Multiple Kernel $k$-means Clustering using Min-Max Optimization with $l_2$ Regularization

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Abstract

As various types of biomedical data become available, multiple kernel learning approaches have been proposed to incorporate abundant yet diverse information collected from multiple sources (or views) to facilitate disease prediction and pattern recognition. Although supervised multiple kernel learning has been extensively studied, until recently, only a few unsupervised approaches have been proposed. Moreover, the existing unsupervised approaches are unable to effectively utilize useful and complementary information especially when signals in some views are weak. We propose a novel multiple kernel $k$-means clustering method which aims to effectively use complementary information from multiple views to identify clusters. It is achieved by optimizing the unsupervised problem using a min$_H$-max$_\theta$ formulation, such that more weights can be assigned to views having weak signal for cluster identification. Moreover, our method avoids dismissing views with informative but weak signals by imposing $l_2$ constraint. Additionally, it allows to distill biological prior knowledge on the clustering by imposing a linear constraint on the kernel coefficients. To evaluate our method, we compare it with seven other clustering approaches on simulated multiview data. The simulation results show that our method outperforms existing clustering approaches especially when there is noise and redundancy in the data.

Availability: R package is available at https://github.com/SeojinBang/MKKC.

1 Introduction

With the advent of various genome-wide technologies, biological samples obtained from patients with complex human diseases are now analyzed in numerous ways. Abnormalities in clinical characteristics, DNA copy numbers, gene expression levels, and epigenomic profiles can be measured and they can provide novel insights into understanding the mechanisms underlying complex diseases. In recent years, an increasing number of machine learning approaches has been developed to help clinicians better diagnose diseases, predict disease outcomes and identify new disease subtypes using supervised and unsupervised learning. However, how to integrate and use abundant yet diverse biological data from different sources remains challenging.

Difficulties for combining different types of data include: (i) data from different sources (or called views) have different statistical properties, and (ii) data from a view with a large number of features

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may dominate those from other views with much smaller number of features (Zhao et al., 2017). As such, a naive approach which simply combines all the data from different sources in a single view, then applies supervised methods such as support vector machines or unsupervised methods such as k-means clustering can lead to biased results.

To overcome the limitations of the single-view approach, Pavlidis et al. (2002) first proposed a multiview learning approach which incorporates different views including DNA microarray expression and phylogenetic profiles into a gene functional classification model. Since then, many multiview learning methods have been developed. In multiview settings, each view is composed of a group of features/variables either measured from the same source of data or sharing similar characteristics. By carefully concatenating different views, diverse characteristics of these views are combined to learn a model. As such, multiview learning approaches can be used to extract useful information from heterogeneous biomedical data sets such as DNA copy number, mRNA gene expression, and DNA methylation profiling data by integrating them in a single learning process (Lin and Lane, 2017).

1.1 Supervised multiple kernel learning

With the advance in the kernel-based methods such as kernel SVMs (Schölkopf, 1997; Schölkopf et al., 1999; Mika et al., 1999) and kernel PCA (Schölkopf et al., 1998), kernel-based learning has demonstrated advantages over traditional linear methods. It projects data points in the input space to a high-dimensional feature space via a nonlinear mapping; hence, different classes of the data points can be separated by linear discriminant boundaries in the feature space (Schölkopf, 1997; Schölkopf et al., 1999). To take advantage of the kernel techniques, Lanckriet et al. (2004) first developed a multiple kernel learning (MKL) approach. Since then, MKL methods have witnessed successes in various domains such as computer vision (Gehler and Nowozin, 2009; Bucak et al., 2014; Joutou and Yanai, 2009) and document classification (Lanckriet et al., 2004; Xu et al., 2007).

MKL is a type of multiview learning approach that calculates similarity of data points with different kernel functions for different types of data (views). The kernel matrices are combined in a single learning process for prediction or pattern recognition. The combined kernel $K_\theta$ is usually a linear combination of the multiple kernels weighted by non-negative coefficients $\theta$. The non-negative coefficients guarantee $K_\theta$ to be a positive semidefinite matrix which ensures inner products of the feature map to be defined in the Hilbert space (Lanckriet et al., 2004; Kloft et al., 2011). By restricting the parameters to be non-negative with at least one parameter be positive, it precludes the positive semidefinite constraint on $K_\theta$ so that the computational burden of the optimization problem is reduced to those of a quadratically constrained programming (Weinberger et al., 2004). In order to deal with heterogeneous data obtained from irrelevant sources and select informative sources, a few MKL methods seeking sparse solutions of the kernel coefficients were developed (Lanckriet et al., 2004). In particular, a MKL method with $l_1$ constraint imposed on the kernel coefficients was proposed to encourage sparsity of views and to devise faster and efficient optimization strategies (Lanckriet et al., 2004). Rakotomamonjy et al. (2007) proposed to use an adaptive 2-norm formulation with $l_1$ constraint on the kernel coefficients to encourage sparsity. Zien and Ong (2007) extended the MKL problem to a multi-class task using a sparsity-promoting regularizer.

However, these methods favoring sparse solutions of the kernel coefficients $\theta$ may not work well with the biomedical data, since sources of biomedical data are often carefully selected, expensive to generate, and biologically informative to the problems of interest. For example, gene expression microarray data and clinical measurements obtained from a cohort of cancer or asthma subjects take years to recruit and collect; a sparse solution tends to dismiss the sources with relatively weak
signals despite they are biologically relevant, which as a result compromises the quality of learning (Yu et al., 2010; Kloft et al., 2011). In this kind of scenarios, the MKL methods with $l_2$ (Cortes et al., 2009) and $l_p$ (Yu et al., 2010; Kloft et al., 2009, 2011; Cortes et al., 2009) regularization have shown that non-sparse solutions actually increase classification performance, especially when different views carry complementary information.

1.2 Unsupervised multiple kernel learning

While MKL in supervised settings has been extensively studied in recent years, only a few unsupervised MKL approaches have been proposed (Yu et al., 2012; Gönen and Margolin, 2014; Liu et al., 2016). Although details vary, the unsupervised approaches iteratively optimize kernel coefficients $\theta$ and a matrix $H$ containing information about clustering assignment. Optimization of the kernel coefficients $\theta$ differs depending on how they formulate objective functions and corresponding constraints.

In particular, Yu et al. (2012) proposed a multiple kernel $k$-means clustering (MKKC) method which determines the kernel coefficients $\theta$ by maximizing between-cluster distance instead of minimizing within-cluster distance. The $m$ multiple views were combined using a linear combination of $m$ multiple kernels weighted by the kernel coefficients $\theta$. The optimization of $\theta$ was formulated as a semi-infinite programming. In order to capture sample specific characteristics of multiple data sources, Gönen and Margolin (2014) combined the multiple kernels using a linear sum weighted by subject-specific squared kernel coefficients. Liu et al. (2016) suggested a MKKC method using a matrix-induced $l_2$ regularization to avoid redundancy and improve the diversity of the kernels. While multiple views are usually combined as a linear sum of multiple kernels weighted by non-negative coefficients $\theta$. Gönen and Margolin (2014) and Liu et al. (2016) used a linear sum of the multiple kernels weighted by squared coefficients $\theta^2$ to avoid sparsity, and formulated the optimization problem as a form of quadratic programming (QP).

However, all these aforementioned methods have a common limitation — algorithmically, they assign more weights to strong views with a smaller within-cluster distance (or larger between-cluster distance for Yu’s OKKC); as a result, important yet weak views with a larger within-cluster distance (or a smaller between-cluster distance for Yu’s OKKC) are assigned with less or negligible weights. It consequently leads to clustering results heavily influenced by strong views. As such, these methods fail to utilize complementary and useful information provided by the weak views.

1.3 Contribution

To overcome the limitation of the aforementioned methods, we develop a novel unsupervised MKKC using $\min_H \max_\theta$ optimization with $l_2$ regularization. It aims to efficiently and robustly utilize complementary information collected from different sources.

Our method is inspired by MKL methods mainly proposed in the supervised settings. Unlike the aforementioned methods, our method aims to assign larger weights to the views having weak signals for cluster identification; this way, all important and complementary information can be used to detect true clusters. To achieve this, kernel coefficients $\theta$ are optimized in a way to maximize the within-cluster distance and the cluster indexes $H$ are optimized in a way to minimize the maximum within-cluster distance. Further, we employ an $l_2$ constraint on the kernel coefficients $\theta$ to avoid a sparse solution, so that sources with informative yet weak signals will not be dismissed. Also, our method allows biological prior knowledge about importance of the views to be incorporated in the optimization process, by imposing additional linear constraints on the kernel coefficients.

