Statistical Inference in Heterogeneous Block Model

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Abstract

There exist various types of network block models such as the Stochastic Block Model (SBM), the Degree Corrected Block Model (DCBM), and the Popularity Adjusted Block Model (PABM). While this leads to a variety of choices, the block models do not have a nested structure. In addition, there is a substantial jump in the number of parameters from the DCBM to the PABM. The objective of this paper is formulation of a hierarchy of block model which does not rely on arbitrary identifiability conditions, treats the SBM, the DCBM and the PABM as its particular cases with specific parameter values and, in addition, allows a multitude of versions that are more complicated than DCBM but have fewer unknown parameters than the PABM. The latter allows one to carry out clustering and estimation without preliminary testing to see which block model is really true.

1 Introduction

Consider an undirected network with \( n \) nodes and no self-loops and multiple edges. Let \( A \in \{0, 1\}^{n \times n} \) be the symmetric adjacency matrix of the network with \( A_{i,j} = 1 \) if there is a connection between nodes \( i \) and \( j \), and \( A_{i,j} = 0 \) otherwise. We assume that \( A_{i,j} \sim \text{Bernoulli}(P_{i,j}) \), \( 1 \leq i \leq j \leq n \), where \( A_{i,j} \) are conditionally independent given \( P_{i,j} \) and \( A_{i,j} = A_{j,i} \), \( P_{i,j} = P_{j,i} \) for \( i > j \). The probability matrix \( P \) has low complexity and can be described by a variety of models.

The classical Erdős-Rényi [6] random graph model assumes that the edges in a random graph are drawn independently with an equal probability, does not allow community structures and is too simplistic for applications. The simplest random graph model for networks with community structure is the Stochastic Block Model (SBM) [20], [1], [10]. Under the \( K \)-block SBM, all nodes are partitioned into communities \( G_k \), \( k = 1, \ldots, K \), and the probability of connection between nodes is completely defined by the communities to which they belong: \( P_{i,j} = B_{z(i), z(j)} \) where \( B_{k,l} \) is the probability of connection between communities \( k \) and \( l \), and \( z : \{1, \ldots, n\} \rightarrow \{1, \ldots, K\} \) is a clustering function. The Erdős-Rényi model can be viewed as the SBM with only one community \( K = 1 \).

Since the real-life networks usually contain a very small number of high-degree nodes while the rest of the nodes have very low degrees, the SBM fails to explain the structure of many networks that occur in practice. The Degree-Corrected Block Model (DCBM), introduced by Karrer and Newman (2011) addresses this deficiency by allowing these probabilities to be multiplied by the node-dependent weights. Under the DCBM, the elements of matrix \( P \) are modeled as

\[
P_{i,j} = h_i B_{z(i), z(j)} h_j, \quad i, j = 1, \ldots, n, \tag{1.1}
\]

where \( h = [h_1, h_2, \ldots, h_n] \) is a vector of the degree parameters of the nodes, and \( B \) is the \((K \times K)\) matrix of baseline interaction between communities. Matrix \( B \) and vector \( h \) in (1.1) are defined up to a scalar factor, which is usually fixed via the so called identifiability condition, that can be imposed
in a variety of ways. For example, Karrer and Newman [14] enforce a constraint of the form

\[ \sum_{i \in G_k} h_i = 1, \quad k = 1, \ldots, K. \]  

(1.2)

The DCBM implies that the probability of connection of a node is uniformly proportional to the degree of this node across all communities. This assumption, however, is violated in a variety of practical applications. For this reason, Sengupta and Chen [26] introduced the Popularity Adjusted Block Model (PABM). The PABM presents the probability of a connection between nodes as a product of popularity parameters, that depend on the communities to which the nodes belong as well as on the pair of nodes themselves:

\[ P_{i,j} = V_{i,z(j)} V_{j,z(i)}. \]  

(1.3)

Although the popularity parameters in (1.3) are defined up to scalar constants and require an identifiability condition for their recovery, clustering of the nodes and fitting the matrix of connection probabilities do not require any constraints. According to [24], if one re-arranged the nodes, so that the nodes in every community are grouped together, then matrix \( P \) of the connection probabilities would appear as \((K \times K)\) block matrix with every block \( P^{(k,l)} \) being of rank one.

Having several types of block models introduces a variety of choices, but also leads to some significant drawbacks. Specifically, although the block models can be viewed as progressively more elaborate with the Erdős-Rényi being the simplest and the PABM the most complex, the simpler models are not necessarily particular cases of the more sophisticated ones. Indeed, with the identifiability condition (1.2), the SBM matrix \( B \) will be different from the one in the DCBM formulation (1.1). For this reason, majority of authors carry out estimation and clustering under the assumption that the model which they use is indeed the correct one. There are only very few papers that study goodness of fit in block models and majority of them are concerned with either testing that there are no distinct communities (\( K = 1 \) in SBM or DCBM) [3], [9], [12], or testing the exact number of communities \( K = K_0 \) in the SBM [8], [16], [22]. To the best of our knowledge, [22] is the only paper testing the SBM versus the DCBM, where the testing is carried out under rather restrictive assumptions. On the other hand, using the most flexible model, the PABM, may not always be the right choice since there is a substantial jump in complexity from the DCBM with \( O(n + K^2) \) parameters to the PABM with \( O(nK) \) parameters.

The objective of the present paper is to provide a unified approach to block models. In what follows, we shall deal only with the graphs where each node belongs to one and only one community; thus, leaving aside the mixed membership models [2], [13]. Specifically, our purpose is formulation of a hierarchy of block model which does not rely on arbitrary identifiability conditions, treats the SBM, the DCBM and the PABM as its particular cases (with specific parameter values) and, in addition, allows a multitude of versions that are more complicated than DCBM but have fewer unknown parameters than the PABM. The aim of this construction is to treat all block models as a part of one paradigm and, therefore, carry out estimation and clustering without preliminary testing to see which block model fits data at hand.

2 The hierarchy of block models

Consider an undirected network with \( n \) nodes that are partitioned into \( K \) communities \( G_k, \ k = 1, \ldots, K \), by a clustering function \( z : \{1, \ldots, n\} \to \{1, \ldots, K\} \) with the corresponding clustering
matrix $Z$. Denote by $B$ the matrix of average connection probabilities between communities, so that for $k, l = 1, 2, \ldots, K$, one has

$$B_{k,l} = \frac{1}{n_k n_l} \sum_{i,j=1}^{n} P_{ij} I(z(i) = k) I(z(j) = l), \quad (2.1)$$

where $n_k$ is the number of nodes in the community $k$.

In order to better understand the relationships between various block models, consider a rearranged version $P(Z)$ of matrix $P$ where its first $n_1$ rows correspond to nodes from class 1, the next $n_2$ rows correspond to nodes from class 2 and the last $n_K$ rows correspond to nodes from class $K$. Denote the $(k_1, k_2)$-th block of matrix $P(Z)$ by $P^{(k_1, k_2)}(Z)$. Then, the block models vary by how dissimilar matrices $P^{(k_1, k_2)}(Z)$ are. Indeed, under the SBM

$$P^{(k_1, k_2)}(Z) = B_{k_1, k_2} 1_{n_{k_1}} 1_{n_{k_2}}^T, \quad (2.2)$$

where $1_k$ is the $k$-dimensional column vector with all elements equal to one. In the DCBM, there exists a vector $h \in \mathbb{R}_{+}^K$, with sub-vectors $h^{(k)} \in \mathbb{R}_{+}^{n_k}$, $k = 1, \ldots, K$, such that, for $k_1, k_2 = 1, 2, \ldots, K$,

$$P^{(k_1, k_2)}(Z) = B_{k_1, k_2} h^{(k_1)} (h^{(k_2)})^T. \quad (2.3)$$

In the PABM, instead of one vector $h$, there are $K$ vectors $\Lambda^{(1)}, \ldots, \Lambda^{(K)}$ with sub-vectors

$$\Lambda^{(k_1, k_2)} \in \mathbb{R}_{+}^{n_k}, \quad k_1, k_2 = 1, 2, \ldots, K. \quad (2.4)$$

In this case, vectors $\Lambda^{(k)}$ form the $(n \times K)$ matrix $\Lambda$ with columns partitioned into sub-columns $\Lambda^{(k_1, k_2)}$, and

$$P^{(k_1, k_2)}(Z) = B_{k_1, k_2} \Lambda^{(k_1, k_2)} (\Lambda^{(k_2, k_1)})^T, \quad (2.5)$$

for every $k_1, k_2 = 1, 2, \ldots, K$. Hence, (2.2) and (2.3) coincide if $h \equiv 1_n$, and (2.5) reduces to (2.3) if all columns of matrix $\Lambda$ are identical, i.e.

$$\Lambda^{(k_1, k_2)} \equiv h^{(k_1)}, \quad k_1, k_2 = 1, 2, \ldots, K. \quad (2.6)$$

Since in the DCBM there is only one vector $h$ that models heterogeneity in probabilities of connections, the ratios $P_{i_1,j_1}/P_{i_2,j_2}$ of the probabilities of connections of two nodes, $i_1$ and $i_2$, that belong to the same community, are determined entirely by the nodes $i_1$ and $i_2$ and are independent of the community with which those nodes interact. On the other hand, for the PABM, each node has a different degree of popularity (interaction level) with respect to every other community, so that $P_{i_1,j_1}/P_{i_2,j_2} \neq P_{i_1,j_2}/P_{i_2,j_2}$ if nodes $j_1$ and $j_2$ belong to different communities. In the PABM, those variable popularities are described by the matrix $\Lambda \in [0, 1]^{n \times K}$ which reduces to a single vector $h$ in the case of the DCBM. One can easily imagine the situation where nodes do not exhibit different levels of activity with respect to every community but rather with respect to some groups of communities, “mega-communities”, so that there are $L$, $1 \leq L \leq K$, different vectors $H^{(l)} \in \mathbb{R}_{+}^K$, $l = 1, 2, \ldots, L$, and each of columns $\Lambda_k$, $k = 1, 2, \ldots, K$, of matrix $\Lambda$ is equal to one of vectors $H^{(l)}$. In other words, there exists a clustering function $c : \{1, \ldots, K\} \rightarrow \{1, \ldots, L\}$ with the corresponding clustering matrix $C$ such that

$$\Lambda_k = H^{(l)}, \quad l = c(k), \quad l = 1, \ldots, L, \quad k = 1, \ldots, K.$$ We name the resulting model the **Heterogeneous Block Model** (HBM) to emphasize that, beyond the average connection probabilities of communities, the mega-communities are determined by the heterogeneity of the probabilities of connections.
3 The Heterogeneous Stochastic Block Model (HBM)

The HBM contains two types of communities, the regular communities that can be distinguished by the average probabilities of connections between them (like in the SBM or the DCBM) and the mega-communities that are described by the heterogeneity of probabilities of connections of individual nodes across the communities.

The idea of mega-communities is not entirely new. It was introduced in [29] and recently appeared in [13]. The difference between the present paper and the above cited publications is that in [29] and [13] the mega-communities are determined by intermediate results of the clustering algorithms while we define them on the basis of the heterogeneous patterns of the connection probabilities of nodes with respect to different communities.

