Optimal Variable Clustering for High-Dimensional Matrix Valued Data

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December 28, 2021

Abstract

Matrix valued data has become increasingly prevalent in many applications. Most of the existing clustering methods for this type of data are tailored to the mean model and do not account for the dependence structure of the features, which can be very informative, especially in high-dimensional settings. To extract the information from the dependence structure for clustering, we propose a new latent variable model for the features arranged in matrix form, with some unknown membership matrices representing the clusters for the rows and columns. Under this model, we further propose a class of hierarchical clustering algorithms using the difference of a weighted covariance matrix as the dissimilarity measure. Theoretically, we show that under mild conditions, our algorithm attains clustering consistency in the high-dimensional setting. While this consistency result holds for our algorithm with a broad class of weighted covariance matrices, the conditions for this result depend on the choice of the weight. To investigate how the weight affects the theoretical performance of our algorithm, we establish the minimax lower bound for clustering under our latent variable model. The practical implementation of our algorithm with the optimal weight is also discussed. Finally, we conduct simulation studies to evaluate the finite sample performance of our algorithm and apply the method to a genomic dataset.

Keywords: Clustering, matrix data, high dimensional estimation, minimax optimality, latent variable model, hierarchical algorithm

1 Introduction

Clustering analysis is one of the most important unsupervised learning techniques and has been widely used to discover the underlying group structure in data, arising in many applications including economics, image analysis, psychology and biomedical science (Everitt et al., 2011; Kogan, 2003).
In these applications, matrix valued data become increasingly prevalent. For example, in genetic studies, one may observe data matrices of dimension \( p \times q \) from \( n \) subjects, where the \((j,k)\)th entry corresponds to the expression value of the \(j\)th gene at the \(k\)th tissue (Zahn et al., 2007). The biologist is often interested in identifying the clusters of genes that may share similar biological functions, and also the clusters of tissues. Similarly, in functional magnetic resonance imaging (fMRI) studies, to understand how brain connectivity structure changes under different tasks/stimuli, researchers can measure the blood oxygen level (BOLD) within each region of interest (ROI) from the brain under a variety of conditions (Mitchell et al., 2008). The data points from each participant can be stacked as a matrix, in which the rows and columns correspond to different ROIs and tasks/stimuli respectively. Given the data from \( n \) participants, it is of interest to simultaneously cluster the ROIs and tasks/stimuli. Such clustering results can be used as a dimension reduction step to further investigate the brain connectivity networks (Eisenach et al., 2020). Driven by these applications, the goal of the paper is to develop a statistical clustering framework for matrix valued data with theoretical guarantees. In particular, assuming that \( n \) i.i.d. samples \( X^{(1)}, \ldots, X^{(n)} \) of a random matrix \( X \in \mathbb{R}^{p \times q} \) are observed, we would like to recover the cluster membership of the rows and the columns of the feature matrix \( X \).

In the literature, clustering a data matrix is often known as biclustering (Hartigan, 1972; Madeira and Oliveira, 2004). Most of the existing biclustering methods can be classified into the following categories: (1) hierarchical approach based on the dendrogram (Hastie et al., 2009); (2) extensions of K-means (Fraiman and Li, 2020); (3) the penalized likelihood approach (Tan and Witten, 2014); (4) convex clustering via fused lasso (Chi et al., 2017); and (5) clustering based on the singular value decomposition (Sill et al., 2011; Lee et al., 2010). In these existing works, the goal is to simultaneously cluster \( n \) samples and \( d \) features stacked as a \( n \times d \) data matrix, whereas in our problem we are interested in clustering a \( p \times q \) feature matrix. Since the features are often correlated, the \( p \times q \) feature matrix induces a sophisticated but informative dependence structure, that is not accounted for in the existing biclustering methods, and therefore these methods are not appropriate in our setting. More recently, multiway clustering, also known as tensor clustering, attracts increasing attention (Mankad and Michailidis, 2014; Zhao et al., 2016; Chi et al., 2018; Sun and Li, 2019; Wang et al., 2019; Wang and Zeng, 2019). Since we observe \( n \) i.i.d \( p \times q \) feature matrices, we can view our data as a 3-way tensor with dimension \( p \times q \times n \). The existing tensor clustering methods aim to cluster each mode of the tensor from the mean model, such as the tensor block model (Wang and Zeng, 2019; Chi et al., 2018). While these approaches enjoy great success in many applications and can be adapted to our setting, they may not perform well when the dependence structure of the features is informative.

In this paper, our first contribution is to propose a new latent variable model for clustering matrix valued data. Assume that the features are stacked as a random matrix \( X \in \mathbb{R}^{p \times q} \), which follows

\[
X = AZB^T + \Gamma, \tag{1.1}
\]

where \( Z \in \mathbb{R}^{K_1 \times K_2} \) is a latent variable matrix with \( \mathbb{E}(Z) = 0 \), \( A \in \mathbb{R}^{p \times K_1} \) and \( B \in \mathbb{R}^{q \times K_2} \) are the
unknown membership matrices for the rows and columns respectively, and $\Gamma \in \mathbb{R}^{p \times q}$ represents the random noise with mean 0 and variance $\sigma_{ab}^2 = \text{Var}(\Gamma_{ab})$. We assume the noise matrix $\Gamma$ is mutually independent and is also independent of $Z$. The entry of the membership matrix $A$ takes values in $\{0, 1\}$, such that $A_{ak} = 1$ if row $a$ belongs to row cluster $k$ and $A_{ak} = 0$ otherwise. In this paper, we focus on the non-overlapping and exhaustive clustering, that is for each row $a$, there exists one and only one cluster $k$ with $A_{ak} = 1$. The same requirement holds for the membership matrix $B$. To see why $A$ and $B$ are interpreted as membership matrices, we note that, for any feature $X_{ab}$, if $A_{ak} = 1$ and $B_{b\ell} = 1$ for some $k$ and $\ell$, then model (1.1) implies $X_{ab} = Z_{k\ell} + \Gamma_{ab}$, that is, the feature $X_{ab}$ is associated with the latent variable $Z_{k\ell}$. For this reason, we say that $X_{ab}$ belongs to the row cluster $k$ and column cluster $\ell$. Under model (1.1), we can formally define the row clusters as the partition

