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Article

Kernel Spectral Clustering for Big Data Networks

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Abstract: This paper shows the feasibility of utilizing the Kernel Spectral Clustering (KSC) method for the purpose of community detection in big data networks. KSC employs a primal-dual framework to construct a model. It results in a powerful property of effectively inferring the community affiliation for out-of-sample extensions. The original large kernel matrix cannot fitinto memory. Therefore, we select a smaller subgraph that preserves the overall community structure to construct the model. It makes use of the out-of-sample extension property for community membership of the unseen nodes. We provide a novel memory- and computationally efficient model selection procedure based on angular similarity in the eigenspace. We demonstrate the effectiveness of KSC on large scale synthetic networks and real world networks like the YouTube network, a road network of California and the Livejournal network. These networks contain millions of nodes and several million edges.

Keywords: kernel spectral clustering; out-of-sample extensions; sampling graphs; angular similarity

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1. Introduction

In the modern era, complex networks are ubiquitous. Their omnipresence is reflected in domains like social networks, web graphs, road graphs, communication networks, biological networks and financial networks. Complex networks can be represented as graphs ($G(V, E)$), where the nodes (V) represent

vertices in the graph and edges (E) depict the relationship between these nodes. These networks exhibit community like structure, where nodes within a community are densely connected and the connections are sparse between the communities. The problem of community detection has also been framed as graph partitioning and graph clustering [1] and has received a lot of attention lately [2–13]. Among the myriad variety of algorithms for community detection, the Kernel Spectral Clustering (KSC) method is related to the spectral clustering methods [10–13]. Spectral clustering methods are standard techniques for graph partitioning. The underlying model is based on eigen-decomposition of the Laplacian matrix derived from the affinity matrix of the nodes in the community. The major drawback of these spectral clustering methods is the construction of the large affinity matrix ($N \times N$), where N is the number of nodes in the network, which requires to calculate the similarity between every pair of nodes in the network. As the size of the network increases, the $O(N^2)$ computation and storage of this affinity $N \times N$ matrix become infeasible.

Recently, a spectral clustering formulation based on weighted kernel PCA with primal-dual framework was proposed in [14]. The formulation resulted in a model with a powerful property of inferring community memberships for out-of-sample nodes. The model is built on a small subset of the big data network that captures the inherent community structure. One then solves an affordable eigenvalue problem on this smaller subgraph and uses the out-of-sample extension property. The KSC method was extended for community detection by [8]. However, the two important steps, the subset selection and the model selection proposed by [8], are computationally expensive and memory inefficient. The two major contributions of the paper are:

- We propose a novel memory-and computationally efficient model selection technique to tune the parameter of the model using angular similarity in the eigenspace between the projected vectors of the nodes in the validation set.
- We show that kernel spectral clustering is applicable for community detection in big data networks.

The authors in [8] utilized Modularity [15] for the purpose of model selection. However, they need to keep a square, non-sparse $N \times N$ matrix for validation of the model using Modularity. This makes the approach infeasible when the networks are large scale. We provide a novel model selection technique based on angular similarity between the projected vectors in the eigen-spectrum. The authors in [8] used Expansion sampling [16] technique for subset selection. The method is based on the principle of expander graphs and optimizes the expansion factor function. However, the method is computationally expensive as shown in [17] and stochastic by nature. Therefore, for the given big data network, for each iteration of Expansion sampling, the obtained subgraph would be different. We use the Fast and Unique Representative Subset (FURS) selection technique [17] for obtaining a representative subset of the big data network. The method is computationally less expensive and is a better representative of the community structure than most of the state-of-the-art sampling techniques like SlashBurn [18], Metropolis [19], Snowball Expansion [16], Random Node [20] sampling, *etc*., as shown through extensive comparisons in [17]. The KSC method was recently extended to evolving networks as described in [21]. In this paper, all considered graphs are unweighted and undirected unless specified otherwise. All the experiments were performed on a machine with 12 GB RAM and 2.4 GHz Intel Xeon processor. The maximum size of the kernel matrix that can be stored in the memory of our PC

is $5,000 \times 5,000$. The approach that we present can be easily implemented in a distributed environment as well and can handle big data networks.

The rest of the paper is organized as the follows. Section 2 provides details about the kernel spectral clustering method. Section 3 describes the angular similarity based model selection procedure. Section 4 gives insight into the FURS selection technique to obtain a representative subgraph. Section 5 describes the experiments undertaken along with the results on big data networks. We conclude in Section 6.

2. Kernel Spectral Clustering

We first provide details about the notations used.

2.1. Notations

(1) A graph is mathematically represented as $G = (V, E)$ where V represents the set of nodes and $E \subseteq V \times V$ represents the set of edges in the network. Physically, the nodes represent the entities in the network and the edges represent the relationship between these entities.
(2) The cardinality of the set V is denoted as N.
(3) The cardinality of the set E is denoted as e.
(4) The matrix A is a $N \times N$ matrix and represents the affinity or similarity matrix.
(5) For unweighted graphs, A is called the adjacency matrix and $A_{ij} = 1$ if $(v_i, v_j) \in E$, otherwise $A_{ij} = 0$.
(6) The subgraph generated by the subset of nodes S is represented as $G(S)$. Mathematically, $\bar{G} = (S, Q)$ where $S \subset V$ and $Q = (S \times S) \cap E$ represents the set of edges in the subgraph.
(7) The degree distribution function is given by $f(V)$. For the graph G it can written as $f(V)$ while for the subgraph S it can be presented as $f(S)$. Each vertex $v_i \in V$ has a degree represented as $f(v_i)$.
(8) The degree matrix is represented as D, a diagonal matrix with diagonal entries $d_{i,i} = \sum_j A_{ij}$.
(9) The adjacency list corresponding to each vertex $v_i \in V$ is given by $A(i, :)$.
(10) The neighboring nodes of a given node v_i are represented by $Nbr(v_i)$.
(11) The median degree of the graph is represented as M.

2.2. General Background

Spectral clustering uses the information contained in the affinity matrix to detect structures in the given network. In case of data points, the similarity between the points is measured with respect to the mutual distance (e.g., Euclidean, cosine, RBF distance) between the points. Thus, the obtained similarity matrix can be considered as a weighted graph where each point has a certain extent of similarity with other points in the dataset. For our case, we already have a weighted graph A, where $A_{ij} = 1$ if $(v_i, v_j) \in E$ else $A_{ij} = 0$. Therefore, in our case the spectral clustering method can be applied directly. However, for the KSC method, we need to build a graph over the network to represent the similarity between the nodes in a kernel based framework.