For any $M$ and $K \leq M$, denote by $M_{M,K}$ the collection of all clustering matrices $Z \in \{0,1\}^{M \times K}$ with the corresponding clustering function $z : \{1, \ldots, M\} \to \{1, \ldots, K\}$ such that $Z_{i,k} = 1$ iff $z(i) = k$, $i = 1, \ldots, M$. Then, $Z^T Z = \text{diag}(n_1, \ldots, n_K)$ where $n_k$ is the size of community $k$, $k = 1, \ldots, K$. The HBM, with $K$ communities and $L \leq K$ mega-communities, is defined by two clustering matrices $Z \in M_{n,K}$ and $C \in M_{K,L}$ with corresponding clustering functions $z$ and $c$ that, respectively, partition the $n$ nodes into $K$ communities, and $K$ communities into $L$ mega-communities. If the $l$-th mega-community consists of $K_l$ communities and the community sizes are $n_k$, then the total number of nodes in mega-community $l$ is $N_l$, where

$$N_l = \sum_{k=1}^{K} n_k I(c(k) = l), \quad \sum_{l=1}^{L} K_l = K, \quad \sum_{l=1}^{L} N_l = n, \quad l = 1, \ldots, L. \quad (3.1)$$

The communities are characterized by their average connection probability matrix with elements $B_{k_1,k_2}$, $k_1, k_2 = 1, 2, \ldots, K$, defined in (2.1). In order to better understand the mega-communities, consider a permutation matrix $P_{Z,C}$ that arranges nodes into communities consecutively, and orders communities so that the $K_l$ blocks within the $l$-th mega-community are consecutive, $l = 1, 2, \ldots, L$. Recall that $P_{Z,C}$ is an orthogonal matrix with $P_{Z,C}^{-1} = P_{Z,C}^T$ and denote

$$P(Z,C) = P_{Z,C}^T P_{Z,C}, \quad P = P_{Z,C} P(Z,C) P_{Z,C}^T.$$ 

According to $Z$ and $C$, matrix $P$ is partitioned into $K^2$ blocks $P^{(k_1,k_2)}(Z,C) \in [0,1]^{n_{k_1} \times n_{k_2}}$, $k_1, k_2 = 1, \ldots, K$, with the block-averages given by (2.1). In addition, blocks $P^{(k_1,k_2)}(Z,C)$ can be combined into the $L^2$ mega-blocks $B^{(l_1,l_2)}(Z,C) \in [0,1]^{N_{l_1} \times N_{l_2}}$, corresponding to probabilities of connections between mega-communities $l_1$ and $l_2$, $l_1, l_2 = 1, \ldots, L$. Consider matrix $H \in \mathbb{R}^{n \times L}$ (Figure 1 top middle), where each column $H_l$, $l = 1, \ldots, L$, can be partitioned into $K$ sub-vectors $h^{(k,l)} \in \mathbb{R}^{n_k}$ of lengths $n_k$, $k = 1, \ldots, K$. Those sub-vectors are combined into $L$ mega sub-vectors $H^{(m,l)} \in \mathbb{R}^{n_m}$ of lengths $N_m$, $m = 1, \ldots, L$, according to matrix $C$, where $N_m$ is defined in (3.1). Similarly, matrix $B \in [0,1]^{K \times K}$ of block probabilities is partitioned into sub-matrices $B^{(l_1,l_2)} \in [0,1]^{K_{l_1} \times K_{l_2}}$, $l_1, l_2 = 1, \ldots, L$. With these notations, for any $l_1, l_2 = 1, \ldots, L$, the $(l_1, l_2)$-th mega-block of $P$ can be presented as

$$\tilde{P}^{(l_1,l_2)}(Z,C) = \left( H^{(l_1,l_2)} (H^{(l_2,l_1)} )^T \circ \left( J^{(l_1)} B^{(l_1,l_2)} (J^{(l_2)} )^T \right) \right), \quad (3.2)$$

where $A \circ B$ is the Hadamard product of $A$ and $B$, and matrices $J^{(l)} \in \{0,1\}^{N_l \times K_l}$, $l = 1, \ldots, L$, are of the form

$$J^{(l)} = \begin{bmatrix} 1_{n_{k_1}} & 0 & \ldots & 0 \\ 0 & 1_{n_{k_2}} & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & 1_{n_{K_l}} \end{bmatrix}. \quad (3.3)$$
In order for the model to be identifiable, we impose the following assumptions:

**A1.** Matrix $B$ is non-singular with $\lambda_{\min}(B) \geq \lambda_0 > 0$.

**A2.** For each $k = 1, \cdots, K$, vectors $H^{(k,l)}$, $l = 1, \cdots, L$, are linearly independent.

By rewriting (3.2) in an equivalent form, one can conclude that each of the mega-blocks $\tilde{P}^{(l_1,l_2)}(Z,C)$ (and, hence, $\tilde{P}^{(l_1,l_2)}$ if we scramble them to the original order) follows the (non-symmetric) DCBM model with $K_{l_1} \times K_{l_2}$ blocks. Specifically, for a pair of sub-vectors $H^{(l_1,l_2)} \in \mathbb{R}_{+}^{N_{l_1}}$ and $H^{(l_2,l_1)} \in \mathbb{R}_{+}^{N_{l_2}}$ of matrix $H$ and a matrix $B^{(l_1,l_2)} \in [0,1]^{K_{l_1} \times K_{l_2}}$ containing average probabilities of connections for each pair of communities within the mega-community $(l_1, l_2)$ one has

$$\tilde{P}^{(l_1,l_2)}(Z,C) = Q^{(l_1,l_2)} J^{(l_1)} B^{(l_1,l_2)} (J^{(l_2)})^T Q^{(l_2,l_1)}.$$

Here, $Q^{(l_1,l_2)} = \text{diag}(H^{(l_1,l_2)})$ and the $(k_1, k_2)$-th block of $P$ is given by

$$P^{(k_1,k_2)}(Z,C) = B_{k_1,k_2} h^{(k_1,l_2)} \left( h^{(k_2,l_1)} \right)^T,$$

where $l_i = c(k_i)$, $i = 1, 2$, and $h^{(k,l)} \in \mathbb{R}_{+}^{N_k}$ is a sub-vector of $H^{(m,l)}$ with $m = c(k)$. Observe that the formulation above imposes a natural scaling on the sub-vectors $h^{(k,l)}$ of $H$, since it follows from equations (2.1) and (3.4), that for any pair of communities $(k_1, k_2)$ which belong to a pair of
The latter implies that for any $k = 1, \ldots, K$ and $l = 1, \ldots, L$,
\[ 1^T_k h^{(k,l)} = n_k, \quad k = 1, \ldots, K, \quad l = 1, \ldots, L. \] (3.5)

Now, it is easy to see that all block models, the SBM, the DCBM and the PABM, can be viewed as particular cases of the HBM introduced above. Indeed, the DCBM is a particular case of the HBM with $L = 1$ while the PABM corresponds to the setting of $L = K$. Finally, due to (3.5), the SBM constitutes a particular case of the HBM with $L = 1$ and matrix $H$ reduced to vector $1_n$, the $n$-dimensional column vector with all entries equal to one. Moreover, the absence of the community structure (whether in the SBM or the DCBM) is equivalent to $K = 1$, and implies that the HBM necessarily reduces to the DCBM.

4 Optimization procedure for estimation and clustering

Note that, in terms of the matrices $J^{(l)}$ defined in (3.3), the scaling conditions (3.5) appear as
\[ (J^{(l)})^T Q^{(l,l')} J^{(l')} = (J^{(l)})^T J^{(l)}, \quad l, l' = 1, \ldots, L. \] (4.1)

Let $\mathcal{P}_{\tilde{Z}, \tilde{C}}$ be the permutation matrix corresponding to $\tilde{Z} \in \mathcal{M}_{n,K}$ and $\tilde{C} \in \mathcal{M}_{K,L}$. Consider the set $\mathcal{M}(n, K, L)$ of matrices $\Theta$ with blocks $\Theta^{(l_1,l_2)} \in [0,1]^{N_{l_1} \times N_{l_2}}$, $l_1, l_2 = 1, \ldots, L$, such that
\[
\Theta = \bigcup_{l_1,l_2} \Theta^{(l_1,l_2)} \Theta^{(l_1,l_2)} = Q^{(l_1,l_2)} J^{(l_1)} B^{(l_1,l_2)} (J^{(l_2)})^T Q^{(l_2,l_1)},
\]
\[ B^{(l_1,l_2)} \in [0,1]^{K_{l_1} \times K_{l_2}}, \quad Q^{(l_1,l_2)} \in \mathcal{D}_{l_1}, \]
\[ Z \in \mathcal{M}_{n,K}, \quad C \in \mathcal{M}_{K,L}, \quad l_1, l_2 = 1, \ldots, L, \] (4.2)
where \( D_m \) the set of diagonal matrices with diagonals in \( \mathbb{R}_+^m \) and conditions (3.1) and (4.1) hold. Then, it is easy to see that \( P = \mathcal{P}^T_{Z,C} \Theta \mathcal{P}^{T}_{Z,C} \), so its estimator can be obtained as

\[
P = \mathcal{P}^T_{Z,C} \Theta (\hat{Z}, \hat{C}) \mathcal{P}^{T}_{Z,C} \tag{4.3}
\]

Here, for given values of \( K \) and \( L \), \((\hat{Z}, \hat{C}, \hat{\Theta})\) is a solution of the following optimization problem

\[
(\hat{Z}, \hat{C}, \hat{\Theta}) \in \text{argmin}_{Z,C,\Theta} \| A(Z,C) - \Theta \|_F^2 \tag{4.4}
\]

subject to conditions \( A(Z,C) = \mathcal{P}^T_{Z,C} A \mathcal{P}^{T}_{Z,C} \), (3.1), (4.1) and (4.2). In real life, however, the values of \( K \) and \( L \) are unknown and need to be incorporated into the optimization problem by adding a penalty \( \text{Pen}(K, L) \) on \( K \) and \( L \):

\[
(\hat{\Theta}, \hat{Z}, \hat{C}, \hat{K}, \hat{L}) \in \text{argmin}_{Z,C,K,L,\Theta} \left\{ \| A(Z,C) - \Theta \|_F^2 + \text{Pen}(K, L) \right\} \tag{4.5}
\]

where optimization is carried out subject to conditions \( A(Z,C) = \mathcal{P}^T_{Z,C} A \mathcal{P}^{T}_{Z,C} \), (3.1), (4.1) and (4.2). After that, the estimator \( \hat{P} \) of \( P \) can be obtained as (4.3). In practice, one would need to solve optimization problem (4.4) for each \( K = 1, \ldots, n \) and \( L = 1, \ldots, K \), and then find the values \((\hat{K}, \hat{L})\) that minimize the right hand side in (4.5). After that, the estimator \( \hat{P} \) of \( P \) is obtained as (4.3). Then, the following statement holds.

**Theorem 1.** Let Assumptions A1 and A2 hold. Let \((\hat{\Theta}, \hat{Z}, \hat{C}, \hat{K}, \hat{L})\) be a solution of optimization problem (4.5) subject to conditions \( A(Z,C) = \mathcal{P}^T_{Z,C} A \mathcal{P}^{T}_{Z,C} \), (3.1), (4.1) and (4.2) with

\[
\text{Pen}(K, L) = C_1 (nL + K^2) \ln n + C_2 n \ln K \tag{4.6}
\]

where \( C_1 \) and \( C_2 \) are absolute constants. Then, for the estimator \( \hat{P} \) given by (4.3), the true matrix \( P_* \) and any \( K, L, Z \in \mathcal{M}_{n,K}, C \in \mathcal{M}_{K,L} \) and any matrix \( P = \mathcal{P}^T_{Z,C} \Theta \mathcal{P}^{T}_{Z,C} \) with \( \Theta \in \mathcal{S}(n, K, L) \), one has

\[
\mathbb{P} \left\{ \| \hat{P} - P_* \|_F^2 \leq 3 \| P - P_* \|_F^2 + \text{Pen}(K, L) \right\} \geq 1 - \left( n^2 \log_2 n + 1 \right) e^{-n/32},
\]

\[
\mathbb{E} \| \hat{P} - P_* \|_F^2 \leq 3 \| P - P_* \|_F^2 + \text{Pen}(K, L) \right\} + n^5 e^{-n/32}.
\]