To evaluate clustering performance of our method, we compare it with seven other MKKC
methods using multiview simulation data. In particular, we systematically assess how robustly our method and the competing methods perform when noise and redundancy are present in the multiview simulation data. Our results demonstrate that our MKKC method outperforms all the competing methods. Also, we show that, with min$_H$-max$_g$ optimization with $l_2$ regularization, our method assigns larger weights to weak yet complementary views; by doing so, signals from these views can be effectively used to identify true clusters.

2 Method

2.1 Kernel $k$-means clustering

Multiple kernel $k$-means clustering (MKKC) methods are developed from kernel $k$-means clustering methods (Girolami, 2002). Kernel $k$-means clustering extends $k$-means clustering (MacQueen et al., 1967; Hartigan and Wong, 1979) to nonlinear partitioning with a nonlinear mapping $\phi : \mathbb{R}^p \rightarrow \mathcal{F}$.

The optimization problem of kernel $k$-means is constructed by replacing $x$ in the input space $\mathbb{R}^p$ with the mapped feature $\phi(x)$ in the feature space $\mathcal{F}$:

$$\text{minimize} \quad \sum_{i=1}^{n} \sum_{c=1}^{k} z_{ic} \left| \phi(x_i) - \mu_c \right|^2$$

subject to $\sum_{c=1}^{k} z_{ic} = 1$

where $Z = [z_{ic}]_{n \times k}$ is the (hard) cluster assignment; $\mu_c = \frac{1}{n_c} \sum_{i=1}^{n} z_{ic} \phi(x_i)$ is the cluster center; $n_c = \sum_{i=1}^{n} z_{ic}$ is a size of the cluster $c$; and $n$ is the number of samples. The optimization problem (OPT1) is reformulated as a trace minimization problem (Zha et al., 2002):

$$\text{minimize} \quad \text{tr} \left( K - L^{1/2}Z^TKZL^{1/2} \right)$$

subject to $Z1_k = 1_n$

where $L = \text{diag}[1/n_1, \cdots, 1/n_k]$, and $K = [\phi(x_i) \cdot \phi(x_j)]_{n \times n}$. Let $H = ZL^{1/2}$ represents the normalized (hard) clustering assignment. Unfortunately, the optimization problem (OPT2) is NP-hard (Michael and David, 1979). Therefore, it is replaced by a relaxed version of the problem that eliminates the discrete constraint on $H$ but keeps the orthogonal constraint on $H$:

$$\text{minimize} \quad \text{tr} \left( K - H^T KH \right)$$

subject to $H^T H = I_k$

Now the optimization problem (OPT3) is solved by a well-known result from Fan (1949) (see Theorem S1 for the result). Fan (1949) showed that the optimal $H^*$ is given by $H^* = U_k Q$ where each column of $U_k = [u_1, \cdots, u_k]$ is eigenvectors of the kernel matrix $K$ involved with $k$ largest eigenvalues $\lambda_1 \geq \cdots \geq \lambda_k$ and $Q$ is an arbitrary orthogonal matrix. That is, the $k$ eigenvalues are one of the continuous solutions to the discrete cluster assignment in the optimization problem (OPT2). Therefore, the solution to kernel PCA is a continuous solution to kernel $k$-means clustering (Ding and He, 2004). Now, the hard clustering assignment $Z$ is recovered by performing QR decomposition on $H^*$ (Zha et al., 2002) or by $k$-means clustering on normalized $H^*$ (Ng et al., 2002).
2.2 A general formula of multiple kernel k-means clustering

MKKC extends kernel k-means clustering by combining multiple kernel matrices calculated from each view. Different sources are combined into a kernel $K_\theta$ during the learning process using $\theta = [\theta(1), \ldots, \theta(m)]^T \in \mathcal{R}^m_+$ which is a vector of kernel coefficients of $m$ views. For example, a linear combination $K_\theta = \sum_{v=1}^{m} \theta^{(v)} K^{(v)}$ or $K_\theta = \sum_{v=1}^{m} \theta^{(v)^2} K^{(v)}$ can be used to combine kernels of multiple views. By replacing the single kernel $K$ in (OPT3) with the combined kernel $K_\theta$, following optimization problem is obtained:

$$\min_{H \in \mathcal{R}^{n \times k}} \max_{\theta} \text{tr} \left( K_\theta - H^T K_\theta H \right)$$ (OPT4)

subject to $H^T H = I_k$, $\theta \geq 0$, $f(\theta) \leq 0$.

where $f(\theta) \leq 0$ is an appropriate constraint on $\theta$. In order to solve (OPT4), the kernel coefficients $\theta$ and the orthogonal matrix $H$ are alternately optimized given each other: (a) $H$ is optimized given $\theta$ in the same manner with (OPT3); and (b) $\theta$ is optimized given $H$ by solving following optimization problem:

$$\max_{\theta} \sum_{v=1}^{m} \theta^{(v)} \text{tr} \left( K^{(v)} - H^T K^{(v)} H \right)$$ (OPT5)

subject to $\theta \geq 0$, $f(\theta) \leq 0$.

Note that if there is no constraint $f(\theta) \leq 0$ on (OPT5), the maximization problem with respect to $\theta$ will be unbounded and the minimization problem with respect to $\theta$ will have a trivial, meaningless solution as $\theta = 0$.

2.3 Related works

Several MKKC methods have been proposed based on the general formula (OPT4). In particular, three MKKC methods (listed below) are similar in that, they combine multiple kernels as: $K_\theta = \sum_{v=1}^{m} \theta^{(v)^2} K^{(v)}$, with $l_1$ constraint on the coefficients $\theta$, and optimize the objective function in (OPT4) using the $\min_H$-$\min_\theta$ framework. These clustering methods include:

- Gonen’s Multiple Kernel k-Means Clustering (Gonen’s MKK, Gönen and Margolin 2014)
- Gonen’s Localized Multiple Kernel k-Means Clustering (Gonen’s LMKK, Gönen and Margolin 2014): This method aims to estimate sample-specific kernel coefficients capturing sample-specific characteristic of multiple data sources.
- Liu’s Multiple Kernel k-Means Clustering with Matrix-Induced Regularization (Liu’s MKK-MIR, Liu et al. 2016): Correlation of each pair of kernels is characterized by integrating a matrix-induced quadratic regularization into the objective function.

Another MKKC method combines the multiple kernels in a different way:

- Yu’s Optimized Kernel k-Means Clustering (Yu’s OKKC): Yu et al. 2012 combines multiple views as $K_\theta = \sum_{v=1}^{m} \theta^{(v)} K^{(v)}$ and uses $l_p$ constraint where $p \geq 1$ on $\theta$, and optimize the objective function in (OPT4) using the $\max_H$-$\max_\theta$ framework. However, rather than minimizing $\text{tr} \left( K_\theta - H^T K_\theta H \right)$ as the general formula (OPT4) does, it maximizes the objective function $\text{tr} \left( H^T K_\theta H \right)$. 

Note that if there is no constraint $f(\theta) \leq 0$ on (OPT5), the maximization problem with respect to $\theta$ will be unbounded and the minimization problem with respect to $\theta$ will have a trivial, meaningless solution as $\theta = 0$.
It can be seen that even though the four MKKC methods described above combine kernels in multiple views in slightly different ways. They either use the minH-minθ framework (the first 3 MKKC methods) or maxH-maxθ framework (Yu’s OKKC) to optimize (OPT4), which can lead to solutions which favor assigning more weights (i.e., higher kernel coefficients θ) to strong views and assigning less and often time negligible weights to weaker yet complementary views. As shown in our simulation results, it leads to clustering results depending entirely on the strong views.

2.4 Multiple kernel k-means clustering using minH-maxθ optimization with l2 regularization

In order to overcome the limitation of the aforementioned methods, we propose a novel multiple kernel k-means clustering (MKKC) method that aims to make a good use of all complementary views. In particular, our approach linearly combines m multiple kernels as \( K_θ = \sum_{v=1}^{m} θ^{(v)} K^{(v)} \) where \( θ \geq 0 \). The corresponding feature representation is \( φ_θ(x_i) = [\sqrt{θ^{(1)}} φ^{(1)}(x_i^{(1)}), \cdots, \sqrt{θ^{(m)}} φ^{(m)}(x_i^{(m)})] \).

Note that the linear combination of the kernel matrices using non-negative kernel coefficients \( θ \) with at least one non-zero coefficient ensures that the combined kernel matrix \( K_θ \) is positive semidefinite.

However, unlike the other 4 existing MKKC methods in Section 2.3, we optimize (OPT4) using a minH-maxθ framework. In particular, we use the maximization framework for the optimization problem (OPT5) with respect to \( θ \). By doing so, the MKKC method we propose is able to make good use of the information from views with noisy or redundant information. As such, signals from all informative and complementary views are utilized to discover true clusters, as we demonstrate in the simulation experiments. Furthermore, by adding an l2 constraint on the kernel coefficients, MKL methods which avoid sparse solutions (Yu et al., 2010; Kloft et al., 2009, 2011; Cortes et al., 2009) outperform the other methods imposing sparsity with l1 regularization as often shown in the supervised settings. In light of these results and to take advantage of signals from all views, we employ l2 regularization in our unsupervised MKKC problem. Thus, we define it as a minH-maxθ problem with an l2 constraint to the optimization problem (OPT4).

