Consistent estimation of dynamic and multi-layer networks

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Abstract

Dynamic networks where edges appear and disappear over time and multi-layer networks that deal with multiple types of connections arise in many applications. In this paper, we consider the \textit{multi-graph stochastic block model} proposed by Holland et al. (1983), which serves as a foundation for both dynamic and multi-layer networks. We extend inference techniques in the analysis of single networks, namely maximum-likelihood estimation, spectral clustering, and variational approximation, to the multi-graph stochastic block model. Moreover we provide sufficient conditions for \textit{consistency} of the spectral clustering and maximum-likelihood estimates. We verify the conditions for our results via simulation and demonstrate that the conditions are practical. In addition, we apply the model to two real data sets: a dynamic social network and a multi-layer social network, resulting in block estimates that reveal network structure in both cases.

1 Introduction

Modeling relational data arising from networks including social, biological, and information networks has received much attention recently. Various probabilistic models have been proposed, such as stochastic block models, latent variable models, mixed membership models, exchangeable graph models, etc. (Goldenberg et al., 2010). However, in many settings, we not only have a single network, but a collection of networks on a common set of nodes, which is often referred to as a
Two types of multi-graph applications are of particular interest. First are dynamic networks with time-evolving edges, for example, time-stamped social networks of interactions between people. Another type consists of multi-layer networks, where interactions are measured in multiple ways such as phone calls, text messages, e-mails, face-to-face contacts, etc.

The main difficulty is to extract the common information across the layers in a concise representation, yet be flexible to allow differences across networks. Motivated by the above examples, we consider the multi-graph stochastic block model, which first appeared in Holland et al. (1983). The key assumption is that nodes share the same block structure over the multiple layers of the multi-graph, but the connection intensities may vary across layers. We believe this model is a flexible and principled way of analyzing multi-graphs and provides a strong foundation for both applications.

The special case of a single type of relation, often referred to as the stochastic block model (SBM), has been studied extensively in recent years (Bickel and Chen, 2009; Rohe et al., 2011; Choi et al., 2012; Celisse et al., 2012; Jin, 2012; Bickel et al., 2013; Amini et al., 2013). However, the more general multi-graph case has not been studied as much. In this paper, we extend inference methods for the SBM, namely maximum-likelihood estimation (MLE), spectral clustering, and variational approximation to the multi-graph SBM. Moreover we explore its asymptotic properties by letting the number of network layers increase to infinity while keeping the number of nodes fixed. Specifically we provide conditions under which the MLE is consistent, which ensures the tractability of this model and paves the way for more sophisticated models and inference techniques. To the best of our knowledge, it is the first such theoretical result in this regime.

The rest of the paper is organized as follows. In section 2, we review the multi-graph stochastic block model and discuss related work. Then in section 3, we discuss two ways to estimate the model. In section 3.1, we study the behavior of spectral clustering on the mean graph. In section 3.2, we discuss in detail the maximum-likelihood estimate and its asymptotic behavior. We provide simulations and experiments on two real data sets to verify the model in section 4. We conclude with some further discussion in section 5.
We present an overview of the multi-graph stochastic block model first proposed by Holland et al. (1983). A single relation is represented by an adjacency matrix \( G_t = (G_{ij}^t) \), \( i, j = 1, \ldots, n \). We focus on symmetric (binary) relations with no self loops. For a multi-graph, we observe an adjacency array \( \vec{G} = \{ G^1, G^2, \ldots, G^T \} \) sharing the same set of nodes. So \( \vec{G} \) is a “vector of matrices”. The same subscripts correspond to the same node pairs for any \( t \). The superscript \( t \) indexes layers of the multi-graph. It may refer to time or type of relation depending on the application. If \( \vec{G} \) is a random adjacency array for \( n \) nodes and \( T \) relations, then the probability distribution of \( \vec{G} \) is called a stochastic multi-graph. Let the edge \( G_{ij}^t \) be a Bernoulli random variable with probability \( \Phi_{ij}^t \). \( \Phi^t = (\Phi_{ij}^t) \in [0, 1]^{n \times n} \) is the probability matrix of graph \( G^t \). Let \( \vec{\Phi} = \{ \Phi^1, \Phi^2 \ldots \Phi^T \} \) be the probability array. We assume the independence of edges within and across layers conditional on the probability array. That is, the adjacency array is generated according to 

\[
G_{ij}^t | \vec{\Phi} \sim \text{Bern}(\Phi_{ij}^t).
\]

The goal is to find a low dimensional representation of \( \Phi_{ij}^t \) that reveals network structure.

The multi-graph stochastic block model is a special case of a stochastic multi-graph. In the multi-graph SBM, networks are generated in the following way. First, each node is assigned to a class with probability \( \pi = \{ \pi_1, \ldots, \pi_K \} \) where \( \pi_k \) is the probability for a node to be assigned to class \( k \). Then, given that nodes \( i \) and \( j \) are in classes \( k \) and \( l \), respectively, an edge between \( i \) and \( j \) in network layer \( t \) is generated with probability \( P_{kl}^t \). In other words, nodes in the same classes in the same layer have the same connection probability governed by \( \vec{P} = \{ P^1, P^2, \ldots, P^T \} \in [0, 1]^{K \times K} \), the class probability array. Let \( c_i \in [1, \ldots, K] \) be the class label of node \( i \). Then 

\[
\Phi_{ij}^t = P_{c_i c_j}^t.
\]

The nodes have class labels \( \vec{c} \) shared by all of the graphs, and in each graph the class connection probabilities \( P_{kl}^t \) may be different. As we consider undirected networks, \( P^t \) is a symmetric matrix with \( K(K + 1)/2 \) free parameters. We can see that the SBM is a special case of multi-graph SBM.
with $T = 1$. Though simple, this multi-graph model has not been formally studied. It serves as a good simplification in many settings, including dynamic networks where nodes rarely change classes. More importantly, it can be theoretically analyzed and thus provides insight on more complicated models.

