Clustering With Multi-Layer Graphs: A Spectral Perspective

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***Abstract*—Observational data usually comes with a multimodal nature, which means that it can be naturally represented by a multi-layer graph whose layers share the same set of vertices (objects) with different edges (pairwise relationships). In this paper, we address the problem of combining different layers of the multi-layer graph for an improved clustering of the vertices compared to using layers independently. We propose two novel methods, which are based on a joint matrix factorization and a graph regularization framework respectively, to efficiently combine the spectrum of the multiple graph layers, namely the eigenvectors of the graph Laplacian matrices. In each case, the resulting combination, which we call a "joint spectrum" of multiple layers, is used for clustering the vertices. We evaluate our approaches by experiments with several real world social network datasets. Results demonstrate the superior or competitive performance of the proposed methods compared to state-of-the-art techniques and common baseline methods, such as co-regularization and summation of information from individual graphs.**

***Index Terms*—Clustering, graph-based regularization, matrix factorization, multi-layer graphs, spectrum of the graph.**

I. Introduction

CLUSTERING on graphs is a problem that has been studied extensively for years. In this task we are usually given a set of objects, as well as an adjacency matrix capturing the pairwise relationships between these objects. This adjacency matrix is either represented by an unweighted graph, where the weight of the edges is always equal to one, or a weighted graph, where the weight can take any real positive values. The goal is to find an assignment of the objects into several subsets, such that the ones in the same subset are similar in some sense. Due to the wide range of applications for this problem, numerous approaches have been proposed in the literature, and we point the readers to the work of Schaeffer [1] for an extensive survey on this topic.

In contrast to the traditional problem, recent applications such as mobile and online social network analyses bring interesting new challenges. In these scenarios, it is common that observational data contains multiple modalities of information reflecting different aspects of human interactions. This can be conveniently represented by a multi-layer graph whose layers share the same set of vertices representing users, but have different sets of edges for different modalities. Fig. 1 [2] illustrates the mobile phone data collected in the MIT Reality Mining Project [3] as such a multi-layer graph. Specifically, the multiple layers represent relationships between mobile phone users in three different aspects: (i) Saturday night proximity, (ii) physical movement similarity, and (iii) interaction with phone communication. Intuitively, each layer should contribute to a meaningful clustering result from its own angle; however, one can expect that a proper combination of the three layers will possibly lead to improved clustering results by efficient merging and completion of data in each layer.

In this paper, we seek for such a good combination and propose two novel clustering methods by studying the spectrum of the graph. In particular, we propose two efficient ways to combine the spectrum of the multiple graph layers, which results in a "joint spectrum" that is eventually used for spectral clustering [4]. In more details, we first propose to generalize the eigen-decomposition process applied on a single Laplacian matrix to the case of multiple graph Laplacian matrices. We design a joint matrix factorization framework in which each graph Laplacian is approximated by a set of joint eigenvectors shared by all the graph layers, as well as its specific eigenvalues from the eigen-decomposition. These joint eigenvectors can then be used to form a joint low dimensional embedding of the vertices in the graph, based on which we perform clustering. In the second approach, we propose a graph regularization method that combines the spectrum of two graph layers. Specifically, we treat the eigenvectors of the Laplacian matrix from one graph as functions on the other graph. By enforcing the "smoothness" of such functions on the graph through a novel regularization framework, we are able to capture the characteristics of both graphs and achieve improved clustering results compared to using any graph alone. We finally propose an information-theoretic approach to generalize this second method to multiple graph layers.

We evaluate the performance of the proposed clustering methods on several real world social network datasets, and compare them with state-of-the-art techniques as well as several baseline methods used for graph-based clustering, such as summation of information from individual graphs. The results show that, in terms of three evaluation measures, our algorithms outperform the baseline methods, and are very competitive with the state-of-the-art technique introduced in Kumar *et al.* [5]. Furthermore, it is important to note that the contribution of this paper is not limited to a better clustering

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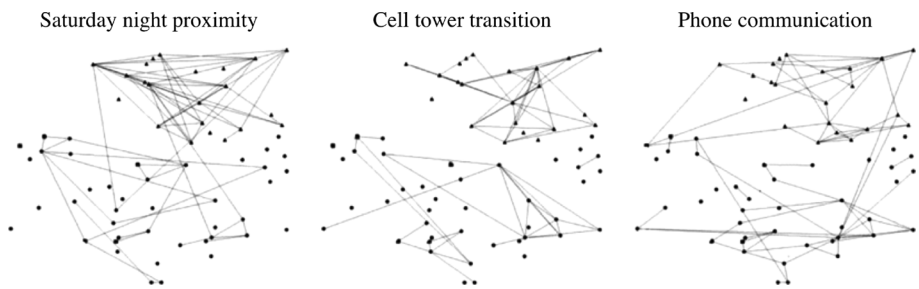

Fig. 1. A multi-layer graph in a mobile social network [2]. On the left, two mobile users are connected with an edge if they were proximate to each other during one Saturday night. In the middle, two are linked to each other if they made the same cell tower transitions at the same time. On the right, we assign an edge between each pair of users who interacted with phone communication.

with multiple graph layers. More generally, the concept of "joint spectrum" is helpful in the analysis of multimodal data that can be conveniently modeled as a multi-layer graph. As an example, it can lead to the generalization of the classical spectral analysis frameworks to multi-dimensional cases.

The rest of the paper is organized as follows. In Section II, we formally introduce the problem of clustering with multi-layer graphs and motivate it from a practical example. In Section III, we review briefly the spectral clustering algorithm, which is one of the building blocks of the methodologies proposed in this paper. Next, we describe in details our novel multi-layer clustering algorithms in Sections IV and V. We then provide experiments in Section VI, where we describe the datasets and present results and comparisons with the existing methods. Finally, we list the related work in Section VII and conclude the paper in Section VIII.

II. Clustering With Multi-Layer Graphs

Consider a multi-layer graph $\mathcal{G}$[1] that contains M individual graph layers $\mathcal{G}^{(i)}$, $i = 1, \ldots, M$, where each layer $\mathcal{G}^{(i)} = \{V, E^{(i)}, \omega^{(i)}\}$ is a weighted and undirected graph consisting of a common vertex set V and a specific edge set $E^{(i)}$ with associated weights $\omega^{(i)}$. Assuming that each layer reveals certain aspect of the intrinsic relationships between the vertices, one can expect that a proper combination of information contained in the multiple graph layers possibly leads to an improved unified clustering of the vertices in V. This can be further demonstrated by the following example.

Let us consider a three-layer graph built from the MIT Reality Mining Dataset [6], where the common vertex set represents 87 participants of the Reality Mining Project and edges represent relationships between these mobile phone users in three different aspects, namely, cell tower proximity, bluetooth proximity and phone call relationship. From these graph layers we form three adjacency matrices and depict them in the spy plots in Fig. 2, where each non-zero entry in the matrices corresponds to a point in the plots[2]. Intuitively, compared to the first two layers, entries in the phone call matrix are stronger indicators of friendship between users, hence the corresponding blue points in the third plot are more reliable. However, the sparse nature of this matrix makes it insufficient for achieving a good global clustering result for all the mobile users. In fact, this graph layer consists of many disconnected components, which makes it very difficult to assign cluster memberships to isolated vertices in the graph. In this case, the first two layers are more informative for achieving the clustering goal: even though single entries in those two matrices are less indicative, they provide richer structural information. This means that, by properly combining layers of different characteristics, we could expect an improved unified clustering result.