Solution of optimization problem (4.5) requires a search over the continuum of matrices \( \Theta \). In order to simplify the estimation, we consider a solution of a somewhat simpler optimization problem. It is easy to observe (see Figure 1) that each of the block columns of matrix \( P \) is a matrix of rank one and, given the clustering, it can be obtained by the rank one projection of the respective adjacency sub-matrix. Denote the block columns of the re-arranged matrices \( P \) and \( A \) by \( P^{(l,k)}(Z,C) \) and \( A^{(l,k)}(Z,C) \). Then, the optimization problem appears as

\[
(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) \in \text{argmin}_{Z,C,K,L} \left\{ \sum_{l=1}^{L} \sum_{k=1}^{K} \| A^{(l,k)}(Z,C) - \Pi_1 \left( A^{(l,k)}(Z,C) \right) \|_F^2 + \text{Pen}(K, L) \right\} \tag{4.7}
\]

s.t. \( A(Z,C) = \mathcal{P}^T_{Z,C} A \mathcal{P}^{T}_{Z,C} \),

where \( \Pi_1 \left( A^{(l,k)}(Z,C) \right) \) is the rank one projection of the matrix \( A^{(l,k)}(Z,C) \). Then, \( \hat{\Theta} \) is the block matrix with blocks \( \hat{\Theta}^{(l,k)} = \Pi_1 \left( A^{(l,k)}(\hat{Z}, \hat{C}) \right), l = 1, \ldots, \hat{L}, k = 1, \ldots, \hat{K} \).
Theorem 2. Let Assumptions A1 and A2 hold. Let $(\hat{\Theta}, \hat{Z}, \hat{C}, \hat{K}, \hat{L})$ be a solution of optimization problem (4.7) with Pen(K, L) of the form

$$\text{Pen}(K, L) = \Psi_1 n K + \Psi_2 K^2 \ln n + \Psi_3 n \ln K,$$

where $\Psi_1$, $\Psi_2$, and $\Psi_3$ are positive absolute constants. Then, for the estimator $\hat{P}$ of $P_*$ given by (4.3) and any $t > 0$, one has

$$\mathbb{P}\left\{ \| \hat{P} - P_* \|_F^2 \leq \tilde{C} \left[ \text{Pen}(n, K_*, L_*) + t \right] \right\} \geq 1 - 3e^{-t},$$

$$\mathbb{E} \| \hat{P} - P_* \|_F^2 \leq \tilde{C} \left[ \text{Pen}(n, K_*, L_*) + 3 \right].$$

Here $K_*$ and $L_*$ are the true number of communities and mega-communities and $\tilde{C} = \tilde{C}(\Psi_1, \Psi_2, \Psi_3) > 0$ is an absolute constant.

Observe that Theorem 2 asserts smaller error rates if $K_*/L_* \ll \ln n$, i.e., if $n$ is large.

5 Implementation of clustering

The optimization procedure in (4.5) is NP-hard. In this section, we describe a computationally tractable clustering procedure that can replace it. Since the model requires identification of mega-communities and communities, naturally, the clustering is carried out in two steps. First, we find the clustering matrix $C$ that arranges the nodes into $L$ mega-communities. Subsequently, we detect communities within each of the mega-communities, obtaining the clustering matrix $Z$.

In order to accomplish the first task, we use the fact that, for a given $L$, under Assumption A2, the columns of matrix $P_*$ lie in the union of $L$ distinct subspaces. Finding those subspaces can be carried out by the subspace clustering. Subspace clustering is widely used in, e.g., computer vision and is designed for separation of points that lie in the union of subspaces. While subspace clustering can be implemented by a variety of techniques, in this paper we use spectral clustering based methods [5], [7], [19], [27]. In particular, we apply the Sparse Subspace Clustering (SSC) [5] which is based on representation of each of the vectors as a sparse linear combination of all other vectors, with the expectation that a vector is more likely to be represented as a linear combination of vectors in its own subspace rather than other subspaces.

If matrix $P_*$ were known, the weight matrix $W$ would be based on writing every data point as a sparse linear combination of all other points by minimizing the number of nonzero coefficients

$$\min_{W_j} \| W_j \|_0 \quad \text{s.t.} \quad (P_*)_j = \sum_{k \neq j} W_{k,j} (P_*)_k$$

(5.1)

where, for any matrix $B$, $B_j$ is its $j$-th column. The affinity matrix of the SSC is the symmetrized version of the weight matrix $W$. Note that since, due to Assumption A2, the subspaces are linearly independent, the solution to the optimization problem (5.1) is $W_j$ such that $W_{k,j} \neq 0$ only if points $k$ and $j$ are in the same subspace. Since the problem (5.1) is NP-hard, one usually solves its convex relaxation

$$\min_{W_j} \| W_j \|_1 \quad \text{s.t.} \quad (P_*)_j = \sum_{k \neq j} W_{k,j} (P_*)_k$$

(5.2)

In the case of data contaminated by noise, the SSC algorithm does not attempt to write data as an
Algorithm 1: The SSC procedure

**Input:** Adjacency matrix $A$, number of clusters $k$, tuning parameters $\gamma_1, \gamma_2$

**Output:** Clustering matrix $C$

**Steps:**
1: For $j = 1, \ldots, n$, find $\hat{W}_j$ in (5.3)
2: Apply spectral clustering to the affinity matrix $|\hat{W}| + |\hat{W}^T|$ to find clustering matrix $C$

Algorithm 2: Spectral clustering with $k$-median

**Input:** Adjacency matrix $A \in \{0, 1\}^{n \times n}$, number of clusters $k$

**Output:** Community assignment

**Steps:**
1: Find $\hat{P} = \Pi_k(A)$, the best rank $k$ approximation of matrix $A$
2: For $j = 1, \ldots, n$, find $\hat{P}_j = \hat{P}_j / \|\hat{P}_j\|_1$
3: Apply spectral clustering to $\hat{P}$ to obtain community assignment

In the first step of clustering, we apply Algorithm 1 to the adjacency matrix $A$ with $k = L$ to find $L$ mega-communities defined by the clustering matrix $C$. In the second step, Algorithm 2 is applied to each of the $L$ mega-communities, obtained at the first step. Specifically, we apply Algorithm 2 with $k = K_l$ and $n = N_l$ to cluster the $l$-th mega-community, $l = 1, \ldots, L$. The union of these communities combined with the clustering matrix $C$, yields the clustering matrix $Z$.
6 Simulations and a real data example

6.1 Simulations on synthetic networks

In the experiments with synthetic data, we generate networks with \( n \) nodes, \( L \) mega-communities and \( K \) communities that fit the HBM. For simplicity, we consider perfectly balanced networks where the number of nodes in each community and mega-community are respectively \( n/K \) and \( n/L \), and there are \( K/L \) communities in each mega-community. First, we generate \( L \) distinct \( n \)-dimensional random vectors with entries between 0 and 1. To this end, we generate a random vector \( Y \in (0,1)^n \) and partition it into \( K \) blocks \( Y^{(k)}, k = 1, \ldots, K \), of size \( n/K \). The vector \( \tilde{h}^{(1)} \) is generated from \( Y \) by sorting each block of \( Y \) in ascending order. After that, we partition each of the \( K \) blocks, \( \tilde{h}^{(k,1)} \) of \( \tilde{h}^{(1)} \), into \( L \) sub-blocks \( \tilde{h}^{(k,1)}_{i}, i = 1, \ldots, L \), of equal size. To generate the \( k \)-th block \( \tilde{h}^{(k,2)} \) of \( \tilde{h}^{(2)} \), we reverse the order of entries in each sub-block \( \tilde{h}^{(k,1)}_{i} \) and rearrange them in descending order. The blocks \( \tilde{h}^{(k,s)} \) of subsequent vectors \( \tilde{h}^{(s)} \), \( s = 3, \ldots, L \), are formed by re-arranging the order of sub-blocks \( \tilde{h}^{(k,2)}_{i} \) in each sub-vector \( \tilde{h}^{(k,2)} \). The \( L \) vectors \( \tilde{h}^{(l)} \), \( l = 1, \ldots, L \), generated by this procedure have different patterns leading to detectable mega-communities. Subsequently, we scale the vectors as \( H^{(k,l)} = (n/K) \tilde{h}^{(k,l)}/\|\tilde{h}^{(k,l)}\|_1 \), \( k = 1, \ldots, K \), \( l = 1, \ldots, L \), obtaining matrix \( H \). After that, we replicate \( K/L \) times each of the columns of \( H \) (Figure 1, top right) and denote the resulting matrix by \( \hat{H} \). Matrix \( B \) has entries

\[
B_{k,l} = \hat{B}_{k,l} ((\hat{H}_{\max})_{k,l})^{-2}, \quad k, l = 1, \ldots, K, \tag{6.1}
\]

where \( \hat{B} \) is a \((K \times K)\) symmetric matrix with random entries between 0.35 and 1 to avoid very sparse networks, and the largest entries of each row (column) are on the diagonal. Matrix \( \hat{H}_{\max} \) is a \( K \times K \) symmetric matrix defined as

\[
(\hat{H}_{\max})_{k,l} = \max \left( \hat{H}^{(k,l)}, \hat{H}^{(l,k)} \right), \quad k, l = 1, \ldots, K,
\]

where \( \hat{H}^{(k,l)} \) is the \((k,l)\)-th block of matrix \( \hat{H} \). The term \(((\hat{H}_{\max})_{k,l})^{-2}\) in (6.1) guarantees that the entries of probability matrix \( P(Z,C) \) do not exceed one. To control how assortative the network is, we multiply the off-diagonal entries of \( B \) by the parameter \( \omega \in (0,1) \). The values of \( \omega \) close to zero produce an almost block diagonal probability matrix \( P(Z,C) \) while the values of \( \omega \) close to one lead to \( P(Z,C) \) with more diverse entries. We obtain the probability matrix \( P(Z,C) \) as

\[
P^{(k,l)}(Z,C) = B_{k,l} \hat{H}^{(k,l)} \left( \hat{H}^{(l,k)} \right)^T, \quad k, l = 1, \ldots, K.
\]

After that, to obtain the probability matrix \( P \), we generate random clustering matrices \( Z \in \mathcal{M}_{n,K} \) and \( C \in \mathcal{M}_{K,L} \) and their corresponding \( n \times n \) permutation matrices \( \mathcal{P}(Z) \) and \( \mathcal{P}(C) \), respectively. Subsequently, we set \( \mathcal{P}_{Z,C} = \mathcal{P}(Z)\mathcal{P}(C) \) and obtain the probability matrix \( P \) as \( P = \mathcal{P}_{Z,C}P(Z,C)(\mathcal{P}_{Z,C})^T \). Finally we generate the lower half of the adjacency matrix \( A \) as independent Bernoulli variables \( A_{i,j} \sim \text{Bern}(P_{i,j}), \ i = 1, \ldots, n, j = 1, \ldots, i - 1 \), and set \( A_{i,j} = A_{j,i} \) when \( j > i \). In practice, the diagonal \( \text{diag}(A) \) of matrix \( A \) is unavailable, so we estimate \( \text{diag}(P) \) without its knowledge.

We apply Algorithm 1 to find the clustering matrix \( \hat{C} \). Since the diagonal elements of matrix \( A \) are unavailable, we initially set \( A_{i,i} = 0, \ i = 1, \ldots, n \). We use \( \gamma_1 = 30\rho(A) \) and \( \gamma_2 = 125(1 - \rho(A)) \) where \( \rho(A) \) is the density of matrix \( A \), the proportion of nonzero entries in \( A \). The spectral clustering in step 2 of the Algorithm 1 is carried out by the normalized cut algorithm [28]. Once the mega-communities are obtained, we apply Algorithm 2 to detect communities inside each mega-community.
The union of detected communities and the clustering matrix $\hat{C}$ yields the clustering matrix $\hat{Z}$. Given $\hat{Z}$ and $\hat{C}$, we generate matrix $A(\hat{Z}, \hat{C}) = \mathcal{P}_k^T A \mathcal{P}_l \hat{Z}$, with blocks $A^{(k,l)}(\hat{Z}, \hat{C})$, $k = 1, \ldots, K$, $l = 1, \ldots, L$, and obtain $\hat{\Theta}^{(k,l)}(\hat{Z}, \hat{C})$ by using the rank one approximation for each of the blocks. Finally, we estimate matrix $P$ by $\hat{P}$ given by formula (4.3).