Also, our method allows a weight tuning based on prior knowledge about importance or reliability of the sources. If it is known in advance some views are more important than other views, it will be beneficial to allow people to hand-tune constraints on weights based on expert knowledge. To provide such flexibility, we additionally allow the weight tuning by imposing a linear constraint on \( θ \). With this constraint, one can readily incorporate biological prior knowledge about the sources in the MKKC learning model.

To summarize, we propose to identify clusters in multiview data using the following optimization problem:

\[
\begin{align*}
\text{minimize} & \quad \text{maximize} \quad \text{tr} \left( K_θ - H^T K_θ H \right) \\
& \quad \text{subject to} \quad H^T H = I_k, \\
& \quad \quad \quad \theta^T θ \leq 1, \theta \geq 0 \\
& \quad \quad \quad A θ \leq b
\end{align*}
\] (OPT6)

where \( A \) and \( b \) are pre-defined constraint matrices based on biological prior knowledge. If no prior knowledge is available, users can choose to set \( A = 0 \) and \( b = 0 \).
3 Algorithm

In order to solve the optimization problem (OPT6), we optimize the vector of kernel coefficients \( \theta \in \mathbb{R}^m \) and the continuous cluster assignment matrix \( H \) alternately given each other: (i) given \( \theta \), \( H \) is optimized in the same manner as (OPT3), and (ii) given \( H \), \( \theta \) is optimized by solving a quadratically constrained linear programming (QCLP) problem. We keep updating \( \theta \) and \( H \) until a stopping criterion is met.

3.1 Estimation of \( \theta \)

For fixed \( H \), we optimize (OPT6) with respect to \( \theta \). It is reformulated as a quadratic constraint linear programming (QCLP):

\[
\begin{align*}
\text{maximize} & \quad \sum_{v=1}^m \theta^{(v)} \text{tr} \left( K^{(v)} - H^T K^{(v)} H \right) \\
\text{subject to} & \quad \frac{1}{2} \theta^T Q_m \theta \leq 1, \theta \geq 0 \\
& \quad A \theta \leq b 
\end{align*}
\]

where \( Q_m = \text{diag}[2, \cdots, 2] \). Since \( Q_m \) is a diagonal matrix, the optimization problem (OPT7) is separable. Hence, the entire problem can be solved as a conic quadratic program (CQP or a second order cone program, SOCP). Even though we can solve the problem using QCLP, the conic formulation usually performs better and is based on more solid duality theory (Andersen, 2016). Thus, we translate (OPT7) by introducing a new variable \( p \) by:

\[
\begin{align*}
\text{maximize} & \quad c^T \theta \\
\text{subject to} & \quad [p, \theta]^T \in K^q, p = 1, \\
& \quad 0 \leq \text{I}_m \theta \\
& \quad A \theta \leq b
\end{align*}
\]

where \( c^T = [\text{tr} \left( K^{(1)} - H^T K^{(1)} H \right), \cdots, \text{tr} \left( K^{(m)} - H^T K^{(m)} H \right)] \) and \( K^q = \left\{ p \geq \sqrt{\sum_{v=1}^m \theta^{(v)}^2} \right\} \). Now, the CQP is analytically solved by existing software such as mosek (MOSEK ApS, 2017).

3.2 Estimation of \( H \)

For fixed \( \theta \), we optimize (OPT6) with respect to \( H \) where \( H \) is a continuous relaxation of the discrete cluster assignment \( ZL^{1/2} \). The problem is reduced to a simple kernel \( k \)-means clustering problem (OPT3) in which the optimal solution is obtained as \( H^* = U_k Q \) where the column of \( U_k \) contains eigenvectors of \( K \) corresponding to \( k \) largest eigenvalues, and \( Q \) is an arbitrary orthogonal matrix. Hence, any spectral clustering methods can be directly applied to restore the binary clustering assignment matrix \( Z \) from the continuous clustering assignment matrix \( H^* \). Here, we use a spectral clustering method proposed by Ng et al. (2002) to restore the binary assignment \( Z \). It normalizes \( H^* \) to make all rows of \( H^* \) to be on the unit sphere as is the binary matrix \( Z \), then performs \( k \)-means clustering on the normalized \( H^* \) to recover the clusters.
3.3 Centering and scaling

Instead of centering directly on the mapping function, the combined mapping function $\phi_\theta(x_i)$ is centered by $K_\theta \leftarrow K_\theta - J_n K_\theta - K_\theta J_n$ where $J_n = 1_n 1_n^T/n$ (Schölkopf et al. 1998). We suggest a following proposition to avoid centering $K_\theta$ at every iteration (see Proposition S1 for proof). Using this proposition, we center $K(v)$ for each view at the beginning of the algorithm instead of centering the combined kernel matrix $K_\theta$ at every iterations.

**Proposition 1.** Let $\tilde{K}_\theta = \sum_{v=1}^{m} \theta^{(v)} K^{(v)}$ where $\tilde{K}^{(v)} = K^{(v)} - J_n K^{(v)} - K^{(v)} J_n + J_n K^{(v)} J_n$ for $v = 1, \cdots, m$. Then $\tilde{K}_\theta = K_\theta$ where $K_\theta = K_\theta - J_n K_\theta - K_\theta J_n + J_n K_\theta J_n$ for any $\theta \in \mathbb{R}^m$.

It is known that estimation of kernel coefficients depends on how the kernel matrices are scaled (Kloft et al. 2011; Ong and Zien 2008). Therefore, scaling of kernel matrices in multiview setting is important for the views comparable to each other. We suggest to scale the kernel matrix for each view $v$ before combining them so that $K^{(v)} \leftarrow K^{(v)}/\text{tr}(K^{(v)})$ where $\text{tr}(K^{(v)}) = \sum_{i=1}^{n} \lambda_i^{(v)}$. By scaling the kernel matrix, we achieves $\text{tr}(K^{(1)}) = \cdots = \text{tr}(K^{(m)}) = 1$ which means each the total variance explained by principal components of the feature space is set to be uniform.

3.4 Discussion of our method

The trace of the centered matrix $\text{tr}(K)$ represents the total variance explained by the feature space, and $\text{tr}(H^{\ast T}KH^{\ast})$ represents the variance explained by principal components of the feature space associated with the $k$ largest eigenvalues where $H^{\ast}$ is the optimal solution of (OPT6). Therefore, $\text{tr}(K) - \text{tr}(H^{\ast T}KH^{\ast})$ is interpreted as the un-explained variance that is not explained by the $k$ principal components, which is also equivalent to $\sum_{i=k+1}^{n} \lambda_i$ (Fan 1949). To support this point, we prove that $\text{tr}(H^{\ast T}KH^{\ast})$ and $\text{tr}(K) - \text{tr}(H^{\ast T}KH^{\ast})$ are always non-negative, consistent with the fact that variances are always non-negative values (see Propositions S2 and S3 for proof). A similar interpretation is applied to the trace formulation $\text{tr}(K^{(v)}) - \text{tr}(H^{\ast T}\tilde{K}^{(v)}H^{\ast})$ for each view $v$.

The optimization problem (OPT7) requires the trace of the weighted combination of the kernels to be maximized. Therefore, as it has a larger un-explained variance, a larger weight $\theta^{(v)}$ will be assigned to a view $v$. After combining the kernels for multiple views, our method minimizes un-explained total variance in the combined view by optimizing the continuous cluster assignment matrix $H$. By doing so, intuitively, our method puts more weights on views having weak signal for cluster information so that we can utilize complementary information collected from all the views to identify clusters. In the simulation experiments, we will show that small weights for strong views are sufficient to extract cluster information from multiview data. Our results demonstrate that our method achieves better clustering performance than other competing methods designed to assign more weights to strong views, largely because the latter methods tend to assign negligible weights to the weak views and thus lead to biased results.