### 2.1 Related work

There are popular static network models other than the stochastic block model, such as exponential random graph models, mixed membership block models, latent variable models, latent feature models, exchangeable random graph models, etc. (Goldenberg et al., 2010; Airoldi et al., 2013; Wolfe and Olhede, 2013; Gao et al., 2014). Previous work on dynamic network models that are concerned specifically with time-varying network structure build upon these static network models and incorporate dynamics by either smoothing or Markov structures. Hanneke et al. (2010); Ahmed and Xing (2009) build upon exponential random graph models. Yang et al. (2011); Xu and Hero (2014); Ho et al. (2011); Ishiguro et al. (2010) build on stochastic block models. Yang et al. (2011) adds independent but shared Markov transition on each node’s class. Ho et al. (2011); Ishiguro et al. (2010) further extend it nonparametrically.

Most of the preceding work assumes the class connection probabilities to be stable over time, which may be unsuitable in many applications. More importantly, the estimation procedure may not be robust to the fixed class connection probability assumption, so more flexible model that can deal with varying probability matrices are required. Xu and Hero (2014) focus on on-time estimation of class connection probabilities via an extended Kalman filter. Sarkar and Moore (2005); Sarkar et al. (2007); Durante and Dunson (2014) use latent space models with smoothing on the latent variables. These models do a good job of link prediction but the change in the abstract latent space is hard to interpret. Foulds et al. (2011); Heaukulani and Ghahramani (2013); Kim and Leskovec (2013) use latent feature models. These models are arguably more interpretable but computationally challenging and difficult to scale.

Multi-layer networks consider multiple type of connections simultaneously. For example, Face-
book users interact by using “likes”, comments, and messages. Multi-layer networks go by many other names like multi-relational networks, multi-dimensional networks and multiplex networks. The analysis of multi-layer networks has a long history (Holland et al., 1983; Fienberg et al., 1985; Szell et al., 2010; Mucha et al., 2010; Magnani and Rossi, 2011; Oselio et al., 2013). Though various models have been proposed, well-established tools for multi-layer network analysis are still lacking.

The statistical properties of the inference algorithms in both dynamic and multi-layer models are not discussed. This means the performance of the model and inference is not guaranteed. Recently there has been a lot of progress on consistency analysis for single networks. Maximum likelihood estimation, variational approximation, and spectral clustering have been proved to be consistent under the stochastic block model (Bickel and Chen, 2009; Rohe et al., 2011; Choi et al., 2012; Celisse et al., 2012; Zhao et al., 2012; Jin, 2012; Bickel et al., 2013; Lei and Rinaldo, 2013) as the number of nodes $n \to \infty$. We extend these ideas to multi-graphs. We note that the asymptotic regime is different in the two cases. For a single network, one typically lets $n \to \infty$, while for multi-graphs, we let $T \to \infty$ with $n$ fixed. Intuitively it means we do not need to observe a very large network to get a correct understanding of the structure. Instead, we can gain the information through multiple samples, which either comes from multiple observations over time or multiple relationships.

3 Consistent estimation

Holland et al. (1983) only discussed estimation of the multi-graph SBM with blocks specified a priori. The sample proportion of each layer $t$ is the maximum-likelihood estimate (MLE) of the class probability matrix $P^t$. However, in most applications, the block structure is unknown. Hence our main goal is to estimate the class memberships and measure its accuracy. We extend inference techniques used for the single network SBM. Specifically we discuss spectral clustering, maximum-likelihood estimation, and variational approximation, all commonly used methods for the single network case.

It is not immediately straightforward how we can utilize these methods. One may imagine inferring $\vec{c}$ independently from each network and averaging across them, but we will see later in
simulations that this ad-hoc method does not work well. We propose spectral clustering on the mean graph as a motivating method for a special case of the model. Then we discuss maximum-likelihood estimation, the most natural way to combine the information contained in the different layers, for the general case.

At the same time we discuss the consistency properties of these methods. We consider a fixed number of nodes $n$ but let the number of slices $T \to \infty$. The theoretical importance of such analysis is to ensure the tractability of the model. In reality, although we do not have infinite layers, we often encounter situations with a large number of layers, such as dynamic networks over long periods of time. The asymptotics may help us to understand the finite sample properties such as the uncertainty of estimates.

### 3.1 Consistency of spectral clustering on the mean graph

Spectral clustering is a popular choice for estimating the block structure of the SBM because it can work on large networks and has shown to be consistent as $n \to \infty$ (Sussman et al., 2012). The method is based on singular value decomposition and K-means clustering on the singular vectors.

We consider two ways to extend spectral clustering from single networks to multi-graphs. The first is to apply spectral clustering on the mean graph $\bar{G} = \frac{1}{T} \sum_{t=1}^{T} G_t$. The second is to apply spectral clustering to each slice of the multi-graph and combine the class estimates by majority vote. That is, each node is assigned the class label that occurs most often. The first method is intuitively appealing as it matches with the fixed class label assumption. We show that under some stationarity conditions, it is indeed a consistent estimate. However, the second method fails, which we demonstrate experimentally in section 4, because majority vote does not cancel the error in the estimation for each slice.

