Simultaneous Dimensionality and Complexity Model Selection for Spectral Graph Clustering

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ABSTRACT
Our problem of interest is to cluster vertices of a graph by identifying underlying community structure. Among various vertex clustering approaches, spectral clustering is one of the most popular methods because it is easy to implement while often outperforming more traditional clustering algorithms. However, there are two inherent model selection problems in spectral clustering, namely estimating both the embedding dimension and number of clusters. This article attempts to address the issue by establishing a novel model selection framework specifically for vertex clustering on graphs under a stochastic block model. The first contribution is a probabilistic model which approximates the distribution of the extended spectral embedding of a graph. The model is constructed based on a theoretical result of asymptotic normality for the informative part of the embedding, and on simulation results providing a conjecture for the limiting behavior of the redundant part of the embedding. The second contribution is a simultaneous model selection framework. In contrast with traditional approaches, our model selection procedure estimates embedding dimension and number of clusters simultaneously. Based on our conjectured distributional model, a theorem on the consistency of the estimates of model parameters is presented, providing support for the utility of our method. Algorithms for our simultaneous model selection (SMS) for vertex clustering are proposed, demonstrating superior performance in simulation experiments. We illustrate our method via application to a collection of brain graphs.

1. Introduction

A mathematical graph encodes the relationships between objects in a network as edges between vertices. The analysis of such networks is of importance in many fields ranging from sociology (Lazer et al. 2009) and ecology (Proulx, Promislow, and Phillips 2005) to political science (Ward, Stovel, and Sacks 2011) and neuroscience (Bullmore and Bassett 2011). One of the most important tasks in the analysis of such a graph is to identify its community structure. This is essentially a vertex clustering problem, in which the set of vertices is to be partitioned into nonoverlapping groups (called clusters) according to their similarities in the underlying network structure. Numerous heuristic methodologies have been proposed for vertex clustering, including divisive approaches by iteratively removing edges based on number of shortest paths (Girvan and Newman 2002; Newman and Girvan 2004), methods of optimizing a function called "modularity" which evaluates the quality of a partition (Newman 2006; Bickel and Chen 2009; Blondel et al. 2008), algorithms employing a random walk to infer structural properties of networks (Pons and Latapy 2005; Rosvall and Bergstrom 2008), to name just a few. Among various vertex clustering approaches, we are interested here in the so-called spectral clustering methods, for their ease of implementation, theoretical consistency and good empirical performance.

Spectral clustering makes use of the spectral decomposition of some kind of similarity matrix that measures the relationship between vertices. Numerous spectral clustering algorithms based on decomposing the adjacency matrix, one natural similarity matrix of the graph, have been proposed to solve the vertex clustering problem (Rohe, Chatterjee, and Yu 2011; Sussman et al. 2012; Qin and Rohe 2013; Lei and Rinaldo 2015). Basically, the so-called adjacency spectral embedding (ASE) is first derived by factorizing the adjacency matrix; then a traditional Gaussian mixture model (GMM) clustering approach is applied on the ASE. Although the GMM o ASE methods exhibit good performance, there are two inherent model selection problems that need to be addressed to perform this clustering. The first is determining the number of eigenvectors whose rows are the low-dimensional points on which the GMM method is applied. Since these top eigenvectors comprise the ASE, we call this number the embedding dimension. The second is determining the number of clusters, essential for the approach of Gaussian mixture modeling.

The first model selection problem of determining the embedding dimension has received much attention over the years. In more general scenarios we call the corresponding eigenvectors "features" or "variables"; thus the problem is one of variable selection. A comprehensive review of variable selection...
approaches in the model-based clustering framework has been provided in Fop and Murphy (2018) and Handcock, Raftery, and Tantrum (2007). The necessity of variable selection is based on the fact that only a subset of the variables of the high-dimensional data are informative and important to the subsequent statistical inference. Using all the variables may lead to unnecessary computational cost, and may also decrease the performance of the clustering due to the irrelevance of extraneous variables. Therefore, the selection of variables which provide access to the clustering structure is of great importance. Considering the overwhelming number of methods for variable selection, we do not attempt to give a concise review of the literature. However, among various techniques for variable selection arguably the best-known methodology of principal component analysis (PCA) (Jolliffe 2011) is worth mentioning. In PCA, singular values of the data matrix measure the (square root of) the variances, which reflect the importance of the variables. Consequently, the variables corresponding to top singular values are retained, as the principle components, according to the desired dimension $d$. While determining the number of principle components $d$ is an essential step before conducting PCA, we refer the readers to Jackson (1993) for a broad review of the many so-called stopping rules. Unfortunately, there are no uniformly best rules for the task of (finite sample) dimension reduction in general due to the bias-variance tradeoff. Roughly speaking, general statistically based heuristic approaches are often inferior in many particular applications—universality is hard to come by, and such approaches necessarily suffer from their intended generality. In contrast, we develop a principled approach based on distributional assumptions that are specific to spectral graph clustering in the stochastic block model (SBM).

The second model selection problem, namely determining the number of clusters, is also a widely studied problem. As numerous approaches have been proposed on this topic, we refer the readers to the detailed reviews in Milligan and Cooper (1985) and Hardy (1996). One substantial category of such methods is the information criterion approach. These methods evaluate and compare a so-called information criterion, since it is a well-studied and easily implemented approach. These methods evaluate and compare a so-called information criterion, usually some kind of penalized likelihood, on finite mixture models with different number of mixture components and various model complexity specifications to perform model selection. Many information criteria have been proposed. To list a few: Akaike information criterion (AIC) (Akaike 1998), Bayesian information criterion (BIC) (Schwarz 1978), an entropy criterion (NEC) (Celeux and Soromenho 1996), integrated completed likelihood (ICL) (Biernacki, Celeux, and Govaert 2000), and cross-validated likelihood (Smyth 2000). Of these, we are mostly interested in BIC, Bayesian information criterion, since it is a well-studied and easily implemented approach. Moreover, the consistency of estimation for number of components using BIC is theoretically supported in Keribin (2000). The practical performance of BIC-based approaches in model selection has also been highly rated by a large number of works (Roeder and Wasserman 1997; Stanford and Raftery 1997; Dasgupta and Raftery 1998; Campbell et al. 1999).

The traditional way to address both of the model selection problems in spectral clustering is to execute the corresponding approaches sequentially. That is, one applies spectral embedding with the dimension given by some dimension reduction technique in the first step, and then one proceeds to the model selection technique on the embedded data to estimate the number of clusters in the second step. This sequential procedure of model selection suffers from two drawbacks. First, there is no one best method for estimating the embedding dimension. Even if we choose one of the modern and commonly used scree plot methods such as (Zhu and Ghodsi 2006), the result is not robust for limited data size. Second, the latter model selection procedure, namely estimating the number of clusters, completely depends on the result of the former one, because no information of the discarded variables will be available. This may cause an accumulation of errors when the former procedure performs poorly, even if the latter procedure is reliable. The original data are truncated before applying the clustering algorithm, which means it will not be possible to take advantage of useful information contained in the discarded dimensions to improve the clustering result. Therefore, jointly addressing these two model selection problems is desirable.

In this article, we propose a novel simultaneous dimensionality and complexity model selection framework for spectral graph clustering. This is inspired by breakthrough work on model selection in the framework of model-based clustering proposed in Raftery and Dean (2006). In that work, all of the variables are taken into consideration in a family of finite mixture models, which describes the distributional behavior of the raw data. The model selection procedure is conducted by comparing different models in the same family via the Bayes factor, the ratio of the posterior probability of the model given the observations. The authors utilize a BIC-based approximation to the Bayes factor that is much easier to compute. A remarkable highlight of this framework is the simultaneity of selecting variables and the number of clusters, which overcomes the drawbacks of the sequential model selection procedure. However, the method is not applicable to the current spectral vertex clustering task in the sense that neither the distributional model nor the greedy variable selection algorithm is appropriate with respect to the graph context. This inspires the development of a reliable model for spectral embedding encompassing both signal and noise dimensions and a novel methodology for vertex clustering on graphs with heterogeneous community structure. Note that our spectral graph clustering setting allows the use of the standard BIC rather than the Bayes factor approximation used in Raftery and Dean (2006).

A simultaneously developed, related approach to ours, using a Bayesian modeling perspective, is presented in Sanna Passino and Heard (2020). The basic model used is the same as in this article, with the extra complexity of the prior distributions on the parameters and their associated hyper-parameters. These are fit using Markov chain Monte Carlo, rather than the frequentist perspective presented herein. One advantage of the frequentist approach is the relative ease in handling very large graphs. We also propose a 2-step procedure which, while it does not produce a maximum likelihood solution, seems empirically to perform as well as the full maximum likelihood procedure. Of course Bayesian inference has its advantages (e.g., uncertainty quantification) and variational methods allow for scalable
Bayesian inference. Still, Sanna Passino and Heard (2020) use our basic distributional model, and we provide an extensive simulation analysis in Section 3.2 to justify our enabling conjecture.