In this paper, we address the following problem. Given a multi-layer graph $\mathcal{G}$ with M individual layers $\mathcal{G}^{(i)}$, $i = 1, \ldots, M$, we want to compute a joint spectrum that properly combines the information provided in different layers. In addition, the joint spectrum shall lead to an effective grouping of the vertices in V with spectral clustering [4].

We propose two novel methods for the construction of a joint spectrum in the multi-layer graph.

III. Spectral Clustering

The idea of working with the spectrum of the graph is inspired by the popular spectral clustering algorithm [4]. In this section, we give a very brief review of this algorithm applied on a single graph, which is the main building block of our novel clustering algorithms. Readers familiar with spectral clustering could skip this section.

Spectral clustering has become increasingly popular due to its simple implementation and promising performance in many graph-based clustering problems. It can be described as follows. Consider a weighted and undirected graph $\mathcal{G}$. The spectrum of $\mathcal{G}$ is represented by the eigenvalues and eigenvectors of the graph Laplacian matrix $L = D - W$ where W is the adjacency matrix and D is the degree matrix containing degrees of vertices along diagonal. Notice that L is also called the unnormalized or combinatorial graph Laplacian matrix. There are two normalized versions of the graph Laplacian defined as follows:

$$L_{\mathrm{sym}} = D^{-\frac{1}{2}}(D - W)D^{-\frac{1}{2}}, \tag{1}$$

$$L_{\mathrm{rw}} = D^{-1}(D - W), \tag{2}$$

where L_{sym} keeps the property of symmetry and L_{rw} has close connection to the random walk process on graphs [7]. Different choices of the graph Laplacian correspond to different versions of the spectral clustering algorithm and detailed discussion on these choices is given in von Luxburg [7]. In this paper, we adopt the normalized spectral clustering algorithm that has been first described in Shi *et al.* [4]. It essentially corresponds to dealing with the eigenvalues and eigenvectors of the graph Laplacian

[1]Throughout the paper, the notation $\mathcal{G}$ without upper index still represents a single graph unless stated differently.

[2]In these plots, the users are ordered according to six ground truth clusters. However, one may find that it is not easy to distinguish the clusters from the observations, which in fact demonstrates the difficulty of this clustering task. Detailed discussions are in Section VI.

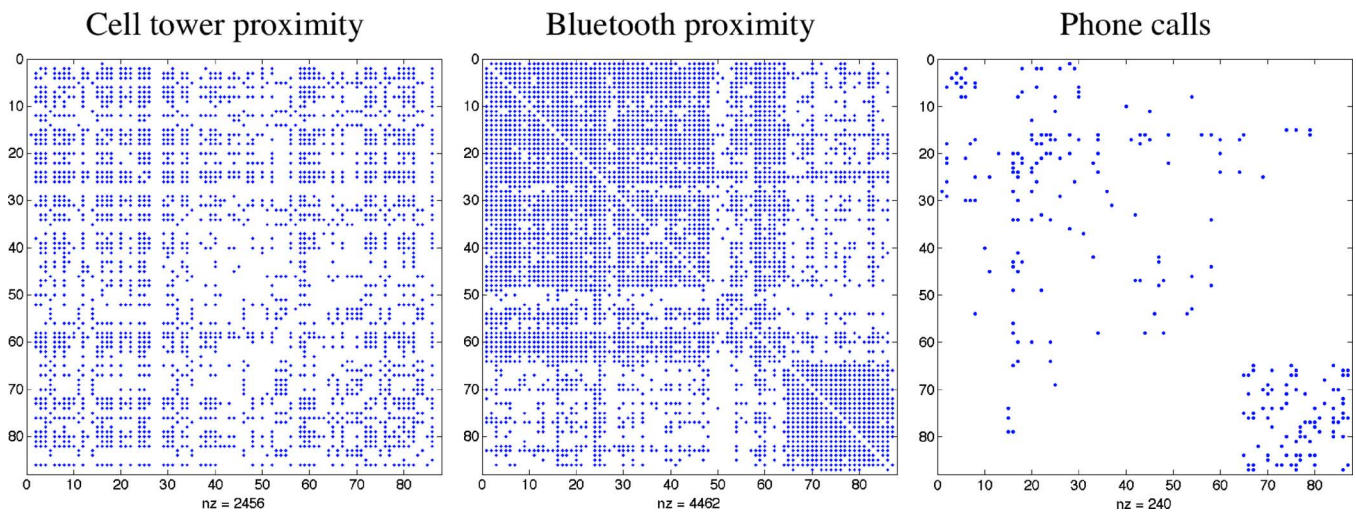

Fig. 2. Spy plots of three adjacency matrices from the MIT dataset. The redundant information contained in the layers for cell tower and bluetooth proximities can compensate the sparse information from the layer for phone call relationship for improved clustering results.

L_{rw}. In practice, the algorithm computes the spectrum of $\mathcal{G}$, and embeds the original vertices in $\mathcal{G}$ to a low dimensional spectral domain formed by the graph spectrum. Due to the properties of the graph Laplacian matrix, this transformation enhances the intrinsic relationships between the original vertices. Consequently, clusters can be eventually detected in the new low dimensional space by many common clustering algorithms, such as the k-means algorithm [8]. An example of such an embedding is illustrated in the toy example shown in Fig. 3. An overview of the algorithm is given in Algorithm 1.

Algorithm 1: Normalized spectral clustering **[4]**

1: **Input:**
W: The $n \times n$ weighted adjacency matrix of graph $\mathcal{G}$ with n vertices
k: Target number of clusters
2: Compute the degree matrix D.
3: Compute the random walk graph Laplacian $L_{\mathrm{rw}} = D^{-1}(D - W)$.
4: Compute the first k eigenvectors $u_1, \ldots, u_k$ (which correspond to the k smallest eigenvalues[3]) of the eigenvalue problem $L_{\mathrm{rw}} u = \lambda u$.
5: Let $U \in \mathbb{R}^{n \times k}$ be the matrix containing $u_1, \ldots, u_k$ as columns.
6: Let $y_i \in \mathbb{R}^k$ $(i = 1, \ldots, n)$ be the i-th row of U to represent the i-th vertex in the graph.
7: Cluster y_i in $\mathbb{R}^k$ into $C_1, \ldots, C_k$ using the k-means algorithm.
8: **Output:**
$C_1, \ldots, C_k$: The cluster assignment

As we can see in Algorithm 1, the spectral embedding matrix U consisting of the first k eigenvectors of the graph Laplacian represents the key idea of spectral clustering. It gives a new representation y_i for each vertex in this low dimensional space, which makes the clustering task trivial with the k-means algorithm. Moreover, as theoretical guarantees, von Luxburg [7] shows that the effectiveness of this approach can be explained from the viewpoint of several mathematical problems, such as the normalized graph-cut problem [4], the random walk process on graphs [9] and problems in perturbation theory [10], [11]. In the following two sections, we will generalize this idea to the case of multi-layer graphs, where we aim at finding a joint spectrum to form the spectral embedding matrix that represents information from all the graph layers.

[3]Throughout the paper, eigenvalues and eigenvectors are always sorted in an ascending order, that is, u_1 is the eigenvector that corresponds to the smallest eigenvalue λ_1 and u_n corresponds to the largest eigenvalue λ_n.

