Late Fusion Multiple Kernel Clustering With Proxy Graph Refinement

Siwei Wang[®], Xinwang Liu[®], Senior Member, IEEE, Li Liu[®], Senior Member, IEEE, Sihang Zhou[®], and En Zhu[®]

Abstract—Multiple kernel clustering (MKC) optimally utilizes a group of pre-specified base kernels to improve clustering performance. Among existing MKC algorithms, the recently proposed late fusion MKC methods demonstrate promising clustering performance in various applications and enjoy considerable computational acceleration. However, we observe that the kernel partition learning and late fusion processes are separated from each other in the existing mechanism, which may lead to suboptimal solutions and adversely affect the clustering performance. In this article, we propose a novel late fusion multiple kernel clustering with proxy graph refinement (LFMKC-PGR) framework to address these issues. First, we theoretically revisit the connection between late fusion kernel base partition and traditional spectral embedding. Based on this observation, we construct a proxy self-expressive graph from kernel base partitions. The proxy graph in return refines the individual kernel partitions and also captures partition relations in graph structure rather than simple linear transformation. We also provide theoretical connections and considerations between the proposed framework and the multiple kernel subspace clustering. An alternate algorithm with proved convergence is then developed to solve the resultant optimization problem. After that, extensive experiments are conducted on 12 multi-kernel benchmark datasets, and the results demonstrate the effectiveness of our proposed algorithm. The code of the proposed algorithm is publicly available at https://github.com/wangsiwei2010/graphlatefusion_MKC.

Index Terms—Data fusion, multiple kernel clustering (MKC), multi-view learning.

I. INTRODUCTION

CLUSTERING is one of the fundamental unsupervised learning tasks in the data science and machine

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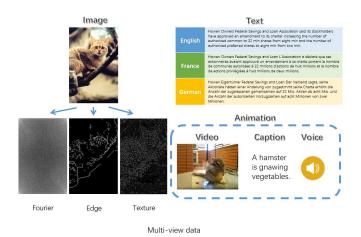


Fig. 1. Example of multi-view data. Images are often described by edge features, Fourier features, and texture features. Text with the same information can be translated into multiple languages. Moreover, videos have vision, text, and voice features.

learning community. In the era of big data, data are often collected from multiple sources or domains as single-view information could not contain comprehensive information, which gives rise to multi-view clustering in literature. For example, for image clustering, images are often described by edge features, HOG features, and local binary pattern (LBP) features (see Fig. 1). Existing multi-view clustering can be roughly categorized into aspects: multiple-view subspace, co-training, multi-view ensemble clustering, and multiple kernel clustering (MKC). Multi-view subspace clustering (MVSC) aims to seek unified subspaces from fused multi-view data representation and then separates data in the corresponding subspace. By capturing nonlinear structure and preserving pairwise similarity in graphs, MVSC has been widely applied in various applications, e.g., image classification, face clustering, and community detection [1]–[7]. Multi-view ensemble clustering optimizes the optimal clustering partition matrix by aggregating a set of given pre-defined multiple partitions [8]-[10]. As an important extension to k-means to handle multi-view data, MKC cooperates a group of weighted kernels from a given library to enhance clustering performances on nonlinearly spreadable data. The existing approaches in literature can be roughly categorized into two strategies from the perspective of different fusion stages, i.e., kernel fusion and late fusion. The kernel fusion methods combine complementary

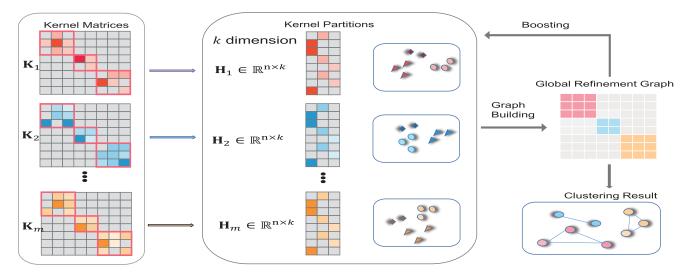


Fig. 2. Illustration of our proposed LFMKC-PGR. The late fusion kernel base partitions are initialized with kernel k-means performed on each kernel matrix. After that, a global self-expressive proxy graph is constructed to capture their complex partition structure. Then the kernel base partitions and proxy graph are alternately boosted until best serving for clustering.

information from multiple kernels and perform kernel k-means on the optimal kernel [11]–[20]. For example, a multiple kernel k-means algorithm is proposed to jointly optimize kernel weights, dimension reduction and clustering task [1]. The work in [2] suggests multiple data-dependent kernels to preserve local structures among different views. Then Liu *et al.* [3] propose multiple kernel k-means with a matrix-induced regularization term to encourage the diversity of selected kernels. Moreover, a multiple kernel k-means method with cluster-aware weighting is introduced in multi-view clustering [21].

Recently, late fusion-based MKC is proposed to utilize underlying shared kernel partition by fusing partition level information, which significantly reduces the computation burden and avoids low-quality solutions [22]–[28]. Wang *et al.* [24] efficiently obtain a unified kernel partition by maximizing its alignments with individual partitions. Comparing to former kernel fusion methods, late fusion variants take advantage of partition information and enjoy considerable algorithm acceleration. Although the proposed late fusion methods enjoy low complexity and considerable promising performance in applications, they can still be improved from the following considerations.

- The kernel base partition learning stage and the subsequent late fusion are separated from each other in the existing mechanism. Therefore, their performance is highly dependent on the quality of pre-calculated kernel partitions in each view, which may contain noises or outliers to degrade performance and lead to suboptimal solutions.
- 2) These methods consider the relationships between kernel base partitions and consensus partition are linear transformation. However, this assumption might fail to handle real multi-kernel applications due to obstructions existing in data.

As consequence, these two major factors inhibit late fusion MKC from obtaining better performance.

To address these issues, in this article, we propose to jointly optimize kernel base partitions and late fusion stage in a unified manner, which is termed as late fusion multiple kernel clustering with proxy graph refinement (LFMKC-PGR) (see Fig. 2). First, we theoretically illustrate the connection between kernel base partition and traditional spectral embedding under certain kernel conditions. Therefore, followed by traditional graph-based methods, we construct a proxy self-expressive graph for individual kernel base partitions and combine them into joint optimization. Moreover, by optimizing a shared selfexpression matrix for base partitions to capture non-linear relationships, they can be jointly negotiated with each other and reach a consensus on partition space best serving for clustering. In addition, extensive experiments on 12 multiple-view benchmark datasets are conducted to evaluate the effectiveness and efficiency of our proposed method. As demonstrated, the proposed algorithm enjoys superior clustering performance in comparison with several state-of-the-art multi-view kernelbased clustering methods.