The article is organized as follows. In Section 2, we review the existing methodology of GMM o ASE, that is, ASE followed by Gaussian mixture modeling. In Section 3, we define an extension of ASE and provide a specific GMM to characterize the potential distribution of the extended ASE based on our simulation results. In Section 4, we propose a SMS framework, as well as two heuristic algorithms specifically tailored for graphs under a SBM. In Section 5, simulation results and an illustrative real data application are presented. We conclude for graphs under a SBM. In Section 6, we work, a well last we heuristic algorithms specific adequately our basic distributional model, and we provide an extension with sequential model selection. We first introduce the existing methodology of GMM. In the context of vertex clustering, vertices from the same latent positions (Hoff, Raftery, and Handcock 2002; Hoff 2005, Laskey, and Leinhardt 1983), in which the set of vertices is partitioned into K groups, called blocks. The connectivity of the graph is parameterized by the block connectivity probability matrix B, which determines the edge probability within and between blocks. The formal definition of SBM is given below:

**Definition 2 (SBM).** Let G be the graph of interest with n vertices, B ∈ [0, 1]^{K×K} be the block connectivity probability matrix, and π = (π(1), . . . , π(K)) ∈ (0, 1)^K be the vector of block membership probabilities such that \( \sum_{k=1}^{K} \pi(k) = 1 \). G is called a K-block SBM graph, denoted by SBM(n, B, π), if there is a random vector \( \tau = (\tau_1, . . . , \tau_n) \), called the block memberships, that assigns vertex i to block k with probability \( \pi(k) \). Mathematically, \( \tau_1, . . . , \tau_n \) are iid categorical random variables distributed according to parameter \( \pi \), that is,

\[
P[\tau_i = k] = \pi(k)
\]

for all \( i \in [n] \) and \( k \in [K] \). Furthermore, the edges are generated according to an edge probability matrix \( P \), whose \( i,j \)th entry equals \( B_{\tau_i, \tau_j} \). Equivalently, \( A_{ij} \), the entry of the adjacency matrix \( A \), is independently Bernoulli distributed with parameter \( P_{ij} = B_{\tau_i, \tau_j} \), that is,

\[
P[A_{ij}] = (B_{\tau_i, \tau_j})^{A_{ij}}(1 - B_{\tau_i, \tau_j})^{1-A_{ij}}
\]

for all \( (i,j) \in [n] \times [n] \).

In addition, it is convenient in some cases to consider that the block membership vector \( \tau \) is not random but fixed. We call such a graph a SBM conditioned on block memberships, denoted by SBM(B, \( \tau \)). If an undirected graph \( G \sim SBM(B, \tau) \) and \( B \) is positive semidefinite, then \( G \) can be represented by an RDPG, the random dot product graph, with at most \( K \) distinct latent positions. In this case, all vertices in the same block have the same latent vectors. This provides the connection between the SBM with positive semidefinite block connectivity probability matrix and the RDPG. For the relationship between an SBM with indefinite block connectivity probability matrix and a generalized RDPG, we refer the reader to Rubin-Delanchy et al. (2017).

### 2.2. Spectral Graph Clustering via ASE

Given an observed SBM graph, our inference task is to identify the underlying memberships of the vertices corresponding to the blocks to which they belong. That is, if \( G \sim SBM(B, \tau) \), our goal is to infer the graph parameter \( \tau \) (in the presence of nuisance parameters \( K \) and \( B \)) from the observed adjacency matrix \( A \). Among various techniques, spectral clustering methods (Von Luxburg 2007) are effective, well-studied and computationally feasible approaches through which the vertices of a graph are mapped to points in Euclidean space. These Euclidean points are the data on which traditional clustering methods can be applied to finalize the clustering procedure. Spectral clustering performs spectral decomposition on some “similarity” matrix that represents the graph. There are two natural similarity matrices, namely the adjacency matrix and the Laplacian matrix of the graph. While the choice between adjacency matrix and Laplacian matrix is always debatable, it has been shown that neither of them dominates the other.
(Tang and Priebe 2018; Cape, Tang, and Priebe 2019; Priebe et al. 2019). Properties of the top eigenvectors of the adjacency matrix, known as the ASE, have been analyzed in the literature (Sussman et al. 2012; Sussman, Tang, and Priebe 2014; Athreya et al. 2016; Lyzinski et al. 2017; see Athreya et al. 2018 for a recent survey) where it has been proven that the rows of ASE converge to the corresponding underlying latent positions. In this article, we focus on the spectral method using the adjacency matrix for ease of analysis.

There are two model selection problems in spectral clustering of an SBM graph. One is to estimate the embedding dimension $d$, while the other is to estimate the number of blocks $K$. The traditional solution of these two model selection problems proceeds sequentially, namely applying variable selection or dimension reduction techniques to estimate $d$ (let the estimate be $\hat{d}$) first, then applying model selection techniques on the data with $\hat{d}$-dimensional ASE to estimate $K$. Since the two model selection procedures are executed in sequence, we refer to this approach as sequential model selection. For example, one can apply any so-called scree plot method (an effective method to locate the “elbow” in the scree plot is proposed in Zhu and Ghodsi (2006); we refer to this method as “ZG” in this article) to estimate the embedding dimension, and then apply the BIC approach (Keribin 2000) on the spectral embedding to select the number of clusters for the subsequent GMM clustering. We denote this sequential model selection approach BIC ◦ ZG for the purpose of comparison.

### 3. Models for Extended ASE

#### 3.1. Extended ASE

In practical settings, the rank of the edge probability matrix $P$, namely the ideal embedding dimension $d$, is unknown, because $P$ is unobserved and we observe only the adjacency matrix $A$ which is a noisy version of $P$. To address the problem of estimating $d$, we hereby define the extended ASE:

**Definition 3 (Extended ASE).** Let $G$ be an undirected graph with $n$ vertices, and $A ∈ \mathbb{R}^{n \times n}$ be its symmetric adjacency matrix. Let the spectral decomposition of $A$ be

$$ A = \hat{U} \hat{\Lambda} \hat{U}^T. \quad (4) $$

Here, $\hat{\Lambda} ∈ \mathbb{R}^{n \times n}$ is a diagonal matrix with eigenvalues of $A$ on its diagonal in descending order. That is, $\hat{\Lambda} = \text{diag}(\hat{\lambda}_1, \ldots, \hat{\lambda}_n)$ with $\hat{\lambda}_1 ≥ \cdots ≥ \hat{\lambda}_n$. $\hat{U}$ is an orthogonal matrix whose columns are the corresponding eigenvectors of $A$. For a given integer $D$ satisfying $1 ≤ D ≤ n$, called the embedding dimension, the extended ASE of $G$ with dimension $D$ is given by

$$ \hat{Z} = \hat{U}_{[D]} \hat{\Lambda}_{[D]}^{\frac{1}{2}}, \quad (5) $$

where $\hat{U}_{[D]} ∈ \mathbb{R}^{n \times D}$ is the submatrix of $\hat{U}$ consisting of its first $D$ columns, and $\hat{\Lambda}_{[D]} ∈ \mathbb{R}^{D \times D}$ is the submatrix of $\hat{\Lambda}$ consisting of its first $D$ rows and columns.

In practice, $D$ can be taken as a loose upper bound for $d$. Because the methodology developed herein allows $D ≫ d$ and allows subsequent post-embedding estimation of $d$, such an upper bound is usually easily obtained either from first principle assumptions about the problem or other external information. Typically one considers the scree plot—the plot of the decreasing eigenvalues against $d$—and looks for an “elbow” using a profile likelihood (Zhu and Ghodsi 2006) or similar method. Since the number of clusters $K$ is a bound on the rank of $P$, one could use the maximum value of $K$ as the choice for $D$. Alternatively, one can look at scatterplots of the embedding to look for dimensions in which no clustering is apparent; this is perilous, but can provide some information to add to that of scree plots or other information. Finally, if one has a Bayesian inclination, and can suggest a reasonable prior on $d$, this prior can be used to determine a reasonable choice for $D$. The number of blocks gives an upper bounded for the rank of $P$, but since this is unavailable, we must rely on other methods. Once again, the information that would be used in a Bayesian prior on the number of blocks can be used to determine an upper bound on $K$. A great advantage of our approach is that we are happy with (perhaps greatly) over-estimating $d$ with $D$, as our methodology allows this first choice to be remedied later, whereas conventional spectral clustering is constrained to proceed with the first embedding dimension.

In this article, we assume $D$, the embedding dimension of the extended ASE, is always given without estimation. From the formula (5), it is immediate that the first $d$ columns of $\hat{Z}$ is the regular ASE, the ASE, $\hat{X}$. The extended ASE $\hat{Z} ∈ \mathbb{R}^{n \times D}$ can be partitioned into two parts as $\hat{Z} = [\hat{X}, \hat{Y}]$, where $\hat{X} ∈ \mathbb{R}^{n \times d}$ and $\hat{Y} ∈ \mathbb{R}^{n \times (D-d)}$. We call the first $d$ dimensions $\hat{X}$ the informative part, while we call the remaining dimensions $\hat{Y}$ the redundant part. If we consider the spectral decomposition of $P$, the unperturbed version of $A$, then all of the latent position information is contained in the first $d$ dimensions, justifying our terminology. We notice that all existing methods using ASE can be applied to the extended ASE simply by truncating to an estimated embedding dimension $\hat{d}$. Moreover, as our main result in the article, the extended ASE can be used to perform SMS and vertex clustering without first estimating the embedding dimension $d$.