We specify sufficient conditions under which spectral clustering on the mean graph is consistent. We consider the case that class connection probabilities $P^t$ fluctuate around some deterministic values that have a stable average. The following theorem shows the consistency of spectral clustering on the mean graph if the mean of the probability matrix converges to an identifiable matrix.
Theorem 1. Assume

\[ P_{kl}^t \overset{\text{ind}}{\sim} N(Q_{kl}^t, \epsilon^2) \]

\[ \frac{1}{T} \sum_t Q_{kl}^t \to \bar{Q}_{kl}, \quad \text{as } T \to \infty \]

Assume \( \bar{Q} \) is identifiable, i.e., \( \bar{Q} \) has no identical rows. Let \( \bar{G} = \frac{1}{T} \sum_{t=1}^T G^t \). Spectral clustering of \( \bar{G} \) gives accurate labels as \( T \to \infty \). That is, let \( U_{N \times K} \) be the first \( K \) right singular vectors in the singular value decomposition of \( \bar{G} \). K-means clustering on the rows of \( U_{N \times K} \) outputs class estimates \( \hat{c}_1, \ldots, \hat{c}_N \). Up to permutation,

\[ \hat{c} = c, \quad \text{a.s. as } T \to \infty. \]

We provide a sketch of the proof; details can be found in Appendix A. Since we have independent error in the probability matrix and also independent error in the Bernoulli observation, averaging cancels the error and so

\[ \bar{G} \to C\bar{Q}C'. \]

Here \( C \) is a rank \( K \) matrix incorporating the class assignment vectors. Therefore, spectral clustering on \( \bar{G} \) clusters the nodes into \( K \) different classes.

Remark 1. To determine the number of classes is a difficult problem even for a single network. We will not discuss this problem in detail. We assume \( K \) is fixed and known in the theorem.

Remark 2. Although random error \( \epsilon \) is allowed, the \( P_{kl}^t \) should be still restricted in \([0, 1]\). Generally we expect \( \epsilon \) to be small enough that we do not need to worry about the boundary issue.

Remark 3. The diagonal of \( G^t \) is always 0. This may not cause a problem as \( N \to \infty \). But for finite \( N \), it causes error in estimating the eigenvectors. We can assume \( N \) is large enough so that the diagonal does not cause a problem. Alternatively, we may directly look for the singular value decomposition that minimizes off-diagonal mean square error. That is,

\[ \arg \min_{U,S} \sum_{i<j} (\bar{G}_{ij} - U_iSU_j')^2 \]
Iterative singular value decomposition can be used to compute it. Scheinerman and Tucker (2010) have a detailed discussion of this problem.

The conditions in theorem 1 can be thought of as stationarity conditions. Because we average the graph first, the essential conditions are on the mean. However, requiring $\bar{Q}$ to be stable and identifiable is restrictive. Spectral clustering on mean graph is not effective in many cases. Consider

$$Q^{2t-1} = \begin{pmatrix} 0.7 & 0.3 \\ 0.3 & 0.7 \end{pmatrix}, \quad Q^{2t} = \begin{pmatrix} 0.3 & 0.7 \\ 0.7 & 0.3 \end{pmatrix}, \quad t \in \mathbb{N}$$

Then $\bar{Q} = \begin{pmatrix} 0.5 & 0.5 \\ 0.5 & 0.5 \end{pmatrix}$ is not identifiable. Spectral clustering on the mean graph cannot work. But there is information contained in this multi-graph. We can use maximum likelihood estimation to estimate the class assignments correctly in this case.

3.2 Consistency of maximum likelihood estimate

Now we focus on the general case where we do not place any structure on $P^t$. The natural way to estimate the class assignment is to use the maximum-likelihood estimate (MLE). We can show that for a large enough fixed $n$, the MLE will estimate the class memberships correctly as $T \to \infty$.

First we define some notation. For any class assignment $z$, let $n_k(z) = \# \{ i : z_i = k \}$ be the number of nodes in class $k$. Let $m(z) = \min_k n_k(z)$ be the minimum number of nodes in any block under labels $z$. Let

$$n_{kl}(z) = \begin{cases} n_k n_l, & k \neq l \\ n_k(n_k - 1)/2, & k = l \end{cases}$$

be the number of total counts in each block connection. We drop the dependency on $z$ whenever it is unambiguous. We also drop the superscript $t$ when we talk about a single layer of the network.

Now let’s define some notation related to the MLE. The complete log-likelihood for parameters $(z, P)$ is

$$l(z, P) = \sum_{i < j} \left( G_{ij} \log(P_{z_iz_j}) + (1 - G_{ij}) \log(1 - P_{z_iz_j}) \right)$$
Here $P$ is a parameter not to be confused with the true class connection probability matrix. In particular, we are interested in the case $P_{kl} = \bar{P}_{kl}(z)$ where

$$\bar{P}_{kl}(z) = \frac{1}{n_{kl}(z)} \sum_{i:z_i=k,j \neq i:z_j=l} P_{c_i c_j}$$

Here $\bar{P}$ is the average of true $P$ under block assignment $z$. To ease notation, let

$$\sigma(p) = p \log(p) + (1 - p) \log(1 - p)$$

(1)

Denote the expectation of log-likelihood of $(z, \bar{P}(z))$ as

$$h(z) = E \log(z, \bar{P}(z)) = \sum_{k \leq l} n_{kl}(z) \sigma(\bar{P}(z))$$

(2)