IV. Clustering With Generalized Eigen-Decomposition

The first method that we propose for clustering with multi-layer graphs is built on the construction of an average spectral embedding matrix, based on which spectral clustering is eventually performed. We compute the average spectral embedding matrix with a generalized eigen-decomposition process. As we know, in order to compute the spectrum of a graph $\mathcal{G}$ with n vertices, namely the eigenvalues and eigenvectors of its Laplacian matrix L_{rw}, one can compute an eigen-decomposition of the matrix L_{rw} as:

$$L_{\mathrm{rw}} = P \Lambda P^{-1}, \tag{3}$$

where P is a $n \times n$ matrix containing eigenvectors of L_{rw} as columns, and Λ is a $n \times n$ diagonal matrix containing the corresponding eigenvalues as the diagonal entries. In case of a multi-layer graph $\mathcal{G}$ with n vertices, we have M Laplacian matrices $L_{\mathrm{rw}}^{(i)}$, $i = 1, \ldots, M$, one for each graph layer $\mathcal{G}^{(i)}$. As a natural extension, we propose to approximate each graph Laplacian $L_{\mathrm{rw}}^{(i)}$ by a set of joint eigenvectors shared by all the graph layers as well as its specific eigenvalue matrix:

$$L_{\mathrm{rw}}^{(i)} \approx P \Lambda^{(i)} P^{-1} \quad \text{for} \quad i = 1, \ldots, M, \tag{4}$$

where P is a $n \times n$ matrix containing the set of joint eigenvectors as columns, and $\Lambda^{(i)}$ is the $n \times n$ eigenvalue matrix of $L_{\mathrm{rw}}^{(i)}$. We now have to compute P, that is the set of eigenvectors that provides a good decomposition of the Laplacian matrix of all layers in the multi-layer graph. To do this, we propose to minimize the following objective function S, written as:

$$\arg \min_{P,Q \in \mathbb{R}^{n \times n}} S = \frac{1}{2} \sum_{i=1}^{M} \|L_{\mathrm{rw}}^{(i)} - P \Lambda^{(i)} Q\|_F^2 + \frac{\alpha}{2}(\|P\|_F^2 + \|Q\|_F^2) + \frac{\beta}{2}\|PQ - I_n\|_F^2, \tag{5}$$

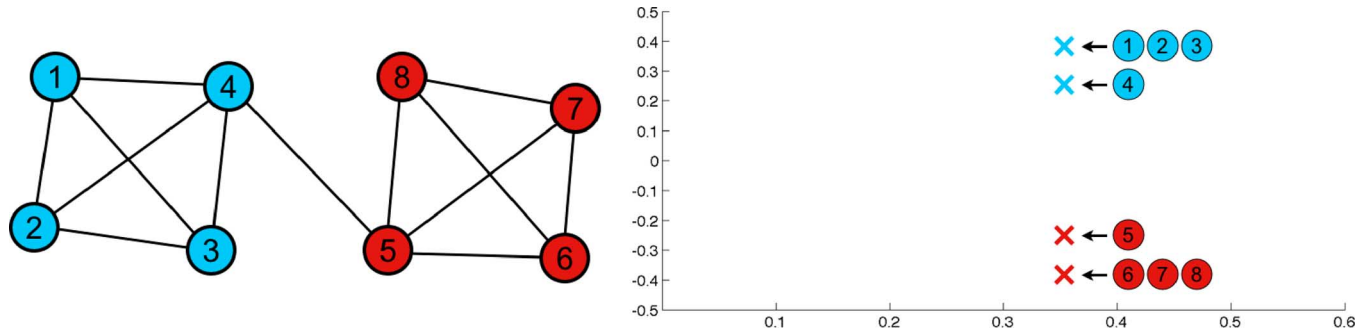

Fig. 3. Toy example to illustrate the spectral embedding. On the left is a simple unweighted graph with eight vertices, which we want to partition into two clusters. On the right is the embedding of the original vertices into a 2-dimensional space using the spectrum of the graph, where the coordinates on the horizontal and vertical axes are determined by the first and second eigenvectors of L_{rw}. In this case, vertices 1, 2 and 3 are embedded into the same point, and so are vertices 6, 7 and 8. It is clear to see that such an embedding helps reveal the intrinsic relationships between the vertices, and k-means can easily find the two clusters.

where P represents the joint eigenvector matrix, Q is enforced to be the inverse matrix of P so that it plays the role of P^{-1} in (4), and $\Lambda^{(i)}$ captures the characteristic of the i-th graph layer $\mathcal{G}^{(i)}$. In addition, I_n represents the identity matrix of dimension n and $\|\cdot\|_F$ denotes the Frobenius norm. Hence, the first term of the objective function S is a data fidelity term to measure the overall approximation error when all layers are decomposed over P; the second term, the sum of the squared Frobenius norms of P and Q, is added to improve numerical stability of the solution; and the third term is a constraint to enforce Q to be the inverse of P. Notice that the purpose of introducing the additional variable Q is purely for the computational convenience of the optimization process. Finally, the regularization parameters α and β balance the trade-offs between the three terms in the objective function.

Now we have to solve the problem in (5) to get P. Since the objective S is not jointly convex in P and Q, it is difficult to find the global minimum solution to (5). Therefore, we adopt an alternating scheme to find a local minimum of the objective function. In the outer loop, we first fix Q and optimize P, and then optimize Q while fixing P. As a consequence, it is important to give a good initialization to our algorithm. In practice, we suggest to compute the eigen-decomposition of $L_{\mathrm{rw}}^{(1)}$ from the most informative graph layer $\mathcal{G}^{(1)}$, and initialize P as the matrix containing its eigenvectors as columns. Q is initialized as the inverse of P. The optimization process is then repeated until the stopping condition is satisfied. In the inner loop, we solve each variable while the other is being fixed. Notice that the objective function S is differentiable with respect to variables P and Q:

$$\frac{\partial S}{\partial P} = -\sum_{i=1}^{M}(L_{\mathrm{rw}}^{(i)} - P\Lambda^{(i)}Q)Q^T\Lambda^{(i)} + \alpha P + \beta(PQ - I_n)Q^T, \tag{6}$$

$$\frac{\partial S}{\partial Q} = -\sum_{i=1}^{M}(L_{\mathrm{rw}}^{(i)} - P\Lambda^{(i)}Q)P\Lambda^{(i)} + \alpha Q + \beta(PQ - I_n)P, \tag{7}$$

where $(\cdot)^T$ denotes the matrix transpose operator. Therefore, we use an efficient quasi-Newton method (Limited-Memory BFGS [12]) to solve each variable.

We have now computed P, which is the set of joint eigenvectors, namely a joint spectrum shared by the multiple graph layers. The average spectral embedding matrix is then formed by the first k joint eigenvectors, that is, the first k columns of P. We then follow the steps 6 and 7 in Algorithm 1 to eventually perform the clustering. The corresponding algorithm is given in Algorithm 2.

Notice that the algorithm proposed in this section is in a sense similar to the approach in Tang *et al.* [13], which introduces a matrix factorization framework to find a low rank matrix that is shared by all the graph layers. However, the matrices they try to approximate in their work are not the graph Laplacian matrices, but the adjacency matrices of all the layers. Moreover, note that the generalized eigen-decomposition process above is essentially based on averaging the information from the multiple graph layers. It tends to treat each layer equally and to build a solution that might smooth out the specificities of each layer. In the next section, we propose a second method based on a regularization process between different layers, which is able to preserve the particularities of each individual layer.