The main contributions of this article can be summarized as follows.

- We theoretically reveal that late fusion kernel partition can be regarded as spectral embedding under certain conditions. Based on that, traditional graph-based methods can be continually applied into late fusion MKC which gives a novel insight into the MKC community.
- 2) We unify the kernel base partition learning and late fusion refinement into one framework. Therefore, they can be jointly promoted and reach a consensus on partition space best serving for clustering. Moreover, we theoretically uncover the proposed method with the existing multiple kernel subspace clustering framework and discuss its pros and cons.
- Extensive experiments are conducted on 12 multi-kernel benchmark datasets. By virtue of the proposed algorithm, LFMKC-PGR shows clear superiority over other multiple kernel state-of-the-art methods.

TABLE I
COMMON KERNEL FUNCTIONS

Name	Expression	Parameter		
Linear kernel	$\kappa (x_i, x_j) = x_i^T x_j$			
Polynomial kernel	$\kappa (x_i, x_j) = (x_i^T x_j)^d$	$d \ge 1$ is the degree of the polynomial		
Gaussian kernel	$\kappa(x_i, x_j) = \exp\left(-\frac{\ x_i - x_j\ ^2}{2\sigma^2}\right)$	$\sigma>0$ is the bandwidth of the Gaussian kernel		
Laplace kernel	$\kappa(x_i, x_j) = \exp\left(-\frac{\ x_i - x_j\ }{\sigma}\right)$	$\sigma > 0$		
Sigmoid kernel	$\kappa\left(x_{i},x_{j} ight)= anh\left(eta x_{i}^{T}x_{j}+ heta ight)$	tanh is the hyperbolic tangent function, $\beta>0, \theta<0$		

The rest of this article is organized as follows. Section II outlines the related work of MKC. Section III presents the proposed optimization objective and the two-step alternate algorithm. Further, we also provide an analysis of the convergence and the computational complexity of our proposed algorithm. Section IV shows the experiment results with evaluation. Section V concludes the article.

II. RELATED WORK

In this section, we introduce existing work most related to our study in this article including kernel clustering and advanced multiple-kernel clustering methods.

A. Multi-Kernel k-Means (MKKM)

In recent years, enormous MKC methods have been proposed to enhance task performance in literature, i.e., the co-training style methods, kernel fusion, and late fusion strategies.

The co-training approaches for MKC iteratively obtain clustering results that can provide predicted clustering indices for the unlabeled data for other views. In this way, besides extracting the specific cluster information from the corresponding view, the clustering results are forced to be consistent across views. These methods may suffer performance degradation when the pseudo-labels obtained from other views are not reliable.

Kernel fusion-based algorithms mainly optimize kernel coefficients for a group of kernel candidates [6], [29]–[32]. Let $\{\mathbf{x}_i\}_{i=1}^n \subseteq \mathcal{X}$ be a collection of n samples, and $\phi_p(\cdot): \mathbf{x} \in \mathcal{X} \mapsto \mathcal{H}_p$ be the p-th feature mapping that maps \mathbf{x} onto a reproducing kernel Hilbert space (RKHS) \mathcal{H}_p $(1 \le p \le m)$. In the multiple kernel setting, each sample is represented as $\phi_{\boldsymbol{\beta}}(\mathbf{x}) = [\beta_1 \phi_1(\mathbf{x})^\top, \dots, \beta_m \phi_m(\mathbf{x})^\top]^\top$, where $\boldsymbol{\beta} = [\beta_1, \dots, \beta_m]^\top$ consists of the coefficients of the m base kernels $\{\kappa_p(\cdot, \cdot)\}_{p=1}^m$. These coefficients will be optimized during learning. The relative commonly used kernel functions are shown in Table I.

Based on the definition of $\phi_{\beta}(\mathbf{x})$, a kernel function can be expressed as

$$\kappa_{\beta}(\mathbf{x}_i, \mathbf{x}_j) = \phi_{\beta}(\mathbf{x}_i)^{\top} \phi_{\beta}(\mathbf{x}_j) = \sum_{p=1}^{m} \beta_p^2 \kappa_p(\mathbf{x}_i, \mathbf{x}_j).$$
 (1)

A kernel matrix \mathbf{K}_{β} is then calculated by applying the kernel function $\kappa_{\beta}(\cdot, \cdot)$ into $\{\mathbf{x}_i\}_{i=1}^n$. Based on the kernel matrix \mathbf{K}_{β} , the objective of multi-kernel k-means (MKKM) can be

written as

$$\min_{\mathbf{H}, \boldsymbol{\beta}} \operatorname{Tr}(\mathbf{K}_{\boldsymbol{\beta}}(\mathbf{I}_{n} - \mathbf{H}\mathbf{H}^{\top}))$$
s.t. $\mathbf{H} \in \mathbb{R}^{n \times k}, \ \mathbf{H}^{\top}\mathbf{H} = \mathbf{I}_{k}$

$$\boldsymbol{\beta}^{\top}\mathbf{1}_{m} = 1, \quad \beta_{p} \geq 0 \quad \forall p \tag{2}$$

where I_k is an identity matrix with size $k \times k$.

The optimization problem in (2) can be solved by alternately updating **H** and β

1) Optimizing **H** Given β : With the kernel coefficients β fixed, **H** can be obtained by solving a kernel k-means clustering optimization problem

$$\max_{\mathbf{H}} \operatorname{Tr}(\mathbf{H}^{\top} \mathbf{K}_{\beta} \mathbf{H})$$
s.t. $\mathbf{H} \in \mathbb{R}^{n \times k}$, $\mathbf{H}^{\top} \mathbf{H} = \mathbf{I}_{k}$. (3)

The optimal **H** for (3) can be obtained by taking the k eigenvectors respecting to the largest eigenvalues of \mathbf{K}_{β} .

2) Optimizing β Given **H**: With **H** fixed, β can be optimized via solving the following quadratic programming with linear constraints:

$$\min_{\boldsymbol{\beta}} \sum_{p=1}^{m} \beta_p^2 \text{Tr} (\mathbf{K}_p (\mathbf{I}_n - \mathbf{H} \mathbf{H}^\top))$$
s.t. $\boldsymbol{\beta}^\top \mathbf{1}_m = 1, \quad \beta_p \ge 0.$ (4)

Along with this line, many variants of MKKM have been proposed in the literature. The work in [1] proposes a three-step alternate algorithm to jointly perform kernel clustering, coefficients and dimension reduction. The work in [3] proposes a multiple kernel k-means clustering algorithm with matrix-induced regularization to reduce the redundancy and enhance the diversity of the pre-defined kernels. Furthermore, the local kernel alignment criterion has been applied to multiple kernel learning to enhance the clustering performance in [33].