Now, as we do not observe the true $P$, the natural step is to estimate it with the empirical mean for any given $z$. So let

$$o_{kl}(z) = \sum_{z_i = k, z_j = l} \begin{cases} G_{ij}, & k \neq l \\ \frac{1}{2} G_{ij}, & k = l \end{cases}$$

be the observed number of edges in block connection. Then the profile log-likelihood is

$$f(z) = \sum_{k \leq l} n_{kl}(z) \sigma \left( \frac{o_{kl}(z)}{n_{kl}(z)} \right)$$

(3)

Let the expectation of $f$ to be

$$g(z) = E(f(z)) = \sum_{k \leq l} n_{kl}(z) E \left( \sigma \left( \frac{o_{kl}(z)}{n_{kl}(z)} \right) \right)$$

(4)

Now we are ready to state the consistency of the MLE for the multi-graph SBM. If all $P^t$ are bounded away from 0 and 1 and their column differences are at least some distance apart, then when we have a sufficient number of nodes in each block, the true label $c$ uniquely maximizes the sum of profile log-likelihoods over the layers.
Theorem 2. Let

\[ C_0 = \inf_{t,k,l} (P_{kl}^t, 1 - P_{kl}^t) \]  
\[ \delta = \inf_t \min_{k,l} \max_m \left( \sigma(P_{km}^t) + \sigma(P_{lm}^t) - 2\sigma\left(\frac{P_{km}^t + P_{lm}^t}{2}\right) \right) \]

Assume \( C_0 > 0 \) and \( \delta > 0 \), if \( m(c) = \min_k n_k(c) \) is sufficiently large,

\[ \hat{c} = \arg \max_z t f^t(z) \rightarrow c, \text{a.s. as } T \rightarrow \infty \]

The idea is that \( \sum_t f^t(z) \) is sum of independent profile log-likelihoods. We want \( N \) to be sufficiently large so that the expectation of the profile log-likelihood at each layer is maximized at the true labels \( c \). Then as \( T \rightarrow \infty \), we have convergence to expectation for \( \sum_t f^t(z) \). We formalize the ideas by establishing the following lemmas.

Lemma 1 (From Choi et al. (2012)). For any label assignment \( z \), let \( r(z) \) count the number of nodes whose true class assignments under \( c \) are not in the majority within their respective class assignment under \( z \). Then let

\[ \delta = \min_{k,l} \max_m \sigma(P_{km}^t) + \sigma(P_{lm}^t) - 2\sigma\left(\frac{P_{km}^t + P_{lm}^t}{2}\right) \]

Then the expectation of log-likelihood \( h \) is maximized by \( h(c) \), and

\[ h(c) - h(z) \geq \frac{r(z)}{2} \delta \min_k n_k(c) \]

In particular, for all \( z \neq c \),

\[ h(c) - h(z) \geq \frac{1}{2} \delta \min_k n_k(c) \]

The lemma shows the expectation of the log-likelihood is maximized at the true parameters, and the difference of the true parameters and any other candidate is at least some distance apart which depends on the column difference of the probability matrix. However, as we work with the profile log-likelihood, we establish lemma 2 and 3 to bound the difference between the expectation.
of the profile log-likelihood and the complete log-likelihood.

**Lemma 2.** \( x \sim \frac{1}{n} \text{Bin}(n, p) \). For \( p \in (0, 1) \),
\[
E(\sigma(x)) \to \sigma(p) + \frac{1}{2n} + O\left(\frac{1}{n^2}\right), \text{ as } n \to \infty
\]

**Lemma 3.** Assume \( C_0 \leq P_{kl} \leq 1 - C_0, C_0 > 0 \). For any \( \delta_0 > 0 \), for any \( z \), if \( \min_k n_k(z) \) large enough, the difference between the expectation of profile log-likelihood \( g(z) \) and the expectation of log-likelihood \( h(z) \) is bounded,
\[
\left| g(z) - h(z) - \frac{K(K+1)}{4} \right| \leq \delta_0
\]

Lemma 3, based on lemma 2, shows that with sufficiently large network size, the difference of the expectation of the profile log-likelihood and complete log-likelihood is \( \frac{K(K+1)}{4} \) and a negligible term \( \delta_0 \). For clearer notation, we use big \( O \) instead of actual bound. Readers can refer to Appendix B for the constants in the bound. Combining the lemmas and using the concentration inequality, we can show that theorem 2 provides sufficient conditions for the consistency of the multi-graph SBM. The proofs of the lemmas and the theorem can be found also in Appendix B.

**Remark 4.** The main difference between the \( n \to \infty \) and \( T \to \infty \) is that for \( n \to \infty \), direct bound is put on \( f \) and \( h \). For \( T \to \infty \), we need only to bound the expectation of \( f \) and \( h \). This is newly studied here. Put in another way, for some particular class connection probability \( P \), the number of nodes required in a single network to have an accurate estimate is much larger than what is needed in a multi-graph with a growing number of layers.

### 3.2.1 Variational approximation

The MLE is computationally unfeasible for large networks because the number of candidate class assignments grow exponentially with the number of nodes. To overcome the computational burden, variational approximation, which replaces the joint distribution with independent marginal distributions, can be used to approximate the MLE. Daudin et al. (2008) has a detailed discussion of variational approximation in the SBM. We adapt it to the multi-graph SBM. The derivation
is straightforward; we provide details in Appendix C. Variational approximation has been shown to be consistent in the SBM (Celisse et al., 2012; Bickel et al., 2013). We conjecture that the performance of variational approximation is also good in our model. Unless otherwise specified we use variational approximation to replace the MLE in all experiments.