Algorithm 2: Clustering with generalized eigen-decomposition (**SC-GED**)

1: **Input:**
$W^{(i)}$ $(i = 1, \ldots, M)$: M $n \times n$ weighted adjacency matrices of a M-layer graph $\mathcal{G}$ with n vertices
k: Target number of clusters
2: For each i, compute the degree matrix $D^{(i)}$.
3: For each i, compute the random walk graph Laplacian $L_{\mathrm{rw}}^{(i)} = (D^{(i)})^{-1}(D^{(i)} - W^{(i)})$.
4: Solve the optimization problem in **(5)** to get the joint eigenvector matrix P.
5: Let $U' \in \mathbb{R}^{n\times k}$ be the matrix containing the first k columns of P.
6: Let $y_i \in \mathbb{R}^k$ $(i = 1, \ldots, n)$ be the i-th row of U' to represent the i-th vertex in the graph.
7: Cluster y_i in $\mathbb{R}^k$ into $C_1, \ldots, C_k$ using the k-means algorithm.
8: 8:**Output:**
$C_1, \ldots, C_k$: The cluster assignment

V. Clustering With Spectral Regularization

In this section, we propose the second novel method for clustering with multi-layer graphs, where we treat all layers

based on their respective importance. As a consequence, this method helps preserve specificities of each layer in the clustering process.

A. Intuition

We first examine the behavior of eigenvectors of the graph Laplacian matrix in more details. Consider a weighted and connected graph $\mathcal{G}$ with vertex set $V = \{v_i,\ i = 1, \ldots, n\}$. From spectral graph theory [14], we know that the eigenvectors $u_1, \ldots, u_n$ of the graph Laplacian matrix L have the following properties:

1) The first eigenvalue λ_1 is 0 and the corresponding eigenvector u_1 is the constant one vector $\mathbf{1}$;
2) For $i = 2, \ldots, n$, u_i satisfies: $u_i \perp \mathbf{1}$ and $\|u_i\| = 1$ (after normalization).

Now consider the problem of mapping the graph $\mathcal{G}$ on a 1-dimensional line such that connected vertices stay as close as possible on the line, with the condition that the mapping vector satisfies the second property above. In other words, we want to find a 1-dimensional mapping (or a scalar function) $f : V \to R$ that minimizes the following term:

$$\arg\min_{f \in \mathbb{R}^n} \left\{ \sum_{i,j}^{n} w_{i,j} (f(v_i) - f(v_j))^2 \right\}, \quad \text{s.t.} \quad f \perp \mathbf{1},\ \|f\| = 1, \tag{8}$$

where $f(v_i)$ and $f(v_j)$ represent the mappings of vertices v_i and v_j respectively, and $w_{i,j}$ is the weight of the edge between the two vertices. The constraints on the norm of f and the orthogonality to the constant one vector $\mathbf{1}$ are introduced to make the solution nontrivial and unique, and can be explained from a graph-cut point of view [7]. Moreover, since eigenvectors of the Laplacian matrix can be viewed as scalar functions defined on the vertices of the graph, these conditions suggest that they can be considered as candidate solutions to the problem in (8). In fact, we can rewrite (8) in terms of the graph Laplacian matrix L so that an equivalent problem is:

$$\arg\min_{f \in \mathbb{R}^n} f^T L f, \quad \text{s.t.} \quad f \perp \mathbf{1},\ \|f\| = 1. \tag{9}$$

It can be shown by the Rayleigh-Ritz theorem [7] that the solution to the problem in (9) is u_2, the eigenvector that corresponds to the second smallest eigenvalue of L, which is usually called the Fiedler vector of the graph.

Illustrative examples of such a mapping can be found in Horaud *et al.* [15]–[17], which shows that the mapping of u_2 indeed keeps the strongly connected vertices as close as possible on the line. More importantly, it is shown in Zhou *et al.* [18] that the quadratic objective in (9) can be viewed as a smoothness measure of the scalar function f defined on the vertices of the graph $\mathcal{G}$, that is, f has similar values on the vertices that are strongly connected in the graph. Therefore, the fact that it minimizes this objective implies that the Fiedler vector u_2 is a smooth function on the graph. In fact, since we have

$$u_i^T L u_i = \lambda_i, \quad \text{for} \quad i = 2, \ldots, n, \tag{10}$$

all the first k eigenvectors tend to be smooth on the graph $\mathcal{G}$ provided that the first k eigenvalues are sufficiently small. Since these first k eigenvectors are used to form the low dimensional embedding U in the spectral clustering algorithm, such smoothness property implies that a special set of smooth functions on the graph, such as eigenvectors of the graph Laplacian matrix, can well represent the graph connectivity and hence help in the clustering process.

This inspires us to combine information from multiple graph layers, with the help of a set of joint eigenvectors that are smooth on all the layers, hence capture all their characteristics. However, instead of treating all the layers equally, we try to highlight the specificities of different layers. Therefore, we propose the following methodology. Consider two graph layers $\mathcal{G}^{(1)}$ and $\mathcal{G}^{(2)}$ in a 2-layer graph. From the smoothness analysis above, we observe that the eigenvectors of the Laplacian matrix from $\mathcal{G}^{(1)}$ are smooth functions on $\mathcal{G}^{(1)}$; in the meantime, since they can also be viewed as scalar functions on $\mathcal{G}^{(2)}$, we try to enforce their smoothness on $\mathcal{G}^{(2)}$ as well. This leads to a set of eigenvectors that are smooth on both layers, namely a jointly smooth spectrum shared by $\mathcal{G}^{(1)}$ and $\mathcal{G}^{(2)}$; this spectrum captures the characteristics of both layers in this 2-layer graph.

B. Jointly Smooth Spectrum Computation

We propose a spectral regularization process to compute a jointly smooth spectrum of two graph layers $\mathcal{G}^{(1)}$ and $\mathcal{G}^{(2)}$ by solving the following optimization problem:

$$\arg\min_{f_i \in \mathbb{R}^n} \left\{ \frac{1}{2} \|f_i - u_i\|_2^2 + \lambda \cdot \Phi_{f_i} \right\} \quad \text{for} \quad i = 2, \ldots, n, \tag{11}$$

where $f_i : V \to R$ is a scalar function on the graph, u_i is the i-th eigenvector from $\mathcal{G}^{(1)}$, and $\Phi_{f_i} = f_i^T L_{\text{sym}}^{(2)} f_i$ is a quadratic term[4] from $\mathcal{G}^{(2)}$ which measures the smoothness of f_i on $\mathcal{G}^{(2)}$. In the problem in (11), we seek for a scalar function f_i such that it is not only close to the eigenvector u_i that comes from $\mathcal{G}^{(1)}$, but also sufficiently smooth on $\mathcal{G}^{(2)}$ in terms of the quadratic smoothness measure. This promotes the smoothness property of our solution f_i on both of the layers, so that f_i can be considered as a joint eigenvector of $\mathcal{G}^{(1)}$ and $\mathcal{G}^{(2)}$. The regularization parameter λ is used to balance the trade-off between the data fidelity term and the regularization term in the objective function.