The spectral graph theory can provide insights into several properties of the graph-like partitions existing in the graph. These insights are obtained by studying the eigen-spectrum of the Laplacian

matrix [10,11,22]. Several Laplacian matrices exist, including the unnormalized Laplacian defined as $L = D - A$, the symmetric normalized Laplacian $L_{SYM} = D^{-1/2}LD^{-1/2} = \mathcal{I}_N - D^{-1/2}AD^{-1/2}$, the non-symmetric normalized Laplacian $L_{RW} = D^{-1}L = \mathcal{I}_N - D^{-1}A$. This Laplacian is related to the random walk on the graph, hence denoted by L_{RW}. For a random walk Laplacian, clustering can be understood as detecting the partitions such that a random walker will spend maximum time in that partition with a few jumps to other clusters. This minimizes the transition probability between the clusters. The transition matrix of the random walker on the graph can be obtained by normalizing the adjacency matrix A such that the sum of its row ends up being 1. Thus the transition matrix can be depicted as $P = D^{-1}A$, where the entry P_{ij} represents the probability of a jump from node v_i to node v_j. The corresponding eigenvalue problem becomes $Pr = \xi r$ and was shown to be the dual problem of a constrained optimization problem typical of least squares support vector machines (LS-SVM) [23].

2.3. Primal-Dual Formulation

The KSC method is described by a primal-dual framework. The model is determined during the training phase, and the parameter of the model, *i.e.*, k (number of clusters), is estimated during the validation stage. Finally, the model is tested on the test data to provide community affiliation to the unseen nodes.

In case of networks, the training data comprises the adjacency list of all the vertices $v_i \in X_{tr}$, where X_{tr} represents the set of nodes used for training the model. Let the cardinality of the set X_{tr} be N_{tr}. Big data networks can be stored into memory in sparse format as these networks are highly sparse. However, if the graph does not fit in the main memory, it can be split into blocks of adjacency lists and stored on the hard disk. We can then iterate over these blocks by selecting the adjacency lists corresponding to the nodes in the training set X_{tr}. This set of adjacency lists can be efficiently stored in the memory as real world networks are highly sparse and there are very few connections for each node $v_i \in X_{tr}$. The maximum length of the adjacency list of a node in the training data can be equal to N, when the node is connected to all the other nodes in the network. During the test phase, the cluster memberships for each of the unseen nodes can be predicted by uploading the adjacency list of the test node in the memory and using the out-of-sample extension property of the model. This makes the approach feasible for big data networks, unlike approaches that require the entire graph to be stored in the main memory. Moreover, the computational complexity of our approach is dominated by the time required to construct the kernel matrix. It is given by $O(N_{tr}^2 N)$, *i.e.*, the time required to calculate the similarity between sparse adjacency lists of the nodes in the training data.

Given X_{tr} training nodes $\mathcal{D} = \{x_i\}_{i=1}^{N_{tr}}$, $x_i \in \mathbb{R}^N$ and $x_i \in X_{tr}$. Here x_i represents the adjacency list of the i^{th} training node and the number of nodes in the training set is N_{tr}. Given $\mathcal{D}$ and the number of communities k, the primal problem of the spectral clustering via weighted kernel PCA is formulated as follows [14]:

$$\begin{aligned} \min_{w^{(l)},e^{(l)},b_l} \quad & \frac{1}{2}\sum_{l=1}^{k-1} w^{(l)\intercal} w^{(l)} - \frac{1}{2N}\sum_{l=1}^{k-1} \gamma_l e^{(l)\intercal} D_\Omega^{-1} e^{(l)} \\ \text{such that} \quad & e^{(l)} = \Phi w^{(l)} + b_l 1_{N_{tr}}, l = 1, \ldots, k-1 \end{aligned} \tag{1}$$

where $e^{(l)} = [e_1^{(l)}, \ldots, e_{N_{tr}}^{(l)}]^\intercal$ are the projections onto the eigenspace, $l = 1, \ldots, k-1$ indicates the number of score variables required to encode the k communities, $D_\Omega^{-1} \in \mathbb{R}^{N_{tr} \times N_{tr}}$ is the inverse of the degree matrix associated to the kernel matrix Ω. Φ is the $N_{tr} \times d_h$ feature matrix, $\Phi = [\phi(x_1)^\intercal; \ldots; \phi(x_{N_{tr}})^\intercal]$ and $\gamma_l \in \mathbb{R}^+$ are the regularization constants. We note that $N_{tr} \ll N$, *i.e.*, the number of nodes in the training set, is much less than the total number of nodes in the big data network. The kernel matrix Ω is the obtained by calculating the similarity between the adjacency list of each pair of nodes in the training set. Each element of Ω, denoted as $\Omega_{ij} = K(x_i, x_j) = \phi(x_i)^\intercal \phi(x_j)$, is obtained by calculating the cosine similarity between the adjacency lists of x_i and x_j, which has been shown to be an effective similarity measure for large scale data [24]. Thus, $\Omega_{ij} = \frac{x_i^\intercal x_j}{\|x_i\| \|x_j\|}$ and can be calculated efficiently using notions of set unions and intersections. This corresponds to using a normalized linear kernel function $K(x, z) = \frac{x^\intercal z}{\|x\| \|z\|}$ [23]. The clustering model is then represented by:

$$e_i^{(l)} = w^{(l)^\intercal} \phi(x_i) + b_l, i = 1, \ldots, N_{tr} \tag{2}$$

where $\phi : \mathbb{R}^N \to \mathbb{R}^{d_h}$ is the mapping to a high-dimensional feature space d_h, b_l are the bias terms, $l = 1, \ldots, k-1$. However, for big data networks we can utilize the explicit expression of the underlying feature map and $d_h = \mathbb{R}^N$. The projections $e_i^{(l)}$ represent the latent variables of a set of $k-1$ binary cluster indicators given by $\mathrm{sign}(e_i^{(l)})$, which can be combined with the final groups using an encoding/decoding scheme. The dual problem corresponding to this primal formulation is:

$$D_\Omega^{-1} M_D \Omega \alpha^{(l)} = \lambda_l \alpha^{(l)} \tag{3}$$

where M_D is the centering matrix, which is defined as $M_D = \mathrm{I}_{N_{tr}} - (\frac{1}{1_{N_{tr}}^\intercal D_\Omega^{-1} 1_{N_{tr}}})(1_{N_{tr}} 1_{N_{tr}}^\intercal D_\Omega^{-1})$. The $\alpha^{(l)}$ are the dual variables and the kernel function $K : \mathbb{R}^N \times \mathbb{R}^N \to \mathbb{R}$ plays the role of similarity function. This dual problem is closely related to the random walk model.