4 Simulation experiments

In order to evaluate our method, we compared the clustering performance of our method with seven existing MKKC methods using simulation data sets. Moreover, to assess how robust each method performs when noise and redundant information are present in the multiview data, we added varying numbers of noise and redundant variables to the simulated data. All simulated data sets were designed to have three clusters, each of which contains 100 samples, hence there are 300 samples in total for all simulated data sets.
4.1 Multiview Scenarios

In order to evaluate our method, we consider three multiview scenarios, A–C, which have increasing levels of difficulty to recover all 3 clusters of samples. The heatmaps illustrating the simulated data in these scenarios can be found in Figure S1. In Scenario A, the simulated data sets are composed of two views: while View 1 is a ‘complete’ view which can be used to separate all 3 clusters, View 2 is a ‘partial’ view which can only distinguish Cluster 1 from Clusters 2 & 3, but unable to separate Clusters 2 & 3. To make the problem more challenging, we added different levels of noise and/or redundant variables to this data. Noise variables are independently generated from Gaussian distribution with zero-mean and unit-variance. The noise level is increased by adding more noise variables ($N_{\text{noise}} = 1, 2, \ldots, 10$) to View 1. The redundancy is increased by adding more pairs of redundant variables to View 1 ($N_{\text{redundPairs}} = 1, 2, \ldots, 5$) with different correlation levels ($\text{cor} = 0.45, 0.72, 0.90, 0.97, 1.00$) between the redundant variables and the original pair of the same variables. In Scenario B, both views are partial views. Neither View 1 nor View 2 alone contains sufficient information to recover all 3 clusters; however, when combined, they provide sufficient and complementary information which allows a ‘good’ MKKC method to recover all 3 clusters. Moreover, different levels of noise and/or redundant variables (as described in Scenario A) are added to the data in this scenario. Furthermore, to test how well our method performs when one of the views contains only noise variables (without any useful information needed to distinguish all 3 clusters), we generated the simulated data in Scenario C by adding an additional ‘noise’ view (View 3) to the data in Scenario B. To summarize, we have 36 simulated data sets for each scenario, and a total number of $3 \times 36$ simulation data sets are used to evaluate our method and compare with the existing approaches.

4.2 Compared methods

We compared our method with seven multiple kernel clustering algorithms: two baseline methods, one variant of our method, and four recently proposed MKKC methods. The baseline methods include (i) **Single Best** which chooses and clusters using the single best view that minimizes the kernel $k$-means objective function in (OPT3); and (ii) **Uniform Weight** which equally assigns all the kernel coefficients $\theta$ to $1/m$ where $m$ is the number of views which takes the combined kernel $K_\theta = \sum_{v=1}^{m} K^{(v)}/m$ as an input $K$ in (OPT3). We also compared our method with a method **MinMax-MinC** which uses the same min$_{\theta}$-max$_{\theta}$ formulation in (OPT6) as our approach does, but with $l_1$ instead of $l_2$ constraint on $\theta$. Additionally, a MinMax-MinC uses $\theta \geq \theta_{\text{min}}$ where $\theta_{\text{min}} = 0.5/m1$ to avoid a sparse solution.

The four MKKC methods we compared with our method were developed and extended from the general formula of MKKC (OPT4) as described in Section 2.3. For **Gonen’s MKK** and **LMKK**, we used a R code publicly available on GitHub [https://github.com/mehmetgonen/lmkkmeans](https://github.com/mehmetgonen/lmkkmeans). For **Liu’s MKK-MIR**, a regularization parameter $\lambda$ was set to 1 and the quadratic coefficient matrix $M$ was defined as suggested in the paper. For **Yu’s OKKC**, the original algorithm iteratively optimizes the kernel coefficients $\theta$ and discrete clustering assignment, which increases computational burden and costs more time. For a fair comparison, we updated the continuous cluster assignment $H$ instead of retaining the discrete assignment at every iteration, and optimized it as QCLP, as proposed by all the other MKKC methods including ours.

4.3 Experimental details

Before processing the data with kernels, all features were standardized so that they are centered around zero with standard deviations of one. The combined kernel matrix $K_\theta$ was centered
Methods

Our Method
Single Best
Uniform Weight
MinMax−MinC
Yu’s OKKC
Liu’s MKK−MIR
Gonen’s MKK
Gonen’s LMKK

Figure 1: Clustering performances of the compared methods. The adjRI values are plotted against the number of the added noise variables in the simulated scenarios (A) A-1, (B) B-1, and (C) C-1, or against the number of the added pairs of redundant variables (correlated with the original pairs with $cor = 0.90$) in the scenarios (D) A-2, (E) B-2, and (F) C-2.

and scaled as we suggested in Section 3.3. A Radial Basis Function (RBF) kernel $k(x, y) = \exp(-0.5||x - y||^2)$ was used for all the views. After obtaining continuous clustering indicator $H^*$, we performed $k$-means clustering on the normalized $H^*$ with 1000 random starts and reported the best result minimizing the objective function. We stopped the iteration if the stopping criteria $||\theta_t - \theta_{t-1}||_2 < 10^{-4}$ is met within maximum iteration 500. We used three metrics for evaluating clustering performance of the compared methods: Adjusted Rand Index (AdjRI, Hubert and Arabie 1985), Normalized Mutual Information (NormMI, Strehl and Ghosh 2002), and Purity (Manning et al., 2008). Note that a higher value of the metrics indicates a better clustering performance.

For comparison purposes, we defined the weight as $\theta / \theta^T 1$ for the methods combining kernels using $K_\theta = \sum_{v=1}^m \theta^{(v)} K^{(v)}$ (such as Uniform Weight, MinMax-MinC, Yu’s OKKC, and our method) and as $\theta^2 / \theta^T 1$ for the methods using $K_\theta = \sum_{v=1}^m \theta^{(v)} 2 K^{(v)}$ (such as Liu’s MIR, Gonen’s MKK and LMKK).

4.4 Simulation results

We evaluated our method and compared with other methods using all 3 clustering evaluation measures: AdjRI, NormMI, and Purity. Our approach achieves the best performance in most of the scenarios. The performances of the methods in different scenarios are shown in Figures 1 & 2. The clustering results for all the compared methods on the simulated data sets in Scenarios A–C as assessed by all three measures adjRI, normMI and purity are summarized in Table S1–S6.
Figure 2: Clustering results generated by different MKKC methods for Scenarios A-1 and B-2. The heatmaps at the top panel of each subfigure illustrate the two-view data for Scenarios (A) A-1 where $N_{\text{noise}} = 3$, and (B) B-2 where $N_{\text{redundantPairs}} = 3$ and $\text{cor} = 0.7$. The rows and columns in the heatmap represent variables and samples, respectively. The tile plots at the bottom panel of each subfigure illustrate the clustering results generated by different MKKC methods. All 3 clusters are labeled in black, light blue and red, respectively. The first tile plot shows the ground truth; the second to the last plots show results for the compared methods.

they all show similar trends.

**Scenario A-1 (with noise added to Scenario A):** This scenario contains a complete view (View 1) and a partial view (View 2). To test the effect of noise on different methods, we added varying levels of noise to the complete view. Figure 1A illustrates the results showing how adjRIs for the compared methods change as noise variables are added to View 1.

In particular, when there is no noise in the view, almost all methods perform perfectly well except for the Single Best. As the noise variables are added to the complete view, our method (Figure 1A) performs as well as when there is no noise in the view up to the third noise. To understand further how different methods work algorithmically, we examined the weights each method assigns to the views. As seen in Figure S2A, our method gradually puts more weight on the complete view (View 1) as it is weakened by the noise variables, consistent with the $\min_{\mathbf{H}} \max_{\mathbf{G}} \theta$ optimization framework in (OPT6). In contrast to our methods, the performances of the four existing MKKC methods (Yu’s OKKC, Liu’s MKK-MIR, Gonen’s MKK and LMKK) sharply decline to the similar levels as those of the Single Best (Figure 1A), which are even worse than Uniform Weight.

Figure 2A illustrates how each method performs when three noise variables are added to the complete view. Our result is well matched with the ground truth, whereas the other MKKC methods cannot distinguish the first two clusters (shown in Figure 2A) indicating that they identify the
clusters mainly based on the view with stronger signal (View 2, the partial view) as the Single Best does. This speculation is confirmed when we examined the weights assigned to the views by different methods. As shown in Figure S2A, the four MKKC methods put less weight on the complete view as its signal is weakened by the noise variables, while putting more weights on the partial view, which as a result leads to inferior results.

Note that as a variant of our method, MinMax-MinC was also designed to put more weights on weak views due to its \( \min H - \max \theta \) optimization framework. However, even though MinMax-MinC puts more weight on the weakened complete view (Figure S2A), the method performs much worse than our method in existence of a larger number of the noise variables (Figures 1A & 2A). This is probably due to the following reason: since the weight assigned to any view cannot be smaller than a heuristically set minimum threshold, the weight of any single view cannot be set large enough to extract sufficient information from the view.

**Scenario A-2 (with redundancy added to Scenario A):** To evaluate the effect of redundant variables on our method and the competing methods, we added pairs of redundant variables to the complete view (View 1) in Scenario A. Figure 1D shows how adjRIs for different methods change as the redundant pairs correlated with the original variables (\( \text{cor} = 0.90 \)) are added to View 1.