B. Late Fusion Multiple Kernel Clustering

Based on the assumption that the multiple kernels are expected to share a consensus partition matrix among partition levels, late fusion methods seek the optimal kernel partition by combing linearly transformed base partitions obtained from single views [22], [24], [25]. Given n samples in k clusters among m views, their optimization goal can be mathematically expressed as

$$\max_{\mathbf{H}^{c}, \{\mathbf{W}_{i}\}_{i=1}^{m}, \boldsymbol{\beta}} \operatorname{Tr} \left(\mathbf{H}^{c\top} \sum_{i=1}^{m} \beta_{i} \mathbf{H}_{i} \mathbf{W}_{i} \right) + \lambda \mathbf{\Omega} \left(\mathbf{H}^{c} \right)$$
s.t.
$$\mathbf{H}^{c\top} \mathbf{H}^{c} = \mathbf{I}_{k}, \quad \mathbf{W}_{i}^{\top} \mathbf{W}_{i} = \mathbf{I}_{k}$$

$$\|\boldsymbol{\beta}\|_{2} = 1, \quad \beta_{i} \geq 0 \quad \forall i$$
(5)

where the first term and $\Omega(\cdot)$ denote the late fusion alignment and regularization term for the consensus partition \mathbf{H}^c respectively. $\mathbf{H}_i \in \mathbb{R}^{n \times k}$ and \mathbf{W}_i are the *i*th kernel partition matrix obtained from *i*-th kernel and its transformation matrix regarding the consensus partition matrix.

Although (5) accomplishes MKC with kernel individual partition matrices fusion via an effective and efficient manner,

its partition presentation learning and late fusion are conducted separately which may lead to suboptimal solutions. Moreover, the linear transformation relationships do not always hold when facing noises or outliers in real-world complex data. As a result, these two factors shadow the representation ability of latent kernel partitions and adversely harm the performance of the model. In the following, we propose a proxy graph to refine the base partitions and optimally optimize them and fusion in a unified manner termed LFMKC-PGR.

III. LATE FUSION MULTIPLE KERNEL CLUSTERING WITH PROXY GRAPH REFINEMENT

In this section, we first describe our proposed LFMKC-PGR in detail. Then an efficient two-step optimization algorithm is proposed to solve the respective optimization formula. Finally, we summarize our algorithm and provide analysis and extensions for LFMKC-PGR.

A. Revisit Kernel k-Means and Spectral Clustering

In this section, we first revisit the popular kernel k-means clustering and mathematically reveal its connection with traditional spectral clustering. Given a similarity matrix **W**, the optimization goal of spectral clustering algorithm can be rewritten as [34]

$$\min_{\mathbf{F}} \operatorname{Tr}(\mathbf{F}^{\top} \mathbf{L}_{\mathbf{W}} \mathbf{F})$$
s.t. $\mathbf{F} \in \mathbb{R}^{n \times k}, \quad \mathbf{F}^{\top} \mathbf{F} = \mathbf{I}_{k}$ (6)

where F is regarded as the spectral embedding of data matrix and L is the Laplacian matrix for the respective affinity matrix W as $L_W = D - W$, where D is the degree matrix.

The traditional kernel k-means clustering can be mathematically written as follows [35]:

$$\max_{\mathbf{H}} \operatorname{Tr}(\mathbf{H}^{\top} \mathbf{K} \mathbf{H})$$
s.t. $\mathbf{H} \in \mathbb{R}^{n \times k}$, $\mathbf{H}^{\top} \mathbf{H} = \mathbf{I}_{k}$. (7)

It seems that there is no significant connection between (6) and (7) at first glance. The following theorem gives a theoretic analysis of kernel k-means and (6).

Theorem 1: Given a normalized kernel matrix \mathbf{K} as the affinity matrix under the condition $\mathbf{D}_K = \mathbf{I}_n$, the optimal solutions of \mathbf{F}^* in (6) and \mathbf{H}^* in (7) satisfy the following equation $\mathbf{F}^* = \mathbf{H}^*$.

Proof: Notice that $\operatorname{Tr}(\mathbf{F}^{\top}\mathbf{L}_{\mathbf{K}}\mathbf{F}) = \operatorname{Tr}(\mathbf{F}^{\top}(\mathbf{D}_{\mathbf{K}} - \mathbf{K})\mathbf{F}) = k - \operatorname{Tr}(\mathbf{F}^{\top}\mathbf{K}\mathbf{F})$, where k is a constant. The optimal solution for (6) is the k smallest eigenvectors of $\mathbf{L}_{\mathbf{K}}$ while the solution for (7) is the k largest eigenvectors of \mathbf{K} . Therefore it is straightforward to see that $\mathbf{F}^* = \mathbf{H}^*$. The equation holds if we set the degree matrix $\mathbf{D}_{\mathbf{K}}$ as \mathbf{I}_n and this could be easily done by normalizing the kernel matrix.

Theorem 1 inspires us a new perspective on (5) that the kernel partitions $\{\mathbf{H}_i\}_{i=1}^m$ can be regarded as the spectral embeddings from individual views under certain conditions. Therefore, they can be refined by the existing graph-based methods and jointly be optimized during the learning process. In the next subsection, we describe our proposed proxy graph

refinement in detail to combine kernel partition and graph constructing into one objective and further improve the existing late-fusion-based strategy.

B. Proposed Formula

Regarding (5), the base partition matrices are learned individually from each kernel with fixed representations during the learning stage and the consensus \mathbf{H}^c is obtained by a linear transformation. Therefore, the kernel representation learning and the fusion procedures are conducted separately which do not satisfy an end-to-end manner. Moreover, we might capture more complicated relationships between each base partition rather than simple linear transformations.

The kernel base partitions $\{\mathbf{H}_i\}_{i=1}^m$ are independently initialized from each kernel in original model of (5). Different from that, the base partitions are refined by a proxy graph regularization term in our new model. Inspired by the self-expressive subspace graph building method [32], [36]–[46], we treat each base partition with refined similarity graph S building as follows:

$$\min_{\mathbf{S}} \sum_{i=1}^{m} \|\mathbf{H}_{i} - \mathbf{S}\mathbf{H}_{i}\|_{F}^{2} + \beta \|\mathbf{S}\|_{F}^{2}$$
s.t. $\mathbf{S} \ge 0$, $\mathbf{S}\mathbf{1} = \mathbf{1}$, $\operatorname{diag}(\mathbf{S}) = 0$ (8)

where **S** is the shared proxy graph for base partitions and represents the complex relationship between each single view representation, and $\|\mathbf{S}\|_F^2$ is the regularization term. $\mathbf{S} \geq 0$ ensures the non-negative of the similarity matrix \S and $\mathbf{S1} = \mathbf{1}$ normalizes the obtained **S**. Moreover, diag(**S**) = 0 avoids the trivial solution.