4 Experiments

In this section, we use simulations to verify the correctness of theorem 2 and apply the model to two data examples.

4.1 Numerical illustration

We begin with a toy example where we investigate empirically how many nodes are needed for the profile MLE to correctly recover the classes as $T \to \infty$. Due to the computational intractability of computing the exact profile MLE, we consider very a small network with $n = 16$ nodes and $K = 2$ classes where each class has 8 nodes. Consider two multi-graph SBMs with the following probability matrices:

Case 1: $P^t \equiv \begin{pmatrix} 0.55 & 0.45 \\ 0.45 & 0.55 \end{pmatrix}$

Case 2: $P^t \equiv \begin{pmatrix} 0.51 & 0.49 \\ 0.49 & 0.51 \end{pmatrix}$

The $\delta$ (defined in theorem 2) corresponding to the row difference of $P^t$ is much smaller in case 2. Empirically the profile MLE succeeds to get the true labels in case 1 while it fails in case 2. Further analysis shows that in order to have consistency given the class connection probability matrix $P^t$ in case 2, the total number of nodes should be at least 40. This toy example demonstrates that conditions on the probability matrices and network size are necessary for consistency. Theorem 2 provides sufficient conditions for consistency.

Next we investigate the tightness of the conditions in theorem 2. The tightness of lemma 1 was
Figure 1: Comparison of bound in lemma 2 to exact values of \( n(E(\sigma(x)) - \sigma(p)) - 1/2 \) for varying \( n \) and \( p \).
studied by Choi et al. (2012). We check the tightness of lemma 2. For different $p$, we can calculate the exact value of $n(E(\sigma(x)) - \sigma(p)) - 1/2$ and compare it to the bound from lemma 2. Figure 1 shows that the bound is loose for small $n$, but has almost the same asymptotic decay as the exact calculation. For small $n$, the remainder in Taylor expansion causes deviation. Also the bounds are looser for $p$ closer to 0 or 1 but still informative in most cases.

For the special case of $K = 2$ classes, we can calculate all of the constants in the sufficient conditions in theorem 2 for different values of $C_0$ and $\delta$ by enumerating cases. Table 1 shows the smallest number of nodes $n$ that is sufficient for consistency of the profile MLE to hold for different values of $C_0$ and $\delta$. The minimum $n$ is in the tens or hundreds, indicating that the bounds in theorem 2 are not overly loose and are indeed of practical significance.

### 4.2 Comparison with other methods

As previously mentioned, majority vote is another way to utilize static network inference methods on multi-graph SBMs. We consider two methods that rely on static estimation by either spectral clustering or variational approximation and combine them using a majority vote. We conduct simulations to compare our proposed methods of spectral clustering on the mean graph and profile maximum-likelihood estimation with heuristic majority voting using the class estimates for each layer by spectral clustering and variational approximation individually for each layer.

We consider a well-studied scenario where we have 128 nodes initialized randomly into 4 classes (Newman and Girvan, 2004). For each layer, the within-class connection probability is 0.0968, and the between class connection probability is 0.0521. We increase the number of time steps (layers) and observe how the accuracy changes over time. Figure 2 shows the accuracy of the two

| $\delta$ | $C_0$ | 0.3 | 0.25 | 0.2 | 0.15 | 0.1 | 0.05 |
|---------|-------|-----|-----|-----|-----|-----|-----|
| 0.165   | 42  | 50 | 64 | 88 | 124 | 184 |
| 0.091   | 44  | 52 | 66 | 92 | 142 | 234 |
| 0.040   | 46  | 56 | 70 | 94 | 148 | 314 |
| 0.010   | 66  | 68 | 74 | 100 | 156 | 330 |
Figure 2: Simulation experiment comparing four methods: profile maximum likelihood estimation (pMLE), spectral clustering on the mean graph (spectral_mean), majority vote by spectral clustering (spectral_vote) and variational approximation (variational_vote). The two proposed methods (pMLE and spectral_mean) have the anticipated increasing accuracy over time while the two heuristic methods fail.

Both profile maximum-likelihood estimation and spectral clustering on the mean graph have the anticipated increasing accuracy over time. But the accuracies of the two heuristic majority vote methods do not improve. Though one may expect the errors in majority vote to be canceled out over time, these results show that, without careful averaging of errors, we cannot gain from the multiple layers.

4.3 MIT reality mining data

Next we apply our model on the MIT Reality Mining data set (Eagle and Pentland, 2006). This data set comprises 93 students and staff at MIT in the 2004-2005 school year during which time their cell phone activities were recorded. We construct dynamic networks based on physical proximity, which was measured using scans for nearby Bluetooth devices at 5-minute intervals. We exclude data near the beginning and end of the experiment where participation was low. Each time step corresponds to a 1-week interval, resulting in 39 time steps between August 2004 and May 2005.

We treat the affiliation of participants as ground-truth class labels and test our proposed methods. Two communities are found: one of 26 Sloan business school students, and one of 67 staff
working in the same building. Since degree heterogeneity may cause problems in detecting communities using the SBM (Karrer and Newman, 2011), we reduce its impact by connecting each participant to the 5 other participants who spent the most time in physical proximity during each week. The class connection probabilities vary significantly over time, which validates the importance of the varying class connection probability assumption in our model. Figure 3 shows the empirical block connection probabilities within and between the two classes, estimated by the profile MLE. Notice that the two communities become well-separated around week 8. The class estimation accuracies for the different methods are shown in Table 2. Since the community structure only becomes clear at around week 8, the spectral and profile MLE methods are initially worse than majority voting but quickly improve and are superior over the remainder of the data trace. By combining
Figure 4: The estimated community structures in the AU-CS multi-layer networks overlaid onto the adjacency matrices of different relations. The dots denote connections, and the grids correspond to blocks.

information across time, the proposed methods successfully reveal the community structure while majority voting continues to improperly estimate the classes of about 20% of the people.