In general, the effect of redundancy on our method and the other MKKC methods is similar to that of noise shown in Scenario A-1. Overall, our method outperforms all other methods even when the five redundant pairs are added to the data (Figure 1D). Similar to Scenario A-1, our method gradually puts more weight (from 64.78% to 81.30% as the number of the added redundant pairs are increased from 1 to 5) on the complete view when the signal of this view becomes weakened by the redundant variables (Figure S3A). On the other hand, the four MKKC methods (Yu’s OKKC, Liu’s MKK-MIR, Gonen’s MKK and LMKK) fail to perform well; they show similar inferior performances as that of the Single Best (Figure 1D). In particular, Gonen’s MKK and LMKK are very sensitive to the redundancy in the data; Figure S3A shows that the weight on View 1 assigned by these methods sharply decreases to less than 3% even when only one redundant pair is added, hence the signal in this view is again barely used to identify the true clusters.

When we varied the correlation level of the redundant variables (\( \text{cor} = 0.45, 0.72, 0.90, 0.97, 1.00 \)) added to the complete view, we observe similar performance trends for the selected methods (see Table S4).

**Scenario B** aims to show how our method uses the complement information in two views when neither of the views alone contains sufficient information to recover all three clusters. As shown in Figure 1B & 1E, our method outperforms all other methods without or with noise/redundancy added to Scenario B, whereas the clustering performances of the four competing MKKC methods are even worse than the baseline methods. MinMax-MinC performs slightly better than the four existing MKKC methods but is still worse than our method.

Figure 2B illustrates the clustering results for Scenario B-2 where three pairs of redundant variables are added to View 1. The clustering results generated by our method match well with the ground truth, indicating that our method effectively utilizes complementary information from both the views. However, the competing MKKC methods cannot distinguish two of the three clusters (shown in light blue and red), suggesting that they identify the clusters mainly based on the uncompromised view (View 2) as Single Best does. As shown in Figure S3B, our method puts more weight (63.08%–80.26%) on the compromised view (View 1), which as a result allows the signal (albeit weak) in this view to be extracted. This result suggests that while a small weight is sufficient to extract useful information from a strong view, a relatively large weight is needed to get useful signals from a weak view.

**Scenario C** aims to investigate further whether our method can robustly use complement information from multiple views even when a view contains noise variables only. We generated a
three-view data in Scenario C by adding a ‘noise’ view to the two-view data in Scenario B.

As seen in Figure 1C & 1F, our method outperforms all the other methods in most of the conditions in Scenario C. Notably, as shown in Figure S2C & S3C, our method puts more weight not only on View 1, but also on the ‘noise’ view (View 3) when an increasing number of the noise or redundant variables are added to View 1. Interestingly, however, the \( l_2 \) norm in (OPT6) ensures that View 2 gets a sufficient amount of weight (14.66%–18.05% for Scenario C-1, and 14.80%–17.66% for Scenario C-2), and hence View 3 is not assigned too much weight (40.74%–59.16% for Scenario C-1, and 41.10%–51.90% for Scenario C-2). Moreover, as more noise variables and redundant pairs are added to View 1, our method raises the weight on View 1 but reduces the weight on the ‘noise’ view (View 3), while keeping the weight on View 2 stable; by doing so, our method is able to extract the weakened signal from View 1 instead of View 3, without losing the signal extracted from View 2. Since the signal from View 3 is much weaker than those from Views 1 and 2, our result is not significantly contaminated by the ‘noise’ view.

Note that MinMax-MinC performs better than the four existing MKKC methods. However, it puts too much weight on View 3 (66.67% for both Scenario C-1 & C-2), and too small weight on View 1 (16.67% for both Scenario C-1 & C-2), possibly due to its ineffective way to estimate weights for the views (i.e., using a minimum constraint to estimate the weights). As a result, MinMax-MinC performs much worse than our method.

Gonen’s MKK and LMKK are successful in dismissing the ‘noise’ view (View 3) by assigning almost zero weight (0.89%–1.86%) on View 3. However, they fail to recover the true clusters because they also assign almost zero weight (0.95%–2.12%) on View 1, while putting most of the weight (96.02%–98.10%) on View 2. As a result, the signal in View 1 is barely used to identify the true clusters, and the clusters are identified almost entirely based on View 2. We observe similar results for Yu’s OKKC and Liu’s MKK-MIR (see Table S3 & S6).

### 5 Conclusion

In this paper, we propose a novel multiple kernel \( k \)-means clustering (MKKC) method which combines multiple views using a linear combination of multiple kernels obtained from different views and identifies clusters using a \( \min_{H} \max_{\theta} \) optimization framework with \( l_2 \) regularization. Our method provides robust estimation of kernel coefficients in existence of noise and redundancy, and flexibly optimizes the kernel coefficients by allowing the weight tuning based on biological prior knowledge.

The \( \min_{H} \max_{\theta} \) framework allows our method to put more weights on weak views; as such, our method aims to identify clusters by taking advantage of useful and complementary signals from views even with noisy and redundant information. By imposing an \( l_2 \) constraint on the kernel coefficients \( \theta \), our method avoids sparse solutions that may dismiss sources which are valuable but having weak signals. Additionally, a linear constraint is imposed on the kernel coefficients to distill biological prior knowledge in the optimization problem.

We systematically evaluated our method and seven competing methods using simulation data. The simulation experiments were designed to assess how well different MKKC approaches utilize complementary information in multiple views and how robustly they perform under the influence of noise and redundancy in the data. The simulation results show that our method outperforms the competing MKKC approaches especially when the noise and redundancy are present in the multiview data, while the performances of the other MKKC methods sharply decrease with a few added noise or redundant variables.
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Supplementary Materials

Theorem S1. (Fan, 1949) Let $K$ is a symmetric matrix where $u_1, \cdots, u_n$ are eigenvectors corresponding to eigenvalues $\lambda_1 \geq \cdots \geq \lambda_n$ of $K$. Then, the optimal solution of the problem

$$ \arg\max_{H \in \mathbb{R}^{n \times k}} tr(H^T KH) \quad \text{subject to } H^T H = I_k $$

is given by $H^* = U_k Q$ where $U_k = [u_1, \cdots, u_k]$ and $Q$ is an arbitrary $k \times k$ orthogonal matrix, and the maximum is given by

$$ \max_{H \in \mathbb{R}^{n \times k}} tr(H^T KH) = tr(H^*^T KH^*) = \sum_{i=1}^{k} \lambda_i $$
Proposition S1. Let \( \tilde{K}_\theta^* = \sum_{v=1}^{m} \theta(v) \tilde{K}^{(v)} \) where \( \tilde{K}^{(v)} = K^{(v)} - J_n K^{(v)} J_n + J_n K^{(v)} J_n \) for \( v = 1, \cdots, m \). Then \( \tilde{K}_\theta^* = \tilde{K}_\theta \) where \( \tilde{K}_\theta = K_\theta - J_n K_\theta J_n + J_n K_\theta J_n \) for any \( \theta \in \mathcal{R}^m \).

Proof.

\[
\tilde{K}_\theta^* = \sum_{v=1}^{m} \theta(v) \tilde{K}^{(v)} \\
= \sum_{v=1}^{m} \theta(v) \left( K^{(v)} - J_n K^{(v)} J_n + J_n K^{(v)} J_n \right) \\
= \sum_{v=1}^{m} \theta(v) K^{(v)} - \sum_{v=1}^{m} \theta(v) J_n K^{(v)} - \sum_{v=1}^{m} \theta(v) K^{(v)} J_n + \sum_{v=1}^{m} \theta(v) J_n K^{(v)} J_n \\
= K_\theta - J_n \left( \sum_{v=1}^{m} \theta(v) K^{(v)} \right) - J_n \left( \sum_{v=1}^{m} \theta(v) K^{(v)} \right) J_n + J_n \left( \sum_{v=1}^{m} \theta(v) K^{(v)} \right) J_n \\
= K_\theta - J_n K_\theta - K_\theta J_n + J_n K_\theta J_n \\
= \tilde{K}_\theta
\]

\(\square\)
Proposition S2. If $K^{(v)}$ is a $n \times n$ positive semidefinite matrix, $\text{tr}(H^T K^{(v)} H)$ is non-negative for any $n \times k$ real valued matrix $H$.

Proof.

A positive semidefinite matrix $K^{(v)}$ satisfies $h^T K^{(v)} h \geq 0$ for every real valued column vector $h$. Let $h_1, \cdots, h_k$ are column vectors of $H$, then $h_i^T K^{(v)} h_i \geq 0$ for $i = 1, \cdots, k$. Therefore, $\text{tr}(H^T K^{(v)} H) = \sum_{i=1}^k h_i^T K^{(v)} h_i \geq 0$ for any $n \times k$ real valued matrix $H$. \hfill $\square$

Proposition S3. If $K^{(v)}$ is a $n \times n$ positive semidefinite matrix, $\text{tr}(K^{(v)} - H^T K^{(v)} H)$ is non-negative for any real valued $n \times k$ matrix $H$ such that $H^T H = I_k$.