#### 3.2. Distributional Results for Extended ASE

We seek a model-based clustering approach to perform vertex clustering directly on the extended ASE. In the framework of model-based clustering, both the informative part and the redundant part need to be jointly parameterized so as to make all models comparable. For this purpose, we need to provide a model for the entire extended ASE. A remarkable distributional result for the informative part of the extended ASE is available (Athreya et al. 2016; Tang and Priebe 2018). In Athreya et al. (2016), a central limit theorem for the rows of ASE for the RDPG, the random dot product graph, is provided. This result justifies GMM clustering for identifying the block memberships in a SBM via ASE. In Tang and Priebe (2018), the central limit theorem of ASE is restated in a stronger version, in the sense that its proof does not need an assumption that has been made in Athreya et al. (2016). Basically, the theorem states that any row of the ASE of an RDPG asymptotically follows a multivariate normal distribution centered at its conditional latent position (up to orthogonal nonidentifiability). Specifically, let
\( G \sim \text{SBM}(n, B, \pi) \), that is, \( G \) is a SBM graph. Considering the latent positions themselves follow an iid categorical distribution into \( K \) distinct possible \( d \)-dimensional vectors according to \( B \), the unconditioned version of the theorem claims that any row of the ASE of the graph \( G \) converges in distribution to a mixture of \( K \) multivariate normals, with mixing probabilities \( \pi \). The theorem gives a complete formula for the covariance matrix of each multivariate normal component, thus fully characterizing the marginal distributional behavior of the informative part of the extended ASE.

To obtain empirical understanding of the distributional behavior of the redundant part of extended ASE, we consider the extended ASE. The observationsof the distributional behavior of the redundant part \( \hat{Y} \) are as follows.

**Observation 1** (The within-block sample mean of rows of \( \hat{Y} \) tends to zero as \( n \) increases). Figure 2 shows the results for the sample mean for the 2-block model. Denoted by \( \hat{\mu}^{(k)} \in \mathbb{R}^{D-d} \), the sample mean of the rows of redundant part \( \hat{Y} \), for all the rows belonging to block \( k \), is calculated by

\[
\hat{\mu}^{(k)} = \frac{1}{n_k} \sum_{i \in \tau_k} \hat{Y}_i,
\]

where \( n_k \) is the number of vertices assigned to block \( k \). We plot the sample mean values \( \hat{\mu}^{(k)} \) \( (k = 1, 2) \) for each dimension from 100 Monte Carlo replicates in Figure 2(a). For larger \( n \), the points are closer to zero in general. The upper tick-mark for the \( n = 200 \) plots is 0.01, while for \( n = 2000 \) it is 0.0002. In Figure 2(b), we plot the means for 100 Monte Carlo replicates for various values of \( n \) for the first redundant vector, \( \hat{\mu}^{(1)} \). While this proves nothing, even for this one simulation setting, the boxplots in Figure 2(b) certainly support our Observation 1.

**Observation 2** (The within-block sample variances of rows of \( \hat{Y} \) (for each dimension) tend to constants as \( n \) increases, but the values of these constants are distinct across different blocks). Figure 3 shows the results for the sample variances. For each dimension \( s \), the sample variance of the rows of \( \hat{Y} \), for all the rows belonging to block-\( k \), is calculated by

Figure 1 depicts the informative part \( \hat{X} \) for the two different block models described above, entirely in agreement with theory. Colors indicate block membership. Each graph was drawn with \( n = 1000 \) vertices.

The observations of the distributional behavior of the redundant part \( \hat{Y} \) are as follows.

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Figure 2. (a) Boxplots of 100 Monte Carlo replicates of the sample mean of the redundant part \( \hat{\gamma}_i \) for all \( i \) in block 1 (top) and block 2 (bottom). The graphs are drawn from the 2-block SBM(\( n, B, \pi \)) with \( B \) and \( \pi \) given in the text. The number of vertices of the graphs is \( n = 200 \) (left) and \( n = 2000 \) (right). The extended ASE is applied with dimension \( D = 80 \). (b) The sample mean of the redundant part of \( \hat{\mu}^{(k)}_1 \) for \( n = 200 \) to \( n = 16,000 \). Again, the top plot corresponds to block 1, the bottom to block 2. In all the simulations, 100 graphs are generated, so each box corresponds to 100 observations.

Figure 3. The within-block sample variance of rows of \( \hat{Y} \) for each redundant dimension. The graphs are drawn from the 2-block SBM(\( n, B, \pi \)) with \( B \) and \( \pi \) given in the text. The number of vertices is varied from 200 to 16,000, denoted by colors. The extended ASE is applied with dimension \( D = 80 \). The sample variance is calculated from dimension 3 to dimension 80. (a) Sample variance values from 100 Monte Carlo replicates for \( n = 1000 \) (top) and \( n = 16,000 \) (bottom). Boxplots are used to indicate the variation of the values. In each of the two panels, the boxes with larger values correspond to Block 1, and the ones with smaller values correspond to Block 2. (b) Curves of the median of 100 Monte Carlo replicates of the sample variance values against the dimensions for the values of \( n \) indicated in the legend. To avoid overplotting and for better comparison across the values of \( n \), we have multiplied the value of \( \hat{\sigma}^2 \) by \( n \) in this plot. The solid curves correspond to the first block, and the dashed curves to the second block.
where \( n_k \) is the number of vertices assigned to block \( k \) and \( \hat{\mu}_i^{(k)} \) is corresponding sample mean in block-\( k \). We plot the sample variance values \( \hat{\sigma}_s^{2(k)} \) for each dimension from 100 Monte Carlo replicates in Figure 3(a). In each panel, the boxplots indicate the variances for the two blocks, the lower set in each panel corresponding to the first block, the upper to the second. For relatively small graphs \((n = 1000, \text{top panel})\), the variances are clearly different across the dimensions, indicating that for these graphs a modified model may be appropriate—although the extra measurement error inherent in these more complex models may argue for using the simpler model of a constant variance, particularly if it is assumed that there are a small number of redundant variables. For larger graphs \((n = 16,000, \text{bottom})\) we see that the variances appear constant and distinct for the different blocks. To investigate the structure of the variance for a range of graph orders, we show in Figure 3(b) the medians of the variances for 100 Monte Carlo replicates for various values of \( n \). Again we see that for small \( n \) there is clearly a difference in the variances for the different dimensions, but this difference becomes less pronounced for larger \( n \). Again, these empirical results, narrow though they may be, certainly support our Observation 2.

**Observation 3** (The within-block sample covariance matrix of rows of \( \hat{\bar{Y}} \) tends to diagonal, and the covariance between informative and redundant dimensions tends to zero, for large \( n \)). Figure 4 shows the results for the sample covariance matrix. The sample covariance matrix of the rows of \( \hat{Z} \), for all the rows belonging to block-\( k \), is calculated by

\[
\hat{\Sigma}^{(k)} = \frac{1}{n_k - 1} \sum_{i \in \tau,=k} \left( \hat{Z}_i - \overline{\hat{Z}}^{(k)} \right) \left( \hat{Z}_j - \overline{\hat{Z}}^{(k)} \right)^T,
\]

where \( n_k \) is the number of vertices assigned to block \( k \), \( \hat{Z}_i \in \mathbb{R}^{D \times 1} \) is the \( i \)th row of extended ASE (but regarded as a column vector), and \( \overline{\hat{Z}}^{(k)} \in \mathbb{R}^{D \times 1} \) is the corresponding sample mean for block \( k \). We plot the sample covariance matrix \( \hat{\Sigma}^{(k)} \) for \( n = 200 \) in Figure 4(a) and \( n = 2000 \) in Figure 4(b). The matrix contains both informative dimensions and redundant dimensions. We observe that the diagonal values in the matrix of redundant dimensions concentrates on a constant for \( n = 2000 \), which is consistent with the result shown in Observation 2 and Figure 3. The off-diagonal values in the matrix of redundant dimensions tend to zero as \( n \) increases. For \( n = 2000 \), the covariance matrix presents a block diagonal structure, partitioned by the true embedding dimension \( d \). These provide evidence that the within-block sample covariance matrix of rows of \( \hat{\bar{Y}} \) tends to be diagonal, and the covariance between informative and redundant dimensions tends to be zero, for large \( n \). Further evidence that the off-diagonal terms are zero is given in Figure 5, depicting boxplots of all the off-diagonal terms in the redundant part for 100 Monte Carlo replicates for the 2-block model, for various values of \( n \) between 200 and 4000.

The above results provide the impetus for several observations about the distribution of the extended ASE of a SBM. Although we do not present results from more extensive simulations, the plot in Figure 1 suggests (and the theoretical results mentioned support) a GMM model with general mean vectors and covariance matrices is appropriate for the informative part of the embedding. For the redundant part, asymptotically, it appears that the block-conditional means are zero, and the block-conditional covariances are diagonal. There is some evidence that (again asymptotically) the block-conditional variances for redundant are the same, although for small \( n \), and in particular for large \( d \), these variances may well be different, as suggested in Figure 3(b). For our simulations, “small \( n \)” seems to be in the thousands, but of course this would depend on the specific structure of the SBM. Since the extra block-conditional information in these variance differences is likely to be small,
we will assume the simpler model where all the redundant variances are equal within blocks, but this is an area for future investigation.