4.4 AU-CS multi-layer network data

We look at another example from a multi-layer network comprising five kinds of self-reported online and off-line relationships between the employees of a research department: Facebook, leisure, work, co-authorship, and lunch (AU-CS ML). We assume the class structure to be invariant across the different types of relations and apply our model. For model selection, we extend the Integrated Completed Likelihood (ICL) (Daudin et al., 2008) to multi-graphs to select the number of blocks $K$. Specifically we maximize the term

$$-2Q(G) + (K - 1) \log N + [TK(K + 1)/2] \log[N(N - 1)/2],$$
where $Q(\tilde{G})$ is the variational approximation to the complete log-likelihood. We start the variational approximation with different randomizations as well as the spectral clustering solution. The criteria is maximized at $K = 4$.

Figure 4 shows the estimated 4 classes overlaid onto the adjacency matrix of each relation. Although we have no ground truth for this data set, we detect well-separated communities in all relations. Notice once again the difference in empirical connection probabilities over the multiple layers of the multi-graph.

5 Discussion

In this paper, we investigate the multi-graph stochastic block model applied to dynamic and multi-layer networks with invariant class structure. Both spectral clustering on the mean graph and maximum-likelihood estimation are proved to be consistent for a fixed number of nodes when we have an increasing number of network layers, provided the class connection probabilities satisfy some identifiability conditions.

There is much room for extension on the multi-graph stochastic block model. First, we can add a layer of probabilistic modeling on the probability matrices if we have additional information. Since dynamic networks usually vary smoothly over time, we can put a state-space model to ensure continuity. Xu and Hero (2014) provide a detailed discussion. We can also use a hierarchical model on the probability matrices. In multiple layers, if we know the types of connections are all stronger within classes than between classes, we can use different hyper means for diagonal and off-diagonal elements in probability matrices.

A limitation of our model is that we assume a fixed number of classes over all layers of the network. However, it is not as restrictive as one may imagine. Consider stochastic block models on two networks over the same set of nodes with $K_1$ and $K_2$ blocks, respectively. Then they can be viewed as a multi-graph network with at most $K_1 \times K_2$ blocks. Therefore, any multi-layer network can be regarded as a multi-graph SBM with at most $K_{\text{max}} = K_1 \times K_2 \times \ldots \times K_T$ blocks, as long as each layer obeys the stochastic block model. Of course $K_{\text{max}}$ gets large quickly, and the classes lose
meaning after a block becomes a singleton. However in many real-world application the number of blocks is mostly of manageable size compared to the number of nodes $n$. In addition, choosing an appropriate $K$ is difficult. One could potentially use Bayesian nonparametrics to determine a posterior distribution of $K$ by extending the infinite relational model (Kemp et al., 2006).

A Proof of theorem 1

**Proof.** Denote the vector latent class label for each node as $\vec{C}_i = (C_{i1}, ..., C_{iK})$ where $C_{ij} = \begin{cases} 0, & c_i \neq j \\ 1, & c_i = j \end{cases}$. Denote $C_{N \times K} = \begin{bmatrix} \vec{C}_1 \\ \vdots \\ \vec{C}_N \end{bmatrix}$. Notice that

$$E(\bar{G}) = E(\bar{\Phi}) = CE(\bar{P})C' = C\bar{Q}C'$$

Intuitively $\bar{G}$ would converge to $C\bar{Q}C'$. Because the eigen decomposition of $C\bar{Q}C'$ only has $K$ distinct rows, the eigen decomposition of $\bar{G}$ would converge to that of $C\bar{Q}C'$ and eventually the rows of eigenvectors will be well separated for nodes in different classes. More formally, we first bound the difference of $\bar{G}$ and $C\bar{Q}C'$.

The Frobenius norm of matrix is $\|A\|_F = (\sum_{i,j} a_{ij}^2)^{1/2}$. We have

$$E(\|\bar{G} - C\bar{Q}C'\|^2_F) = \sum_{i,j} \text{Var}(G_{ij})$$

$$= \sum_{i,j} E(\text{Var}(\bar{G}_{ij} | \bar{\Phi}_{ij})) + \text{Var}(E(\bar{G}_{ij} | \bar{\Phi}_{ij}))$$

$$\text{Var}(\bar{G}_{ij} | \bar{\Phi}_{ij}) = \bar{\Phi}_{ij}(1 - \bar{\Phi}_{ij})/T \leq \frac{1}{4T}$$

$$\text{Var}(E(\bar{G}_{ij} | \bar{\Phi}_{ij})) = \text{Var}(\bar{\Phi}_{ij})$$

$$= \text{Var}(\bar{P}_{zizj})$$

$$= \epsilon^2/T$$
Therefore,

\[ E(\|\tilde{G} - C\bar{Q}C'\|_F^2) \leq \frac{N^2(1 + 4\epsilon^2)}{4T} \]

By Markov inequality, for any \( \delta \),

\[ P(\|\tilde{G} - C\bar{Q}C'\|_F^2 > \delta) \leq \frac{N^2(1 + 4\epsilon^2)}{4T\delta} \rightarrow 0, \text{ as } T \rightarrow \infty \]