We evaluated the accuracy of estimation and clustering in the setting above with $K = 6$, two values of $L$, $L = 2$ and $L = 3$, and the number of nodes ranging from $n = 180$ to $n = 720$ with the increments of 180. The proportion of misclustered nodes was evaluated as

$$\text{Err}(Z, \hat{Z}) = (2n)^{-1} \min_{\mathcal{P}_K \in \mathcal{P}_K} \|Z \mathcal{P}_K - \hat{Z}\|_F$$

where $\mathcal{P}_K$ is the set of permutation matrices $\mathcal{P}_K : \{1, \ldots, K\} \to \{1, \ldots, K\}$. The accuracy of estimating the probability matrix $P$ by $\hat{P}$ is measured as $n^{-2} \|\hat{P} - P\|_F^2$.

Figure 3 displays the accuracies of the two-step clustering procedure and the estimated probability matrix $\hat{P}$ in the above settings. We compare the results obtained by the two-step clustering procedure (solid lines) with the clustering results obtained by using only Algorithm 2 (dashed lines), where the post-clustering estimation is based on rank one approximations. The top panels present the clustering errors $\text{Err}(\hat{C}, C)$, the middle ones show the clustering errors $\text{Err}(\hat{Z}, Z)$, and the bottom panels exhibit the estimation errors $n^{-2} \|\hat{P} - P\|_F^2$, as functions of the number of nodes, for three different values of the parameter $\omega$: $\omega = 0.35$ (red lines), 0.55 (blue lines), and 0.75 (black lines). One can see from Figure 3 that since mega-communities are detected first, the accuracy of detecting $K$ communities (middle panels) depends on the precision of detecting $L$ mega-communities (top panels). Furthermore, the estimation errors (bottom panels) in turn depend on the accuracy of detecting $K$ communities (middle panels). Therefore, improved clustering precision leads to smaller estimation errors with finding the mega-communities being the key task.

### 6.2 Real data examples

In this section, we describe application of the two-step clustering procedure of Section 5 to two real life networks, a butterfly similarity network and a human brain network.

We consider the butterfly similarity network extracted from the Leeds Butterfly dataset [30], which contains fine-grained images of 832 butterfly species that belong to 10 different classes, with each class containing between 55 and 100 images. In this network, the nodes represent butterfly species and edges represent visual similarities (ranging from 0 to 1) between them, evaluated on the basis of butterfly images. We extract the five largest classes and draw an edge between two nodes if the visual similarity between them is greater than zero, obtaining a simple graph with 462 nodes and 28799 edges. We carry out clustering of the nodes, employing the two-step clustering procedure, first finding $L = 4$ mega-communities by Algorithm 1 and then using Algorithm 2 to find communities within mega-communities. We conclude that the first mega-community has two communities, while the other three mega-communities have one community each. We also applied Algorithms 1 and 2 separately for detection of five communities. Here, Algorithms 1 and 2 correspond, respectively, to the PABM and the DCMB settings with $K = 5$. Subsequently, we compare the clustering assignments with the true class specifications of the species. Algorithms 1 and 2 lead to 74% and 77% accuracy, respectively, while the two-step clustering procedure provides better 84% accuracy, thus, justifying the application of the HBM. The better results are due to the higher flexibility of the HBM.

The second example deals with analysis of a human brain functional network, based on the brain connectivity dataset, derived from the resting-state functional MRI (rsfMRI) [4]. In this dataset, the brain is partitioned into 638 distinct regions and a weighted graph is used to characterize the network topology. For a comparison, we use the Asymptotical Surprise method [23] which is applied
Figure 3: The clustering errors $\text{Err}(\hat{C}, C)$ (top panels) and $\text{Err}(\hat{Z}, Z)$ (middle panels) defined in (6.2) and the estimation errors $n^{-2}\|\hat{P} - P\|^2_F$ (bottom panels) for $K = 6$ communities and $L = 2$ (left) and $L = 3$ (right) mega-communities. The errors are evaluated over 50 simulation runs. The number of nodes ranges from $n = 180$ to $n = 720$ with the increments of 180. Dashed lines represent the results using Algorithm 2 for clustering and solid lines represent the results using the two-step clustering procedure; $\omega = 0.35$ (red), $\omega = 0.55$ (blue) and $\omega = 0.75$ (black).
Figure 4: The adjacency matrices of the butterfly similarity network with 57598 nonzero entries and 5 clusters (left) and the brain network with 33140 nonzero entries and 7 clusters (right) after clustering.

for clustering the GroupAverage rsfMRI matrix in [3]. Asymptotical Surprise detects 47 communities with sizes ranging from 1 to 133. Since the true clustering as well as the true number of clusters are unknown for this dataset, we treat the results of the Asymptotical Surprise as the ground truth. In order to generate a binary network, we set all nonzero weights to one in the GroupAverage rsfMRI matrix, obtaining a network with 18625 undirected edges. For our study, we extract 7 largest communities derived by the Asymptotical Surprise, obtaining a network with 450 nodes and 16570 edges. Similarly to the previous example, we apply Algorithms 1 and 2 separately to detect seven communities, obtaining, respectively, 88% and 73% accuracy. We also use the two-step clustering procedure above, detecting six mega-communities and seven communities, attaining 92% accuracy.

Figure 4 (right) shows the adjacency matrices of the butterfly similarity network (left) and the human brain network after clustering.

7 Discussion

The present paper examines the hierarchy of block models with the purpose of treating all existing singular membership block models as a part of one formulation, which is free from arbitrary identifiability conditions. The blocks differ by the average probability of connections and can be combined into mega-blocks that have common heterogeneity patterns in the connection probabilities.

The hierarchical formulation proposed above (see Figure 2) can be utilized for a variety of purposes. Since the HBM treats all other block models as its particular cases, one can carry out estimation and clustering without assuming that a specific block model holds, by employing the HBM with K communities and L mega-communities, where both K and L are unknown. The values of K and L can later be derived on the basis of penalties. Furthermore, in the framework above, one can easily test one block model versus another. For instance, \( L = K \) suggests the PABM while \( L = 1 \) implies the DCBM. If, additionally, \( H = 1_n \), then DCBM reduces to SBM. Finally, one can see from Figure 2 that absence of distinct communities \( (K = 1) \) always leads to DCBM, which reduces to Erdős-Rényi model if \( H = 1_n \).
8 Appendix

8.1 Proof of Theorem

Let \( \Xi = A - P \). We let \( \mathcal{P}_{Z,C,K,L} \) denote the permutation matrix that arranges mega-blocks consecutively and also blocks all mega-blocks consecutively. For simplicity, let

\[
\tilde{P} \equiv \mathcal{P}_{Z,C,K,L}, \quad P_* \equiv \mathcal{P}_{Z_*,C_*,K_*,L_*}, \quad \hat{P} \equiv \mathcal{P}_{\hat{Z},\hat{C},\hat{K},\hat{L}}.
\]

For any matrix \( S \), denote

\[
S(Z,C,K,L) = \mathcal{P}_{Z,C,K,L}^T S \mathcal{P}_{Z,C,K,L} \quad (8.1)
\]

Then, for any \( Z, C, K, \) and \( L \):

\[
\| \hat{P} - P_* \|^2 \leq \| P - P_* \|^2 + \text{Pen}(n, K, L) - \text{Pen}(n, \hat{K}, \hat{L}). \quad (8.2)
\]

Subtracting and adding \( P_* \) in the norms in both sides of (8.2), we rewrite it as

\[
\| \hat{P} - P_* \|^2 \leq \| P - P_* \|^2 + 2\langle \Xi, \hat{P} - P \rangle + \text{Pen}(n, K, L) - \text{Pen}(n, \hat{K}, \hat{L}). \quad (8.3)
\]

Denote

\[
P_0(K, L) = \inf_{P \in \mathcal{I}(n,K,L)} \| P - P_* \|^2_F,
\]

\[
(K_0, L_0) = \inf_{K,L} \left\{ \| P_0(K, L) - P_* \|^2_F + \text{Pen}(n, K, L) \right\}.
\]

Then, for \( \hat{P} \equiv \hat{P}(\hat{K}, \hat{L}) \) and \( P_0 \equiv P_0(K_0, L_0) \), one has

\[
\| \hat{P} - P_* \|^2 \leq \| P_0 - P_* \|^2 + 2\langle \Xi, \hat{P} - P \rangle + \text{Pen}(n, K_0, L_0) - \text{Pen}(n, \hat{K}, \hat{L}).
\]

Denote

\[
\tau(n, K, L) = n \ln K + K \ln L + (K^2 + 2nL) \ln (9nL) \quad (8.5)
\]

and consider two sets \( \Omega \) and \( \Omega^c \)

\[
\Omega = \left\{ \omega : \| \hat{P} - P_* \|^2 \geq C_0 2^{s_0} \sqrt{\tau(n, K_0, L_0)} \right\},
\]

\[
\Omega^c = \left\{ \omega : \| \hat{P} - P_* \|^2 \leq C_0 2^{s_0} \sqrt{\tau(n, K_0, L_0)} \right\} \quad (8.6)
\]