The above simulations illustrate well the reasons for our assumptions about the model. To see that these assumptions are not unique to the specific cases we consider, we ran a much more extensive set of simulations. Just one representative example is depicted in Figure 6. In this model, we draw a random probability matrix

$$P = \begin{pmatrix} p_1 & q \\ q & p_2 \end{pmatrix}$$

with $q \sim U[0, 0.1]$ and $p_1 \sim U[q, 0.2]$, ordered so that $p_1 \geq p_2$.

If our observations are correct, we should expect that the first two means are arbitrary but different, and that the $\Sigma_{s,t}$ are different for $s = 1, 2$. We also expect to see $\mu_s = 0$ for $s > 2$, and off-diagonal covariances are 0 for $s_1, s_2 > 2$. For comparison, the gray boxes in the bottom right are a simulation in which for each graph and each block, 5000 independent normal variates are drawn from an 18-dimensional Gaussian with mean 0 and diagonal covariance equal to the diagonal of the covariance for that block. All off-diagonal terms in the covariance fitted to the data are then collected into the gray box. This shows that the range of variation that we observe in our model is well within that which we would expect for data drawn from the model.

### 3.3. Probability Models for Extended ASE

For the extended ASE of an SBM graph, the theoretical result for its informative part and the conjecture for its redundant part are discussed above. There are few theoretical results about the redundant part in the literature. However, a distributional model is important and necessary for model-based clustering. So we provide a finite mixture model for the extended ASE.

Although it has not been proven analytically at this point, we believe the model is asymptotically close to the truth—wrong but potentially useful, in George Box’s aphorism—based on both our observations of the large sample behavior of the redundant part and the performance based on this model on the subsequent inference task.

We first state mathematically our conjectures regarding the distribution of the redundant part $\hat{Y}$ of the extended ASE. We consider a $K$-block SBM($n, B, \pi$). Any row of $\hat{Y}$ is asymptotically multivariate Gaussian distributed conditioned on its block membership. That is, for any $i \in [n]$,

$$\hat{Y}_i | \tau_i = k \approx N(\mu^{(k)}, \Sigma^{(k)})$$

if $n$ is sufficiently large. If we consider the sample statistics from the simulations to be a good estimation of the Gaussian parameters, we can further specify the model. By Observation 1, we may assume $\mu^{(k)} = 0$ for all $k \in [K]$; by Observation 2 and Observation 3, we assume $\Sigma^{(k)} = \hat{\sigma}^{(k)} I$, where $I$ is the identity matrix. So now our conjecture becomes

$$\hat{Y}_i | \tau_i = k \approx N(0, \hat{\sigma}^{(k)} I).$$

By combining this conjecture with the theoretical results for the informative dimensions, we propose a GMM as follows.

**Model 1 (GMM for extended ASE of undirected graphs).** Let

$$f(\cdot; \theta(d, K)) = \sum_{k=1}^{K} \pi^{(k)} \varphi(\cdot; \mu^{(k)}, \Sigma^{(k)})$$

be a family of density functions for a $D$-dimensional GMM random vector, where $\{\pi^{(k)}\}$ are the mixing probabilities, $\{\mu^{(k)}\}_{k=1}^{K}$ are the mean vectors, and $\{\Sigma^{(k)}\}_{k=1}^{K}$ are the covariance matrices. Furthermore, these parameters satisfy

$$\sum_{k=1}^{K} \pi^{(k)} = 1,$$

$$\mu^{(k)} = [\mu_1^{(k)}, \ldots, \mu_d^{(k)}, 0, \ldots, 0]^T,$$
For $n = 5000$, 10,000 random symmetric $2 \times 2$ probability matrices are computed (see the text) and a stochastic block model with $n_1 = 2500$ and $n_2 = 2500$ nodes is drawn, and the embedding to $D = 20$ is computed. In all plots, the superscript corresponds to block (community) and subscripts denote dimension (variante). The top left plot shows the means for the two blocks for dimensions one and two. The top right plot shows the means for the two blocks for dimensions $s > 2$. The variances for $s = 1, 2$ are shown in the bottom left, first two boxes, and for $s > 2$ in the other two blocks. The off-diagonal covariances are shown in the bottom right plot. The two to the left of the dotted vertical line are for the informative dimensions, $s = 1, 2$, the others are for $s = 2, 3$ and $s > 2$. The gray boxes show the covariance for Gaussian variates drawn from the corresponding model. See the text.

$$\Sigma^{(k)} = \begin{bmatrix} \hat{\Sigma}^{(k)} & 0 \\ 0 & \sigma^{2(k)} I \end{bmatrix},$$

where $\hat{\Sigma}^{(k)}$ is a $d \times d$ positive semidefinite matrix, and $I$ is a $(D - d) \times (D - d)$ identity matrix. In this notation, $\theta(d, K)$ denotes the parameters $\{\pi^{(k)}, \mu^{(k)}, \Sigma^{(k)}\}_{k=1}^{K}$, specifically $\theta(d, K) = \{\pi^{(k)}, [\mu^{(k)}_1, \ldots, \mu^{(k)}_d], \hat{\Sigma}^{(k)}, \sigma^{2(k)} I\}_{k=1}^{K}$, which belongs to the parameter space $\Theta(d, K)$ for GMM model $F_{d,K}$. Our GMMs $F_{d,K}$ are models for data of a given dimensionality $D$ and posit a mixture of $K D$-variate normals for that data. Because we are claiming consistency only for the model complexity parameter estimates $d$ and $K$—that is, our SMS yields $(\hat{d}, \hat{K}) \rightarrow (d_0, K_0)$ as per Theorem 1—and are making no claims about the parameters of the GMM itself—the parameters of the individual multivariate normals themselves, and the mixing coefficients — nonidentifiability within a model $F_{d,K}$ does not concern us; we just need identifiability in terms of the model complexity parameters $d$ and $K$.

Identifiability Assumption. For any $(d, K) \neq (d', K')$ there does not exist $f \in F_{d,K}$ and $f' \in F_{d', K'}$ such that $f = f'$. This is ensured by noting that none of the informative dimensions have spherical covariances and 0 means. Therefore, $d$ is identifiable as the smallest value such that the latter $D - d$ components all have spherical covariances and 0 means. Furthermore, by specifying that all mixing coefficients $\pi^{(k)} > 0$ and that if $\mu^{(k)}_1 = \mu^{(k)}_2$ then $\Sigma^{(k_1)} = \Sigma^{(k_2)}$, we guarantee that $K$ is identifiable as the smallest value such that any equivalent mixture components have been merged — the “index of the economical representation” from James, Priebe, and Marchette (2001).

We establish our probability model for the extended ASE of $G \sim \text{SBM}(n, B, \pi)$. Let the extended ASE be $\hat{Z} \in \mathbb{R}^{n \times D}$, then
our conjecture states, for any \( i \in [n] \),

\[
\hat{Z}_i \sim f(\cdot; \theta^*(d_0, K_0))
\]

approximately for sufficiently large \( n \), where \( f(\cdot; \theta(d, K)) \) is the density function defined in Model 1, \( d_0 \) is the true dimension of latent positions, \( K_0 \) is the true number of blocks, and \( \theta^*(d, K) \) is the true underlying collection of parameters of the GMM. This conjecture states that the rows of the extended ASE are identically distributed as in the GMM. In fact, it has been shown that the rows of ASE are not independent (Athreya et al. 2016; Tang and Priebe 2018). (See Tang, Cape, and Priebe (2017) for one recent treatment of the dependency.) However, for ease of analysis we will proceed in the consistency theorem and in the calculation of BIC by ignoring dependency, because the independence assumption makes the estimation tractable and simulation results demonstrate acceptable performance.

The GMMs from ASE are also curved families (Athreya et al. 2016; Tang and Priebe 2018); we ignore this complexity here, but see Pisano et al. (2020) for an estimation algorithm which takes curvature into account (but still ignores dependence).

4. Simultaneous Model Selection

4.1. SMS Framework

The idea of SMS is inspired by the model comparison presented in Raftery and Dean (2006). Assume \( M_1 \) and \( M_2 \) are models that both describe the same random vector. By Bayes’ theorem, the posterior probability of the model is proportional to the product of the prior and the integrated likelihood, that is, for \( t = 1, 2 \)

\[
P(M_t | X) \propto P(M_t) P(X | M_t),
\]

where we call \( P(X | M_t) \) the integrated likelihood because it can be obtained by integrating over all the unknown parameters in the model, that is,

\[
P(X | M_t) = \int P(X | \theta_t, M_t) P(\theta_t | M_t) d\theta_t.
\]

Since usually we assume no preference between the models, we can ignore the prior probability term \( P(M_t) \) and just compare the integrated likelihoods. However, computing the integrated likelihood is impractical. Thus, we use the Bayesian information criterion (BIC).