Proof.

From Theorem $[S1]$

$$\min_{H \in \mathbb{R}^{n \times k}, H^T H = I_k} \text{tr}(K^{(v)} - H^T K^{(v)} H) = \text{tr}(K^{(v)}) - \max_{H \in \mathbb{R}^{n \times k}, H^T H = I_k} \text{tr}(H^T K^{(v)} H)$$

$$= \sum_{i=1}^n \lambda_i - \sum_{i=1}^k \lambda_i$$

$$= \sum_{i=k+1}^n \lambda_i$$

Since $K^{(v)}$ is positive semidefinite, all its eigenvalues are non-negative. Therefore,

$$\min_{H \in \mathbb{R}^{n \times k}, H^T H = I_k} \text{tr}(K^{(v)} - H^T K^{(v)} H) = \sum_{i=k+1}^n \lambda_i \geq 0$$

Finally, for any real valued $n \times k$ matrix $H$ such that $H^T H = I_k$,

$$\text{tr}(K^{(v)} - H^T K^{(v)} H) \geq \min_{H \in \mathbb{R}^{n \times k}, H^T H = I_k} \text{tr}(K^{(v)} - H^T K^{(v)} H) \geq 0$$

$\square$
Figure S1: **Multi-view Scenarios.** (A) Scenario A is composed of a complete view and a partial view. (B) Scenario B is composed of two partial views. (C) Scenario C is composed of two partial views and a ‘noise’ view. In our simulation experiments, we modified each scenario by (1) adding numbers of noise variables ($N_{\text{noise}} = 1, 2, \cdots$), or (2) adding numbers of redundant pairs to the first view ($N_{\text{redunPairs}} = 1, 2, \cdots$) as well as increasing correlation level between the first pair and the redundant pairs ($\text{cor} = 0.45, 0.72, 0.90, 0.97, 1$). Each of the noise variables are independently sampled from Gaussian distribution with zero-mean and unit-variance. The samples in the heatmaps are ordered by their true cluster index.
Figure S2: Weights given by the compared methods to the views when Scenarios A-1, B-1, and C-1 were used to identify clusters. The weights on the views are plotted against the number of the noise variables $N_{\text{noise}}$ added to the first view in each scenario. The x-axis represents the number of noise variables added to the first view. The y-axis represents the relative weight given by the compared methods. The methods are identified by different colors.
(A) Scenario A-2

Figure S3: Weights given by the compared methods to the views when Scenario A-2, B-2, and C-2 were used to identify clusters. The weights on the views are plotted against the number of the pairs of the redundant variables $N_{\text{redundPairs}}$ where $\text{cor} = 0.90$ added to the first view in each scenario. The x-axis represents the number of noise variables added to the first view. The y-axis represents the relative weight given by the compared methods. The methods are identified by different colors.
Table S1: Evaluation of the Clustering Methods on Scenario A-1

| Scenario A-1 | N_{\text{noise}} | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|--------------|------------------|---|---|---|---|---|---|---|---|---|---|----|
|              | adjRI            | 0.497 | 0.497 | 0.497 | 0.497 | 0.497 | 0.497 | 0.497 | 0.497 | 0.497 | 0.497 | 0.497 |
|              | normMI           | 0.837 | 0.837 | 0.837 | 0.837 | 0.837 | 0.837 | 0.837 | 0.837 | 0.837 | 0.837 | 0.837 |
|              | purity           | 0.680 | 0.680 | 0.680 | 0.680 | 0.680 | 0.680 | 0.680 | 0.680 | 0.680 | 0.680 | 0.680 |
| Single Best  | adjRI            | 1.000 | 1.000 | 0.795 | 0.522 | 0.502 | 0.500 | 0.499 | 0.499 | 0.497 | 0.498 | 0.497 |
|              | normMI           | 1.443 | 1.443 | 1.137 | 0.858 | 0.840 | 0.839 | 0.838 | 0.838 | 0.837 | 0.837 | 0.837 |
|              | purity           | 1.000 | 1.000 | 0.923 | 0.740 | 0.700 | 0.693 | 0.687 | 0.687 | 0.687 | 0.680 | 0.680 |
| Uniform Weight | adjRI            | 1.000 | 1.000 | 0.923 | 0.740 | 0.700 | 0.693 | 0.687 | 0.687 | 0.687 | 0.680 | 0.680 |
|              | normMI           | 1.443 | 1.443 | 1.137 | 0.858 | 0.840 | 0.839 | 0.838 | 0.838 | 0.837 | 0.837 | 0.837 |
|              | purity           | 1.000 | 1.000 | 0.923 | 0.740 | 0.700 | 0.693 | 0.687 | 0.687 | 0.687 | 0.680 | 0.680 |
| MinMax MinC  | adjRI            | 1.000 | 1.000 | 0.795 | 0.522 | 0.502 | 0.500 | 0.499 | 0.499 | 0.497 | 0.498 | 0.497 |
|              | normMI           | 1.443 | 1.443 | 1.137 | 0.858 | 0.840 | 0.839 | 0.838 | 0.838 | 0.837 | 0.837 | 0.837 |
|              | purity           | 1.000 | 1.000 | 0.923 | 0.740 | 0.700 | 0.693 | 0.687 | 0.687 | 0.687 | 0.680 | 0.680 |
| Yu's OKKC    | adjRI            | 1.000 | 1.000 | 0.795 | 0.522 | 0.502 | 0.500 | 0.499 | 0.499 | 0.497 | 0.498 | 0.497 |
|              | normMI           | 1.443 | 1.443 | 1.137 | 0.858 | 0.840 | 0.839 | 0.838 | 0.838 | 0.837 | 0.837 | 0.837 |
|              | purity           | 1.000 | 1.000 | 0.923 | 0.740 | 0.700 | 0.693 | 0.687 | 0.687 | 0.687 | 0.680 | 0.680 |
| Liu's MKK-MIR| adjRI            | 1.000 | 1.000 | 0.795 | 0.522 | 0.502 | 0.500 | 0.499 | 0.499 | 0.497 | 0.498 | 0.497 |
|              | normMI           | 1.443 | 1.443 | 1.137 | 0.858 | 0.840 | 0.839 | 0.838 | 0.838 | 0.837 | 0.837 | 0.837 |
|              | purity           | 1.000 | 1.000 | 0.923 | 0.740 | 0.700 | 0.693 | 0.687 | 0.687 | 0.687 | 0.680 | 0.680 |
| Gonen's MKK  | adjRI            | 1.000 | 1.000 | 0.795 | 0.522 | 0.502 | 0.500 | 0.499 | 0.499 | 0.497 | 0.498 | 0.497 |
|              | normMI           | 1.443 | 1.443 | 1.137 | 0.858 | 0.840 | 0.839 | 0.838 | 0.838 | 0.837 | 0.837 | 0.837 |
|              | purity           | 1.000 | 1.000 | 0.923 | 0.740 | 0.700 | 0.693 | 0.687 | 0.687 | 0.687 | 0.680 | 0.680 |
| Gonen's LMKK | adjRI            | 0.980 | 0.948 | 0.948 | 0.948 | 0.948 | 0.948 | 0.948 | 0.948 | 0.948 | 0.948 | 0.948 |
|              | normMI           | 1.400 | 0.837 | 0.837 | 0.837 | 0.837 | 0.837 | 0.837 | 0.837 | 0.837 | 0.837 | 0.837 |
|              | purity           | 0.993 | 0.683 | 0.683 | 0.683 | 0.683 | 0.683 | 0.683 | 0.683 | 0.683 | 0.683 | 0.683 |
| Our Method   | adjRI            | 1.000 | 1.000 | 1.000 | 0.951 | 0.666 | 0.649 | 0.548 | 0.508 | 0.503 | 0.501 | 0.498 |
|              | normMI           | 1.443 | 1.443 | 1.443 | 1.355 | 0.993 | 0.976 | 0.882 | 0.846 | 0.841 | 0.840 | 0.837 |
|              | purity           | 1.000 | 1.000 | 1.000 | 0.983 | 0.860 | 0.850 | 0.773 | 0.717 | 0.703 | 0.697 | 0.683 |