By minimizing (8), S_{ij} can be regarded as the similarity score between i-th and j-th sample. The larger value S_{ij} is, the more likely two samples belong to the same cluster. After getting the global graph S, we refine the kernel base partition with the guidance of kernel matrices and the learned global graph. Our idea can be mathematically expressed as follows:

$$\min_{\{\mathbf{H}_i\}_{i=1}^m, \mathbf{S}} \sum_{i=1}^m \underbrace{\operatorname{Tr}(\mathbf{K}_i(\mathbf{I} - \mathbf{H}_i \mathbf{H}_i^\top))}_{\text{Kernel clustering}} + \underbrace{\lambda \|\mathbf{H}_i - \mathbf{S}\mathbf{H}_i\|_F^2}_{\text{Graph Refinement}} + \beta \|\mathbf{S}\|_F^2$$
s.t. $\mathbf{S} \ge 0$, $\mathbf{S}\mathbf{1} = \mathbf{1}$, $\operatorname{diag}(\mathbf{S}) = 0$, $\mathbf{H}_i^\top \mathbf{H}_i = \mathbf{I}_k$. (9)

From the above formula, we summarize the differences between our MKL methods and MVSC as follows.

- Methods of MVSC are facing raw data or extracted features while the MKL method optimizes the multiple kernel matrices (similarity matrices). Further, it is quite straightforward to combine MKL and feature selection into a unified framework. With an adequate feature selection strategy, the base kernels can be dynamically constructed from the selected features rather than raw data.
- 2) The advantage of MKL is to handle nonlinear-separable data. MKL adopts several kernel functions to transfer original data to their new representations in Hilbert Space. While they are not easy to be clustered in original space.

3) MKL can naturally handle heterogeneous source information regardless of the data items. Whatever the data types are, the kernels can be defined once the similarity measure is defined. Therefore, MKL is widely applied in Biology and Chemistry. Other methods will conduct graph alignment to handle in-heterogeneous multi-view information.

Our proposed LFMKC-PGR model jointly optimizes the individual kernel representations and the consensus proxy graph into a unified formula, which avoids the former separate two-step late fusion strategy. Although the formula is quite simple and straightforward, LFMKC-PGR has the following merits: 1) it addresses MKC via a refined late fusion manner which simultaneously combines kernel partition learning and graph refinement in a joint framework; 2) view-specific correlations are captured in graph structure making it more robust to noises or corrupted multi-view data; and 3) more considerations of graph constructions in kernel partition space can be easily adjusted into this framework with prior knowledge.

C. Connections With the Existing Multiple Kernel Subspace Clustering

Comparing with conventional MKC algorithms, ours is the first attempt to combine kernel k-means and the latter graph regularization which has not been studied in the existing literature. The equation seems much such as with the combination of kernel self-expressive subspace clustering [14], [47]–[49].

The kernel self-expressive subspace clustering extends traditional subspace clustering with kernel tricks to handle nonlinearly separable subspaces [47]. The original formula is that

$$\min_{\mathbf{S}} \operatorname{Tr} \left(\mathbf{K} \left(\mathbf{I} - 2\mathbf{S} + \mathbf{S} \mathbf{S}^{\top} \right) \right) \tag{10}$$

where **S** is the learned kernel graph.

We summarize the differences of our new MKC framework comparing to the kernel subspace algorithms. As we mentioned in our article, the original space may be infinitedimensional (e.g., Gaussian kernel) and contain noise or outliers, which could better capture information at the partition level. However, in our article, we directly start from the kernel k-means and therefore the subsequent graph is constructed in the partition space rather than the former in the original RKHS. As can be seen, the graph S in [47] is only reflected by the original kernel K while ours is both influenced by the kernel and the partition matrix **H** respectively. These lead to two different formulations in [47] and ours. To the best of our knowledge, it is also the first practice within the MKC domain. By following this new framework, more interesting approaches could be introduced into MKC and can greatly contribute to the MKC community.

D. Optimization

The optimization problem in (9) is a non-convex problem when regarding the two variables. In this section, we develop an alternate optimization algorithm which separates the resultant problem into two subproblems such that each is convex when the other variable is fixed.

1) Update $\{\mathbf{H}_i\}_{i=1}^m$: By fixing \mathbf{S} , $\{\mathbf{H}_i\}_{i=1}^m$ can be solved individually with each of the m sub-problems. The optimization

problem regarding of \mathbf{H}_i can be simplified as

$$\min_{\mathbf{H}_{i}} \operatorname{Tr}(\mathbf{K}_{i}(\mathbf{I} - \mathbf{H}_{i}\mathbf{H}_{i}^{\top})) + \lambda \|\mathbf{H}_{i} - \mathbf{S}\mathbf{H}_{i}\|_{F}^{2}$$
s.t. $\mathbf{H}_{i}^{\top}\mathbf{H}_{i} = \mathbf{I}_{k}$ (11)

which can be further converted into

$$\max_{\mathbf{H}_{i}} \operatorname{Tr}(((\mathbf{K}_{i} - \lambda(\mathbf{I} - 2\mathbf{S} + \mathbf{S}\mathbf{S}^{\top}))\mathbf{H}_{i}\mathbf{H}_{i}^{\top}))$$
s.t. $\mathbf{H}_{i}^{\top}\mathbf{H}_{i} = \mathbf{I}_{k}$. (12)

By denoting $\mathbf{G} = \mathbf{K}_i - \lambda(\mathbf{I} - 2\mathbf{S} + \mathbf{S}\mathbf{S}^{\top})$, the optimal \mathbf{H}_i in (11) can be obtained by taking the k largest eigenvectors corresponding to the largest k eigenvalues of \mathbf{G} .