Now we consider \( d \) and \( K \) as the model parameters in the vertex clustering problem. Let \( f(\cdot; \theta(d, K)) \) be the probability density function of the model which characterizes the distribution of \( \hat{Z}_i \), the rows of extended ASE. We assume two models differ from each other if and only if they have distinct model parameters—our Identifiability Assumption. (GMMs have well-known non-identifiabilities—in particular, labeling of components is arbitrary—which are of no practical concern in most GMM inference tasks and do not concern us here.) So selecting a model from the family is equivalent to determining the model parameters. Now we can recast the model selection problem in the SMS framework as follows. Provided we have a family of \( D \)-dimensional distributional models, each with a distinct pair of model parameters \( (d, K) \) that determine the structure of the model, the model selection problem is to choose a model from amongst all \( (d, K) \) pairs by comparing the values \( BIC(\hat{Z}; d, K) \) evaluated on the observed \( \hat{Z} \).

In the framework of SMS, a probability model \( f(\cdot; \theta(d, K)) \) for the rows of the extended ASE is needed. The model parameter \( d \) should play a similar role to the embedding dimension, which separates the informative dimensions and redundant dimensions in the extended ASE. The model parameter \( K \) should be the number of mixture components in the mixture model. If we have such a family of models that well approximates the distribution of the extended ASE with an appropriate \( (d, K) \), we can apply our SMS procedure. Fortunately, Model 1 exactly satisfies these requirements. To see this, let \( G \sim SBM(n, b, \pi) \) be the random graph and \( \hat{Z} \in \mathbb{R}^{n \times D} \) be the corresponding extended ASE. Let \( d_0 = \text{rank}(b) \) be the dimension of the latent position vectors, and let \( K_0 \) given by the dimension of \( B \) be the number of blocks in the SBM. In Model 1, \( d \) is the model parameter which determines the dimensionality of the informative part and \( K \) is the model parameter which determines the number of components. Most importantly, the rows of \( \hat{Z} \) approximately follow the distribution \( f(\cdot; \theta(d_0, K_0)) \) by the existing theorem and our conjecture. Therefore, if we use this family of models in SMS, we expect maximizing BIC will provide good estimates of the model parameters \( (d_0, K_0) \). In fact, if we assume that the rows of \( \hat{Z} \) do asymptotically follow the distribution in the model, we can prove the consistency of the model parameter estimates obtained via our SMS procedure.

4.2. Consistency of Model Parameter Estimates

We first define some notation. Let

\[
f(\cdot; \theta(d, K)) = \sum_{k=1}^{K} \pi(k) \varphi(\cdot; \mu(k), \Sigma(k))
\]

be a family of GMM density functions for a \( D \)-dimensional random vector, as defined in Model 1, where \( (d, K) \) are the model parameters which determine a specific class of densities. For given constants \( d_0 \) and \( K_0 \), let \( \theta^*(d_0, K_0) \) be a set of given parameters in the density function (18). We define

\[
\theta^*(d, K) = \arg \min_{\theta(d,K) \in \Theta(d,K)} D_{KL}[f(\cdot; \theta^*(d_0, K_0)) || f(\cdot; \theta(d, K))]
\]

for all \( d, K \). Here, \( D_{KL}[g||h] \) is the Kullback–Leibler divergence of density \( h \) from density \( g \), defined as

\[
D_{KL}[g||h] = E_{g(\cdot)} \left[ \log \left( \frac{g(X)}{h(X)} \right) \right] = \int \log \left( \frac{g(x)}{h(x)} \right) g(x) dx.
\]
BIC evaluated on $\hat{Z}$ with model $f(\cdot; \theta(d, K))$, that is,

$$
\text{BIC}(\hat{Z}; d, K) = 2 \sum_{i=1}^{n} \log f(\hat{Z}_i; \hat{\theta}(\hat{Z}; d, K)) - \eta(d, K) \log(n),
$$

(21)

where $\eta(d, K)$ is the number of parameters in the model, $n$ is the number of rows in $\hat{Z}$, and $\hat{\theta}(\hat{Z}; d, K)$ is the maximum likelihood estimator (MLE) of the parameters from optimizing the log-likelihood

$$
\hat{\theta}(\hat{Z}; d, K) = \arg \max_{\theta(d, K) \in \Theta(d, K)} \frac{1}{n} \sum_{i=1}^{n} \log f(\hat{Z}_i; \theta(d, K)),
$$

(22)

where $\Theta(d, K)$ is the parameter space of the model with given $(d, K)$.

Using the notation defined above, we here state our theoretical result as follows.

**Theorem 1 (Consistency of model parameter estimates).** Let $(\hat{Z}^{(n)}_i)_{n=1}^{\infty}$ be a sequence of random matrices, where each element $\hat{Z}^{(n)}_i \in \mathbb{R}^{n \times D}$ is a matrix with $n$ rows of $D$-dimensional random vectors. If

(a) the rows of $\hat{Z}^{(n)}_i$ are independently identically distributed according to (18), with parameter $\theta^*(d_0, K_0)$, that is, for an arbitrary $n$,

$$
\hat{Z}^{(n)}_i \sim f(\cdot; \theta^*(d_0, K_0))
$$

(23)

iid for all $i \in [n]$;
(b) the model $f(\cdot; \theta(d, K))$ satisfies our Identifiability Assumption on density $f(\cdot; \theta^*(d_0, K_0))$;
(c) for all $(d, K)$, the parameter space $\Theta(d, K)$ is a compact metric space; then the estimates of model parameters given by

$$
(\hat{d}^{(n)}, \hat{K}^{(n)}) = \arg \max_{d \in [D], K \in [K_{\text{max}}]} \text{BIC}(\hat{Z}^{(n)}; d, K)
$$

(24)

(with a constant $K_{\text{max}} \geq K_0$) will converge to the truth, that is,

$$
(\hat{d}^{(n)}, \hat{K}^{(n)}) \xrightarrow{p} (d_0, K_0)
$$

(25)

as $n \to \infty$.

We leave the proof of the theorem for the Appendix. This theoretical support together with the practical advantages of SMS motivate us to conduct vertex clustering via SMS.

### 4.3. Algorithms for SMS

We present a model-based clustering algorithm via SMS with the GMM. The entire procedure consists of three phases. First, the “parameter fitting” phase. We compute the MLE—the maximum likelihood estimator—in the GMM for each pair $(d, K)$. The MLEs are used to complete the density function while evaluating the likelihood on the data. Second, the “model selection” phase. We compute the BIC values for all $(d, K)$ pairs, then choose the one with the largest BIC as the model parameter estimate given the data. Finally, the “clustering” phase. The likelihoods of all the data points are evaluated on the selected model with fitted parameters. Labels are assigned to each point by the maximization a posterior (MAP) rule. A summary of the SMS algorithm is provided in the Algorithm 1 display.

Although we believe that SMS has advantages compared to its sequential counterpart, it is unclear whether including the redundant dimensions of the extended ASE in the clustering phase is preferable. The reasoning can be explained by two aspects. First, the redundant dimensions may contain little information for the clustering—as indicated by the model, and by the simulations in the preceding section, only a single variance term contains potential clustering information. Second, choosing a smaller dimension in the clustering task may lead to better performance, especially for a small number of observations, due to the bias-variance tradeoff (Jain, Duin, and Mao 2000). This motivates a variation in the third phase of the SMS algorithm. To be specific, in phase 1 and phase 2, Model 1 and the extended ASE $\hat{Z}$ are used just to find the estimate of embedding dimension. In phase 3, we can now truncate the extended ASE to the dimension $\hat{d}$ which is estimated by SMS. In this alternative context, redundant dimensions do not take part in the clustering procedure. Thus, we may apply the traditional model-based clustering algorithm with regular GMM on the truncated embedding $\hat{Z}^{(n)}_{\hat{d}}$. Notice that the embedding dimension is determined by the SMS procedure, so the clustering results could be remarkably different than the algorithm under a sequential model selection framework. We call this algorithm SMS-reduced, inspired by model-based clustering by GMM with reduced embedding dimension determined via SMS. The outline of the steps of SMS-reduced is provided in the Algorithm 2 display.