As a result, the spectral norm \( \|\tilde{G} - C\bar{Q}C'\| \leq \|\tilde{G} - C\bar{Q}C'\|_F \) goes to 0 too. Based on lemma A.2 of (Oliveira, 2009), if \( \bar{Q} \) has \( K \) distinct eigenvalues, then the eigenvectors of \( \tilde{G} \) is close to the corresponding eigenvectors of \( C\bar{Q}C' \). That is, let \( u_i \) be the \( i \)th eigenvectors corresponding to the \( i \)th largest eigenvalues of \( \tilde{G} \). Let \( \theta_i \) be the counterpart of \( C\bar{Q}C' \). If \( \|\tilde{G} - C\bar{Q}C'\| < \epsilon \), then \( \|u_iu_i^T - \theta_i\theta_i^T\| < \delta\epsilon \). This implies that \( 1 - (u_i^T\theta_i)^2 < \delta\theta \). That is, \( u_i \) is close to \( \theta_i \) or \(-\theta_i\). But \( C\bar{Q}C' \) has only \( K \) distinct rows. So the results show a spectral clustering on \( \tilde{G} \) will eventually lead to perfect labeling.

\[ \square \]

B Proof of theorem 2

We begin with the lemmas.

**Proof of lemma 1.** This is from lemma A1 and A2 of (Choi et al., 2012). To recap, the arguments are, \( h \), the expectation of log likelihood, is always maximized at true parameter. For any partition of \( P \), any refinement of the partition increases \( h \). For any label assignment \( z \), we can find a refinement that has at least \( \frac{r(z)}{2} \) pairs of nodes that connect to at least \( \min_k n_k(c) \) of nodes that differ at least \( \delta \) to the truth.

\[ \square \]

**Proof of lemma 2.** Because of symmetry, we only consider \( p \in (0, \frac{1}{2}] \). Let \( C_0 = p/2 \). Then \( C_0 < p < 1 - C_0 \). Let region \( C = [C_0, 1 - C_0] \). By Chernoff bound, \( P(|x - p| > \epsilon) \leq 2\exp(-2n\epsilon^2) \). Therefore, \( P(x \notin C) \leq 2\exp(-\frac{np^2}{2}) \). Denote \( E_C(x) = \sum_{x \in C} xp(x) \). So the subscript \( C \) means any
operation restricted on region C. We can get the following bounds.

\[ \sigma(p) = p \log(p) + (1 - p) \log(1 - p); \quad M_0 = \max_{p \in C} |\sigma(p)| = -\sigma(0.5) \leq 0.7 \]

\[ \sigma'(p) = \log(p) - \log(1 - p); \quad M_1 = \max_{p \in C} |\sigma'(p)| = \log(1 - C_0) - \log(C_0) \]

\[ \sigma''(p) = \frac{1}{p} + \frac{1}{1 - p}; \quad M_2 = \max_{p \in C} |\sigma''(p)| = \frac{1}{C_0} + \frac{1}{1 - C_0} \]

\[ \sigma'''(p) = -\frac{1}{p^2} + \frac{1}{(1 - p)^2}; \quad M_3 = \max_{p \in C} |\sigma'''(p)| = \frac{1}{C_0^2} - \frac{1}{(1 - C_0)^2} \]

\[ \sigma^{(4)}(p) = \frac{1}{2p^3} + \frac{1}{2(1 - p)^3}; \quad M_4 \max_{p \in C} |\sigma^{(4)}(p)| = \frac{1}{2C_0^3} + \frac{1}{2(1 - C_0)^3} \]

\[ |E_C \sigma(x)| \leq M_0 P(x \notin C) \leq 2 \exp(-\frac{np^2}{2}) \]

\[ E(x - p)^3 = \frac{p(1-p)(1-2p)}{n^2} \leq \frac{1}{4n^2} \]

\[ E(x - p)^4 = \frac{p(1-p)^3 + p^3(1-p)}{n^3} + \frac{3(n-1)p^2(1-p)}{n^3} \leq \frac{1}{2n^3} + \frac{1}{4n^2} \]

By Taylor expansion, on region C,

\[ \sigma(x) = \sigma(p) + \sigma'(p)(x - p) + \frac{\sigma''(p)}{2}(x - p)^2 + \frac{\sigma'''(p)}{6}(x - p)^3 + R(x) \]

\[ |R(x)| \leq \max_{x \in C} |\sigma^{(4)}(x)(x - p)^4/24| \]

\[ n[E(\sigma(x)) - \sigma(p)] - \frac{1}{2} \]

\[ = nE[\sigma(x) - \sigma(p) - \sigma'(p)(x - p) - \frac{\sigma''(p)}{2}(x - p)^2] \]

\[ \leq nE_C[\sigma(x) - \sigma(p) - \sigma'(p)(x - p) - \frac{\sigma''(p)}{2}(x - p)^2] + n(2M_0 + 2M_1)P(x \notin C) \]

\[ \leq nE_C[\frac{\sigma'''(p)}{6}(x - p)^3] + \max_{x \in C} |\sigma^{(4)}(x)(x - p)^4/24| + n(2M_0 + 2M_1)P(x \notin C) \]

\[ \leq \frac{M_3}{24n} + \frac{M_4}{24} \left( \frac{1}{2n^2} + \frac{1}{4n} \right) + 2n(1 + M_1 + \frac{M_3}{6}) \exp(-\frac{np^2}{2}) \]

\[ \rightarrow 0, \text{ as } n \rightarrow \infty \]
Proof of lemma 3. For any $z$, as $\bar{P}$ averages $P$, $C_0 \leq \bar{P}_{kl}(z) \leq 1 - C_0$. We have

$$g(z) - h(z) = \sum_{k \leq l} n_{kl}(z)[E(x_{kl}(z)) - \sigma(\bar{P}_{kl})]$$

where $x_{kl}(z) = \frac{O_{kl}(z)}{n_{kl}(z)} \sim \frac{1}{n_{kl}}\text{Bin}(n_{kl}, \bar{P}_{kl})$.