Clustering performance of the methods are evaluated by three widely-used metrics: Adjusted Rand Index (adjRI), Normalized Mutual Information (normMI), and purity. A higher value of the metrics indicates better clustering performance. Each column represents a simulated data set where the corresponding number indicates the number of the noise variables (N_{\text{noise}}) added to the complete view (View 1). The bolded numbers are the maximum value for each the evaluation measure within a simulation data set.
### Scenario B-1

| N_{noise} | 0   | 1   | 2   | 3   | 4   | 5   | 6   | 7   | 8   | 9   | 10  |
|-----------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| **Single** |     |     |     |     |     |     |     |     |     |     |     |
| **Best**  | adjRI     | 0.497 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 |
|           | normMI    | 0.837 | 0.811 | 0.811 | 0.811 | 0.811 | 0.811 | 0.811 | 0.811 | 0.811 | 0.811 | 0.811 |
|           | purity    | 0.667 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 |
| **Uniform** |     |     |     |     |     |     |     |     |     |     |     |
| **Weight** | adjRI | 1.000 | 1.000 | 0.980 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 |
|           | normMI | 1.443 | 1.443 | 1.400 | 0.811 | 0.811 | 0.811 | 0.811 | 0.811 | 0.811 | 0.811 | 0.811 |
|           | purity | 1.000 | 1.000 | 0.993 | 0.670 | 0.663 | 0.663 | 0.663 | 0.677 | 0.663 | 0.663 | 0.663 |
| **MinMax** |     |     |     |     |     |     |     |     |     |     |     |
| **MinC**  | adjRI | 1.000 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 |
|           | normMI | 1.443 | 0.811 | 0.811 | 0.811 | 0.811 | 0.811 | 0.811 | 0.811 | 0.811 | 0.811 | 0.811 |
|           | purity | 1.000 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 |
| **Yu's**  |     |     |     |     |     |     |     |     |     |     |     |
| **OKKC**  | adjRI | 1.000 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 |
|           | normMI | 1.443 | 0.811 | 0.811 | 0.811 | 0.811 | 0.811 | 0.811 | 0.811 | 0.811 | 0.811 | 0.811 |
|           | purity | 1.000 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 |
| **Liu's** |     |     |     |     |     |     |     |     |     |     |     |
| **MKK-MIR** | adjRI | 1.000 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 |
|           | normMI | 1.443 | 0.811 | 0.811 | 0.811 | 0.811 | 0.811 | 0.811 | 0.811 | 0.811 | 0.811 | 0.811 |
|           | purity | 1.000 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 |
| **Gonen's** |     |     |     |     |     |     |     |     |     |     |     |
| **MKK**   | adjRI | 1.000 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 |
|           | normMI | 1.443 | 0.811 | 0.811 | 0.811 | 0.811 | 0.811 | 0.811 | 0.811 | 0.811 | 0.811 | 0.811 |
|           | purity | 1.000 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 |
| **Gonen's** |     |     |     |     |     |     |     |     |     |     |     |
| **LMKK**  | adjRI | 0.552 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 |
|           | normMI | 0.832 | 0.812 | 0.811 | 0.811 | 0.811 | 0.811 | 0.811 | 0.811 | 0.811 | 0.811 | 0.811 |
|           | purity | 0.820 | 0.670 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 |
| **Our Method** |     |     |     |     |     |     |     |     |     |     |     |
|           | adjRI | 1.000 | 1.000 | 1.000 | 0.951 | 0.789 | 0.510 | 0.490 | 0.493 | 0.490 | 0.487 | 0.487 |
|           | normMI | 1.443 | 1.443 | 1.443 | 1.355 | 1.159 | 0.847 | 0.814 | 0.817 | 0.814 | 0.812 | 0.811 |
|           | purity | 1.000 | 1.000 | 1.000 | 0.983 | 0.920 | 0.720 | 0.687 | 0.700 | 0.690 | 0.673 | 0.670 |

Clustering performance of the methods are evaluated by three widely-used metrics: Adjusted Rand Index (adjRI), Normalized Mutual Information (normMI), and purity. A higher value of the metrics indicates better clustering performance. Each column represents a simulated data set where the corresponding number indicates the number of the noise variables (N_{noise}) added to the first partial view (View 1). The bolded numbers are the maximum value for each the evaluation measure within a simulation data set.
| Scenario C-1                  | \( N_{\text{noise}} \)\( \quad 0\quad 1\quad 2\quad 3\quad 4\quad 5\quad 6\quad 7\quad 8\quad 9\quad 10 \) |
|----------------------------|--------------------------------------------------|
| **Single Best**             | AdjRI                | 0.497 0.487 0.487 0.487 0.487 0.487 0.487 0.487 0.487 0.487 |
|                            | NormMI               | 0.837 0.811 0.811 0.811 0.811 0.811 0.811 0.811 0.811 0.811 |
|                            | Purity               | 0.667 0.663 0.663 0.663 0.663 0.663 0.663 0.663 0.663 0.663 |
| **Uniform Weight**          | AdjRI                | 1.000 0.990 0.878 0.500 0.487 0.487 0.487 0.487 0.487 0.487 |
|                            | NormMI               | 1.443 1.418 1.234 0.839 0.811 0.812 0.811 0.811 0.811 0.812 |
|                            | Purity               | 1.000 0.997 0.957 0.693 0.667 0.670 0.677 0.677 0.677 0.677 |
| **MinMax MinC**             | AdjRI                | 1.000 0.990 0.878 0.500 0.487 0.487 0.487 0.487 0.487 0.487 |
|                            | NormMI               | 1.443 1.418 1.234 0.839 0.811 0.812 0.811 0.811 0.811 0.812 |
|                            | Purity               | 1.000 0.997 0.957 0.693 0.667 0.670 0.677 0.677 0.677 0.677 |
| **Yu’s OKKC**               | AdjRI                | 1.000 0.545 0.487 0.487 0.487 0.487 0.487 0.487 0.487 0.487 |
|                            | NormMI               | 1.443 0.879 0.811 0.811 0.811 0.811 0.811 0.811 0.811 0.811 |
|                            | Purity               | 1.000 0.770 0.663 0.663 0.663 0.663 0.663 0.663 0.663 0.663 |
| **Liu’s MKK-MIR**           | AdjRI                | 1.000 0.980 0.487 0.487 0.487 0.487 0.487 0.487 0.487 0.487 |
|                            | NormMI               | 1.443 1.394 0.811 0.811 0.811 0.811 0.811 0.811 0.811 0.811 |
|                            | Purity               | 1.000 0.993 0.663 0.663 0.663 0.663 0.663 0.663 0.663 0.663 |
| **Gonen’s MKK**            | AdjRI                | 1.000 0.487 0.487 0.487 0.487 0.487 0.487 0.487 0.487 0.487 |
|                            | NormMI               | 1.443 0.811 0.811 0.811 0.811 0.811 0.811 0.811 0.811 0.811 |
|                            | Purity               | 1.000 0.663 0.663 0.663 0.663 0.663 0.663 0.663 0.663 0.663 |
| **Gonen’s LMKK**           | AdjRI                | 0.500 0.490 0.490 0.490 0.490 0.490 0.490 0.490 0.490 0.490 |
|                            | NormMI               | 0.775 0.814 0.814 0.814 0.814 0.814 0.814 0.814 0.814 0.814 |
|                            | Purity               | 0.790 0.683 0.683 0.683 0.683 0.683 0.683 0.683 0.683 0.683 |
| **Our Method**             | AdjRI                | 1.000 0.990 0.923 0.869 0.556 0.515 0.498 0.498 0.499 0.498 0.497 |
|                            | NormMI               | 1.443 1.418 1.300 1.223 0.890 0.852 0.838 0.837 0.838 0.838 0.837 |
|                            | Purity               | 1.000 0.997 0.973 0.953 0.780 0.730 0.680 0.680 0.690 0.683 0.677 |

Clustering performance of the methods are evaluated by three widely-used metrics: Adjusted Rand Index (adjRI), Normalized Mutual Information (normMI), and purity. A higher value of the metrics indicates better clustering performance. Each column represents a simulated data set where the corresponding number indicates the number of the noise variables (\( N_{\text{noise}} \)) added to the first partial view (View 1). The bolded numbers are the maximum value for each the evalution measure within a simulation data set.
Table S4: Evaluation of the Clustering Methods on Scenario A-2