There is another implementation that we consider here, which we refer to as the “two-step” algorithm. It is nearly equivalent to the reduced algorithm—and in fact is identical to it in those cases where the two models produce the same $\hat{d}, \hat{K}$. The loop in Algorithm 3 is over $d$ alone. There is indeed a loop over $K$ in the model-based clustering, which halts when the BIC value decreases. Note that this approach does not necessarily produce the maximum likelihood solution; however, in the event the
Algorithm 2 SMS-reduced

Input: The adjacency matrix $A \in \mathbb{R}^{n \times n}$; an upper bound $D$ on embedding dimension; an upper bound $K_{\text{max}}$ on mixture complexity

1: function SMS-REDUCED($A, D, K_{\text{max}}$)
2: Apply extended ASE on $A$ with dimension $D$: $\hat{Z} \leftarrow \hat{U}_{|D|}\hat{\Lambda}_{|D|}^{1/2}$
3: loop
4: Compute MLEs $\hat{\theta}(\hat{Z}; d, K)$ for Model 1
5: $d \leftarrow \arg \max_{d \in [D], K \in [K_{\text{max}}]} \text{BIC}(\hat{Z}; d, K)$
6: Truncate the ASE: $\tilde{Z}_{[d]} \leftarrow \hat{U}_{[d]}\hat{\Lambda}_{[d]}^{1/2}$
7: $(\hat{\tau}_1, \ldots, \hat{\tau}_n) \leftarrow \text{GMM} \circ \text{BIC}(\tilde{Z}_{[d]})$
8: end function

Output: The clustering labels $(\hat{\tau}_1, \ldots, \hat{\tau}_n)$

Algorithm 3 SMS two-step

Input: The adjacency matrix $A \in \mathbb{R}^{n \times n}$; an upper bound $D$ on embedding dimension; an upper bound $K_{\text{max}}$ on mixture complexity

1: function TWO_STEP($A, D, K_{\text{max}}$)
2: Apply extended ASE on $A$ with dimension $D$: $\hat{Z} \leftarrow \hat{U}_{|D|}\hat{\Lambda}_{|D|}^{1/2}$
3: loop
4: Step 1: Compute GMM on $\hat{Z}_d$ using model based clustering to choose $\hat{K}$ (Fraley and Raftery 2002)
5: Step 2: Use the fitted mixture to estimate the $\sigma_d^2$ of the redundant part. Compute BIC for the resulting model
6: end loop
7: $d \leftarrow \arg \max_{d \in [D], K \in [K_{\text{max}}]} \text{BIC}(\hat{Z}; d, K)$
8: $(\hat{\tau}_1, \ldots, \hat{\tau}_n) \leftarrow \text{GMM} \circ \text{BIC}(\tilde{Z}_{[d]})$
9: end function

Output: The clustering labels $(\hat{\tau}_1, \ldots, \hat{\tau}_n)$

We compare our methods with the sequential BIC $\circ$ ZG method, first choosing the dimension a la Zhu and Ghodsi (2006) and then using BIC in the GMM to choose the number of clusters. Deciding which scree plot elbow to use is always subjective in practice, so we will consider ZG1, ZG2, and ZG3, the ZG algorithm which takes the 1st, 2nd, and 3rd elbows, respectively. For $\ell = 1, 2, 3$ we use the notation ZG$\ell$; hence, BIC $\circ$ ZG$\ell$ provides three sequential model selection competitors. Notice that even if one ZG$\ell$ (or corresponding BIC $\circ$ ZG$\ell$) method outperforms our proposed simultaneous methods in a specific setting, this does not mean that the ZG algorithm is superior to ours because the optimal $\ell$ will be different in a different setting. We will see this in the simulations. We apply the mclust R package (Scrucca et al. 2016) to perform the BIC selection, always using the “full covariance” model for consistency throughout. Additionally, we also consider three well-known heuristic vertex clustering methods for comparison: the Louvain algorithm proposed in Blondel et al. (2008); the Walktrap algorithm proposed in Pons and Latapy (2005); and the infinite relational model (IRM) (Kemp et al. 2006).

There are numerous criteria to evaluate the performance of a clustering result, including Jaccard (Jaccard 1912), Rand index (Hubert and Arabie 1985), normalized mutual information (Danon et al. 2005) and variation of information (Meila 2007). Of these, we choose the well-known adjusted Rand index (ARI) as the measure of the similarity between the clustering result and the ground truth labels—in the simulations the ground truth is known, and it is this that is used to compute the ARI. As a corrected-for-chance version of the Rand index, ARI normalizes the Rand index so that the expected value between a random cluster and the ground truth is zero. The maximum value of ARI is 1, which indicates perfect agreement of two partitions. So a larger ARI means the clustering is performing better.

5.1. Numerical Results on Synthetic Data

First, we consider Monte Carlo simulation for the two- and three-block models described in Section 3.2. Recall that both models have a full-rank $B$ matrix, so $K = d = 2$ for the former and $K = d = 3$ for the latter. We used $(D, K_{\text{max}}) = (6, 6)$ in this simulation, with 100 Monte Carlo replicates. The results are depicted in Figure 7. There is a tendency for the SMS method to choose $\hat{d}$ slightly larger than the rank of $B$. (This is an acceptable bias: underestimating $d$ can have catastrophic consequences for subsequent inference, while overestimating $d$ has a relatively minor impact. However, the correct $K$ is chosen nearly always (all but once for the 2-block model, and all but 11 times for the 3-block model, out of a total of 400 simulations for each model.)

Next we generate a graph $G$ from a SBM($n, B, \pi$) by specifying the block probability matrix $B$, prior block probability $\pi$, and number of vertices $n$. The adjacency matrix $A \in \mathbb{R}^{n \times n}$ represents $G$. Then we apply the extended ASE on the graph, denoted by $\tilde{Z} \in \mathbb{R}^{n \times D}$. For simplicity, we fix $D = 8$. Let $n = 500,

$$B = \begin{bmatrix} 0.2 & p \\ p & 0.1 \end{bmatrix}$$

and $\pi = (0.5, 0.5)$. We vary $p$ to change the angle between two latent vectors.
Figure 7. Simultaneous model selection (SMS) simulation results from 100 Monte Carlo trials with the 2- and 3-block models described in Section 3.2.

For this experiment, we consider the SMS-reduced algorithm, which we refer to as “our algorithm.” Figure 8 shows the difference of ARI (computed using the ground truth provided by the simulations) between our algorithm and the BIC ◦ ZG methods in boxplots—100 Monte Carlo trials each produces paired results allowing for analysis of differences. A value larger than 0 means our algorithm has a higher ARI than the corresponding BIC ◦ ZG method in that Monte Carlo replicate. Figure 8 (left panel) shows the result under the setting with \( p = 0.095 \). We find our algorithm outperforms BIC ◦ ZG1 and BIC ◦ ZG3, and performs nearly the same as BIC ◦ ZG2. We perform a sign test for the paired differences of ARI, where the null hypothesis is that the two methods are equally good or BIC ◦ ZG is better (\( \theta \leq 0.5 \) with respect to Binomial distribution), and the alternative hypothesis is that our method is better (\( \theta > 0.5 \)). The \( p \)-values for our algorithm comparing to BIC ◦ ZG1, BIC ◦ ZG2, and BIC ◦ ZG3 are < 10^{-6}, 0.04 and < 10^{-6}, respectively. The small \( p \)-values suggest that our algorithm is superior, surely, to BIC ◦ ZG1 and BIC ◦ ZG3. In Figure 8 (right panel), we use \( p = 0.115 \) in the \( B \) matrix. In this case, the \( p \)-values of a sign test for our algorithm compared to BIC ◦ ZG1, BIC ◦ ZG2, and BIC ◦ ZG3 are 0.34, <10^{-6}, and <10^{-6}, respectively. In this case, our algorithm has similar performance to BIC ◦ ZG1, but outperforms BIC ◦ ZG2 and BIC ◦ ZG3. In both cases, our algorithm has joint best performance with respect to ARI. In contrast, none of the BIC ◦ ZG methods win in both cases. The analogous \( t \)-test \( p \)-values agree across the board. Considering that in practice we need to fix an elbow in BIC ◦ ZG methods without knowing the ground truth, the SMS algorithm provides a robust solution.

Figure 9 shows the distribution of ARI for the SMS algorithm for a range of values \( p \) in the \( B \) matrix. The gray boxes in the figure indicate those for which more extensive experiments are reported, comparing the reduced and full algorithms to other methods. The reason for the first low box with median near 50% is the fact that for very small \( p \) there is a high probability of the graphs being disconnected, in which case simple spectral embedding is inappropriate.

Figure 10 shows the mean of ARI for all methods, including the existing heuristic Louvain, Walktrap, and IRM algorithms. The random graph with \( n = 500 \) vertices is generated from a 2-block SBM with block probability matrix [0.2, \( p \); \( p \), 0.1]. The parameter \( p \) is varying from 0.09 to 0.115. We observe that the Louvain, Walktrap, and IRM algorithms do not perform well for large \( p \), so we may conclude that these three heuristic vertex clustering algorithms are not suitable for specific SBM graphs. To have a detailed look, Figure 11 shows the mean of ARI for SMS and the ZGs. For small \( p \) ZG1 is the best of the ZGs, while for large \( p \) ZG2 is the best of the ZGs; in all cases, SMS is as good as the best ZG. This demonstrates precisely the robustness
Figure 9. Boxplots of adjusted Rand index (ARI) of 100 Monte Carlo trials for the simultaneous model selection (SMS) method. The random graph with \( n = 500 \) vertices is generated from a 2-block SBM with block probability matrix \([0.2, p; p, 0.1]\). The parameter \( p \) is varied from 0.005 to 0.2. The gray boxes correspond to the region of the \( p \) parameter used in the subsequent experiment described in Figure 10.

Figure 10. The mean of adjusted Rand index (ARI) of 100 Monte Carlo trials for different methods. The random graph with \( n = 500 \) vertices is generated from a 2-block SBM with block probability matrix \([0.2, p; p, 0.1]\). The parameter \( p \) is varying from 0.09 to 0.115.