2.4. Encoding/Decoding Scheme

In ideal situations when the communities are non-overlapping, we will obtain k well separated clusters and the matrix $D^{-1} M_D \Omega$ has $k-1$ piece-wise constant eigenvectors. This is because the multiplicity of the largest eigenvalue (*i.e.*, 1) is $k-1$ as depicted in [22]. In the eigenspace every cluster A_p, $p = 1, \ldots, k$ is a point and is represented with a unique codebook $c_p \in \{-1, 1\}^{k-1}$. To obtain this codebook $\mathcal{CB} = \{c_p\}_{p=1}^k$ we transform the rows of the projected vector matrix obtained from the training data by binarizing it, *i.e.*, $[\mathrm{sign}(e^{(1)}, \ldots, e^{(k-1)})]$. However, in real world networks, the communities do overlap and we have nearly piece-wise constant eigenvectors. The codebook set $\mathcal{CB}$ is also obtained by selecting the top k most frequent codebook vectors. Due to the centering matrix M_D, the eigenvectors have zero mean and the optimal threshold for binarizing the eigenvectors is self-determined (equal to 0). Taking into account that the first eigenvector $\alpha^{(1)}$ already provides a binary clustering, the number of score variables needed to encode k clusters is $k-1$. The decoding scheme consists of comparing the cluster indicators obtained in the validation/test stage with the codebook and selecting the nearest codebook based on Hamming distance. This scheme corresponds to the ECOC decoding procedure [25] and is used in out-of-sample extensions as well. The proposed extension is based on the score variables, which correspond to the projections of the mapped out-of-sample points onto the eigenvectors found

in the training stage. The cluster indicators can be obtained by binarizing the score variables for the out-of-sample points as follows:

$$\text{sign}(e_{test}^{(l)}) = \text{sign}(\Omega_{test}\alpha^{(l)} + b_l 1_{Ntest}) \tag{4}$$

where $l = 1, \ldots, k-1$, Ω_{test} is the $N_{test} \times N_{tr}$ kernel matrix evaluated using the test points with entries $\Omega_{test,ri} = K(x_r^{test}, x_i)$, $r = 1, \ldots, N_{test}$ and $i = 1, \ldots, N_{tr}$. Here N_{test} represents the number of nodes in the test set. This natural extension to out-of-sample points is the main advantage of the kernel spectral clustering framework. In this way the clustering model can be trained, validated and tested in an unsupervised learning procedure. If the Ω_{test} cannot fit the memory, then we divide the test set into blocks and perform the testing operations iteratively on a single computer. However, this operation can easily be performed in parallel in a distributed environment.

3. Model Selection by Means of Angular Similarity

Model selection is a crucial step in KSC. In order to obtain correct cluster parameters for the model, we propose a novel and computationally efficient mechanism using the concept of angular similarity. In [8], the authors used Modularity as a model selection criterion. However, the validation matrix required for Modularity calculation can blow up as the size of the network becomes large and might be infeasible to store into memory. Therefore, we need to work with the sparse adjacency lists of the nodes in the validation set instead of creating a square validation matrix. Since we are using the cosine similarity metric to estimate each element of the kernel matrix Ω, the model is free of a tuning parameter σ, unlike the original formulation of KSC [14] when using a Gaussian RBF kernel. Thus, the only parameter to be determined for our procedure is the number of clusters k in the network.

We propose a criterion *Balanced Angular Fit* for estimating the number of clusters $k > 2$ in the network. This criterion exploits the projections of the training and validation nodes in the eigenspace. For a given value of $k > 2$, we estimate the cluster memberships of the nodes in the training set X_{tr} based on the codebook $\mathcal{CB}$. We assign each training node to the cluster corresponding to the codebook vector for which its Hamming distance is the minimum. Thus, for a given value of $k > 2$, we can obtain the clustering $\Delta = \{P_1, \ldots, P_k\}$, where P_i contains the set of training nodes belonging to the i^{th} cluster. We calculate the cluster mean (μ_i) for each cluster w.r.t. to the projections of the training nodes belonging to the i^{th} cluster in the eigenspace.

Once we obtain the cluster means for all the clusters, we use the projections of the validation nodes in the eigenspace. The idea is to calculate the angular similarity between the projection of each validation node and each of the cluster means. The cluster mean that makes the least angle with the projection of the validation node is the closest or most similar for that node. Thus, we assign the cluster corresponding to that cluster mean to the given validation node. For each validation node ($valid_i$), we want to obtain $\max_j \cos(\theta_{j,valid_i})$, where

$$cos(\theta_{j,valid_i}) = \frac{\mu_j^T e_{valid_i}}{\|\mu_j\| \|e_{valid_i}\|}, j = 1, \ldots, k. \tag{5}$$

The closer the projection of the validation node is to that of a given cluster mean, the smaller the angle it has with it and the larger the cosine value of that angle. Therefore, for each validation node we have

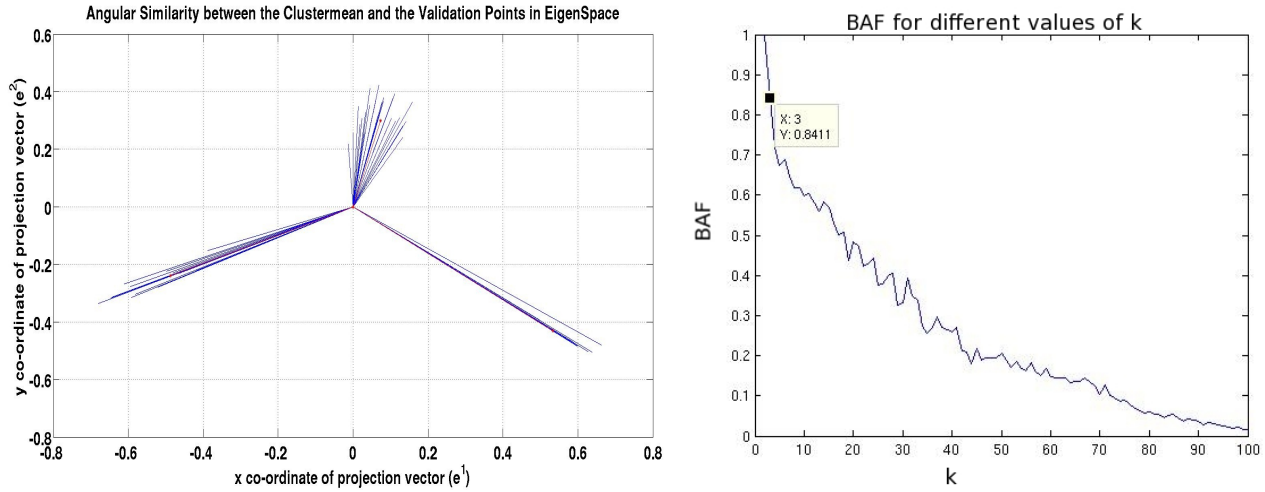
the cluster to which it is assigned along with the maximum cosine similarity value. We maintain the maximum cosine similarity value for each validation node in a dictionary $MaxSim$. The dictionary is maintained as $MaxSim(valid_i) = \cos(\theta_{j,valid_i})$, where $\cos(\theta_{j,valid_i}) = \max_j \cos(\theta_{j,valid_i}), j = 1, \ldots, k$ is the maximum cosine similarity value for the validation node ($valid_i$). The obtained clustering is $\Delta_{valid} = \{Q_1, \ldots, Q_k\}$, where Q_i contains the set of validation nodes belonging to cluster i. We now define *Balanced Angular Fit* (BAF) as:

$$BAF(k) = \sum_{i=1}^{k} \sum_{valid_j \in Q_i} \frac{1}{k} . \frac{MaxSim(valid_j)}{|Q_i|} \tag{6}$$