where \( s_0 \) is a constant. If \( \omega \in \Omega^c \), then

\[
\| \hat{P} - P_* \|^2 \leq C_0^2 2^{2s_0} \tau(n, K_0, L_0) \quad (8.7)
\]
Consider the case when $\omega \in \Omega$. It is known [15] that for any fixed matrix $G$, any $\alpha > 0$ and any $t > 0$ one has
\[
P \left\{ 2 \langle \Xi, G \rangle \geq \alpha \|P_s - P_0\|_F^2 + 2t/\alpha \right\} \leq e^{-t}. \quad (8.8)
\]
Then, there exists a set $\hat{\Omega}$ such that $P(\hat{\Omega}_Z) \geq 1 - e^{-t}$ and for $w \in \hat{\Omega}$
\[
2 \langle \Xi, P_\ast - P_0 \rangle \leq \alpha \|P_\ast - P_0\|_F^2 + 2t/\alpha \quad (8.9)
\]
Note that the set $\Omega$ can be partitioned as $\Omega = \bigcup_{K,L} \Omega_{K,L}$, where
\[
\Omega_{K,L} = \left\{ \omega : \left( \|\hat{P} - P_\ast\|_F \geq C_02^{s_0} \sqrt{\tau(n, K, L_0)} \right) \cap (\hat{K} = K, \hat{L} = L) \right\} \quad (8.10)
\]
with $\Omega_{K_1, L_1} \cap \Omega_{K_2, L_2} = \emptyset$ unless $K_1 = K_2$ and $L_1 = L_2$. Denote
\[
\Delta(n, K, L) = C_0^2 C_2 \tau(n, K, L) + n, \quad (8.11)
\]
where $\tau(n, K, L)$ is defined in (8.5). Then,
\[
\begin{align*}
&\P\left\{ \left[ 2 \langle \Xi, \hat{P}(n, K, L) - P_s \rangle - \frac{1}{2} \left\| \hat{P}(n, K, L) - P_\ast \right\|_F^2 - 2\Delta(n, K, L) \right] \geq 0 \right\} \\
\leq &\sum_{K=1}^{n} \sum_{L=1}^{K} \P\left\{ \sup_{P \in \Omega_{K,L}} \left[ 2 \langle \Xi, \hat{P} - P_\ast \rangle - \frac{1}{2} \left\| \hat{P} - P_\ast \right\|_F^2 - 2\Delta(n, K, L) \right] \geq 0 \right\}
\end{align*}
\]
By Lemma 3 in Section 8.3 there exist sets $\tilde{\Omega}_{K,L} \subseteq \Omega_{K,L} \subseteq \Omega$ such that $\P(\tilde{\Omega}_{K,L}^c) \leq 2 \log_2 n \cdot \exp \left( -n \cdot 2^{s_0 - 7} \right)$ and, for $\omega \in \Omega_{K,L}$, one has
\[
\left\{ 2 \langle \Xi, \hat{P} - P_\ast \rangle \leq \frac{1}{2} \left\| \hat{P} - P_\ast \right\|_F^2 + 2\Delta(n, K, L) \right\} \cap \left\{ \hat{K} = K, \hat{L} = L \right\}
\]
Denote
\[
\tilde{\Omega} = \left( \bigcap_{K,L} \tilde{\Omega}_{K,L} \right) \cap \tilde{\Omega}_t \quad (8.12)
\]
and observe that
\[
\P(\tilde{\Omega}) \geq 1 - n^2 \log_2 n \cdot \exp \left( -n \cdot 2^{s_0 - 7} \right) - e^{-t}.
\]
Then, for $\omega \in \tilde{\Omega}$, one has
\[
2 \langle \Xi, \hat{P} - P_\ast \rangle \leq \frac{1}{2} \left\| \hat{P} - P_\ast \right\|_F^2 + 2\Delta(n, \hat{K}, \hat{L}) \quad (8.13)
\]
and it follows from (8.9) with $\alpha = 1/2$ that
\[
2 \langle \Xi, P_\ast - P_0 \rangle \leq \frac{1}{2} \left\| P_\ast - P_0 \right\|_F^2 + 4t \quad (8.14)
\]
Plugging (8.13) and (8.14) into (8.4), obtain that for $\omega \in \Omega$ one has
\[
\begin{align*}
\left\| \hat{P} - P_\ast \right\|_F^2 \leq &\left\| P_0 - P_\ast \right\|_F^2 + \text{Pen}(n, K_0, L_0) + \frac{1}{2} \left\| \hat{P} - P_\ast \right\|_F^2 + 2\Delta(n, \hat{K}, \hat{L}) + \frac{1}{2} \left\| P_\ast - P_0 \right\|_F^2 + 4t - \text{Pen}(n, \hat{K}, \hat{L})
\end{align*}
\]
Finally, setting
\[ \text{Pen}(n, K, L) = 2\Delta(n, K, L) = 2 \left[ C_0^2 \tau(n, K, L) + n \right], \]
obtain that for any \( t > 0 \), for \( \omega \in \hat{\Omega} \), one has
\[ \left\| \hat{P} - P_s \right\|_F^2 \leq 3 \left\| P_0 - P_s \right\|_F^2 + 2\text{Pen}(n, K_0, L_0) + 8t, \]
for any \( \omega \in \Omega \). Now, for \( \omega \in \Omega^c \), it follows from (8.7) that
\[ \left\| \hat{P} - P_s \right\|_F^2 \leq C_0^2 2^s \tau(n, K_0, L_0) \leq 2^{2s \omega} \text{Pen}(n, K_0, L_0) \]
Setting \( s_0 = 1 \) and \( t = n/32 \), obtain
\[ \mathbb{P}\left\{ \left\| \hat{P} - P_s \right\|_F^2 \leq 3 \left\| P_0 - P_s \right\|_F^2 + 2\text{Pen}(n, K_0, L_0) \right\} \geq 1 - \left( n^2 \log_2 n + 1 \right)e^{-\frac{n}{32}}, \]
so that
\[ \mathbb{P}\left\{ \left\| \hat{P} - P_s \right\|_F^2 \leq \inf_{P \in \mathcal{A}(n, K, L)} \left\| P - P_s \right\|_F^2 + \text{Pen}(n, K, L) \right\} \geq 1 - \left( n^2 \log_2 n + 1 \right)e^{-\frac{n}{32}}. \]
Since \( \left\| \hat{P} - P_s \right\|_F^2 \leq n^2 \), obtain
\[ \mathbb{E}\left\| \hat{P} - P_s \right\|_F^2 \leq 3 \min_{P \in \mathcal{A}(n, K, L)} \left\| P - P_s \right\|_F^2 + \text{Pen}(n, K, L) \right\} + n^5 e^{-n/32}. \]

8.2 Proof of Theorem 2

Let
\[ F_1(n, K, L) = C_1 nK + C_2 K^2 \ln(nK) + C_3 \left( \ln n + (n + 1) \ln K + K \ln L \right) \]
\[ F_2(n, K, L) = 2 \ln n + 2(n + 1) \ln K + 2K \ln L, \]
where \( C_1, C_2, \) and \( C_3 \) are absolute constants. Denote \( \Xi = A - P_s \) and recall that, given matrix \( P_s \), entries \( \Xi_{i,j} = A_{i,j} - (P_s)_{i,j} \) of \( \Xi \) are the independent Bernoulli errors for \( 1 \leq i \leq j \leq n \) and \( A_{i,j} = A_{j,i} \). Then, following notation (8.1), for any \( Z, C, \) and \( L \)
\[ \Xi(Z, C, K, L) = \mathcal{P}^T \Xi \mathcal{P} \]
\[ P_s(Z, C, K, L) = \mathcal{P}^T P_s \mathcal{P}, \]
where \( \mathcal{P} \equiv \mathcal{P}_{Z,C,K,L} \). Then it follows from (4.7) that
\[ \left\| \mathcal{P}^T A \hat{\Theta} - \hat{\Theta}(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) \right\|_F^2 + \text{Pen}(n, \hat{K}, \hat{L}) \leq \left\| \mathcal{P}_s^T A P_s - \mathcal{P}_s^T P_s \mathcal{P}_s \right\|_F^2 + \text{Pen}(n, K_s, L_s) \]
where \( \mathcal{P}_s \equiv \mathcal{P}_{Z_s,C_s,K_s,L_s} \). Using the fact that permutation matrices are orthogonal, we can rewrite the previous inequality as
\[ \left\| A - \hat{\Theta}(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) \mathcal{P}^T \right\|_F^2 + \text{Pen}(n, \hat{K}, \hat{L}) \leq \left\| A - P_s \right\|_F^2 + \text{Pen}(n, K_s, L_s). \] (8.15)
Hence, (8.15) and (4.3) yield
\[ \left\| A - \hat{P} \right\|_F^2 \leq \left\| A - P_s \right\|_F^2 + \text{Pen}(n, K_s, L_s) - \text{Pen}(n, \hat{K}, \hat{L}) \] (8.16)
Subtracting and adding $P_*$ in the norm of the left-hand side of (8.16), we rewrite (8.16) as

$$\|\hat{P} - P_*\|_F^2 \leq \Delta(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) + \text{Pen}(n, K_*, L_*) - \text{Pen}(n, \hat{K}, \hat{L}),$$

where

$$\Delta \equiv \Delta(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) = 2\text{Tr}\left[\Xi^T(\hat{P} - P_*)\right].$$

Again, using orthogonality of the permutation matrices, we can rewrite

$$\Delta = 2\langle \Xi(\hat{Z}, \hat{C}, \hat{K}, \hat{L}), (\hat{\Theta}(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) - P_*(\hat{Z}, \hat{C}, \hat{K}, \hat{L})) \rangle,$$

where $\langle A, B \rangle = \text{Tr}(A^T B)$. Then, in the block form, $\Delta$ appears as

$$\Delta = \sum_{l=1}^{\hat{L}} \sum_{k=1}^{\hat{K}} \Delta^{(l,k)}$$

where

$$\Delta^{(l,k)} = 2\langle \Xi^{(l,k)}(\hat{Z}, \hat{C}, \hat{K}, \hat{L}), \Pi_{\hat{u}, \hat{v}}(A^{(l,k)}(\hat{Z}, \hat{C}, \hat{K}, \hat{L})) - P_*^{(l,k)}(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) \rangle$$

and $\Pi_{\hat{u}, \hat{v}}$ is defined in (8.52) of Lemma 4.

Let $\hat{u} = \hat{u}^{(l,k)}(\hat{Z}, \hat{C}, \hat{K}, \hat{L})$ and $\hat{v} = \hat{v}^{(l,k)}(\hat{Z}, \hat{C}, \hat{K}, \hat{L})$ be the singular vectors of $P_*^{(l,k)}(\hat{Z}, \hat{C}, \hat{K}, \hat{L})$ corresponding to the largest singular value of $P_*^{(l,k)}(\hat{Z}, \hat{C}, \hat{K}, \hat{L})$. Then, according to Lemma 4

$$\Pi_{\hat{u}, \hat{v}}(P_*^{(l,k)}(\hat{Z}, \hat{C}, \hat{K}, \hat{L})) = \hat{u}^{(l,k)}(\hat{u}^{(l,k)})^T P_*^{(l,k)}(\hat{v}^{(l,k)}(\hat{v}^{(l,k)})^T$$

Recall that

$$\Pi_{\hat{u}, \hat{v}}(A^{(l,k)}(\hat{Z}, \hat{C}, \hat{K}, \hat{L})) = \Pi_{\hat{u}, \hat{v}}\left[ P_*^{(l,k)}(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) + \Xi^{(l,k)}(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) \right],$$

Then, $\Delta^{(l,k)}$ can be partitioned into the sums of three components

$$\Delta^{(l,k)} = \Delta_1^{(l,k)} + \Delta_2^{(l,k)} + \Delta_3^{(l,k)}, \quad l = 1, 2, \ldots, \hat{L}, \quad k = 1, 2, \ldots, \hat{K}$$

where

$$\Delta_1^{(l,k)} = 2\langle \Xi^{(l,k)}(\hat{Z}, \hat{C}, \hat{K}, \hat{L}), \Pi_{\hat{u}, \hat{v}}(\Xi^{(l,k)}(\hat{Z}, \hat{C}, \hat{K}, \hat{L})) \rangle$$

$$\Delta_2^{(l,k)} = 2\langle \Xi^{(l,k)}(\hat{Z}, \hat{C}, \hat{K}, \hat{L}), \Pi_{\hat{u}, \hat{v}}(P_*^{(l,k)}(\hat{Z}, \hat{C}, \hat{K}, \hat{L})) - P_*^{(l,k)}(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) \rangle$$

$$\Delta_3^{(l,k)} = 2\langle \Xi^{(l,k)}(\hat{Z}, \hat{C}, \hat{K}, \hat{L}), \Pi_{\hat{u}, \hat{v}}(P_*^{(l,k)}(\hat{Z}, \hat{C}, \hat{K}, \hat{L})) - \Pi_{\hat{u}, \hat{v}}(P_*^{(l,k)}(\hat{Z}, \hat{C}, \hat{K}, \hat{L})) \rangle$$

With some abuse of notations, for any matrix $B$, let $\Pi_{\hat{u}, \hat{v}}\left( B(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) \right)$ be the matrix with blocks $\Pi_{\hat{u}, \hat{v}}\left( B^{(l,k)}(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) \right)$ and $\Pi_{\hat{u}, \hat{v}}\left( B(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) \right)$ be the matrix with blocks

$$\Pi_{\hat{u}, \hat{v}}\left( B^{(l,k)}(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) \right), \quad l = 1, 2, \ldots, \hat{L}, \quad k = 1, 2, \ldots, \hat{K}$$
. Then, it follows from (8.21)–(8.24) that
\[ \Delta = \Delta_1 + \Delta_2 + \Delta_3 \] (8.25)
where
\[ \Delta_1 = 2(\langle \Xi(\hat{Z}, \hat{C}, \hat{K}, \hat{L}), \Pi_{\hat{u}, \hat{v}}(\Xi(\hat{Z}, \hat{C}, \hat{K}, \hat{L})) \rangle) \] (8.26)
\[ \Delta_2 = 2(\langle \Xi(\hat{Z}, \hat{K}), \Pi_{\hat{u}, \hat{v}}(P_s(\hat{Z}, \hat{C}, \hat{K}, \hat{L})) - P_s(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) \rangle) \] (8.27)
\[ \Delta_3 = 2(\langle \Xi(\hat{Z}, \hat{C}, \hat{K}, \hat{L}), \Pi_{\hat{u}, \hat{v}}(P_s(\hat{Z}, \hat{C}, \hat{K}, \hat{L})) - \Pi_{\hat{u}, \hat{v}}(P_s(\hat{Z}, \hat{C}, \hat{K}, \hat{L})) \rangle) \] (8.28)

Observe that
\[ \Delta_1^{(l,k)} = 2(\langle \Xi(l,k)(\hat{Z}, \hat{C}, \hat{K}, \hat{L}), \Pi_{\hat{u}, \hat{v}}(\Xi(l,k)(\hat{Z}, \hat{C}, \hat{K}, \hat{L})) \rangle) \]
\[ = 2 \left\| \Pi_{\hat{u}, \hat{v}}(\Xi(l,k)(\hat{Z}, \hat{C}, \hat{K}, \hat{L})) \right\|^2_F \]
\[ \leq 2 \left\| \Xi(l,k)(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) \right\|^2_{op} \] (8.29)