It is shown that the problem in (11) has a closed form solution [18]:

$$f_i^* = \mu (L_{\text{sym}}^{(2)} + \mu I_n)^{-1} u_i, \tag{12}$$

where $\mu = \frac{1}{\lambda}$. Furthermore, notice that for each u_i there is an associated optimization problem (except for $i = 1$ since the first eigenvector is a constant vector), hence by solving all these problems we get a set of joint eigenvectors f_i, $i = 2, \ldots, n$. Therefore, they together can be viewed as a jointly smooth spectrum of $\mathcal{G}^{(1)}$ and $\mathcal{G}^{(2)}$. The first k joint eigenvectors can then be used to form a spectral embedding matrix, based on which we perform clustering. The overall clustering algorithm is summarized in Algorithm 3.

It is worth noting that $\mathcal{G}^{(1)}$ and $\mathcal{G}^{(2)}$ play different roles in our framework. Specifically, $\mathcal{G}^{(1)}$ is used for the eigen-decomposition process to get the eigenvectors, and $\mathcal{G}^{(2)}$ is used as the graph structure for the regularization process. It is natural to choose

[4]Since the smoothness analysis in Section V-A can be easily generalized from L to L_{sym}, here we follow Zhou et al. [18] to use L_{sym} instead of L for a better implementation of the algorithm.

the more informative layer as $\mathcal{G}^{(1)}$. Moreover, we can generalize the above framework to multi-layer graphs with more than two layers. Specifically, we propose to start with the most informative graph layer $\mathcal{G}^{(1)}$, and search for the next layer $\mathcal{G}^{(2)}$ that maximizes the mutual information between $\mathcal{G}^{(1)}$ and $\mathcal{G}^{(2)}$. More clearly, the mutual information between two graph layers is introduced by interpreting clustering from each individual layer as a discrete distribution of the cluster memberships of the vertices. Therefore, it can be calculated by measuring the mutual information between two distributions using (20). Next, after having the combination of the first two layers, we can repeat the process by maximizing the mutual information between the current combination and the next selected layer, until we include all the layers in the end. This provides a greedy approach to compute a jointly smooth spectrum of all layers in the multi-layer graph.

Algorithm 3: Clustering with spectral regularization (**SC-SR**)

1: **Input:**
$W^{(i)}$ $(i = 1, 2)$: $n \times n$ weighted adjacency matrices of two graph layers $\mathcal{G}^{(1)}$ and $\mathcal{G}^{(2)}$
k: Target number of clusters
2: For $\mathcal{G}^{(1)}$, compute the degree matrix $D^{(1)}$.
3: Compute the random walk graph Laplacian $L_{\mathrm{rw}}^{(1)} = (D^{(1)})^{-1}(D^{(1)} - W^{(1)})$.
4: Compute the first k eigenvectors $u_1, \ldots, u_k$ of $L_{\mathrm{rw}}^{(1)}$.
5: Let $U \in \mathbb{R}^{n \times k}$ be the matrix containing $u_1, \ldots, u_k$ as columns.
6: For $i = 2, \ldots, k$, solve the spectral regularization problem in **(11)** for each u_i and replace it with the solution f_i in U to form the new low dimensional embedding U''.
7: Let $y_i \in \mathbb{R}^k$ $(i = 1, \ldots, n)$ be the i-th row of U'' to represent the i-th vertex in the graph.
8: Cluster y_i in $\mathbb{R}^k$ into $C_1, \ldots, C_k$ using the k-means algorithm.
9: **Output:**
$C_1, \ldots, C_k$: The cluster assignment

C. Discussion

In addition to the intuition provided above, we further explain in this subsection why the spectral regularization process is considered as a good way of combining the spectrum of two graph layers.

We first interpret the combination of multiple layers from the viewpoint of label propagation [19]–[22], which is proven to be an effective approach for graph-based semi-supervised learning. In label propagation, one usually has a similarity graph whose vertices represent objects and edges reflect the pairwise relationships between them. We let the initial labels of the vertices propagate towards their neighboring vertices to make inference, based on the strength of relationships between them and their neighbors. This is exactly what the spectral regularization process in (11) does. More clearly, the optimization problem in (11) can be solved through an iterative process, where in each iteration we have for every vertex $v \in V$:

$$(f_i(v))^{[t+1]} \leftarrow \alpha((I - L_{\mathrm{sym}}^{(2)})f_i^{[t]})(v) + (1-\alpha)u_i(v), \quad (13)$$

where u_i contains the initial values at the vertices and $f_i^{[t]}$ represents f_i at iteration t [18]. The parameter α is defined as $\alpha = \frac{\lambda}{1+\lambda}$ while λ is the regularization parameter in (11). In other words, the value at each vertex is updated by a convex combination of the initial value $u_i(v)$ and the values at its neighboring vertices at the current iteration, where the parameter α balances the trade-off between the two portions. Notice that the initial values $\{u_i\}_{i=1}^k$ from $\mathcal{G}^{(1)}$ form the continuous-valued solver of a relaxed discrete graph-cut problem [7]. Therefore, $\{u_i\}_{i=1}^k$ can be viewed as labels indicating the cluster memberships derived from $\mathcal{G}^{(1)}$. Consequently, the spectral regularization process in (11) can be interpreted as a label propagation process, where the cluster labels derived from $\mathcal{G}^{(1)}$ are linearly propagated on $\mathcal{G}^{(2)}$. In this way, both of the graph structures have been taken into account hence making the resulting combination meaningful.

Another interpretation is based on disagreement minimization [5], [23], which has been proposed for the task of learning with multiple sources of data. The basic idea is to minimize the disagreement between information from the multiple sources so that we get a good combination of all the sources. For example, Kumar *et al.* [5] suggests a clustering algorithm that minimizes the disagreement between information from multiple graphs. Similarly, since we aim at finding a unified clustering result from multiple graph layers, it is natural to enforce the consistency between the clustering result and the information from all the graph layers, or in other words, to minimize the disagreement between them. Such a disagreement is again reflected in the objective function of the optimization problem in (11). More specifically, the data fidelity term explicitly measures the disagreement between the solution f_i and the initial vector u_i that comes from $\mathcal{G}^{(1)}$, while the regularization term implicitly represents the inconsistency of the information contained in f_i with the structure of $\mathcal{G}^{(2)}$. Indeed, the regularization term Φ_f can be expressed in the following form:

$$\Phi_f = \frac{1}{2}\sum_{i,j}^{n} w_{i,j}\left(\frac{f(v_i)}{\sqrt{d(v_i)}} - \frac{f(v_j)}{\sqrt{d(v_j)}}\right)^2, \quad (14)$$

where $d(v_i)$ and $d(v_j)$ are the degrees of v_i and v_j, respectively. This means that Φ_{f_i} will only be small if the two end-point vertices of a large-weight edge in $\mathcal{G}^{(2)}$ have similar function values normalized by their degrees. Therefore, minimizing the objective function in (11) can be considered as minimizing the total disagreement between the solution f_i and the information from multiple graph layers. Notice that in this formation the disagreement is modeled from two different viewpoints for the two individual layers, whose respective importance is controlled by the parameter λ.

VI. Experimental Results

In this section we present the experimental results. We first describe the datasets and different clustering algorithms used in the experiments, and then compare their performances in terms of three evaluation measures for clustering.