2) Update S: When \mathbf{H}_i being fixed, (9) can be rewritten as

$$\min_{\mathbf{S}} \sum_{i=1}^{m} \lambda \|\mathbf{H}_{i} - \mathbf{S}\mathbf{H}_{i}\|_{F}^{2} + \beta \|\mathbf{S}\|_{F}^{2}$$
s.t. $\mathbf{S} \ge 0$, $\mathbf{S}\mathbf{1} = \mathbf{1}$, $\operatorname{diag}(\mathbf{S}) = 0$. (13)

Specially, we design a two-step algorithm to quickly solve (13). In the first step, we solve (13) without constraints, which can be written as

$$\hat{\mathbf{S}} = \arg\min_{\mathbf{S}} \sum_{i=1}^{m} \lambda \|\mathbf{H}_i - \mathbf{S}\mathbf{H}_i\|_F^2 + \beta \|\mathbf{S}\|_F^2.$$
 (14)

Equation (14) is a constraint-free problem. By taking the derivation of (14) with respect to S to zero, we can get the closed-form solution to (14)

$$\hat{\mathbf{S}} = \left(\mathbf{C} + \frac{\beta}{\lambda}\mathbf{I}\right)^{-1}\mathbf{C} \tag{15}$$

where $\mathbf{C} = \sum_{i}^{m} \mathbf{H}_{i} \mathbf{H}_{i}^{\top}$.

Then, we can obtain the approximate solution of **S** by projecting $\hat{\mathbf{S}}_i$ through the following minimization problem with proper constraints:

$$\min_{\mathbf{S} \ge 0, \ \mathbf{S} = \mathbf{1}, \text{diag}(\mathbf{S}) = 0} \|\mathbf{S} - \hat{\mathbf{S}}\|_F^2.$$
 (16)

This problem yields a close-formed solution that

$$\mathbf{S}_{j,:} = \max(\hat{\mathbf{S}}_{j,:} + \alpha_j \mathbf{1}, 0), \quad \mathbf{S}_{jj} = 0, \ \alpha_j = \frac{1 + \hat{\mathbf{S}}_{j,:}^{\top} \mathbf{1}}{n}.$$
 (17)

Proof: The problem of (16) can be easily rewritten into n row-formed independent optimization problems as follows:

$$\min_{\mathbf{S}_{j,:} \geq 0, \ \mathbf{S}_{j,:}^{\top}, 1=1, \ \mathbf{S}_{j,:} = 0} \|\mathbf{S}_{j,:} - \mathbf{\hat{S}}_{j,:}\|_F^2$$
 (18)

where $S_{j,:}$ is the *j*-th row of S. We write the Lagrangian function of (18) as

$$\mathcal{L}(\mathbf{S}_{j,:}, \alpha, \beta) = \|\mathbf{S}_{j,:} - \hat{\mathbf{S}}_{j,:}\|_F^2 - \alpha_j (\mathbf{S}_{j,:}^\top \mathbf{1} - 1) - \eta_j^\top \mathbf{S}_{j,:}$$
(19)

where α and η_j are the respective Lagrangian multipliers. Then the KKT conditions are written as

$$\begin{cases} \mathbf{S}_{j,:} - \hat{\mathbf{S}}_{j,:} - \alpha_j \mathbf{1} - \eta_j = 0 \\ \eta_j \bigodot \mathbf{S}_{j,:} = 0. \end{cases}$$
 (20)

Therefore with $\mathbf{S}_{i,1}^{\top} \mathbf{1} = 1, \mathbf{S}_{jj} = 0$, we can easily obtain that

$$\mathbf{S}_{j,:} = \max(\hat{\mathbf{S}}_{j,:} + \alpha_j \mathbf{1}, 0), \mathbf{S}_{jj} = 0, \alpha_j = \frac{1 + \hat{\mathbf{S}}_{j,:}^{\perp} \mathbf{1}}{n}.$$
 (21)

This completes the proof.
$$\Box$$

Algorithm 1 Late Fusion Multiple Kernel Clustering With Proxy Graph Refinement (LFMKC-PGR)

Input: Base kernel matrices $\{\mathbf{K}_i\}_{i=1}^m$, clustering number k, Hyper-parameters λ , β .

Initialize: S

while not converged do

Update $\{\mathbf{H}_i\}_{i=1}^m$ by solving (12);

Update S by obtaining (17);
end

Output: Performing spectral clustering on S.

E. Analysis and Discussions

Computational Complexity: With the optimization process outlined in Algorithm 1, the total time complexity consists of two parts referring to the alternate steps. The first step mentioned in (12), actually needs singular value decomposition (SVD) for **G** and therefore needs $\mathcal{O}(mn^2k)$. As for the third step, we design a two-step approximate algorithm for solving S. Its time complexity is $\mathcal{O}(n^2k)$. The key issue in time complexity in the algorithm is to solve the inverse of $C + (\beta/\lambda)I$ with the size n * n. Note that to obtain C needs $O(n^2k)$. Then we formalize $C = UU^{\top}(O(n^2k))$, with the size n * k). We apply the Woodbury formulation which is widely applied in ridge regression to accelerate the inverse problem into $O(n^2k)$ with the following equation. $(\mathbf{C} + (\beta/\lambda)\mathbf{I}_n)^{-1} =$ $(\lambda/\beta)((\lambda/\beta)\mathbf{C} + \mathbf{I}_n)^{-1} = (\lambda/\beta)(\mathbf{U}\mathbf{U}^\top + \mathbf{I}_n)^{-1} = (\lambda/\beta)(\mathbf{I}_n - \mathbf{I}_n)^{-1}$ $\mathbf{U}(\mathbf{I}_k + \mathbf{U}^{\mathsf{T}}\mathbf{U})^{-1}\mathbf{U}^{\mathsf{T}}$). Hence for each iteration, the whole time complexity of our proposed algorithms is $\mathcal{O}(mn^2k + n^2k)$.

Convergence: It is easy to obtain that the whole optimization function is lower bounded to 0. As the two subproblems are strictly convex when optimizing one variable and keeping the others fixed. The objective of Algorithm 1 is monotonically increased when optimizing one variable with the others fixed at each iteration. As a result, the proposed algorithm can be verified to be convergent according to [50].

Extensions: LFMKC-PGR offers a novel insight on the connection between kernel partitions and traditional spectral embedding. More interesting graph-based methods can be introduced to this framework. For example, a local graph structure building strategy can be applied to further enhance the clustering performances by exploiting local structures among different views.

IV. EXPERIMENT

In this section, we evaluate the effectiveness and efficiency of the proposed method for 12 widely used multiview benchmark datasets with strong competitors from the perspectives of clustering performance, parameter sensitivity, and convergence.

A. Datasets

The proposed algorithm is experimentally evaluated on 12 widely used multiple kernel benchmark datasets shown in Table II. They are AR10P, Oxford Flower17 and

TABLE II

DATASETS USED IN OUR EXPERIMENTS

Dataset	#Samples	#Kernels	#Classes	
AR10P	130	6	10	
YALE	165	5	15	
ProteinFold	694	12	27	
Flower17	1360	7	17	
Nonplant	2732	69	3	
Flower102	8189	4	102	
Caltech102-5	510	48	102	
Caltech102-10	1020	48	102	
Caltech102-15	1530	48	102	
Caltech102-20	2040	48	102	
Caltech102-25	2550	48	102	
Caltech102-30	3060	48	102	

Flower102,² ProteinFold,³ YALE Face,⁴ Nonplant and Caltech102.⁵ For these datasets, all kernel matrices are precomputed and can be publicly downloaded from the above websites. Further, followed by [22], we have downloaded the last six Caltech102 datasets where Caltech102-5 denotes the number of samples belonging to each cluster is 5 and so on.