Now, fix \( t \) and let \( \Omega_1 \) be the set where \( \sum_{l=1}^{L} \sum_{k=1}^{K} \left\| \Xi(l,k)(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) \right\|^2_{op} \leq F_1(n, \hat{K}, \hat{L}) + C_3 t \). According to Lemma 7
\[ \mathbb{P}(\Omega_1) \geq 1 - \exp(-t), \] (8.30)
and, for \( \omega \in \Omega_1 \), one has
\[ |\Delta_1| \leq 2 \sum_{l=1}^{L} \sum_{k=1}^{K} \left\| \Xi(l,k)(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) \right\|^2_{op} \leq 2F_1(n, \hat{K}, \hat{L}) + 2C_3 t \] (8.31)

Now, consider \( \Delta_2 \) given by (8.27). Note that
\[ |\Delta_2| = 2 \left\| \Pi_{\hat{u}, \hat{v}} \left( P_s(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) \right) - P_s(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) \right\|^2_F \left| \langle \Xi(\hat{Z}, \hat{C}, \hat{K}, \hat{L}), H_{\hat{u}, \hat{v}}(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) \rangle \right| \] (8.32)
where
\[ H_{\hat{u}, \hat{v}}(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) = \frac{\Pi_{\hat{u}, \hat{v}} \left( P_s(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) \right) - P_s(\hat{Z}, \hat{C}, \hat{K}, \hat{L})}{\left\| \Pi_{\hat{u}, \hat{v}} \left( P_s(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) \right) - P_s(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) \right\|^2_F} \]

Since for any \( a, b, \) and \( \alpha_1 > 0 \), one has \( 2ab \leq \alpha_1 a^2 + b^2 / \alpha_1 \), obtain
\[ |\Delta_2| \leq \alpha_1 \left\| \Pi_{\hat{u}, \hat{v}} \left( P_s(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) \right) - P_s(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) \right\|^2_F + \]
\[ 1 / \alpha_1 \left| \langle \Xi(\hat{Z}, \hat{C}, \hat{K}, \hat{L}), H_{\hat{u}, \hat{v}}(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) \rangle \right|^2 \] (8.33)

Observe that if \( K, L, Z \in \mathcal{M}_{\hat{u}, \hat{v}}, \) and \( C \in \mathcal{M}_{\hat{u}, \hat{v}} \) are fixed, then \( H_{\hat{u}, \hat{v}}(Z, C, K, L) \) is fixed and, for any \( K, L, Z, \) and \( C, \) one has \( \left\| H_{\hat{u}, \hat{v}}(Z, C, K, L) \right\|^2_F = 1 \). Note also that, for fixed \( K, L, Z, \) and \( C, \) permutated matrix \( \Xi(Z, C, K, L) \in [0,1]^{n \times n} \) contains independent Bernoulli errors. It is well known
that if \( \xi \) is a vector of independent Bernoulli errors and \( h \) is a unit vector, then, for any \( x > 0 \), Hoeffding’s inequality yields

\[ \Pr(|\xi^T h|^2 > x) \leq 2\exp(-x/2) \]

Since

\[ \langle \Xi(Z, C, K, L), H_{\tilde{a}, \tilde{\nu}}(Z, C, K, L) \rangle = [\text{vec}(\Xi(Z, C, K, L))]^T \text{vec}(H_{\tilde{a}, \tilde{\nu}}(Z, C, K, L)), \]

obtain for any fixed \( K, L, Z, \) and \( C \):

\[ \Pr \left( |\langle \Xi(Z, C, K, L), H_{\tilde{a}, \tilde{\nu}}(Z, C, K, L) \rangle|^2 - x > 0 \right) \leq 2\exp(-x/2) \]

Now, applying the union bound, derive

\[ \Pr \left( |\langle \Xi(Z, \hat{C}, \hat{K}, \hat{L}), H_{\tilde{a}, \tilde{\nu}}(Z, \hat{C}, \hat{K}, \hat{L}) \rangle|^2 - F_2(n, \hat{K}, \hat{L}) > 2t \right) \]

\[ \leq \Pr \left[ \max_{1 \leq K \leq n} \max_{1 \leq L \leq K} \max_{Z \in \mathcal{M}_{n,K}} \max_{C \in \mathcal{M}_{K,L}} (|\langle \Xi(Z, C, K, L), H_{\tilde{a}, \tilde{\nu}}(Z, C, K, L) \rangle|^2 - F_2(n, K, L)) > 2t \right] \]

\[ \leq 2nK^n L^K \exp \{-F_2(n, K, L)/2 - t\} = 2\exp(-t), \]

where \( F_2(n, K, L) = 2n + 2(n + 1) \ln K + 2K \ln L \). By Lemma 5 one has

\[ \left\| \Pi_{\tilde{a}, \tilde{\nu}} \left( P_*(\tilde{Z}, \hat{C}, \hat{K}, \hat{L}) \right) - P_*(\tilde{Z}, \hat{C}, \hat{K}, \hat{L}) \right\|_F^2 \leq \left\| \hat{P} - P_* \right\|_F^2. \]

Denote the set on which (8.33) holds by \( \Omega^C_2 \), so that

\[ \Pr(\Omega_2) \geq 1 - 2\exp(-t). \] (8.34)

Then inequalities (8.32) and (8.33) imply that, for any \( \alpha_1 > 0, t > 0 \) and any \( \omega \in \Omega_2 \), one has

\[ |\Delta_2| \leq \alpha_1 \left\| \hat{P} - P_* \right\|_F^2 + 1/\alpha_1 F_2(n, \hat{K}, \hat{L}) + 2t/\alpha_1. \] (8.35)

Now consider \( \Delta_3 \) defined in (8.28) with components (8.24). Note that matrices

\[ \Pi_{\tilde{a}, \tilde{\nu}}(P_*^{(l,k)}(\tilde{Z}, \hat{C}, \hat{K}, \hat{L})) - \Pi_{\tilde{a}, \tilde{\nu}} \left( P_*^{(l,k)}(\tilde{Z}, \hat{C}, \hat{K}, \hat{L}) \right) \]

have rank at most two. Use the fact that (see, e.g., Giraud (2014), page 123)

\[ \langle A, B \rangle \leq \|A\|_{(2,r)} \|B\|_{(2,r)} \leq 2 \|A\|_{op} \|B\|_F, \quad r = \min\{\text{rank}(A), \text{rank}(B)\}. \] (8.36)

Here \( \|A\|_{(2,q)} \) is the Ky-Fan (2, q) norm

\[ \|A\|_{(2,q)}^2 = \sum_{j=1}^q \sigma_j^q(A) \leq \|A\|_F^2, \]

where \( \sigma_j(A) \) are the singular values of \( A \). Applying inequality (8.36) with \( r = 2 \) and taking into account that for any matrix \( A \) one has \( \|A\|_{(2,2)}^2 \leq 2 \|A\|_{op}^2 \), derive

\[ |\Delta_3^{(l,k)}| \leq 4 \|\Xi^{(l,k)}(\tilde{Z}, \hat{C}, \hat{K}, \hat{L})\|_{op} \left\| \Pi_{\tilde{a}, \tilde{\nu}}(P_*^{(l,k)}(\tilde{Z}, \hat{C}, \hat{K}, \hat{L})) - \Pi_{\tilde{a}, \tilde{\nu}} \left( P_*^{(l,k)}(\tilde{Z}, \hat{C}, \hat{K}, \hat{L}) \right) \right\|_F. \]
Then, for any $\alpha_2 > 0$, obtain
\begin{equation}
|\Delta_3| \leq \sum_{l=1}^{L} \sum_{k=1}^{K} |\Delta_3^{(l,k)}| \leq \frac{2}{\alpha_2} \sum_{l=1}^{L} \sum_{k=1}^{K} \left\| \Xi^{(l,k)}(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) \right\|_{op}^2 + 2\alpha_2 \sum_{l=1}^{L} \sum_{k=1}^{K} \left\| \Pi_{\hat{a}, \hat{v}}(P_*(l,k)(\hat{Z}, \hat{C}, \hat{K}, \hat{L})) - \Pi_{\hat{a}, \hat{v}} \left( P_*(l,k)(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) \right) \right\|_{F}^2.
\end{equation}

Note that, by Lemma 5,
\begin{align*}
\left\| \Pi_{\hat{a}, \hat{v}}(P_*(l,k)(\hat{Z}, \hat{C}, \hat{K}, \hat{L})) - \Pi_{\hat{a}, \hat{v}} \left( P_*(l,k)(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) \right) \right\|_{F}^2 &\leq 2 \left\| \Pi_{\hat{a}, \hat{v}}(P_*(l,k)(\hat{Z}, \hat{C}, \hat{K}, \hat{L})) - P_*(l,k)(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) \right\|_{F}^2 + 2 \left\| \Pi_{\hat{a}, \hat{v}}(P_*(l,k)(\hat{Z}, \hat{C}, \hat{K}, \hat{L})) - P_*(l,k)(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) \right\|_{F}^2 \leq 4 \left\| \Pi_{\hat{a}, \hat{v}}(A(l,k)(\hat{Z}, \hat{C}, \hat{K}, \hat{L})) - P_*(l,k)(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) \right\|_{F}^2
= 4 \left\| \hat{\Theta}(l,k)(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) - P_*(l,k)(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) \right\|_{F}^2.
\end{align*}

Therefore,
\begin{equation}
\sum_{l=1}^{L} \sum_{k=1}^{K} \left\| \Pi_{\hat{a}, \hat{v}}(P_*(l,k)(\hat{Z}, \hat{C}, \hat{K}, \hat{L})) - \Pi_{\hat{a}, \hat{v}} \left( P_*(l,k)(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) \right) \right\|_{F}^2 \leq 4 \left\| \hat{\Theta}(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) - P_*(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) \right\|_{F}^2 = 4 \left\| \hat{P} - P_* \right\|_{F}^2.
\end{equation}

Combine inequalities (8.37) and (8.38) and recall that
\begin{equation}
\sum_{l=1}^{L} \sum_{k=1}^{K} \left\| \Xi^{(l,k)}(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) \right\|_{op}^2 \leq F_1(n, \hat{K}, \hat{L}) + C_3 t
\end{equation}
for $\omega \in \Omega_1$. Then, for any $\alpha_2 > 0$ and $\omega \in \Omega_1$, one has
\begin{equation}
|\Delta_3| \leq 8\alpha_2 \left\| \hat{P} - P_* \right\|_{F}^2 + 2/\alpha_2 F_1(n, \hat{K}, \hat{L}) + 2C_3 t/\alpha_2.
\end{equation}

Now, let $\Omega = \Omega_1 \cap \Omega_2$. Then, (8.29) and (8.34) imply that $\mathbb{P}(\Omega) \geq 1 - 3\exp(-t)$ and, for $\omega \in \Omega$, inequalities (8.30), (8.35) and (8.39) simultaneously hold. Hence, by (8.25), derive that, for any $\omega \in \Omega$,
\begin{equation}
|\Delta| \leq (2 + 2/\alpha_2) F_1(n, \hat{K}, \hat{L}) + 1/\alpha_1 F_2(n, \hat{K}, \hat{L}) + (\alpha_1 + 8\alpha_2) \left\| \hat{P} - P_* \right\|_{F}^2 + 2(C_3 + 1/\alpha_1 + C_3/\alpha_2) t.
\end{equation}

Combination of the last inequality and (8.17) yields that, for $\alpha_1 + 8\alpha_2 < 1$ and any $\omega \in \Omega$,
\begin{align*}
(1 - \alpha_1 - 8\alpha_2) \left\| \hat{P} - P_* \right\|_{F}^2 &\leq \left( 2 + \frac{2}{\alpha_2} \right) F_1(n, \hat{K}, \hat{L}) + \frac{1}{\alpha_1} F_2(n, \hat{K}, \hat{L}) + \text{Pen}(n, K_*, L_*) - \text{Pen}(n, \hat{K}, \hat{L}) + 2(C_3 + 1/\alpha_1 + C_3/\alpha_2) t.
\end{align*}
Setting \( \text{Pen}(n, K, L) = (2 + 2/\alpha_2)F_1(n, K, L) + 1/\alpha_1 F_2(n, K, L) \) and dividing by \((1 - \alpha_1 - 8\alpha_2)\), obtain that
\[
\mathbb{P} \left\{ \| \hat{P} - P_* \|_F^2 \leq (1 - \alpha_1 - 8\alpha_2)^{-1} \text{Pen}(n, K_*, L_*) + \tilde{C} t \right\} \geq 1 - 3e^{-t}
\]
for \( t > 0 \), where
\[
\tilde{C} = 2 (1 - \alpha_1 - 8\alpha_2)^{-1} (C_3 + 1/\alpha_1 + C_3/\alpha_2)
\]
Moreover, note that for \( \xi = \| \hat{P} - P_* \|_F^2 - (1 - \beta_1 - \beta_2)^{-1} \text{Pen}(n, K_*, L_*) \), one has \( \mathbb{E}\| \hat{P} - P_* \|_F^2 = (1 - \beta_1 - \beta_2)^{-1} \text{Pen}(n, K_*, L_*) + \mathbb{E}\xi \), where
\[
\mathbb{E}\xi \leq \int_0^\infty \mathbb{P}(\xi > z)dz = \tilde{C} \int_0^\infty \mathbb{P}(\xi > \tilde{C}t)dt \leq \tilde{C} \int_0^\infty 3e^{-t} dt = 3\tilde{C},
\]
By rearranging and combining the terms, the penalty \( \text{Pen}(n, K, L) \) can be written in the form (4.8), completing the proof.

