427	0.434	0.425
eARI	0.311	0.320	0.285	0.303	0.331	0.275
Iterations(I)	5.820	30.440	51.420	30.120	34.440	29.260
Time(T)	0.616	3.135	5.365	3.124	20.331	17.450

2) Cosine similarity.

$$\kappa_{cs}(\overrightarrow{t_{d_i}}, \overrightarrow{t_{d_j}}) = \frac{\overrightarrow{t_{d_i}} \cdot \overrightarrow{t_{d_j}}}{|\overrightarrow{t_{d_i}}||\overrightarrow{t_{d_j}}|},$$

3) Jaccard coefficient.

$$\kappa_{jc}(\overrightarrow{t_{d_i}}, \overrightarrow{t_{d_j}}) = \frac{\overrightarrow{t_{d_i}} \cdot \overrightarrow{t_{d_j}}}{|\overrightarrow{t_{d_i}}|^2 + |\overrightarrow{t_{d_j}}|^2 - \overrightarrow{t_{d_i}} \cdot \overrightarrow{t_{d_j}}},$$

4) Pearson correlation coefficient.

$$\kappa_{pcc}(\overrightarrow{t_{d_i}}, \overrightarrow{t_{d_j}}) = \frac{m \times (\overrightarrow{t_{d_i}} \cdot \overrightarrow{t_{d_j}}) - TF_i \times TF_j}{\sqrt{I \times J}},$$

where

$$TF_i = \sum_{t=1}^{m} tf\text{-}idf\,(d_i, t)\,,$$

$$TF_j = \sum_{t=1}^{m} tf\text{-}idf\,(d_j, t)\,,$$

$$I = m \sum_{t=1}^{m} tf\text{-}idf\,(d_i, t)^2 - {TF_i}^2,$$

$$J = m \sum_{t=1}^{m} tf\text{-}idf\,(d_j, t)^2 - {TF_j}^2.$$

Finally, we normalized the value of each kernel function. We denote as KFC$_{ed}$, KFC$_{cs}$, KFC$_{jc}$ and KFC$_{pcc}$ the resulting four kernels, respectively.

Tables VIII and IX show the ARI, NMI, EARI, the average number of iterations, and the average total time in seconds for 20 Newsgroups and Reuters-21578, respectively. The kernel weights determined by MKFC were 0.249, 0.250, 0.248,and 0.253 for 20 Newsgroups and 0.248, 0.252, 0.247, and 0.253 for Reuters-21578. Note that documents are represented with the bag-of-word model and these four kernels essentially have quite similar clustering capability. Nevertheless, MKFC was still able to assign the weights appropriately to improve the clustering performance.

VI. CONCLUSIONS

We extended the fuzzy c-means algorithm to MKFC. The proposed algorithm is easy to implement and provides soft clustering results that are immune to irrelevant, redundant, ineffective, and unreliable features or kernels. Experiments show that the method effectively incorporates multiple kernels and yields better overall performance. These characteristics make it useful for real-world applications. In the future, we expect to devote our efforts to related open topics, such as strategies for setting the fuzzification degree or choosing the basis kernels.

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Hsin-Chien Huang received the B.S. and M.S. degree in computer and information science from National Chiao Tung University, Hsinchu, Taiwan, in 2001 and 2003, respectively. He is currently pursuing the Ph.D. degree in computer science and information engineering at National Taiwan University, Taipei, Taiwan. His research interests include image processing, computer vision, pattern recognition and multimedia.

Yung-Yu Chuang (M'04) received his B.S. and M.S. from National Taiwan University in 1993 and 1995 respectively, Ph.D. from University of Washington at Seattle in 2004, all in Computer Science. He is currently an associate professor in the Department of Computer Science and Information Engineering, National Taiwan University. His research interests include computational photography, content analysis, computer vision and rendering. He is a member of the IEEE and a member of the ACM.

Chu-Song Chen (S'94-M'96) received a B.S. degree in Control Engineering from National Chiao-Tung University, Taiwan, in 1989. He received an M.S. degree in 1991 and a Ph.D. degree in 1996, respectively, both from the Department of Computer Science and Information Engineering, National Taiwan University. He is now a deputy director of Research Center for Information Technology Innovation (CITI), Academia Sinica, and a research fellow of Institute of Information Science (IIS), Academia Sinica, Taiwan. He is also an adjunct professor of the Graduate Institute of Networking and Multimedia, National Taiwan University. Dr. Chen's research interests include pattern recognition, computer vision, signal/image processing, and multimedia analysis. In 2007-2008, he served as the Secretary-General of the IPPR Society, Taiwan, which is one of the regional societies of the International Association of Pattern Recognition (IAPR). Dr. Chen has served as the program co-chairs of the conferences *ICDAT 2005* and *ICDAT 2006*, theme chair of *PSIVT 2009*, and area chairs of *ACCV 2009*, *ACCV 2010*, and *NBiS 2010*. He is on the editorial board of *Journal of Multimedia* (Academy Publisher), *Machine Vision and Applications* (Springer), and *IPSJ Trans. on Computer Vision and Applications*.