B. Compared Algorithms

In the experiments, our proposed algorithm is compared with the following state-of-the-art multiple kernel or subspace clustering methods.

- 1) Best Single Kernel k-Means (BSKM).
- 2) *MKKM* [51]: The algorithm alternatively performs kernel k-means and updates the kernel coefficients.
- Co-Regularized Spectral Clustering (CRSC) [52]: CRSC provides a co-regularization way to perform spectral clustering on multiple views.
- 4) Robust Multiple Kernel k-Means (RMKKM) Using $\ell_{2,1}$ Norm [53]: RMKKM simultaneously finds the clustering label, the cluster membership, and the optimal combination of multiple kernels by adding $\ell_{2,1}$ norm.
- 5) Robust Multi-View Spectral Clustering (RMSC) [54]: RMSC constructs a transition probability matrix from each single view, and then use recover a shared low-rank transition probability matrix as an input to the standard Markov chain for clustering.
- 6) Multiple Kernel k-Means With Matrix-Induced Regularization (MKMR) [3]: MKMR fulfills the multiple kernel k-means clustering with a matrix-induced regularization to reduce the redundancy and enhance the diversity of the kernels.
- 7) Multiple Kernel Clustering With Local Kernel Alignment Maximization (MKAM) [33]: The algorithm maximizes the proposed local kernel alignment and therefore captures local structure among kernels.
- 8) Multi-View Clustering via Late Fusion Alignment (MLFA) Maximization [24]: MLFA maximizes the alignment of individual kernel partitions and consensus one, and reach an agreement on partition level information.

¹http://featureselection.asu.edu/old/datasets.php

²http://www.robots.ox.ac.uk/~vgg/data/flowers/

³http://mkl.ucsd.edu/dataset/protein-fold-prediction

⁴www.cs.yale.edu/cvc/projects/yalefaces/yalefaces.html

⁵http://www.vision.caltech.edu/archive.html

TABLE III

ACC, NMI, AND PURITY COMPARISON OF DIFFERENT CLUSTERING ALGORITHMS ON 12 BENCHMARK DATASETS.

THE BEST RESULT IS HIGHLIGHTED AND BOLDFACED WITH UNDERLINES

Dataset	Metric	BSKM	MKKM	CRSC	RMKKM	RMSC	MKMR	MKAM	MLFA	FMR	Proposed
	ACC	43.08	40.00	38.46	30.77	30.77	39.23	27.69	41.54	51.23	56.15
AR10P	NMI	42.61	39.53	39.82	26.62	27.87	40.11	24.72	39.15	45.52	$\overline{51.82}$
	Purity	43.08	40.00	39.23	32.31	33.08	39.23	28.46	41.54	51.23	56.15
YALE	ACC	56.97	52.12	56.97	56.36	58.03	60.00	46.67	54.55	61.21	62.42
	NMI	58.42	54.16	57.69	59.32	57.58	62.87	53.51	59.86	60.31	63.48
	Purity	57.58	52.73	57.58	58.18	57.24	60.00	49.09	55.76	61.33	62.42
	ACC	33.86	27.23	34.87	30.98	33.00	36.46	37.90	35.88	34.96	40.06
ProteinFold	NMI	42.03	37.16	43.32	38.78	43.91	45.32	44.46	44.00	43.68	48.72
	Purity	41.21	33.86	40.78	36.60	42.36	42.65	43.95	41.93	42.22	$\underline{45.97}$
	ACC	42.06	45.37	52.35	53.38	51.10	58.82	57.87	60.16	58.78	62.28
Flower17	NMI	45.14	45.35	50.42	52.56	54.39	57.05	56.06	59.79	56.98	61.72
	Purity	44.63	46.84	53.01	55.07	54.12	60.51	59.26	62.13	59.66	63.60
	ACC	49.38	54.32	55.56	49.33	60.65	56.59	59.57	50.07	36.70	67.50
Nonplant	NMI	16.55	15.83	17.44	16.55	20.35	23.43	23.04	16.55	0.50	25.56
	Purity	72.18	71.45	73.17	72.18	70.50	73.33	74.34	72.18	60.36	75.29
	ACC	33.13	21.96	37.26	28.17	32.97	39.91	40.84	42.73	35.24	46.78
Flower102	NMI	48.99	42.30	54.18	48.17	53.36	57.27	57.60	57.59	57.42	60.30
	Purity	38.78	27.61	44.08	33.86	40.24	46.39	48.21	49.73	41.62	53.07
	ACC	36.86	28.63	36.08	32.75	33.73	38.04	32.16	37.45	36.27	43.73
Caltech-5	NMI	68.64	65.97	70.60	66.76	68.93	71.08	67.18	71.87	70.25	73.69
	Purity	36.24	29.80	37.65	33.92	34.90	39.02	33.92	39.61	37.29	45.49
	ACC	30.88	22.75	33.43	26.67	29.80	33.73	28.33	32.45	28.73	40.78
Caltech-10	NMI	59.77	55.80	62.10	57.28	59.86	62.76	58.51	61.99	59.09	66.90
	Purity	31.24	24.22	35.29	28.82	31.47	35.88	30.39	34.22	29.80	43.73
	ACC	29.11	20.39	31.18	24.90	25.49	32.29	27.32	31.11	17.12	39.93
Caltech-15	NMI	53.66	49.27	57.73	52.04	54.57	58.25	55.20	57.66	46.81	63.01
	Purity	31.81	21.63	33.14	26.21	27.12	34.25	28.89	33.14	17.71	41.83
	ACC	28.20	18.73	30.98	24.51	23.87	32.55	25.88	30.44	9.71	37.25
Caltech-20	NMI	53.19	45.61	54.84	48.66	50.34	56.06	51.42	54.33	37.74	59.58
	Purity	31.91	20.39	32.50	26.13	25.59	34.66	27.84	32.60	10.22	39.85
	ACC	26.41	16.63	29.69	21.92	24.08	30.12	26.16	29.45	8.23	36.47
Caltech-25	NMI	49.92	41.86	52.04	45.53	48.35	52.94	50.12	52.00	33.43	57.04
	Purity	30.41	18.00	31.57	23.45	25.80	32.20	28.75	31.49	8.64	$\overline{38.75}$
	ACC	25.91	16.31	28.53	21.41	22.58	31.31	24.54	28.56	7.50	36.37
Caltech-30	NMI	49.31	39.92	50.42	43.72	46.04	51.55	47.39	50.12	30.38	$\overline{55.98}$
	Purity	28.71	18.04	30.07	23.50	24.15	33.20	26.76	29.87	7.75	38.40

9) Flexible Multi-View Representation Learning for Subspace Clustering (FMR) [55]: FMR optimizes subspace clustering via encoding complementary latent representations and their nonlinear or high-order correlations from multiple views.