### 8.3 Supplementary statements and their proofs

**Lemma 1.** The logarithm of the cardinality of a \( \delta \)-net on the space of non-symmetric DCBMs of size \( n_1 \times n_2 \) with \( K_1 \times K_2 \) blocks is
\[
(K_1K_2 + n_1 + n_2) \ln \left( \frac{9}{\delta} \right) + \left( K_1K_2 + \frac{n_1 + n_2}{2} \right) \ln(n_1n_2)
\]

**Proof.** Let \( Z_1 \) and \( Z_2 \) be fixed. Then by rearranging \( \Theta \), rewrite it as \( \Theta = Q_1BQ_2^T \), where \( B \) and \( Q_i \), \( i = 1, 2 \), have the sizes \( K_1 \times K_2 \) and \( n_i \times K_i \), respectively. Here, \( Q_i \) is of the form
\[
Q_i = \begin{bmatrix}
q_{i,1} & 0 & \cdots & 0 \\
0 & q_{i,2} & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & q_{i,K_i}
\end{bmatrix},
\]
(8.42)
We re-scale components of matrices \( Q_1, Q_2 \) and \( B \), so that vectors \( q_{i,j} \in \mathbb{R}^{n_i,j}, j = 1, \ldots, K_i, i = 1, 2 \), have unit norms \( \| q_{i,j} \|_2 = 1 \), and \( \sum_{j=1}^{K_i} n_{i,j} = n_i \). Let \( \Theta^{(k_1,k_2)} \in \mathbb{R}^{n_1k_1 \times n_2k_2} \) be the \((k_1,k_2)\)-th block of \( \Theta \). Then,
\[
\Theta^{(k_1,k_2)} = B_{k_1,k_2}q_{1,k_1}q_{2,k_2}^T
\]
and
\[
\| \Theta^{(k_1,k_2)} \|_F^2 = B_{k_1,k_2}^2 \| q_{1,k_1} \|_2^2 \| q_{2,k_2} \|_2^2 = B_{k_1,k_2}^2 \leq n_{k_1} \cdot n_{k_2},
\]
due to \( \| ab^T \|_F^2 \leq \| a \|_2^2 \| b \|_2^2 \) (for any vectors \( a \) and \( b \)) and \( \| \Theta \|_\infty \leq 1 \). Hence, \( B_{k_1,k_2} \leq \sqrt{n_{k_1} \cdot n_{k_2}} \leq \sqrt{n_1 \cdot n_2} \).

Let \( \mathcal{D}_1(\delta_1), \mathcal{D}_2(\delta_2), \) and \( \mathcal{D}_B(\delta_B) \) be the \( \delta_1 \), \( \delta_2 \), and \( \delta_B \) nets for \( Q_1 \), \( Q_2 \), and \( B \), respectively. The nets \( \mathcal{D}_i(\delta_i) \) are essentially constructed for \( K_i \) vectors of length 1 in \( \mathbb{R}^{n_i,j} \), hence, by [25]
\[
\text{card}(\mathcal{D}_i(\delta_i)) \leq \Pi_{j=1}^{K_i} (3/\delta_i)^{n_{i,j}} = (3/\delta_i)^{n_i}, i = 1, 2.
\]
Let \( b = \text{vec}(B) \). Then, \( b \in \mathbb{R}^{K_1K_2} \) and \( \| b \| \leq \sqrt{n_1n_2} \) since
\[
\| b \|^2 = \| B \|_F^2 = \sum_{k_1,k_2} B_{k_1,k_2}^2 = \sum_{k_1,k_2} n_{k_1}n_{k_2} = n_1n_2.
\]
Therefore,

$$\text{card}(\mathcal{D}_B(\delta_B)) \leq \left(\frac{3n_1n_2}{\delta_B}\right)^{K_1K_2}$$

Now, let us check what values of $\delta_1$, $\delta_2$, and $\delta_B$ result in a $\delta$-net. Let $\Theta = Q_1BQ_2^T$ and $\tilde{\Theta} = \tilde{Q}_1\tilde{B}\tilde{Q}_2^T$. Then

$$\begin{align*}
\left\|\tilde{\Theta} - \Theta\right\|_F &= \left\|\tilde{Q}_1\tilde{B}\tilde{Q}_2^T - Q_1BQ_2^T\right\|_F \\
&\leq \left\|\tilde{Q}_1 - Q_1\right\|_F \left\|\tilde{B}\right\|_F \left\|\tilde{Q}_2^T\right\|_F + \left\|Q_1B\left(\tilde{B} - B\right)\tilde{Q}_2^T\right\|_F + \left\|Q_1B\left(\tilde{Q}_2 - Q_2\right)^T\right\|_F
\end{align*}$$

Note that

$$\|A_1A_2\|_F \leq \min\left(\|A_1\|_F \|A_2\|_{op}, \|A_1\|_{op} \|A_2\|_F\right)$$

for any matrices $A_1$ and $A_2$, and that also

$$Q_i^TQ_i = \text{diag}\left(\|q_{i,1}\|^2, \cdots, \|q_{i,K}\|^2\right) = I_{K_i}, \ i = 1, 2.$$  

Hence

$$\|Q_i\|_{op} = 1; \quad \|Q_i\|_F = \sqrt{K_i}, \ i = 1, 2.$$  

Similarly, if $\tilde{Q}_i, Q_i \in \mathcal{D}_i(\delta_i)$, then

$$(\tilde{Q}_i - Q_i)^T(\tilde{Q}_i - Q_i) = \text{diag}\left(\|	ilde{q}_{i,1} - q_{i,1}\|^2, \cdots, \|	ilde{q}_{i,K_i} - q_{i,K_i}\|^2\right)$$

Thus

$$\|\tilde{Q}_i - Q_i\|_{op} = \delta_i; \quad \|\tilde{Q}_i - Q_i\|_F \leq \sqrt{K_i}\delta_i, \ i = 1, 2.$$  

Also, for $i = 1, 2$

$$\text{Tr}(B^TQ_i^TQ_iB) = \|Q_iB\|_F^2 = \|B\|_F^2 = n_1n_2.$$  

Hence,

$$\begin{align*}
\left\|\tilde{\Theta} - \Theta\right\|_F &\leq \|\tilde{Q}_1 - Q_1\|_{op} \|\tilde{B}\tilde{Q}_2^T\|_F \\
&\quad + \|Q_1B\|_F \|\tilde{Q}_2\|_{op} + \|Q_1\|_{op} \|\tilde{B} - B\|_F \|\tilde{Q}_2\|_{op} \\
&= (\delta_1 + \delta_2)\sqrt{n_1n_2} + \delta_B \leq \delta
\end{align*}$$

Set $\delta_B = \frac{\delta}{3}$ and $\delta_1 = \delta_2 = \frac{\delta}{\sqrt{n_1n_2}}$. Then

$$\begin{align*}
\text{card}(\mathcal{D}_B(\delta_B)) &= \left(\frac{9n_1n_2}{\delta}\right)^{K_1K_2}, \\
\text{card}(\mathcal{D}_i(\delta_i)) &= \left(\frac{9\sqrt{n_1n_2}}{\delta}\right)^{n_i}
\end{align*}$$

which completes the proof.

**Lemma 2.** Consider the set of matrices $P$ which can be transformed by a permutation matrix $\mathcal{P}_{Z,C}$ into a block matrix $\Theta \in \mathcal{Z}(n, K, L)$ where $\mathcal{Z}(n, K, L)$ is defined in (4.2). Let $\mathcal{Y}(\epsilon, n, K, L)$ be an $\epsilon$-net on the set $\mathcal{Z}(n, K, L)$ and $|\mathcal{Y}(\epsilon, n, K, L)|$ be its cardinality. Then, for any $K$ and $L$, $1 \leq K \leq n$, $1 \leq L \leq K$, one has

$$|\mathcal{Y}(\epsilon, n, K, L)| \leq n \ln K + K \ln L + (K^2 + 2nL) \ln \left(\frac{9nL}{\epsilon}\right) \quad (8.43)$$

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Proof. First construct nets on the set of matrices $Z$ and $C$ with the respective the cardinalities $K^n$ and $L^K$. After that, validity of the lemma follows from Lemma 1.

Lemma 3. Let $C_0^2 = 3009$, $C_2 = 1$, $s_0 > 0$ be an arbitrary constant and $\Omega_{K,L}$ be defined in (8.10). Then,

$$\mathbb{P}\left\{ \sup_{\hat{P} \in \Omega_{K,L}} \left[ 2\langle \Xi, \hat{P} - P_\ast \rangle - \frac{1}{2} \left\| \hat{P} - P_\ast \right\|_F^2 - 2\Delta(n, K, L) \right] \geq 0 \right\} \leq \log_2 n \cdot \exp \left( -n \cdot 2^{2s_0 - 7} \right)$$

where $\Delta(n, K, L)$ is defined in (8.11).

Proof. Consider sets

$$\chi_s(K, L) = \left\{ \exists Z, C : P(Z, C) \in \Im(n, K, L); \right\}$$

$$C_0 2^s \sqrt{\tau(n, K_0, L_0)} \leq \left\| P - P_\ast \right\|_F \leq C_0 2^{s+1} \sqrt{\tau(n, K_0, L_0)} \right\},$$

and

$$\mathcal{J}_s(K, L) = \left\{ \exists Z, C : P(Z, C) \in \Im(n, K, L); \left\| P - P_\ast \right\|_F \leq C_0 2^s \sqrt{\tau(n, K_0, L_0)} \right\}$$

Note that the set $\Omega$ can be partitioned as

$$\Omega = \bigcup_{K,L} \Omega_{K,L}$$

where $\Omega_{K,L}$ are defined in (8.10). Then

$$\mathbb{P}\left\{ \sup_{\hat{P} \in \chi_s(K,L)} \left[ \langle \Xi, \hat{P} - P_\ast \rangle - \frac{1}{4} \left\| \hat{P} - P_\ast \right\|_F^2 - \Delta(n, K, L) \right] \geq 0 \right\} \leq$$

$$\sum_{s=0}^{s_{\max}} \mathbb{P}\left\{ \sup_{\hat{P} \in \chi_s(K,L)} \left[ \langle \Xi, \hat{P} - P_\ast \rangle - \frac{1}{4} \left\| \hat{P} - P_\ast \right\|_F^2 - \Delta(n, K, L) \right] \geq 0 \right\} \leq$$

$$\sum_{s=0}^{s_{\max}} \mathbb{P}\left\{ \sup_{\hat{P} \in \mathcal{J}_s(K,L)} \langle \Xi, \hat{P} - P_\ast \rangle \geq C_0^2 2^{2s-2} \tau(n, K_0, L_0) + \Delta(n, K, L) \right\} \leq$$

$$\sum_{s=0}^{s_{\max}} \mathbb{P}\left\{ \sup_{\hat{P} \in \mathcal{J}_{s+1}(K,L)} \langle \Xi, \hat{P} - P_\ast \rangle \geq C_0^2 2^{2s-2} \tau(n, K_0, L_0) + \Delta(n, K, L) \right\}$$

Here, $s_{\max} \leq \log_2 n$ since $\left\| \hat{P} - P_\ast \right\|_F \leq n$.