A. Datasets

We adopt three real world social network datasets to compare the clustering performances between our proposed methods and the existing approaches. Two of them are mobile phone datasets,

and the third one is a bibliographic dataset. In this section, we give a brief description on each dataset and explain how we construct multiple graph layers in each case.

The first dataset is a subset of the MIT Reality Mining Dataset[5], which includes mobile phone data of 87 mobile users on the MIT campus. We select three types of information to build a multi-layer graph: physical locations, bluetooth scans and phone calls. More specifically, for physical locations and bluetooth scans, we measure how many times two users are under the service of the same cell tower, and how many times two have scanned the same bluetooth device, within a 30-minute time window. Aggregating results from such windows throughout a 10-month period gives us two weighted adjacency matrices. In addition, a phone call matrix is generated by assigning weight of the edge between any two users as how many times one has established or received calls from the other. In this dataset, we take the ground truth of the clusters as the self-reported affiliations of the subjects. The clustering objective is to partition all the users into six groups with the 3-layer graph and compare them with the six ground truth clusters.

The second dataset in our experiments is the mobile phone dataset that is currently being collected by Nokia Research Center (NRC) Lausanne [24], which includes data of around 200 mobile users living or working in the area of Lausanne, Switzerland. We construct a multi-layer graph from the same information as that in the MIT dataset, with the only difference being that we measure the physical proximity between every pair of users directly using their GPS coordinates. In the Nokia dataset, we take the ground truth of the clusters as eight groups divided by their email affiliations. The goal is to find the ground truth clusters with the 3-layer graph constructed.

The third dataset we adopt is the Cora dataset[6]. Although the objects in this bibliographic dataset are research papers rather than people, it still reflects human interactions in research and publishing activities. In our experiments, we select 292 research papers that roughly come from three different fields: Natural Language Processing, Data Mining and Robotics. Each paper has been manually labeled with one of the categories and we consider this information as the ground truth of the clusters. To build the first two graph layers, we represent the title and abstract of each paper as vectors of nontrivial words, and take the cosine similarity between each pair of vectors as the corresponding entry in the adjacency matrices. In addition, we include a citation graph as the third layer that reflects the citation relationships of these papers. Finally, the goal is to cluster these papers based on the three graph layers we create.

It can be noted that the Cora dataset is considered quite easy to cluster while the MIT and Nokia datasets are much more difficult. The reason is that it is not straightforward to define the ground truth clusters for a group of human users, and observational data does not necessarily correspond well to the intended clusters. In these two datasets, both the academic and e-mail affiliations are not fully reflected by the physical proximity and phone communication between the mobile users, which makes the tasks difficult. Moreover, as we can imagine, the Nokia dataset is expected to be even more difficult to cluster than the MIT dataset as e-mail affiliations is less trustworthy. Nevertheless, we still choose the ground truth clusters in these ways as they are the best indicative information available in the datasets. After all, these two datasets are representative for analyses of activities of mobile phone users, and they can serve as challenging tasks in the experiments compared to the easier one from the Cora dataset.

[5]Available online at "http://reality.media.mit.edu/download.php".

[6]Available online at "http://www.cs.umass.edu/~mccallum/data.html" under category "Cora Research Paper Classification".

B. Clustering Algorithms

In this section, we explain briefly the clustering algorithms that are included in the performance comparisons, along with some implementation details. First of all, we describe some implementation details of the two proposed methods:

- **SC-GED**: Spectral clustering with generalized eigen-decomposition described in Section IV. In **SC-GED**, there are two regularization parameters α and β to balance the trade-off between the approximation error and the stability and conditions on the solution. In our experiments, we set β to be rather large, for example 100, to enforce the inverse relationship between P and Q. We choose α to be 0.5 for the Nokia dataset and around 10 for the other two datasets.
- **SC-SR**: Spectral clustering with spectral regularization described in Section V. Since **SC-SR** is a recursive approach, we need to select two graph layers to fit in the regularization framework at each time. As discussed in Section V-B, we investigate the mutual information between different graph layers. As an example, in the MIT dataset, the "cell tower" and "bluetooth" layers have the highest mutual information between them. Therefore we choose to first combine these two layers. We select the "bluetooth" layer to act as $\mathcal{G}^{(1)}$ in the spectral regularization framework, as it is considered more informative than the "cell tower" layer. After the first combination, the third layer "phone call" is incorporated to get the final solution. In addition, at each combination step, there is a regularization parameter λ in the optimization problem in (11) to control the relative importance of the two graph layers. Intuitively, the choice of this parameter at each step should loosely reflect the mutual information between the two layers being considered. We use this as a rule of thumb to set the parameters in the first and second combination steps, which are denoted by λ_1 and λ_2, respectively. As an example, we set $\lambda_1 = 2$ and $\lambda_2 = 1$ for the MIT dataset.

Next, we introduce five competing schemes as follows. The first three are common baseline methods for clustering with multiple graphs, and the last two are representative techniques in the literature:

- **SC-SUM**: Spectral clustering applied on the summation of the adjacency matrices:

$$\sum_{i=1}^{M} W^{(i)}. \tag{15}$$

If the weights of edges are of different scales across the multiple layers, we use the summation of the normalized adjacency matrices:

$$\sum_{i=1}^{M} (D^{(i)})^{-\frac{1}{2}} W^{(i)} (D^{(i)})^{-\frac{1}{2}}. \tag{16}$$

- **K-Kmeans**: Kernel k-means applied on the summation of the spectral kernels of the adjacency matrices [13]:

$$\sum_{i=1}^{M} K^{(i)} \quad \text{with} \quad K^{(i)} = \sum_{k=1}^{d} u_k^{(i)} (u_k^{(i)})^T, \tag{17}$$

  where $d \ll n$ (number of vertices) and $u_k^{(i)}$ represents the k-th eigenvector of the Laplacian $L_{\text{sym}}^{(i)}$ from $\mathcal{G}^{(i)}$.
- **SC-AL**: Spectral Clustering applied on the averaged random walk graph Laplacian matrix:

$$\frac{1}{M} \sum_{i=1}^{M} L_{\text{rw}}^{(i)}. \tag{18}$$

- Co-regularization (**CoR**): The co-regularization approach proposed in Kumar *et al.* [5] is the latest state-of-the-art technique aimed at combing information from multiple graphs. In this work, the authors have proposed to enforce the similarity between information from two different graphs where the similarity is measured by a linear kernel. In our experiments, we generalize their approach to multiple graphs and tune the hyperparameter λ in their work to achieve the best clustering performance.
- Community detection via modularity maximization (**CD**): In addition to spectrum-based clustering algorithms, modularity maximization is a different approach proposed by Newman *et al.* [25]–[27] for community detection. We adopt the algorithm described in Nefedov [28], which applies modularity maximization [27] using fast greedy search algorithm [29]. It uses the summation of the normalized adjacency matrices to combine information from different graph layers.