By lemma 2, we see

$$n_{kl}(z)[E(x_{kl}(z)) - \sigma(\bar{P}_{kl})] \rightarrow \frac{1}{2} + O\left(\frac{1}{n_{kl}(z)}\right)$$

Therefore,

$$g(z) - h(z) = \frac{K(K+1)}{4} + O\left(\frac{K^2}{m(z)}\right)$$

Proof of Theorem 2. We want to show that there exists $\delta_0$ such that

$$Ef(c) - Ef(z) \geq \delta_0$$  \hspace{1cm} (7)

for all $z \neq c$. Then by Bernstein’s inequality, we have

$$\frac{1}{T} \left| \sum_t [f^t(z) - Ef^t(z)] \right| \rightarrow 0 \text{ as } T \rightarrow \infty$$

Therefore,

$$\frac{1}{T} \sum_t f^t(c) - \frac{1}{T} \sum_t f^t(z) \rightarrow \frac{1}{T} \sum_t (Ef(c) - Ef(z)) \geq \delta_0$$

for all $z \neq c$. Then we get the conclusion that $c$ is the unique maximizer of $\sum_t f^t(z)$. To show Equation 7, we know

$$Ef(c) - Ef(z) = g(c) - g(z)$$

$$= (h(c) - h(z)) + (g(c) - h(c)) - (g(z) - h(z))$$

$$\geq \delta m(c)r(z) + (g(c) - h(c)) - (g(z) - h(z))$$

by lemma 1.
Let \( n_0 \) to be the threshold that for all \( n \geq n_0 \), \(|g(z) - h(z) - \frac{K(K+1)}{4}| \leq \delta_1 \) if \( m(z) \geq n_0 \). Then for \( m(c) \geq n_0 \),

\[ g(c) - h(c) \geq \frac{K(K+1)}{4} - \delta_1 \]

For any \( z \), the total number of nodes are \( N \geq m(c) * K \). The total number of nodes that do not satisfy \( n_k(z) \geq n_0 \) is at most \( n_0(K - 1) \). And for the rest of nodes, we still have the bounded feature as in lemma 3. Therefore,

\[ g(z) - h(z) \leq \delta_2 n_0(K - 1) + \frac{K(K+1)}{4} + \delta_1 \]

Therefore,

\[ Ef(c) - Ef(z) \geq \delta m(c) r(z) - 2\delta_1 - \delta_2 n_0(K - 1) \]

This is an increasing function of \( m(c) \). So we can find large enough \( m(c) \) that \( \delta m(c) r(z) - 2\delta_1 - \delta_2 n_0(K - 1) \geq \delta_0 \) as we need.

\[ \Box \]

C Details of variational approximation

Denote vector \( \tilde{z}_i = (z_{i1}, \ldots, z_{iK}) \) for each node \( i \) the class assignment vector.

\[ z_{ik} = \begin{cases} 
1 & \text{if } i \text{ in class } k \\
0 & \text{otherwise} 
\end{cases} \]

So \( \tilde{z}_i \) has all 0 except one 1 indicating its class. This notation is easier for writing down the likelihood. We further let the initial class assignment probability to be \( \tilde{\pi} = (\pi_1, \ldots, \pi_K) \). This is the multinomial parameter of \( \tilde{z}_i \). The likelihood is

\[ l = \prod_{i,k} \pi_k^{z_{ik}} \prod_{i<j,k \leq l} \left[ (p_{kl}^{t})^{g_{ij}^{t}} (1 - p_{kl}^{t})^{1-g_{ij}^{t}} \right]^{z_{ik}z_{jl}} \]

It is difficult to maximize because \( \tilde{z} \) cannot be integrated out. Instead we use variational approximation to decompose the likelihood into independent marginal distributions and apply expectation-
maximization technique to search for maximum. Let $\tilde{z}_i$ be independent multinomial distribution, $\tilde{z}_i \sim \text{Multi}(b_{i1}, \ldots, b_{iK})$, $E[z_{ik}] = b_{ik}$.

In the variational E-step, the approximate marginal distribution $q(z_i)$ is

$$
\ln q(z_i) = \sum_k z_{ik} \ln \pi_k + \sum_{j \neq i, l, t} E[z_{jl}] \left( g_{ij}^t \ln P_{kl}^t + (1 - g_{ij}^t) \ln (1 - P_{kl}^t) \right) + \text{Const.} \quad (8)
$$

We update $b_{ik}$ according to (8). In the M-step, we maximize $\pi$ and $P^t$.

$$
\pi_k \propto \sum_i E[z_{ik}] = \sum_i b_{ik}
$$

$$
P_{kl}^t = \frac{\sum_{i \neq j} E[z_{ik}] E[z_{jl}] g_{ij}^t}{\sum_{i \neq j} E[z_{ik}] E[z_{jl}]} = \frac{\sum_{i \neq j} b_{ik} b_{jl} g_{ij}^t}{\sum_{i \neq j} b_{ik} b_{jl}}
$$

Iterate between the 2 steps until convergence.

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