Construct a 1-net $\mathcal{Y}_s(n, K, L)$ on the set of matrices in $\mathcal{J}_{s+1}(K, L)$ and observe that, for any $\hat{P} \in \mathcal{J}_s(K, L)$, there exists $\tilde{P} \in \mathcal{Y}_s(n, K, L)$ such that $\left\| \hat{P} - \tilde{P} \right\|_F \leq 1$. Then,

$$\sup_{\hat{P} \in \mathcal{Y}_{s+1}(n, K, L)} \langle \Xi, \hat{P} - P_\ast \rangle \leq$$

$$\max_{\hat{P} \in \mathcal{Y}_s(n, K, L)} \left[ \langle \Xi, \hat{P} - P_\ast \rangle + \langle \Xi, \hat{P} - \tilde{P} \rangle \right] \leq$$

$$\max_{\hat{P} \in \mathcal{Y}_s(n, K, L)} \langle \Xi, \hat{P} - P_\ast \rangle + n$$

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Below we shall use the following version of Bernstein inequality (see, e.g., [15]): if Ξ is a matrix of independent Bernoulli errors and G is an arbitrary matrix of the same size, then for any $t > 0$ one has

$$P \{ \langle \Xi, G \rangle > t \} \leq \max \left( e^{-\frac{t^2}{4\|G\|_F^2}}, e^{-\frac{t}{4\|G\|_\infty}} \right).$$  \hfill (8.44)

We apply (8.44) with $G = \hat{P} - P_*$ and

$$t = C_0^2 \left[ 2^{2s-2}\tau(n, K_0, L_0) + C_2\tau(n, K, L) \right]. \hfill (8.45)$$

Then, $\|G\|_\infty = 1$ and $\|G\|^2 \leq C_0^2 2^{2s+2}\tau(n, K_0, L_0)$ due to $\hat{P} \in \mathcal{F}_s(n, K, L) \subseteq \mathcal{J}_{s+1}(K, L)$. Denote

$$d_{K,L}^{(s)} = \max \left\{ e^{-\frac{t^2}{4C_0^2 2^{2s+2}\tau(n, K_0, L_0)}}, e^{-\frac{t}{4}} \right\}$$  \hfill (8.46)

$$d_{K,L} = \sum_{s=s_0}^{s_{max}} d_{K,L}^{(s)} \cdot \exp \{ \tau(n, K, L) \} \hfill (8.47)$$

Obtain

$$P \{ \sup_{\hat{P} \in \Omega_{K,L}} [\langle \Xi, \hat{P} - P_* \rangle - \frac{1}{4} \|\hat{P} - P_*\|_F^2 - \Delta(n, K, L) \geq 0] \leq d_{K,L} \} \hfill (8.48)$$

Observe that

$$\exp \left\{ -\frac{t^2}{4C_0^2 2^{2s+2}\tau(n, K_0, L_0)} \right\} \geq \exp \left\{ -\frac{3t}{4} \right\}$$

is equivalent to $t \leq 3C_0^2 2^{2s+2}\tau(n, K_0, L_0)$ which can be rewritten as

$$C_2\tau(n, K, L) \leq 47 \cdot 2^{2s-2}\tau(n, K_0, L_0) \hfill (8.49)$$

Now, consider two cases: when (8.49) holds and when it does not.

**Case 1:** If (8.49) holds, then

$$d_{K,L}^{(s)} \leq \exp \left\{ -C_0^2 \left[ 2^{2s-8}\tau(n, K_0, L_0) + \frac{C_2^2 \tau^2(n, K, L)}{2^{2s+4}\tau(n, K_0, L_0)} \right] \right\},$$

so that

$$d_{K,L}^{(s)} \exp \{ \tau(n, K, L) \} \leq \exp \left\{ -\left[ C_0^2 2^{2s-8}\tau(n, K_0, L_0) - \frac{47 \cdot 2^{2s-2}}{C_2} \tau(n, K_0, L_0) \right] \right\} \leq \exp \left\{ -\tau(n, K_0, L_0) \cdot 2^{2s-8} \left[ C_0^2 - \frac{47 \cdot 64}{C_2} \right] \right\}.$$
Thus, it follows from (8.46) and (8.47) that
\[ d_{K,L} \leq \log_2 n \cdot \exp\left\{ -\tau(n, K_0, L_0)2^{2s_0-8}\hat{C} \right\} \] (8.50)
where \(\hat{C} = (C_0^2C_2 - 47 \cdot 64)/C_2\), provided \(C_0C_2 \geq 47 \cdot 64\).

Case 2: If (8.49) does not hold, then
\[ d_{K,L} \leq \exp\left\{ -3\left[\frac{C_0^2}{4}(2^{2s-2}\tau(n, K_0, L_0) + C_2\tau(n, K, L))\right] - \tau(n, K, L)\left(\frac{3C_0^2C_2}{4} - 1\right) \right\} \]

Hence, if \(3C_0^2C_2 > 4\), then
\[ d_{K,L} \leq \log_2 n \cdot \exp\left\{ -\tau(n, K, L)\left(\frac{3C_0^2C_2 - 4}{4}\right) \right\}. \] (8.51)

Combine (8.50) and (8.51) and observe that for \(C_2 = 1\) and \(C_0^2 = 47 \cdot 64 + 1 = 3009\) inequalities \(C_0C_2 \geq 47 \cdot 64\) and \(3C_0^2C_2 > 4\) hold. Then, due to \(\tau(n, K, L) \geq 2n\), for any \((K, L)\)
\[ d_{K,L} \leq \log_2 n \cdot \exp\left\{ -2n \cdot 2^{2s_0-8} \right\}, \]
so that validity of the lemma follows from (8.48).

**Lemma 4.** For any matrices \(A, B \in \mathbb{R}^{m \times n}\) and any unit vectors \(u \in \mathbb{R}^m\) and \(v \in \mathbb{R}^n\), let
\[ \Pi_{u,v}(A) = (uu^T)A(vv^T) \] (8.52)
denote the projection of matrix \(A\) on the vectors \((u, v)\). Then,
\[ \langle \Pi_{u,v}(B), A - \Pi_{u,v}(A) \rangle = 0. \] (8.53)
Furthermore, if we let \(\hat{u}\) and \(\hat{v}\) be the singular vectors of matrix \(A\) corresponding to its largest singular value \(\sigma\), the best rank one approximation of \(A\) is given by
\[ \Pi_{\hat{u},\hat{v}}(A) = (\hat{u}\hat{u}^T)A(\hat{v}\hat{v}^T) = \sigma\hat{u}\hat{v}^T. \] (8.54)

**Lemma 5.** Let \((\hat{u}, \hat{v})\) and \((u, v)\) denote the pairs of singular vectors of matrices \(A\) and \(P\), respectively, corresponding to their largest singular values. Then,
\[ \|\Pi_{u,v}(P) - P\|_F \leq \|\Pi_{\hat{u},\hat{v}}(P) - P\|_F \leq \|\Pi_{\hat{u},\hat{v}}(A) - P\|_F \] (8.55)
where \(\Pi_{u,v}(\cdot)\) is defined in (8.52).

**Proof.** The first inequality in (8.55) is true because \(\Pi_{u,v}(P)\) is the best rank one approximation of \(P\). Now let \(A = P + \Xi\). Then
\[ \|\Pi_{\hat{u},\hat{v}}(A) - P\|_F^2 = \|\Pi_{\hat{u},\hat{v}}(P) - P + \Pi_{\hat{u},\hat{v}}(\Xi)\|_F^2 = \|\Pi_{\hat{u},\hat{v}}(P) - P\|_F^2 + \|\Pi_{\hat{u},\hat{v}}(\Xi)\|_F^2 \]
which leads to the second inequality in (8.55).
Lemma 6. Let elements of matrix $\Xi \in (-1, 1)^{n \times n}$ be independent Bernoulli errors and matrix $\Xi$ be partitioned into $KL$ sub-matrices $\Xi^{(l,k)}$, $l = 1, \cdots, L$, $k = 1, \cdots, K$. Then, for any $x > 0$

$$
\mathbb{P} \left\{ \sum_{l=1}^{L} \sum_{k=1}^{K} \left\| \Xi^{(l,k)} \right\|_{op}^2 \leq C_1 nK + C_2 K^2 \ln(n) + nK + C_3 x \right\} \geq 1 - \exp(-x), \quad (8.56)
$$

where $C_1$, $C_2$, and $C_3$ are absolute constants independent of $n, K$, and $L$.

**Proof.** See [24] for the proof.

Lemma 7. For any $t > 0$,

$$
\mathbb{P} \left\{ \sum_{l=1}^{L} \sum_{k=1}^{K} \left\| \Xi^{(l,k)}(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) \right\|_{op}^2 - F_1(n, \hat{K}, \hat{L}) \leq C_3 t \right\} \geq 1 - \exp(-t). \quad (8.57)
$$

where $F_1(n, K, L) = C_1 nK + C_2 K^2 \ln(n) + C_3 (\ln n + (n + 1) \ln K + K \ln L)$.

**Proof.** Using Lemma 6, for any fixed $K$, $L$, $Z \in \mathcal{M}_{n,K}$, and $C \in \mathcal{M}_{K,L}$, we have

$$
\mathbb{P} \left\{ \sum_{l=1}^{L} \sum_{k=1}^{K} \left\| \Xi^{(l,k)}(Z, C, K, L) \right\|_{op}^2 - C_1 nK - C_2 K^2 \ln(n) \right\} \leq \exp(-x).
$$

Application of the union bound over $Z \in \mathcal{M}_{n,K}$, $C \in \mathcal{M}_{K,L}$, $K \in \{1, \ldots, n\}$, and $L \in \{1, \ldots, K\}$ and setting $x = t + \ln n + (n + 1) \ln K + K \ln L$ yield

$$
\mathbb{P} \left\{ \sum_{l=1}^{L} \sum_{k=1}^{K} \left\| \Xi^{(l,k)}(\hat{Z}, \hat{C}, \hat{K}, \hat{L}) \right\|_{op}^2 - F_1(n, \hat{K}, \hat{L}) \right\} \geq C_3 t
$$

$$
\leq \mathbb{P} \left\{ \max_{1 \leq K \leq n} \max_{1 \leq L \leq K} \max_{Z \in \mathcal{M}_{n,K}} \max_{C \in \mathcal{M}_{K,L}} \left( \sum_{l=1}^{L} \sum_{k=1}^{K} \left\| \Xi^{(l,k)}(Z, C, K, L) \right\|_{op}^2 - F_1(n, K, L) \right) \right\} \geq C_3 t
$$

$$
\leq \sum_{i=1}^{n} \sum_{j=1}^{K} \sum_{Z \in \mathcal{M}_{n,K}} \sum_{C \in \mathcal{M}_{K,L}} \mathbb{P} \left\{ \sum_{l=1}^{L} \sum_{k=1}^{K} \left\| \Xi^{(l,k)}(Z, C, K, L) \right\|_{op}^2 - F_1(n, K, L) \right\} \geq C_3 t
$$

$$
\leq n K n L \exp \left\{ -t + \ln n + (n + 1) \ln K - K \ln L \right\} = \exp(-t),
$$

which completes the proof.

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