The BAF simply sums up the cosine similarity values of all the validation nodes belonging to each cluster divided by the cardinality of that cluster. It then divides this overall value by the total number of clusters k in the network. The range of values that BAF can take is $[-1, 1]$. This is because the maximum similarity value that a validation node can have w.r.t. a cluster mean is 1 (*i.e.*, the angle between them is zero). Because we sum up the cosine similarity values of all the validation nodes in a cluster and divide it by the cardinality of that cluster, the metric is inherently balanced and this fraction cannot exceed one. This process is repeated for each cluster, and in order to normalize the metric, we divide it by the number of clusters in the network. In the worst case scenario, when all the validation nodes are wrongly assigned to clusters with whose cluster mean it makes an angle of π, the BAF can end up being -1. However, we observed empirically that the BAF value ranges between $[0, 1]$ in all our experiments. Higher values of BAF indicate better graph partitions found in the validation set. To estimate the parameter k, we iteratively increase the value of k from 3 till a maximum value and select the value of k for which the BAF is maximum. The BAF will not work for $k = 2$ as the cluster mean obtained are one-dimensional, one value is positive and the other is negative. The projections of validation nodes are also one-dimensional and either positive or negative and thus the minimum angle between the projections of the validation nodes and the best cluster mean will always be zero. Thus, the BAF value will turn out to be 1. The BAF measure can not only be used as a model selection criterion but also serve the purpose of an evaluation metric for testing the quality of the clustering. There can be several values of k for which the BAF values can be high. If the interval between these values of k is large, then it can be identified with the underlying hierarchy in the network.

In Figure 1, the red colored "*" marked points represent the cluster means in 2-D projected eigenspace where the number of cluster k in the network is equal to 3. The projections of the validation nodes are represented as blue colored "." points in 2-D. From Figure 1, one can easily conclude the presence of three clusters and the same can be inferred by BAF. We can observe that angle between the projections of the validation points and the corresponding best cluster mean is quite small. This is also inferred from the high BAF value of 0.8411 for $k = 3$. We also observe that the nodes in the validation set whose projections are in the first quadrant have maximum deviation from their cluster mean, which affects the overall BAF value. From the figure on the right, we observe that for $k = 2$, the BAF value is equal to 1 as suggested earlier and thus ignored while reporting the correct number of clusters.

Figure 1. Model Selection for KSC based on BAF.



4. Selecting a Representative Subgraph

An inherent requirement of the KSC method is to generate a model on the training set. Since, KSC generates a $N_{tr} \times N_{tr}$ size kernel matrix, if the size of N_{tr} becomes too large then the KSC procedure would become infeasible. Thus, we need to select a subset of nodes that is representative for the underlying community structure. The obtained subgraph allows to build a model on it during the training phase and provides a meaningful out-of-sample extension to nodes that are not present in the training set. State-of-the-art techniques for sampling large scale graphs include SlashBurn algorithm [18], Snowball Expansion sampling [16], Metropolis [19] and random sampling techniques. An exhaustive comparison of these methods with Fast and Unique Representative Subset (FURS) selection approach was done in [17]. FURS is computationally less expensive and preserves the inherent community structure as evaluated on the various quality metrics like computation time, clustering coefficient, degree distribution, coverage, fraction of communities preserved and variation of information metric, as described in [17].

The motivation is to select a subset of nodes that approximately maximizes the coverage of the graph under the constraint that the selected nodes belong to different dense regions in the graph. Coverage is defined as the ratio of the number of unique nodes directly reachable from the nodes in the selected subset to the total number of nodes in the graph. Coverage is determined by the degree distribution of the nodes in the graph. The idea is to first sort the nodes based on their degree in descending order during each iteration and pick the node with highest degree. Once such a node is selected, its immediate neighbors are deactivated (as they can be reached directly from this node) during that iteration and the node is placed in the selected subset without affecting the graph topology. We then select the node with highest degree among the active nodes and the process is repeated until either all the nodes are deactivated or we reach the subset size. If all nodes are deactivated before we reach the desired subset size, a new iteration is started and the deactivated nodes are reactivated. They are sorted according to their degree in descending order and the process of node selection, deactivation and reactivation is repeated till we obtain the desired subset. FURS results in a subset of nodes that span *most* or *all* of the communities in the network. We outline the FURS approach in Algorithm 1.

Algorithm 1: FURS Algorithm

Data: A list of nodes with their corresponding degree values $L = (V, f(V))$, the median degree M and the adjacency matrix A containing information about neighbors $Nbr(v_i), \forall v_i \in V$.

Result: A subset of representative nodes S whose cardinality is N_S

$L := (V, f(V)), \forall v_i \in V$ such that $f(v_i) > M$

$L :=$ sort(L) // Based on the degree values in descending order

while $|S| < N_S$ **do**

  // **REACTIVATION** Step

  if $L == \{\}$ **then**

    $L := L \cup \{v_i, f(v_i)\}, \forall v_i \in V$ that was deactivated.

    $L :=$ sort(L) // Based on the degree values in descending order

  end

  // **HUB SELECTION**

  $v_1 := L.pop()$ // pop out the highest degree node

  $S := S \cup v_1$ // Add to output set S

  $Nb \leftarrow Nbr(v_1)$ // Neighboring nodes of v_1

  // Create a temporary list and add Nb along with their corresponding degree, if $Nbr(v_1)$ is not already present in the list.

  // **DEACTIVATION** Step

  $L := L.deactivate(Nb, f(Nb))$ // Deactivate the neighbors of v_1

  .

end

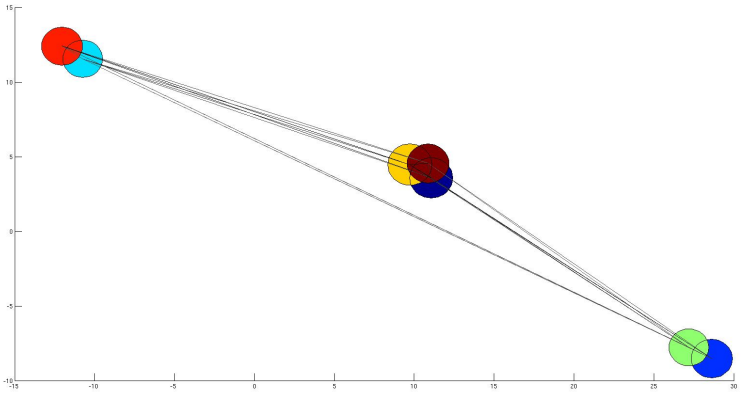
For big data networks, which cannot fit into memory, FURS can be applied to each individual block of the network that can be stored into memory. Thus, the obtained subset would approximately maximize the coverage of the network and capture the inherent community structure.