C. Experimental Setting

For all the above-mentioned algorithms, we have downloaded their public MATLAB code implementations from original websites. The hyper-parameters are set according to the suggestions of the corresponding literature. For the proposed algorithm LFMKC-PGR, the trade-off parameters λ and β are chosen from $[2^{-2}, 2^{-1}, \dots, 2^2]$ by grid search. For all datasets, we assumed that the true number of clusters is given. The widely used clustering accuracy (ACC), normalized mutual information (NMI), and purity are applied to evaluate the clustering performance. For all algorithms, we repeat each experiment for 50 times with random initialization to reduce the effect of randomness caused by k-means and report the best result. All our experiments are conducted on a desktop

computer with a 2.5-GHz Intel Platinum 8269CY CPU and 48-GB RAM, MATLAB 2019b (64 b).

D. Experimental Results

Table III presents the ACC comparison of the above algorithms on the 12 benchmark datasets. The best result is highlighted with underlines. Based on the results, we have the following observations.

- 1) Our proposed algorithm shows clear advantages over other multi-kernel clustering baselines, with 12 best out of the total 12 datasets; in particular, the margins for the nine datasets: AR10P, Nonplant, Flower102, and the six Caltech are very impressive, outperforming the second-best algorithm 9.61%, 11.29%, 9.48%, 14.95%, 14.85%, 15.94%, 10.47%, and 6.90% on ACC respectively. These results verify the effectiveness of the proposed method comparing to existing state-of-the-art approaches.
- Comparing with the FMR [55], the proposed LFMKC-PGR consistently further improves the clustering performance and achieves better results among the

TABLE IV

ACC, NMI, AND PURITY COMPARISON OF MULTI-KERNEL SUBSPACE
CLUSTERING, DEEP MULTI-VIEW CLUSTERING
METHODS AND OURS

Dataset	SPMKC	DAMC	Proposed				
ACC(%)							
CCV	23.64	20.51	26.89				
NonPlant	13.50	54.90	67.50				
Flower17	50.07	30.29	62.28				
Flower102	36.55	22.50	46.78				
NMI(%)							
CCV	28.11	22.50	20.72				
NonPlant	1.27	16.64	25.56				
Flower17	51.28	34.38	61.72				
Flower102	52.73	27.80	60.30				
Purity(%)							
CCV	25.46	28.60	29.57				
NonPlant	14.15	69.78	75.29				
Flower17	47.65	35.10	63.60				
Flower102	38.76	21.25	53.07				

benchmark datasets. Both of them adopt the self-expressive subspaces for graph building. The clustering results clearly demonstrate that adapting kernel representations into proxy graphs might capture non-linearly separable data comparing to existing subspace methods.

3) Mentioned before, our LFMKC-PGR originates from MLFA [24] which separates kernel base partition learning and the late fusion stage. As can be seen, the newly proposed algorithm significantly surpasses MLFA in real experiments. Therefore, it is vital to jointly combine the kernel base partition learning and late fusion refinement in MKC.

We also report the NMI and purity in Table III. Again, we observe that the proposed algorithm significantly outperforms other MKC algorithms. These results are consistent with our observations in Table III.

In summary, the above experimental results have well demonstrated the effectiveness of our proposed method comparing to other state-of-the-art methods. We attribute the superiority of the proposed algorithm to two aspects.

- LFMKC-PGR incorporates kernel base partition learning and proxy graph refinement into a unified framework. By the virtue of it, kernel partitions are refined by a global proxy graph and subsequently contributing to construct better graphs. Therefore the two processes are mutually promoted serving for clustering.
- Compared with the existing late fusion multiple kernel methods, the proposed LFMKC-PGR adopts graph structure to capture complex relationships between multiple partitions which is more suitable in real applications.

These two factors contribute to significant improvements in clustering performance.

E. Comparing With Existing Multiple Kernel Subspace Clustering

As mentioned in Section III-C, our proposed LFMKC-PGR has a close relationship with the existing multiple kernel subspace clustering methods which also construct a graph from

TABLE V

ACC, NMI, AND PURITY COMPARISON OF MULTI-VIEW
ENSEMBLE CLUSTERING METHODS AND OURS

Datasets	MVEC	M2VEC	Ours			
ACC(%)						
Caltech-5	25.13	25.37	43.73			
Caltech-10	19.55	20.08	40.78			
Caltech-15	15.97	16.64	39.93			
Flower17	36.51	31.84	62.28			
YALE	26.55	27.52	62.42			
AR10P	20.62	20.15	56.15			
	NMI(%)				
Caltech-5	61.34	62.47	73.69			
Caltech-10	49.61	50.24	66.90			
Caltech-15	42.06	43.88	63.01			
Flower17	40.19	36.80	61.72			
YALE	36.43	34.90	63.48			
AR10P	10P 15.60 16.00		51.82			
Purity(%)						
Caltech-5	28.44	29.64	45.49			
Caltech-10	21.71	22.05	43.73			
Caltech-15	17.44	18.23	41.83			
Flower17	38.58	34.56	63.60			
YALE	31.15	33.46	62.42			
AR10P	21.46	22.54	56.15			

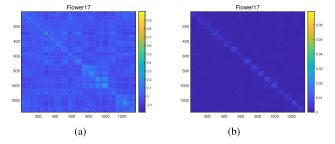


Fig. 3. Illustration of the learned affinity matrix on Flower17: (a) MLFA and (b) our proposed LFMKC-PGR.

kernels. Therefore we also conduct comparison experiments on the existing STOA multi-kernel subspace clustering methods [14], which we refer to it SPMKC in Table IV. And the representative deep multi-view clustering method DAMC [56] is also shown in the table.

We conduct experiments on computer vision datasets CCV,⁶ which contains 6773 YouTube videos over 20 semantic categories. We show our results in Table IV. The superiority experimental results of ours outperform existing SOTA kernel subspace clustering and even deep multi-view algorithm. It is noticed that the comparing method FMR in our article is also a deep-based strong baseline as [31] and [57]. And [14] is considered to be a strong baseline for multiple kernel self-expressive subspace clustering. As can be seen, our method significantly outperforms theirs and the results clearly demonstrate the effectiveness of our proposed method.