| Method          | adjRI  | normMI | purity   | adjRI  | normMI | purity   | adjRI  | normMI | purity   | adjRI  | normMI | purity   | adjRI  | normMI | purity   |
|-----------------|--------|--------|----------|--------|--------|----------|--------|--------|----------|--------|--------|----------|--------|--------|----------|
| Single Best     |        |        |          |        |        |          |        |        |          |        |        |          |        |        |          |
| purity          | 0.497  | 0.497  | 0.497    | 0.497  | 0.497  | 0.497    | 0.497  | 0.497  | 0.497    | 0.497  | 0.497  | 0.497    | 0.497  | 0.497  | 0.497    |
| purity          | 0.680  | 0.680  | 0.680    | 0.680  | 0.680  | 0.680    | 0.680  | 0.680  | 0.680    | 0.680  | 0.680  | 0.680    | 0.680  | 0.680  | 0.680    |
| Liu's MKK-MIR   |        |        |          |        |        |          |        |        |          |        |        |          |        |        |          |
| purity          | 0.497  | 0.497  | 0.497    | 0.497  | 0.497  | 0.497    | 0.497  | 0.497  | 0.497    | 0.497  | 0.497  | 0.497    | 0.497  | 0.497  | 0.497    |
| purity          | 0.680  | 0.680  | 0.680    | 0.680  | 0.680  | 0.680    | 0.680  | 0.680  | 0.680    | 0.680  | 0.680  | 0.680    | 0.680  | 0.680  | 0.680    |
| Gonen's MKK     |        |        |          |        |        |          |        |        |          |        |        |          |        |        |          |
| purity          | 0.497  | 0.497  | 0.497    | 0.497  | 0.497  | 0.497    | 0.497  | 0.497  | 0.497    | 0.497  | 0.497  | 0.497    | 0.497  | 0.497  | 0.497    |
| purity          | 0.680  | 0.680  | 0.680    | 0.680  | 0.680  | 0.680    | 0.680  | 0.680  | 0.680    | 0.680  | 0.680  | 0.680    | 0.680  | 0.680  | 0.680    |
| Gonen's LMKK    |        |        |          |        |        |          |        |        |          |        |        |          |        |        |          |
| purity          | 0.497  | 0.497  | 0.497    | 0.497  | 0.497  | 0.497    | 0.497  | 0.497  | 0.497    | 0.497  | 0.497  | 0.497    | 0.497  | 0.497  | 0.497    |
| purity          | 0.680  | 0.680  | 0.680    | 0.680  | 0.680  | 0.680    | 0.680  | 0.680  | 0.680    | 0.680  | 0.680  | 0.680    | 0.680  | 0.680  | 0.680    |
| Uniform Weight  |        |        |          |        |        |          |        |        |          |        |        |          |        |        |          |
| purity          | 0.497  | 0.497  | 0.497    | 0.497  | 0.497  | 0.497    | 0.497  | 0.497  | 0.497    | 0.497  | 0.497  | 0.497    | 0.497  | 0.497  | 0.497    |
| purity          | 0.713  | 0.680  | 0.680    | 0.680  | 0.680  | 0.680    | 0.923  | 0.683  | 0.677    | 0.680  | 0.680  | 0.680    | 0.993  | 0.983  | 0.730    |
| MinMax MinC     |        |        |          |        |        |          |        |        |          |        |        |          |        |        |          |
| purity          | 0.497  | 0.497  | 0.497    | 0.497  | 0.497  | 0.497    | 0.980  | 0.951  | 0.515    | 0.497  | 0.497  | 0.497    | 1.000  | 1.000  | 1.000    |
| purity          | 0.713  | 0.680  | 0.680    | 0.680  | 0.680  | 0.680    | 1.132  | 0.689  | 0.636    | 0.537  | 0.837  | 0.837    | 1.000  | 1.000  | 1.000    |
| Liu's OKKC      |        |        |          |        |        |          |        |        |          |        |        |          |        |        |          |
| purity          | 0.497  | 0.497  | 0.497    | 0.497  | 0.497  | 0.497    | 0.497  | 0.497  | 0.497    | 0.497  | 0.497  | 0.497    | 0.950  | 0.950  | 0.950    |
| purity          | 0.680  | 0.680  | 0.680    | 0.680  | 0.680  | 0.680    | 0.680  | 0.680  | 0.680    | 0.680  | 0.680  | 0.680    | 0.993  | 0.993  | 0.993    |
| Gonen's LMKK    |        |        |          |        |        |          |        |        |          |        |        |          |        |        |          |
| purity          | 0.497  | 0.497  | 0.497    | 0.497  | 0.497  | 0.497    | 0.497  | 0.497  | 0.497    | 0.497  | 0.497  | 0.497    | 0.950  | 0.950  | 0.950    |
| purity          | 0.680  | 0.680  | 0.680    | 0.680  | 0.680  | 0.680    | 0.680  | 0.680  | 0.680    | 0.680  | 0.680  | 0.680    | 0.993  | 0.993  | 0.993    |

Clustering performance of the methods are evaluated by three widely-used metrics: Adjusted Rand Index (adjRI), Normalized Mutual Information (normMI), and purity. A higher value of the metrics indicates better clustering performance. Each column represents a simulated data set, where the corresponding number indicates the number of the redundant pairs (N_redunPairs) added to the complete view (N View 1) and correlation between each redundant pairs and the original first pair. The bolded numbers are the maximum value for each the evaluation metric within a simulation data set.
### Table S5: Evaluation of the Clustering Methods on Scenario B-2

| Scenario B-2 | cor | 0.45 | 0.72 | 0.90 | 0.97 | 1 (View 2) |
|--------------|-----|------|------|------|------|------------|
|               | 1   | 2    | 3    | 4    | 5    | 1          | 2          | 3          | 4          | 5          |
| **N_{redunPairs}** |     |      |      |      |      |            |            |            |            |            |
| Single Best   | adjRI | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 |
|               | normMI | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 |
| Uniform Weight| adjRI | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.491 | 0.487 | 0.487 | 0.487 |
|               | normMI | 0.670 | 0.670 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 |
| MinMaxMinC    | adjRI | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 |
|               | normMI | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 |
| Yu's OKKC     | adjRI | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 |
|               | normMI | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 |
| Liu's MKK-MIR | adjRI | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 |
|               | normMI | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 |
| Gonen's MKK   | adjRI | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 |
|               | normMI | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 | 0.663 |
| Our Method    | adjRI | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 | 0.487 |
|               | normMI | 0.840 | 0.673 | 0.667 | 0.663 | 0.987 | 0.980 | 0.989 | 0.980 | 0.994 |
|               | purity |      |      |      |      |      |      |      |      |      |

Clustering performance of the methods are evaluated by three widely-used metrics: Adjusted Rand Index (adjRI), Normalized Mutual Information (normMI), and purity. A higher value of the metrics indicates better clustering performance. Each column represents a simulated data set where the corresponding number indicates the number of the redundant pairs (\(N_{redunPairs} \)) added to the first partial view (View 1) and correlation between each the redundant pairs and the original, first pair. The bolded numbers are the maximum value for each evaluation measure within a simulation data set.
Table S6: Evaluation of the Clustering Methods on Scenario C-2

| Scenario C-2 | cor   | 0.45 | 0.72 | 0.90 | 0.97 | 1   |
|--------------|-------|------|------|------|------|-----|
|              | 1    | 2    | 3    | 4    | 5    |     |
| N_redunPairs|       |      |      |      |      |     |
| Single Best  | adjRI| 0.487| 0.487| 0.487| 0.487| 0.487|
|              | normMI| 0.663| 0.663| 0.663| 0.663| 0.663|
|              | purity| 0.663| 0.663| 0.663| 0.663| 0.663|
| Uniform Weight| adjRI| 0.488| 0.487| 0.487| 0.487| 0.487|
|              | normMI| 0.673| 0.673| 0.673| 0.673| 0.673|
|              | purity| 0.673| 0.673| 0.673| 0.673| 0.673|
| MinMax MinC | adjRI| 0.488| 0.487| 0.487| 0.487| 0.487|
|              | normMI| 0.663| 0.663| 0.663| 0.663| 0.663|
|              | purity| 0.663| 0.663| 0.663| 0.663| 0.663|
| Liu’s MKK-MIR| adjRI| 0.487| 0.487| 0.487| 0.487| 0.487|
|              | normMI| 0.663| 0.663| 0.663| 0.663| 0.663|
|              | purity| 0.663| 0.663| 0.663| 0.663| 0.663|
| Gonen’s MKK | adjRI| 0.487| 0.487| 0.487| 0.487| 0.487|
|              | normMI| 0.683| 0.683| 0.683| 0.683| 0.683|
|              | purity| 0.683| 0.683| 0.683| 0.683| 0.683|
| Gonen’s LMKK| adjRI| 0.592| 0.498| 0.498| 0.498| 0.498|
|              | normMI| 0.614| 0.614| 0.614| 0.614| 0.614|
|              | purity| 0.614| 0.614| 0.614| 0.614| 0.614|
| Our Method   | adjRI| 0.592| 0.498| 0.498| 0.498| 0.498|
|              | normMI| 0.813| 0.680| 0.680| 0.680| 0.680|
|              | purity| 0.813| 0.680| 0.680| 0.680| 0.680|

Clustering performance of the methods are evaluated by three widely-used metrics: Adjusted Rand Index (adjRI), Normalized Mutual Information (normMI), and purity. A higher value of the metrics indicates better clustering performance. Each column represents a simulated data set where the corresponding number indicates the number of the redundant pairs (N_redunPairs) added to the complete view and correlation between each the redundant pairs and the original, first pair. The bolded numbers are the maximum values for each the evolution measure within a simulation data set.
References

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