4.1. Subset Selection from Synthetic Network

We first demonstrate the FURS selection technique on a small synthetic network. The synthetic graph was generated by the software provided by Fortunato as mentioned in [6]. This software is used to generate an undirected and unweighted synthetic graph of $5,000$ nodes with $125,020$ edges and 7 communities. The software allows to set a mixing parameter μ that reflects the extent of overlap among the communities. We set the mixing parameter to a moderate value of $\mu = 0.1$ (higher values of mixing parameter lead to highly overlapped communities). Figure 2 depicts the communities as discs of different colors and reflects the extent of overlap between these communities.

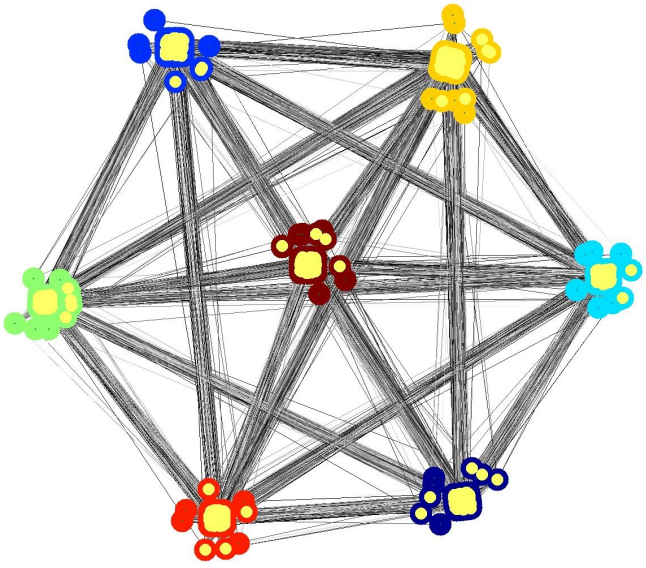
In Figure 2, we do not highlight all the nodes and all the edges. Rather, we show the communities as discs. The communities that are overlapping have more connections among themselves as in comparison with their connections to the other communities.

Figure 2. Communities and their extent of overlap in the synthetic network.



Some of the statistics about the network are that the minimum degree of a node is 17, the maximum degree is 40 and the median degree of the graph is 23. The minimum number of nodes in a community is 603 and the maximum number of nodes in a community is 913. We then perform our subset selection technique resulting in the sample set S. The subset size is set as 15% of the nodes in the network as suggested by the authors in [20]. Figure 3 represents the network $G = (V, E)$ with all the vertices and the edges between these vertices. It also captures the set of representative nodes S as the yellow colored "o" shaped vertices within the network.

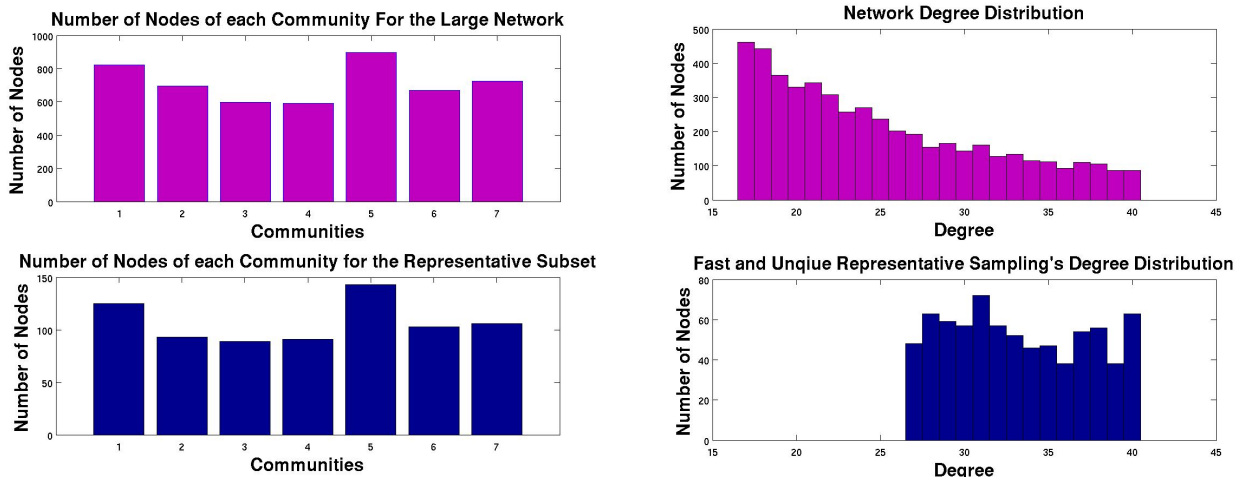
Figure 3. Network along with its representative subset of nodes.



The FURS selection technique concurs with our claim that the representative subset consists of members of *all* or *most* of the communities of the graph. This can be observed easily from Figure 3 where we see that the yellow colored "o" shaped nodes, which are a by-product of FURS selection technique and span all the communities. We further show this explicitly in Figure 4, where we depict that the fraction of nodes selected from each community are nearly proportional to the size of the community

in the original graph. In order to show that the selected nodes have high degree, we present the degree distribution of the entire data network and compare it with the degree distribution of the subset obtained via FURS in Figure 4. From Figure 4, we observe that all the selected nodes have degree greater than M (median degree).

Figure 4. Comparison of data and degree distribution for the synthetic network and the FURS selected subgraph.



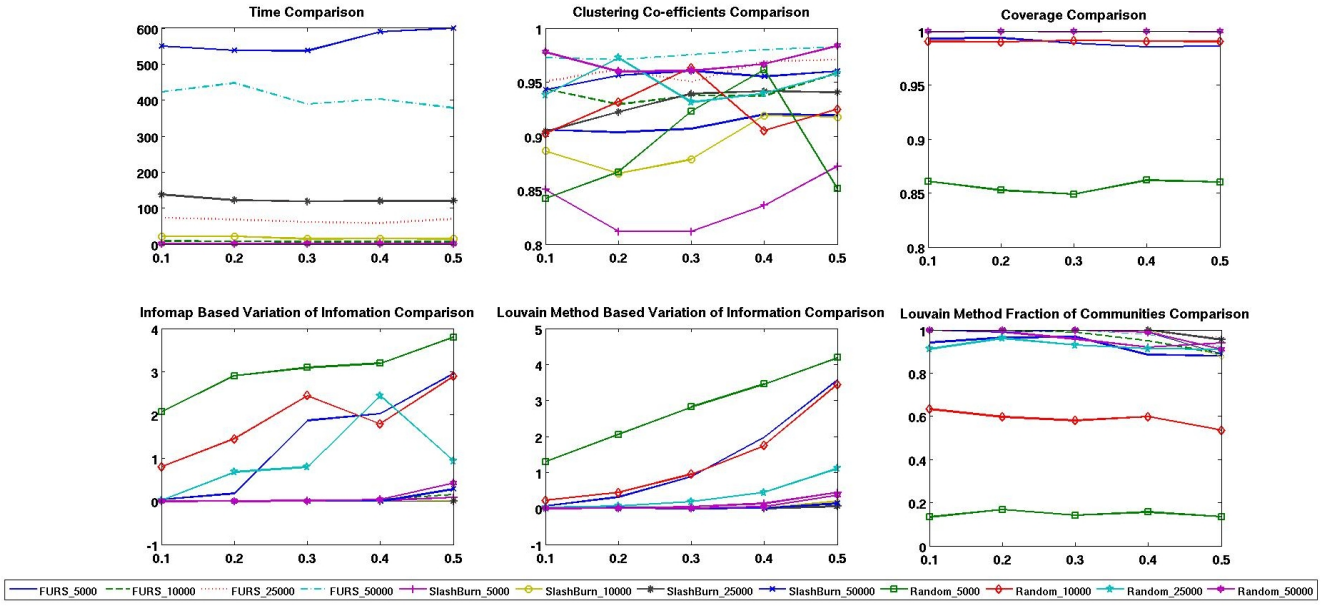
4.2. Comparison with other Techniques on Synthetic Networks