5.2. Demonstration on Connectomes

We demonstrate the performance of the SMS procedure on a real dataset of human connectomes. A connectome represents the brain as a network consisting of neurons (or collections thereof) as vertices and synapses (or structural connections) as edges. It is fundamentally helpful to unlock the structural and functional unknowns in the human brain in cognitive neuroscience and neuropsychology by studying the topological properties of connectomes. For this demonstration, the raw data is collected by diffusion magnetic resonance imaging (dMRI), which can represent the structural connectivity within the brain. The macro-scale connectomes are estimated by NeuroData’s MRI to graphs (NDMG) pipeline (Kiar et al. 2018), which is designed to produce robust and biologically plausible connectomes across studies, individuals and scans. As the output of the NDMG

sought. In Figure 11(a), all methods have decreasing ARI as \( p \) increases. This is because the angle between two latent vectors become smaller, so the cluster centers get closer. Out of all the methods, our algorithm performs well for all \( p \)’s. In Figure 11(b), the mean of \( \hat{d} - d \) is plotted. We can see that the SMS algorithm is the closest one to zero, which means it estimates \( \hat{d} \) better than the other methods.

Figure 11. The mean of ARI and \( \hat{d} \) for varying \( p \): (a) mean of adjusted Rand index (ARI); (b) mean of \( \hat{d} - d \). The random graph with \( n = 500 \) vertices is generated from a 2-block SBM with block probability matrix \([0.2, p; p, 0.1]\). The parameter \( p \) is varying from 0.09 to 0.115.
pipeline, the brain graphs are generated. The vertices of the graph represent regions of interest identified by spatial proximity, and the edges of the graph represent the connection between regions via tensor-based fiber streamlines. Specifically, there is an edge for a pair of regions if and only if there is a streamline passing between them. The graph is undirected since the raw dMRI data has no direction information. For more details, we refer the readers to Kiar et al. (2018).

This specific dataset consists of 114 connectomes (57 subjects with 2 scans each), with 1215 vertices for each graph. There are two attributes for each vertex (region of interest): hemisphere, either left or right; and tissue type, either gray or white. (In fact, the attributes can also take value “other”; for ease of illustration, we consider only regions labeled left or right hemisphere and gray or white tissue, yielding an induced subgraph from the original connectome by deleting the vertices with label “other” in hemisphere or tissue attributes.) Then, we extract the largest connected component of that subgraph so as to facilitate the spectral embedding. This yields 114 connected undirected graphs, with approximately 760 vertices for each graph. As described, each vertex is assigned two labels, hemisphere and tissue type. These are treated as ground truth for the structure in the graphs. We note that these labels do not necessarily correspond to cluster structure of the vertices, and so it is difficult to claim that one method is better than another for any true clustering structure. At most we can claim that clustering the brain regions without using anatomical information provides results in agreement with the anatomy. This does not necessarily translate to any true clustering structure that might be at odds with anatomy. This issue is inherent in clustering the nodes of these graphs, a la the “Two Truths” phenomenon described in Priebe et al. (2019).

We apply clustering methods on the 114 graphs to compare our SMS algorithms (both full and reduced) with the sequential BIC ○ ZG. The ARI is calculated by comparing the clustering results with three separate versions of ground truth, namely hemisphere, tissue, and the combination of the two. Specifically, each vertex of a connectome is assigned a label left or right from the 2-cluster attribute hemisphere, and a label gray or white from the 2-cluster attribute tissue. We also assign a label (left-gray, left-white, right-gray, or right-white) from combining the hemisphere and tissue.

Figure 12 presents the estimates of the model parameter pair \((\hat{d}, \hat{K})\) for the 114 connectomes. The red dots represent the results from SMS, and other colors are the results from BIC ○ ZG. Consequently, there are four points for each graph, representing the pair of estimates by SMS, BIC ○ ZG1, BIC ○ ZG2, and BIC ○ ZG3, respectively.

For each graph and each specific algorithm, we have three ARIs indicating the clustering accuracy for three different cases. We are interested in how well our SMS algorithms perform compared with the traditional BIC ○ ZG algorithms. As an example, Figure 13 shows the result of the paired difference of ARIs between SMS and the BIC ○ ZG methods. Attribute hemisphere (left or right) is considered when computing ARI. Fixing two algorithms in competition, the differences of ARI are taken pairwise for all 114 graphs. We plot the histogram of those differences. More positive values in the histogram indicate stronger evidence that SMS outperforms BIC ○ ZG, since higher ARI indicates that the clustering result is closer to the ground truth. From Figures 13(a)–(c), we claim that the full SMS algorithm, dominates all BIC ○ ZGs, following the observation that obviously more difference values are positive. In Figures 13(d)–(f), although the number of positive values is close to that of negative ones, the reduced SMS algorithm still wins against the BIC ○ ZGs slightly because of higher ARIs on average. Table 1 gives the results on all three attributes, where the number of graphs (out of 114) on which ARI of SMS is strictly larger than the sequential methods is reported in the column "#win." Here, we also consider the Louvain, Walktrap, and IRM methods in the competition. We again calculate \(p\)-values via the sign test. The results show that the full simultaneous algorithm dominates in all cases against the BIC ○ ZGs. Notice that the Louvain method demonstrates good performance for the hemisphere attribute, but it does not work well (with very small ARI values) for the tissue attribute. An analogous “Two Truths” phenomenon has been discovered in the work of Priebe et al. (2019), where the authors find that Laplacian spectral embedding (LSE) better captures the hemisphere affinity structure while ASE better captures the tissue core-periphery structure. Here we see that Louvain, like LSE, is good for detecting the hemisphere affinity structure but not for detecting the tissue core-periphery structure. On the other hand, IRM performs well for the tissue attribute but poorly otherwise.

### 5.3. Computational Considerations

Naively, the eigenvector computation seems to have a cubic cost in the number of vertices. In fact, spectral graph inference never needs the full spectrum; rather, only a few—constant, or at most \(o(n)\)—eigenpairs are required. (This is both a design
Figure 13. Illustration of the difference of adjusted Rand index (ARI) between simultaneous model selection (SMS) and the sequential BIC \( \circ \) ZG. The ARIs are computed against the ground truth in attribute hemisphere. The differences are taken pairwise for all 114 graphs. (a)–(c) The histogram of the 114 differences between SMS and BIC \( \circ \) ZGs, while (d)–(f) the histogram of those between SMS-reduced and BIC \( \circ \) ZGs. More positive values in the histogram indicates stronger evidence that SMS outperforms BIC \( \circ \) ZG. While SMS dominates in all cases, SMS-reduced wins slightly with higher average ARI.

In summary: for fixed \( D \) and \( K_{\text{max}} \) the spectral dominates theoretically even at \( O(n^2) \), but this is a case where the theoretical "Big-O" analysis is misleading with respect to practice: the MLEs dominate our computational complexity in practice. However, our approach is the only computationally feasible simultaneous option. (The MCMC approach of Sanna Passino and Heard (2020) is, at present, not scalable.)

6. Conclusion

This article presents a novel SMS framework—dimensionality and cluster complexity—specifically for vertex clustering on SBM graphs.

In the first part of the article, we propose the extended ASE, in which the embedding is performed with a fixed (large) dimension. Under the framework of model-based clustering, we propose a family of GMM to parameterize the entire extended ASE. The basis of the model is a state-of-the-art distributional result for the informative dimensions, as well as a conjecture founded on evidence from principled simulations for the redundant dimensions.
The evidence that simultaneous model selection (SMS) outperforms the sequential BIC or ZG in terms of adjusted Rand index (ARI), which is evaluated by three different versions of ground truth: hemisphere, tissue and the combination of the two (4-block).

Table 1. The effectiveness of the algorithms is demonstrated in simulations and areal data experiment. The heuristicalgorithms to solvethe vertex clustering problem. The in our proposed model. Based on SMS, we also develop two large graphs, provided the extended ASE followsthe distribution given by our SMS method converge to the underlying truth for or the consistency of model parameter estimates. The theorem claims that the estimates in the model selection procedure given by our SMS method converge to the underlying truth for large graphs, provided the extended ASE follows the distribution in our proposed model. Based on SMS, we also develop two heuristic algorithms to solve the vertex clustering problem. The effectiveness of the algorithms is demonstrated in simulations and a real data experiment.

In the second part of the article, we propose a SMS framework to improve upon sequential model selection. The framework is specifically tailored for the vertex clustering task on SBM graphs. In contrast with sequential model selection, our approach identifies the embedding dimension and mixture complexity simultaneously. Moreover, we state and prove a theorem on the consistency of model parameter estimates. The theorem claims that the estimates in the model selection procedure given by our SMS method converge to the underlying truth for large graphs, provided the extended ASE follows the distribution in our proposed model. Based on SMS, we also develop two heuristic algorithms to solve the vertex clustering problem. The effectiveness of the algorithms is demonstrated in simulations and a real data experiment.

Note that the rank of $B$, the “best” embedding dimension for clustering, and the number of clusters interact in a rather complex manner. In Figure 1, the right plot shows that $d = 2$ is likely to be the correct embedding dimension (and this will be even more obvious for larger values of $n$) and yet both the rank of the $B$ matrix and the number of blocks is 3. Directly utilizing a measure of clustering performance in the parameter selection and modeling is an area for further research.

We have focused on the so called “hard clustering” procedure in which each vertex is assigned to a unique cluster. However, the use of GMM clustering allows for “soft clustering” whereby the likelihood ratio is used as the assignment probability, rather taking the arg max to provide a hard threshold.