C. Evaluation Measures and Results

To quantitatively evaluate the clustering performance, we compare the clusters $\Omega = \{\omega_1, \ldots, \omega_k\}$ we have computed with the intended ground truth classes $C = \{c_1, \ldots, c_k\}$. We adopt *Purity*, *Normalized Mutual Information (NMI)* and *Rand Index (RI)* [30] as three measures to evaluate the clustering performance from different angles. More specifically, *Purity* is defined as:

$$Purity(\Omega, C) = \frac{1}{n} \sum_{k} \max_{j} |\omega_k \cap c_j|, \tag{19}$$

where n is the total number of objects, and $|\omega_k \cap c_j|$ denotes the number of objects in the intersection of ω_k and c_j. Next, *NMI* is defined as:

$$NMI(\Omega, C) = \frac{I(\Omega; C)}{\frac{[H(\Omega)+H(C)]}{2}}, \tag{20}$$

where I is the mutual information between clusters Ω and classes C, and $H(\Omega)$ and $H(C)$ represent the entropies of the clusters and classes, respectively. Finally, when interpreting clustering as a series of binary decisions on each pair of objects, *RI* is defined as:

$$RI(\Omega, C) = \frac{TP + TN}{TP + FP + FN + TN}, \tag{21}$$

where TP, TN, FP, FN represent true positive, true negative, false positive and false negative decisions, respectively.

Fig. 4 shows the performance of different clustering algorithms applied on the three datasets we adopt. As we can see, clustering with the Cora dataset is indeed much easier than the other two datasets as the evaluation scores are much higher. Regarding the performance of the algorithms, it is clearly shown that proper combinations of multiple graph layers indeed lead to improved clustering results compared to using layers independently. In general, our proposed algorithm **SC-SR** achieves superior or competitive performances in all the evaluation measures, while **SC-GED** does not perform as well as **SC-SR**. Among the competitors, **CoR** presents impressive evaluation scores, while **CD** and the three baseline combination methods show intermediate results in general. As we can imagine, this is mainly due to the simple averaging of the information from different graph layers.

In more details, we can see that the regularized combinations in **SC-SR** consistently lead to better clustering results as more layers are combined, particularly in terms of the *NMI* scores. This comes from the way we combine the multiple graph layers in order to maximize the mutual information. Compared to the state-of-the-art algorithm **CoR**, **SC-SR** maintains competitive results while the computational complexity is significantly reduced. Indeed, **CoR** needs to compute extremal eigenvectors of the (original and modified) Laplacian matrices for MN times in total, where M is the number of different graphs and N is the number of iterations the algorithm needs to converge. In contrast, **SC-SR** only needs to implement the same process once, namely for the most informative layer. Therefore, with state-of-the-art eigensolvers [31], **SC-SR** has a complexity usually lower than $O(n^3)$, where n is the number of vertices. Finally, notice that the *NMI* score shows difference from the other two measures in the Nokia dataset, since the ground truth clusters in this dataset are quite unbalanced.

Compared to **SC-SR**, the performance of **SC-GED** is somewhat disappointing, as it only provides limited improvements on the clustering results achieved by individual layers. This is mainly due to the nature of the algorithm: unlike **SC-SR** which is implemented recursively, it resorts to a joint matrix factorization framework to find the set of joint eigenvectors all at once. Therefore, it can be essentially considered as a way to average the information from the multiple graph layers, but without paying much attention to the specific characteristics in each layer. Moreover, the computational complexity of **SC-GED** is higher than that of **SC-SR**, as we need to compute a complete eigen-decomposition and a matrix inversion (both with a complexity of $O(n^3)$) for the initialization, as well as for the evaluations of derivatives in (6) and (7) in the L-BFGS algorithm.

Finally, in addition to the evaluation scores, the confusion matrices for different clustering methods on the MIT dataset are shown in Table I as an illustrative example of the clustering qualities. The columns of the confusion matrices represent the predicted clusters while the rows represent the intended classes. From the diagonal entries of these matrices (which are the numbers of objects that have been correctly identified for each class), it is clear that **SC-SR** best reveals the six classes in the ground truth data.

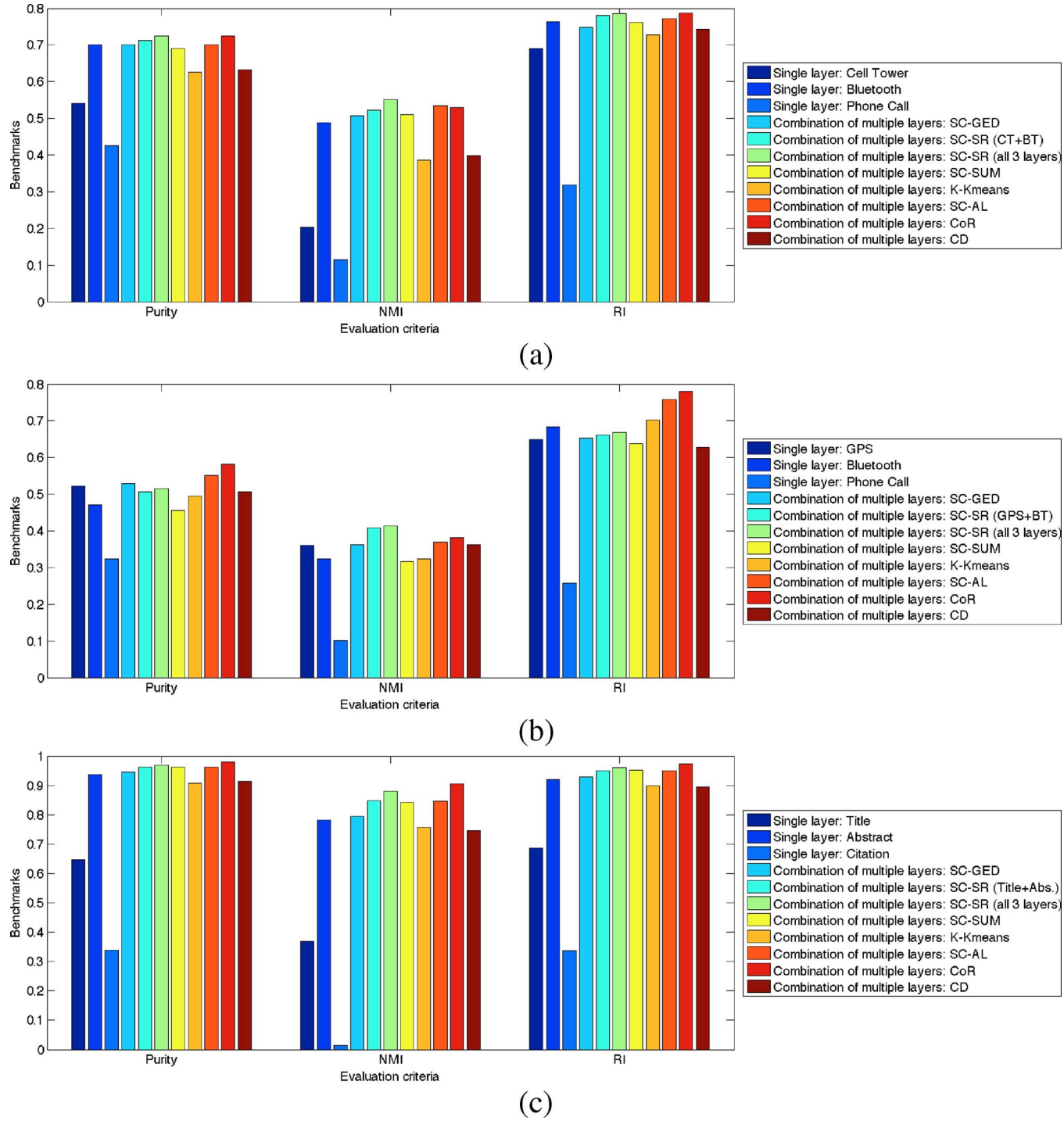

Fig. 4. Performance evaluation of different clustering algorithms. (a) Clustering performance on the MIT dataset. (b) Clustering performance on the Nokia dataset. (c) Clustering performance on the Cora dataset.