We also compare the FURS selection technique with SlashBurn and Random sampling methods on a variety of synthetic networks of increasing size and using multiple mixing parameters as depicted in Figure 5. These synthetic networks were also generated by the software provided by Fortunato as mentioned earlier. We maintain the size of the subset as 15% of the nodes in the network based on experimental findings in [20] and set the k for "k-hubset" for SlashBurn as 0.5% of the nodes as recommended in [18]. For the Infomap [7] and Louvain [9] community detection techniques, we evaluate the subset obtained by FURS on various metrics such as computation time, clustering coefficients (CCF), coverage, variation of information (VI). We also evaluate the ratio of the number of communities in the large network to the number of communities obtained in the subgraph for the different sampling techniques using Louvain method (fraction of communities preserved). These metrics and a bunch of other metrics are described in detail along with their evaluations on several community detection algorithms in [17].

In Figure 5 the lines determine the value of evaluation metrics like time required, clustering coefficient, coverage, variation of information and fraction of communities covered for each value of mixing parameter $\mu \in \{0.1, 0.2, 0.3, 0.4, 0.5\}$. These lines correspond to 3 different sampling algorithms including the FURS selection, SlashBurn and Random sampling methods on synthetic networks containing $5,000$, $10,000$, $25,000$ and $50,0000$ nodes respectively. Several of these values are exactly the same and hence some of these lines completely overlap as observed from Figure 5. From Figure 5, we observe that Random sampling is the least expensive computationally but doesn't preserve the original community structure. This can be observed from the variation of information (VI) for Louvain and

Infomap method (lower values of VI are better) and also the fraction of communities preserved for Louvain method. Surprisingly, the coverage value turns out to be high for Random sampling except for networks with 5000 nodes. The SlashBurn algorithm is computationally expensive and doesn't capture the CCF as well as FURS and Random sampling techniques. However, the SlashBurn approach is highly consistent w.r.t. the other evaluation metrics. The FURS selection technique is computationally less intensive than SlashBurn and better preserves the CCF. With the exception of synthetic networks with 5000 nodes, the FURS technique preserves the community structure of larger networks even with high mixing parameter as depicted in Figure 5. So, for large scale networks it is better to use the FURS selection technique.

Figure 5. Comparison of FURS, SlashBurn and Random sampling techniques for various evaluation metrics on synthetic networks with $5,000$, $10,000$, $25,000$, $50,000$ nodes, with mixing parameter μ varying from 0.1 to 0.5 along the x-axis and the value of the metric plotted on the y-axis.



We provide an algorithm that summarizes the KSC approach for big data networks in Appendix A.

5. Experiments and Analysis

We conducted experiments on several big datasets, including a synthetic network with $500,000$ nodes, a social network with about 4 million nodes, a road network of city with around 2 million nodes, and YouTube network with more than 1 million nodes. These real world datasets are obtained from [26].

5.1. Dataset Description

- Synthetic Network: The synthetic network is generated from the software provided in [6] with a mixing parameter of 0.1. The number of nodes in the network is $500,000$, the number of edges in the network is $23,563,412$ and the number of communities in the network is 6.

- YouTube Network: In YouTube social network, users form friendship with each other and the users can create groups that others can join. This network has more than 1 million nodes and around 2.5 million edges. Thus the network is highly sparse.
- roadCA Network: A road network of California. Intersections and endpoints are represented by nodes and the roads connecting these intersections are represented as edges. The number of nodes in the network is around 2 million and the number of edges in the network is more than 5.5 million.
- Livejournal Network: It is a free online social network where users are bloggers and they declare friendship among themselves. The number of nodes in the network is around 4 million and the network has around 35 million edges.

5.2. FURS on these Datasets

We first apply the FURS technique on these datasets to select a training set and validation set of nodes. As mentioned earlier, the maximum number of nodes that we select using FURS selection technique is $5,000$ nodes in order to have a kernel matrix that adheres to the memory restrictions. The step that we follow is to first select the training set using FURS, then these set of nodes are removed from the graph. We then run another iteration of FURS to select the validation set of nodes. Table 1 highlights the values of various evaluation metrics for these datasets for the FURS selection technique for the training set of nodes.

Table 1. Various evaluation metrics on FURS for each dataset.

Dataset	Nodes	Edges	Time	Coverage	Clustering Coefficient	Degree Distribution
Synthetic	500,000	23,563,412	103.49	0.44	0.906	0.786
YouTube	1,134,890	2,987,624	20.546	0.28	0.975	0.959
roadCA	1,965,206	5,533,214	30.816	0.135	0.89	0.40
Livejournal	3,997,962	34,681,189	181.21	0.173	0.92	0.953

From Table 1, we can observe that even after selecting just $5,000$ nodes, which is equivalent to 0.01, 0.0045, 0.0025, 0.00125 fraction of nodes in the four networks respectively, the coverage value is quite high. The clustering coefficient and degree distribution values have been converted into similarity metric as described in [16]. The maximum value for the clustering coefficient and degree distribution can be 1. Hence, the higher the value, the better the quality of the subset selected. We observe from Table 1 that these quality metrics have quite high values with the exception of 0.4 value of degree distribution for roadCA network. We also notice that the time required for subset selection for the Synthetic network is more than that for networks like YouTube and roadCA, which have more nodes. However, this is because the Synthetic network is much denser than these real world networks with around 23 million edges in comparison with nearly 2.5 and 5.5 million edges in the YouTube and roadCA networks respectively.

5.3. Results and Analysis

The kernel spectral clustering results in a model based on the subgraph selected by the FURS subset selection technique and uses its out-of-sample extension property to provide cluster labels for new unseen nodes. Since most of the spectral clustering methods, graph partitioning methods and graph clustering methods require to take into consideration the full network into the main memory, it would be unfair to compare KSC with these methods. There are several graph clustering techniques like Louvain method, Infomap method, CNM [4], which can scale up to million nodes on a single computer. However, if the size of the network increases such that it can no longer fit in the memory, then these methods would become infeasible.

Figure 6. BAF for different values of k for the various big data networks.