### Appendix

For the proof of Theorem 1, we begin with the following lemma.

**Lemma 1.** Following the notation in Theorem 1, for all $d, K$,

\[
\frac{1}{n} \sum_{i=1}^{n} \log \left( \frac{f(\hat{Z}_i^{(n)}; \hat{\theta}(d, K))}{f(\hat{Z}_i^{(n)}; \hat{\theta}(d, K))} \right) \rightarrow D_{KL}[f(\cdot; \theta^*(d_0, K_0))|f(\cdot; \theta^*(d, K))]
\]

as $n \rightarrow \infty$.

**Proof.** By the definition of Kullback–Leibler divergence in (20),

\[
D_{KL} \left[ f(\cdot; \theta^*(d_0, K_0))|f(\cdot; \theta^*(d, K)) \right] = \mathbb{E} \left[ \log \left( \frac{f(\hat{Z}_i^{(n)}; \theta^*(d_0, K_0))}{f(\hat{Z}_i^{(n)}; \theta^*(d, K))} \right) \right]
\]

\[
= \mathbb{E} \left[ \log (f(\hat{Z}_i^{(n)}; \theta^*(d_0, K_0))) \right] - \mathbb{E} \left[ \log (f(\hat{Z}_i^{(n)}; \theta^*(d, K))) \right].
\]

So we can prove the lemma by showing

\[
\frac{1}{n} \sum_{i=1}^{n} \log \left( \frac{f(\hat{Z}_i^{(n)}; \theta^*(d_0, K_0))}{f(\hat{Z}_i^{(n)}; \theta^*(d_0, K_0))} \right) \rightarrow \mathbb{E}[\log(f(\hat{X}_i; \theta^*(d_0, K_0)))]
\]

and

\[
\frac{1}{n} \sum_{i=1}^{n} \log \left( \frac{f(\hat{Z}_i^{(n)}; \hat{\theta}(d, K))}{f(\hat{Z}_i^{(n)}; \hat{\theta}(d, K))} \right) \rightarrow \mathbb{E}[\log(f(\hat{X}_i; \theta^*(d, K)))]
\]

as $n \rightarrow \infty$. (A.3) is the direct result of the law of large numbers. (A.4) is the result of theorem 2.2 in White (1982) then followed by Slutzky’s theorem. 

Now we show the proof of Theorem 1 as follows.

**Proof of Theorem 1.** Since $\hat{d}^{(n)}$ and $\hat{K}^{(n)}$ are both integer random variables, showing

$(\hat{d}^{(n)}, \hat{K}^{(n)}) \xrightarrow{P} (d_0, K_0)$ is equivalent to showing

\[
\mathbb{P} \left[ (\hat{d}^{(n)}, \hat{K}^{(n)}) = (d_0, K_0) \right] \rightarrow 1.
\]

By the definition of $\hat{d}^{(n)}$ and $\hat{K}^{(n)}$ in (24), the event $\{ (\hat{d}^{(n)}, \hat{K}^{(n)}) = (d_0, K_0) \}$ is equivalent to the event $\{ (d_0, K_0) = \arg \max_{d \in [D], K \in [K_{max}]} \text{BIC}(\hat{Z}^{(n)}; d, K) \}$, which is equivalent to $\bigcap_{d, K} \text{BIC}(\hat{Z}^{(n)}; d_0, K_0) \geq \text{BIC}(\hat{Z}^{(n)}; d, K)$, so

\[
\mathbb{P} \left[ (\hat{d}^{(n)}, \hat{K}^{(n)}) = (d_0, K_0) \right]
\]

\[
= \mathbb{P} \left[ \bigcap_{d \in [D], K \in [K_{max}]} \big( \text{BIC}(\hat{Z}^{(n)}; d_0, K_0) \geq \text{BIC}(\hat{Z}^{(n)}; d, K) \big) \right]
\]

\[
= 1 - \mathbb{P} \left[ \bigcup_{d \in [D], K \in [K_{max}]} \big( \text{BIC}(\hat{Z}^{(n)}; d_0, K_0) < \text{BIC}(\hat{Z}^{(n)}; d, K) \big) \right]
\]

\[
\geq 1 - \sum_{d \in [D], K \in [K_{max}]} \mathbb{P} \left[ \text{BIC}(\hat{Z}^{(n)}; d_0, K_0) < \text{BIC}(\hat{Z}^{(n)}; d, K) \right].
\]

(A.6)

Thus to show (A.5), it is sufficient to show

\[
\mathbb{P} \left[ \text{BIC}(\hat{Z}^{(n)}; d_0, K_0) < \text{BIC}(\hat{Z}^{(n)}; d, K) \right] \rightarrow 0
\]

(A.7)
as \( n \to \infty \) for all \((d, K) \neq (d_0, K_0)\). By the notation in (21) and (22), we notice

\[
\frac{1}{2n} \left[ \text{BIC}(\hat{Z}^{(n)}; d_0, K_0) - \text{BIC}(\hat{Z}^{(n)}; d, K) \right]
\]

\[
= \frac{1}{2n} \left\{ \sum_{i=1}^{n} \log \left[ f(\hat{Z}_i^{(n)}; \hat{d}(d_0, K_0)) \right] - \eta(d, d_0, K_0) \log(n) \right\} - \frac{1}{2n} \left\{ \sum_{i=1}^{n} \log [f(\hat{Z}_i^{(n)}; \hat{d}(d, K))] - \eta(d, K) \log(n) \right\}
\]

\[
= \sum_{i=1}^{n} \log \left[ \frac{f(\hat{Z}_i^{(n)}; \hat{d}(d_0, K_0))}{f(\hat{Z}_i^{(n)}; \hat{d}(d, K))} \right] - \frac{1}{2n} \left\{ \sum_{i=1}^{n} \log \left[ \frac{f(\hat{Z}_i^{(n)}; \hat{d}(d_0, K_0))}{f(\hat{Z}_i^{(n)}; \hat{d}(d, K))} \right] \right\}
\]

For (A.9), by Lemma 1,

\[
\frac{1}{n} \sum_{i=1}^{n} \log \left[ \frac{f(Z_i^{(n)}; \theta^*(d_0, K_0))}{f(Z_i^{(n)}; \theta^*(d, K_0))} \right] \]

\[
\stackrel{P}{\longrightarrow} \text{D}_{\text{KL}}[f(\cdot ; \theta^*(d_0, K_0)) || f(\cdot ; \theta^*(d, K))] = 0 \quad (A.18)
\]

so

\[
\mathbb{P} \left[ \frac{1}{n} \sum_{i=1}^{n} \log \left[ \frac{f(Z_i^{(n)}; \theta^*(d_0, K_0))}{f(Z_i^{(n)}; \theta^*(d, K_0))} \right] < -\epsilon \right] \longrightarrow 0 \quad (A.19)
\]

For (A.10), also by Lemma 1,

\[
\frac{1}{n} \sum_{i=1}^{n} \log \left[ \frac{f(Z_i^{(n)}; \theta^*(d_0, K_0))}{f(Z_i^{(n)}; \theta^*(d, K))} \right] \]

\[
\stackrel{P}{\longrightarrow} \text{D}_{\text{KL}}[f(\cdot ; \theta^*(d_0, K_0)) || f(\cdot ; \theta^*(d, K))] \quad (A.20)
\]

so

\[
\mathbb{P} \left[ \frac{1}{n} \sum_{i=1}^{n} \log \left[ \frac{f(Z_i^{(n)}; \theta^*(d_0, K_0))}{f(Z_i^{(n)}; \theta^*(d, K))} \right] < -\epsilon \right] \longrightarrow 0 \quad (A.21)
\]

For (A.11), if \((d, K) \neq (d_0, K_0)\), then by the identifiability assumption (b), we know

\[
\text{D}_{\text{KL}}[f(\cdot ; \theta^*(d_0, K_0)) || f(\cdot ; \theta^*(d, K))] > 0 \quad (A.22)
\]

Thus, if we take \( \epsilon = \frac{1}{2} \text{D}_{\text{KL}}[f(\cdot ; \theta^*(d_0, K_0)) || f(\cdot ; \theta^*(d, K))] \), then we have

\[
\mathbb{P} \left[ \frac{1}{n} \sum_{i=1}^{n} \log \left[ \frac{f(Z_i^{(n)}; \theta^*(d_0, K_0))}{f(Z_i^{(n)}; \theta^*(d, K))} \right] < -\epsilon \right] \longrightarrow 0 \quad (A.23)
\]

because \( \frac{\log(n)}{n} \to 0 \) as \( n \to \infty \). Combining (A.19), (A.21), and (A.23), we have

\[
\mathbb{P} \left[ \frac{1}{2n} [\text{BIC}(\hat{Z}^{(n)}; d_0, K_0) - \text{BIC}(\hat{Z}^{(n)}; d, K)] < 0 \right] \longrightarrow 0 \quad (A.24)
\]

as \( n \to \infty \) for all \( d \in [D] \) and \( K \in K_{\max} \). So we have shown (A.7), which finishes the proof of

\[
(\hat{Z}^{(n)}; \hat{K}^{(n)}) \to (d_0, K_0) \quad (A.25)
\]

as \( n \to \infty \).

\[
\square
\]

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