VII. Related Work

In this section we give a review of the literature that is related to our work. We start with techniques in the general field of graph-based data processing and learning problems. Next, we move onto spectral methods applied on graphs. Finally, we discuss several existing works that involve the framework of combining information from multiple graphs.

Nowadays, graph theory is widely considered as a powerful mathematical tool for data modeling and processing, especially when the pairwise relationships between objects are of interest. Over the last two decades, graph-based data mining and analysis have become extremely popular. In Cook *et al.* [32] the authors have described the recent developments on the theoretical and practical aspects of graph-based data mining problems together with some practical applications. Especially, clustering on graphs has attracted a large amount of interests due to its numerous applications. In Schaeffer [1] the author has investigated the state-of-the-art techniques and recent advances in this active field, from hierarchical clustering to graph cuts, spectral methods and Markov chain based methods. These are certainly the foundations of our work. From a methodology point

TABLE I
CONFUSION MATRICES FOR SEVEN COMBINATION METHODS ON THE MIT DATASET

SC-GED

4	7	0	1	3	0
7	**15**	0	5	7	0
0	1	**5**	0	0	0
0	3	0	**0**	0	0
0	6	0	0	**0**	0
0	1	0	0	0	**22**

SC-SR (all 3 layers)

6	3	0	1	5	0
7	**10**	0	4	13	0
0	0	**6**	0	0	0
1	0	0	**0**	2	0
1	0	0	0	**5**	0
0	0	0	0	0	**23**

CoR

6	4	0	1	4	0
10	**9**	0	5	10	0
0	0	**6**	0	0	0
1	0	0	**0**	2	0
2	1	0	0	**3**	0
0	0	0	0	0	**23**

CD

6	2	3	1	3	0
6	**10**	5	3	10	0
0	2	**4**	0	0	0
1	0	1	**1**	0	0
0	0	2	0	**3**	1
0	0	0	0	0	**23**

SC-SUM

2	9	3	1	0	0
8	**20**	3	1	2	0
0	0	**6**	0	0	0
0	2	1	**0**	0	0
0	5	1	0	**0**	0
0	0	0	0	0	**23**

K-Kmeans

2	6	1	2	3	1
3	**16**	5	1	5	4
1	0	**4**	0	1	0
0	1	1	**1**	0	0
0	4	0	0	**1**	1
0	0	0	0	0	**23**

SC-AL

3	3	0	0	9	0
5	**10**	2	2	15	0
0	0	**6**	0	0	0
1	0	0	**0**	2	0
1	0	0	0	**5**	0
0	0	0	0	0	**23**

of view, regularization theory on graphs is of particular interest. In Smola *et al.* [33], the authors have developed the regularization theory for learning on graphs using the canonical family of kernels on graphs. In Zhou *et al.* [18], the authors have defined a family of differential operators on graphs, and used them to study the "smoothness" measure of functions defined on graphs. They have then proposed a regularization framework based on the developed smoothness measure. These works provide the main inspirations that lead to our second approach.

In addition to general graph-based data processing, we are especially interested in a unique branch in graph theory that is devoted to analyzing the spectrum of the graphs, namely, spectral graph theory. The manuscript of Chung [14] gives a good introduction to this field. Among various methods that have been developed, we particularly emphasize the so-called spectral clustering algorithm, which has become one of the major graph-based clustering techniques. Due to its promising performance and close links to other well-studied mathematical problems, a large number of variants of the original algorithm has been proposed, such as the constrained spectral clustering algorithms [34]–[38]. In general, these works have suggested different ways to incorporate constraints in the clustering task. Among them, Li *et al.* [36] has proposed a regularization framework in the graph spectral domain, which provides the closest methodology to our work.

Recently, data that can be represented by multiple graphs has attracted increasing attention. In the literature of the learning community this is sometimes referred to as "multiple views" or "multiple kernels", which intuitively means we investigate data from different viewpoints. In this setting, the general problem is how to efficiently combine information from multiple graphs for the learning objectives. In this sense, the following research efforts have the closest ideas to our presented work. In Argyriou *et al.* [39], the authors have proposed a method to compute an "optimal combined kernel" for combining graphs. Their idea is essentially based on averaging the graph Laplacian matrices. In Zhou *et al.* [40], the authors have modeled spectral clustering on a single graph as a random walk process, and then proposed a mixed random walk when two graphs are given. However, the way they make the combination is still based on a convex combination of the two graphs. In Muthukrishnan *et al.* [41], the authors have presented a novel way to exploit the relationships between different graph layers, which permits efficient combination of multiple graphs by a regularization framework in the signal domain. In Cheng *et al.* [42], the authors have proposed to achieve the final clustering result by post-processing the results from individual graph layers. In Savas *et al.* [43] and Vasuki *et al.* [44], the authors have worked with very similar settings to our work, however the problems they have tackled there are not clustering. Finally, the work of Tang *et al.* [13] is the closest to our first algorithm **SC-GED** in the sense that they have also proposed a unified matrix factorization framework to find a joint low dimensional representation shared by the multiple graphs, which inspired us to develop our first approach. Very recently, Kumar *et al.* [5] has proposed the co-regularization framework which is conceptually similar to our second algorithm **SC-SR**, and is adopted as a competing method in our experiments.

To summarize, although some of the works mentioned above are closely related to what we have presented in this paper, there are still noticeable differences that can be summarized as follows. First, despite the nature of the spectral clustering algorithm, most of the existing efforts to combine information from multiple graph layers are done in the signal domain, while the well-developed spectral techniques are mostly applied on a single graph. In contrast, our proposed methods provide novel ways for the same task in the graph spectral domain. Second, to the best of our knowledge, in almost all the state-of-the-art algorithms for combining multiple graphs, different graph layers are either treated equally or combined through a weighted summation. However, we propose **SC-SR** based on a spectral regularization process, in which individual graph layers play different roles in the combination process. In addition, we suggest to quantitatively measure the respective importance of different graph layers from an information-theoretic point of view, which could be beneficial for processing multiple graphs in general. Third, there are only a few works that address the problem of clustering with multiple graph layers, especially in the context of mobile social network analysis. We believe that our efforts to work with rich mobile phone datasets are good attempts in this emerging field.

VIII. CONCLUSION

In this paper we study the problem of clustering with data that can be represented by multi-layer graphs. We have shown

that generalizations of the well-developed spectral techniques applied on a single graph are of great potential in such emerging tasks. In particular, we have proposed two novel methodologies to find a joint spectrum that is shared by all the graph layers: a joint matrix factorization approach and a graph-based spectral regularization framework. In the second approach, we suggest to treat individual graph layers based on their respective importance, which is measured from an information-theoretic point of view. In addition to the improvements we get in the evaluation scores with three social network datasets, we believe that the concept of a joint spectrum shared by multiple graphs is of broad interest in graph-based data processing tasks, as it suggests one way to generalize the classical spectral analysis to multi-dimensional cases. This is certainly one of the focuses in our future work.

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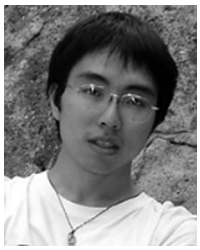

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