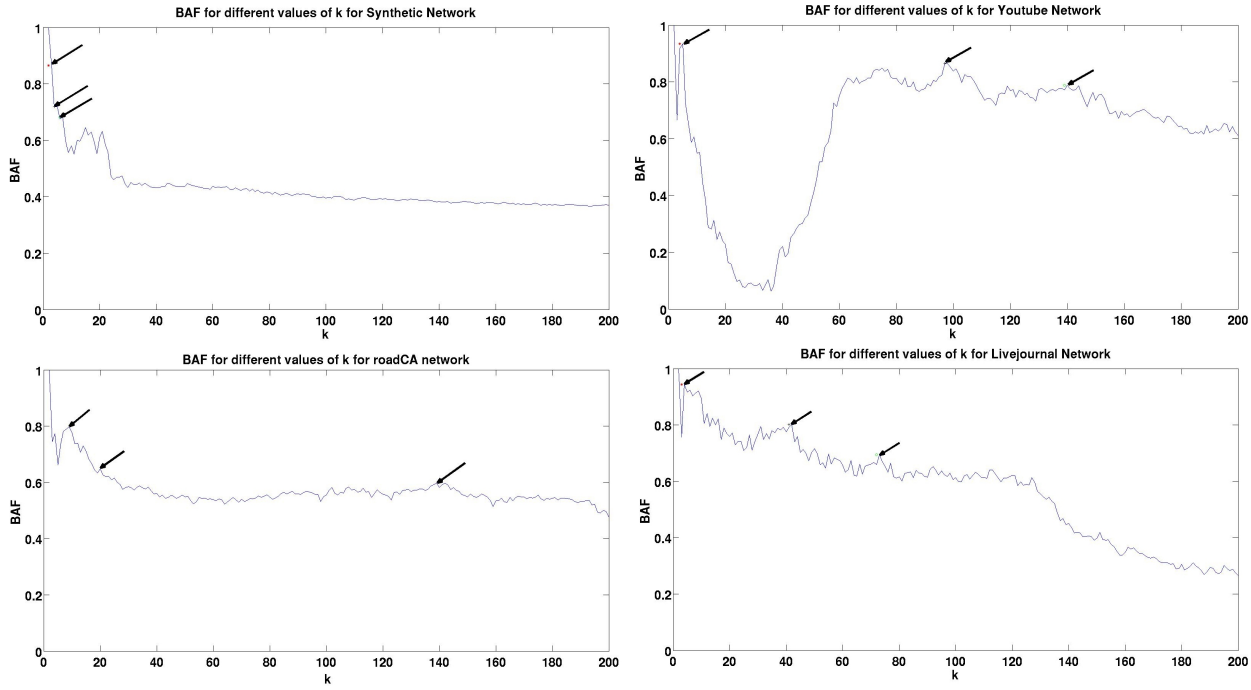


Figure 6 shows the model selection or identification of the number of clusters k for the different datasets. We plot 3 dominant peaks for each of the 4 datasets. Currently, we select the peaks based on an adhoc procedure. We sort BAF values and select the maximum and restrict from selecting peaks in the immediate neighborhood as we might miss the hierarchical structure in that case. As mentioned earlier, the BAF metric is not only suitable for model selection but can also be used as an effective cluster evaluation metric. The higher the BAF value, the better the partitioning of the network. We observe that for the Synthetic network the BAF values are high for small number of clusters. Thus, in this case we make an exception and select the peaks close to each other. For the Synthetic network we do locate a peak at $k = 6$ with $BAF = 0.6817$, which is the actual number of clusters present in the network. For the YouTube network, we observe that we reach the first dominant peak at $k = 9$ and then the BAF value starts to decrease before it starts to increase again and locates the next dominant peak at $k = 97$. This shows the effectiveness of the BAF metric for identification of hierarchical structure in the big data network. For the YouTube network the BAF values decrease initially as the value of k increases indicating that the clusters are not well-formed. However, its value start to increase from $k = 40$ as we are now obtaining the second level of hierarchy. The BAF value is 0.8654 for $k = 97$ which indicates

that there are 97 well partitioned clusters at the second level of hierarchy for the YouTube network. For the roadCA and Livejournal networks, the BAF generally follows a decreasing trend with the increment in the number of clusters with a few spurious dominant peaks as depicted in Figure 6. The maximum number of clusters in the network was fixed as 200 in our experiments and we observe that it is sufficient to provide a general trend for BAF versus the number of clusters (k) curve.

Table 2 provides details about three dominant peaks, time required for training, *i.e.*, time required for building the kernel matrix and obtaining the model $(\alpha^{(l)}, b_l)$, validation time and the time required for testing. For testing, we use the entire big data network as test set. We noticed that it is not possible to store the big Ω_{test} in the main memory and we divided the test data into blocks containing adjacency list of maximum $5,000$ nodes as described in Algorithm 2 in Appendix A. The maximum number of nodes we selected for training set is $5,000$, taking into account the memory constraints.

Table 2. Experimental results for various Big Data Networks

Dataset	**Peak**$_1$	***BAF***$_1$	**Peak**$_2$	***BAF***$_2$	**Peak**$_3$	***BAF***$_3$	**Train Time (Seconds)**	**Validation Time (Seconds)**	**Test Time (Seconds)**
Synthetic	3	0.8605	4	0.719	6	0.6817	103.45	111.42	10234.5
YouTube	5	0.9348	97	0.8654	139	0.7877	88.64	97.86	20055.45
roadCA	9	0.798	20	0.6482	138	0.5917	97.412	105.13	38960
Livejournal	4	0.94355	41	0.8014	73	0.6951	121.43	134.56	97221.4

From Table 2, we observe that the training time for building the model for these big data networks is quite small. The training time comprises of constructing the kernel matrix (Ω) and performing eigen-decomposition to obtain the model $(\alpha^{(l)}, b_l)$. The validation time comprises of creating Ω_{valid}, using out-of-sample extensions to obtain $e^{(l)}_{valid}$ and obtain the model parameter, *i.e.*, the number of clusters k using the BAF metric. The maximum time required is the test time, *i.e.*, time required to create Ω_{test} and cluster memberships using out-of-sample extensions for each block of the large network. We observe that the number of blocks into which the Synthetic network, YouTube network, roadCA network and Livejournal network are divided is 100, 227, 394 and 800 respectively. The average testing time for each block of each dataset is nearly the same as the time required for training the model for that dataset. The testing operation can easily be performed in a distributed environment. Thus, the time required for testing can be scaled down by a factor of 20–40 depending on the number of computers in the cluster of the distributed environment. We observe that the time required for training the Synthetic network is more than that of YouTube and roadCA networks, although they have more number of nodes. This is because the Synthetic network is much denser than these two real world datasets.

We also compare the proposed KSC method using BAF metric (BAF-KSC) with original KSC formulation using BLF criterion (BLF-KSC), Louvain, Infomap and CNM on evaluation metrics like Modularity (Q) and conductance (Con) for several small scale real world networks to provide a comparison of the performances. We have considered a wide range of networks varying from flight network (Openflights), network based on trust (PGPnet), biological network (Metabolic), citation networks (HepTh, HepPh), communication network (Enron), review based network (Epinion) to collaboration network (Condmat). Most of these networks can be found at [26].