F. Comparing With Existing Multi-View Ensemble Clustering

We also conduct experiments comparing to existing multiview ensemble clustering algorithms [8]–[10]. Multi-view ensemble clustering optimizes the optimal clustering partition matrix by aggregating a set of given pre-defined multiple

⁶https://www.ee.columbia.edu/ln/dvmm/CCV/



Fig. 4. Illustration of the learned data distribution with t-sne algorithm on mfeat datasets. (a) 1st iteration. (b) 3rd iteration. (c) 5th iteration. (d) 10th iteration.

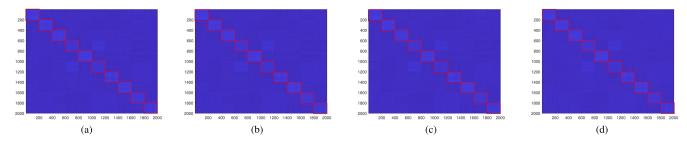


Fig. 5. Illustration of the learned affinity matrix on mfeat datasets. (a) 1st iteration. (b) 3rd iteration. (c) 5th iteration. (d) 10th iteration.

TABLE VI
TIME COMPARISON OF REPRESENTATIVE MKC ALGORITHMS ON
THREE LARGE BENCHMARK DATASETS (IN SECONDS)

Datasets	MKAM	MLFA	FMR	Proposed
Flower102	1027.4	90.71	1805.2	365.1
Nonplant	2694.29	21.18	464.8	148.0
Caltech102-30	620.07	59.76	459.9	143.76

partitions. As can be seen in Table V, our method significantly outperforms the competitors. We attribute the superiority to the following reasons: 1) more flexible similarity measure. Ensemble clustering jointly fuses multiple partitions to reach a consensus partition that heavily relies on the quality of base partitions; and 2) capture nonlinear information. Kernel methods capture the nonlinear relationship with data items which is more practical in real applications.

G. Running Time Comparison

To compare the computational efficiency of the proposed algorithms, we record the running time of various algorithms on these benchmark datasets and report them in Table VI.

From this table, we have two aspects of observations. First, it can be observed that the time complexity of MKAM and FMR are relatively expensive over the other compared methods. Second, the proposed algorithm ranks second best in existing methods. Although MLFA achieves better in terms of efficiency, the proposed method exceeds much better clustering performance as shown in Table III. Therefore, it is clear to see that the total computational cost of the proposed method is less or much less than MKAM, FMR in our experiments. This is probably the main reason that our method is able to cost less time than the compared methods in most cases (as shown in Table VI).

H. Graph Refinement

To directly illustrate the effectiveness of the proxy graph refinement on the late fusion base kernel partitions, we visualize the affinity matrix in Fig. 3. As can be observed, our proposed method refines the base partitions and optimally be fused with the proxy graph. The noises in the affinity matrix shown in Fig. 3(a) are eliminated and the clustering structure becomes clearer in Fig. 3(b). After adding constraint into the MKC optimization goal, the learned similarity graph is constructed in the kernel latent space rather than the original RKHS space.

We have also shown the t-sne visual results on the mfeat datasets in Fig. 4 of the learned data representation on the 1st, 3rd, 5th, and 10th iterations. The figures clearly show the separation of different clusters. Also, it can be observed from Fig. 5, the learned affinity matrices show a clearer block clustering structure with the variation of iterations.

I. Convergence and Parameter Sensitivity

Our algorithm is theoretically guaranteed to converge to a local minimum according to [50]. We also conduct experiments to demonstrate the convergence of the proposed algorithm. The examples of the evolution of the objective value on the experimental results are shown in Fig. 6. In the above experiments, we observe that the objective values of our algorithm monotonically decrease at each iteration. These results clearly verify our proposed algorithm's convergence.

Fig. 7 shows an example of the sensitivity experimental results on AR10P and Flower17. From these figures, we observe that: 1) LFMKC-PGR is practically stable against these parameters that it achieves competitive performance in a wide range of parameter settings and 2) the ACC first increases

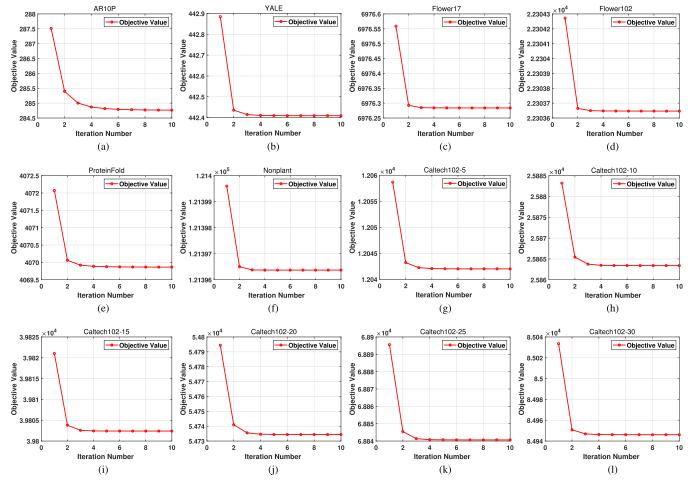


Fig. 6. Convergence of the proposed LFMKC-PGR on the entire 12 datasets. (a) AR10P. (b) YALE. (c) Flower17. (d) Flower102. (e) ProteinFold. (f) NonPlant. (g) Caltech102-5. (h) Caltech102-10. (i) Caltech102-15. (j) Caltech102-20. (k) Caltech102-25. (l) Caltech102-30.

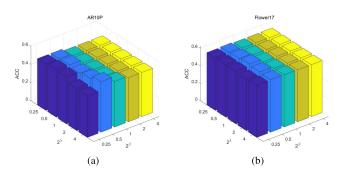


Fig. 7. Sensitivity of the proposed method with the variation of λ and β on benchmark datasets. (a) AR10P. (b) Flower17.

to a high value and generally maintains it up to slight variation with values of two hypermeters. However, it still outperforms the second-best algorithm in most of the benchmarks.

V. CONCLUSION

In this article, we propose a novel MKC method termed LFMKC-PGR which simultaneously optimize kernel base partitions and graph refinement. The kernel base partitions can be refined by the proposed proxy graph and negotiated with each other. Extensive experiments are conducted on 12 multikernel benchmark datasets, demonstrating the effectiveness of our proposed algorithm. In the future, we will consider how to

preserve multi-view local information in the kernel partition space and further improve clustering performance.

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