Table 3. Performance comparison of BAF-KSC method with BLF-KSC, Louvain, Infomap and CNM methods on quality metrics like Modularity (Q) and Conductance (Con) for several real world networks.

Dataset	BAF-KSC			BLF-KSC [14]			Louvain [9]			Infomap [7]			CNM [4]		
	Clusters	Q	Con	Clusters	Q	Con	Clusters	Q	Con	Clusters	Q	Con	Clusters	Q	Con
Openflights	5	0.533	**0.002**	5	0.523	0.002	109	**0.61**	0.02	18	0.58	0.005	84	0.60	0.016
PGPnet	8	0.58	**0.002**	9	0.53	0.002	105	**0.88**	0.045	84	0.87	0.03	193	0.85	0.041
Metabolic	10	0.22	0.028	5	0.215	**0.012**	10	**0.43**	0.03	41	0.41	0.05	11	0.42	0.021
HepTh	6	0.45	**0.0004**	5	0.432	0.0004	172	**0.65**	0.004	171	0.3	0.004	6	0.423	0.0004
HepPh	5	0.56	**0.0004**	5	0.41	0.001	82	**0.72**	0.007	69	0.62	0.06	6	0.48	0.0007
Enron	10	0.4	0.002	7	0.21	**0.001**	1272	**0.62**	0.05	1099	0.37	0.27	6	0.25	0.0045
Epinion	10	**0.22**	0.0003	10	0.22	**0.0**	33	0.006	0.0003	17	0.18	0.0002	10	0.14	**0.0**
Condmat	6	0.28	**0.0002**	13	0.43	0.0003	1030	**0.79**	0.03	1086	0.79	0.025	8	0.38	0.0003

From Table 3 we observe that the BAF-KSC and BLF-KSC methods results in small number of clusters. This is because we consider the first peak corresponding to the highest BAF and BLF value respectively. We also observe that since the KSC method results in small number of clusters the conductance (Con) value is the quite low for most of the networks. The lower the conductance value the better the quality of the clusters. We also observe that the Modularity (Q) metric value is generally high for the BAF-KSC and BLF-KSC methods but less in comparison to Louvain method. We also observe the Q value is higher for the proposed KSC method (BAF-KSC) over the original KSC formulation (BLF-KSC) for 7 real world networks. Higher values of Modularity (Q) mean more modular graph partitions. The Louvain method is the best w.r.t. the Q metric as it optimizes the Modularity function. However, the conductance for the Louvain method for the various real world networks is generally 10 times more than the conductance for the KSC method. The CNM and BLF-KSC methods results in best conductance for Epinion networks as it identifies small number of well separated clusters for these networks.

6. Conclusions

In this paper we showed that the Kernel Spectral Clustering (KSC) method is a powerful tool for community detection in big data networks. While the problem of community detection has received a lot of attention in the past, the state-of-the-art approaches work under the assumption that the entire network can fit in the main memory. However, with the increasing amount of information, the size of the networks will only increase and big data networks may not necessarily fit in the main memory.

The KSC method employs an optimization based framework to construct the model, which has a very useful out-of-sample extension property. However, the model that is constructed should be such that it adheres to the memory restrictions. Therefore, there is a need to select a representative subgraph of the big data network on which the model can be built. We use the FURS selection procedure for this purpose. It selects nodes from different dense regions of the graph while maximizing the coverage and preserves the inherent community structure of the big data network.

In order to obtain the model parameters (*i.e.*, the number of clusters k in the network in case of large complex networks), we propose a novel metric *Balanced Angular Fit*. The BAF metric works with a codebook $\mathcal{CB}$ and the projections of the validation set to determine the ideal number of

clusters k in the big data network. The metric is both memory- and computationally efficient, unlike the previously proposed Modularity metric. The out-of-sample extensions property allows inferring community affiliation for unseen nodes. It is because of this property that we can handle large scale networks relatively easily. Finally, we show that the KSC method works effectively on a big Synthetic Network and several real world big data networks. Future work may focus on automatically determining the dominant peaks in BAF *versus* number of clusters curve.

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Appendix A

Algorithm 2: KSC Algorithm for Big Data Networks

Data: Given a graph $G = (V, E)$, which might not necessarily be stored in the memory.

Result: The partitions of the graph G, *i.e.*, divide graph into k clusters.

Convert and store the graph G in sparse format.

if *If G fits in the main memory* **then**

- Select the training set of nodes X_{tr} (*i.e.*, maximum size $= 5,000$ nodes) using FURS.
- Select the validation set of nodes (same size as X_{tr}) after removing the subgraph S corresponding to X_{tr} using FURS.
- Calculate the kernel matrix Ω by applying cosine similarity operations on sparse adjacency lists of $\forall i, j$ $v_i, v_j \in X_{tr}$.
- Perform eigen-decomposition of Ω to obtain the model, *i.e.*, $\alpha^{(l)}, b_l$.
- Use out-of-sample extension property to obtain the projection values for the validation set, *i.e.*, $e^{(l)}_{valid}$.
- Use BAF and $e^{(l)}_{valid}$ to estimate the number of clusters k.
- After estimating k, use the out-of-sample property and the decoding scheme to assign clusters to unseen test nodes (We use the entire network as test data).

else

- Divide G into blocks where each block contains an adjacency list of maximum $5,000$ nodes.
- To obtain training and validation nodes from all parts of the graph, divide the size of the subset to be selected by the number of blocks used to store G. For example, if the subset size is $5,000$ nodes, the number of blocks required to store the G is 10, then divide the subset size by 10 to estimate a value of 500.
- Select this estimated number of training nodes from each block by running the FURS selection technique on each block. This results in a subset of nodes that approximately maximizes the coverage of the graph.
- Run an iteration over all the blocks and remove all the edges corresponding to the selected subset of training nodes.
- Calculate the kernel matrix Ω by applying cosine similarity operations on sparse adjacency lists of $\forall i, j$ $v_i, v_j \in X_{tr}$.
- Perform eigen-decomposition of Ω to obtain the model, *i.e.*, $\alpha^{(l)}, b_l$.
- Re-perform the operations specified for selecting training nodes to select the validation set.
- If the validation set size $\gg$ training set size, it might become infeasible to store Ω_{valid} in the main memory. To overcome this problem, divide the validation set into blocks containing adjacency list of maximum $5,000$ nodes. The maximum size of Ω_{valid} would be $5,000 \times 5,000$, which can be stored in memory as mentioned earlier.
- Use out-of-sample extension property to obtain the projection values for each block of validation set, *i.e.*, $e^{(l)}_{valid_{block_i}}$.
- Use BAF on all the blocks of $e^{(l)}_{valid_{block_i}}$ to estimate the number of clusters k.
- After estimating k, use the out-of-sample property and the decoding scheme to assign clusters to unseen test nodes.
- Each block of G is used as test data and cluster memberships are assigned to the nodes in the corresponding blocks.

end

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