$$G^{(r)} = \{G_1^{(r)}, ..., G_{K_1}^{(r)}\} \text{ of } \{1, ..., p\}, \text{ where } G_k^{(r)} = \{a : A_{ak} = 1\}$$

for any $1 \leq k \leq K_1$, and $K_1$ is the unknown number of row clusters. When the context is clear, $G$ will be used for notation simplicity. Without loss of generality, we focus on how to recover the unknown membership matrix $A$ for the rows (or equivalently $G^{(r)}$) up to label switching.

Model (1.1) can be viewed as the extension of the G-block model for clustering a random vector in Bunea et al. (2018) to matrix valued data. Indeed, if we vectorize the matrix $X$, model (1.1) is equivalent to $\text{vec}(X) = M \text{vec}(Z) + \text{vec}(\Gamma)$ with $M = B \otimes A$, where $\text{vec}(X)$ denotes the vectorization of $X$, formed by stacking the columns of $X$ into a single column vector, and $\otimes$ denotes the Kronecker product. Thus, compared to Bunea et al. (2018) which allows $M$ to be any unstructured $(pq) \times (K_1K_2)$ membership matrix, we impose the Kronecker product structure to the membership matrix $M$. While our model for $\text{vec}(X)$ is more restrictive than Bunea et al. (2018), it actually comes with two advantages for matrix clustering. First, as seen above, $A$ and $B$ are interpreted as the membership matrices for the rows and columns. Ignoring the Kronecker product structure and directly applying the model in Bunea et al. (2018) would no longer produce interpretable results for matrix clustering. Second, the Kronecker product of $A$ and $B$ provides a more parsimonious parametrization for the unknown membership matrix $M$, leading to stronger theoretical guarantees on clustering. In particular, we show that under our model (1.1) the cluster separation condition required for clustering consistency is weaker than that required in Bunea et al. (2018). Finally, we note that, unlike the aforementioned works on tensor clustering, our model (1.1) implies $\mathbb{E}(X) = 0$ and the clustering structure is informed by the dependence structure of $X$ due to the latent variable matrix $Z$. Thus, our paper complements these works and provides a new approach to clustering matrix valued data.

To recover the unknown membership matrix $A$ (and similarly for $B$), our second contribution is to propose a class of hierarchical clustering methods based on the weighted covariance matrix $\Sigma_{p,W} = \mathbb{E}(XWX^T)$, for some positive semi-definite matrix $W \in \mathbb{R}^{q \times q}$ to be chosen. We use the difference of this weighted covariance matrix as the dissimilarity measure in the hierarchical algorithm to recover the membership matrix $A$. To establish the theoretical guarantees of our algorithm, we introduce the following metric $\text{MCOD}(\Sigma_{p,W})/\|X\|_W$ to quantify how clusters are
separated; see Section 3.1 for the precise definition. Theoretically, we develop a general result on the clustering consistency of our hierarchical algorithm, which allows a broad class of weight matrices $W$. To attain clustering consistency, we require the cluster separation metric $\frac{\text{MCOD}(\Sigma_p, W)}{\|X\|_W}$ to be no smaller than the order of $(\log \frac{p}{nK_2})^{1/2}$, where $K_2$ is the number of column clusters. The implication is that, with the help of a larger $K_2$, clustering the rows of $X$ becomes easier.

To investigate the optimality of our algorithm, we establish the minimax lower bound for clustering under our latent variable model. While the clustering consistency property holds with a broad class of weight matrices $W$, our algorithm with a generic weight $W$ may not be minimax optimal. To derive an optimal clustering algorithm for the rows, the key is to account for the information from the column clusters. The intuition is that with a more accurate column clustering result (i.e., estimate of $B$), we can decorrelate the dependence structure of $X$ and reduce the noise induced by $\Gamma$, which in turn improves the clustering accuracy for the rows. Following this argument, we identify the optimal weight as $\hat{B}(\hat{B}^T \hat{B})^{-2} \hat{B}^T / s$, where $\hat{B}$ is an estimate of the column membership matrix $B$ and $s$ denotes the estimated number of clusters from $\hat{B}$. Under mild conditions, we show that the proposed algorithm with the optimal weight attains the minimax lower bound, and therefore is rate-optimal for clustering. To the best of our knowledge, our paper is the first one that formally establishes the minimax optimality for clustering matrix valued data. From the technical aspect, to show the optimality of our algorithm, the main challenge is to quantify the “stability” of the algorithm with respect to an imperfect estimate $\hat{B}$ in the weight matrix. We provide sufficient conditions to show the stability of the algorithm under some additional modeling assumptions. In practice, the hierarchical algorithm can be applied iteratively to cluster the rows and columns. Finally, we conduct extensive numerical studies to support our theoretical results.

The rest of the paper is organized as follows. In Section 2, we propose the hierarchical algorithm. In Section 3, we establish the clustering consistency of our algorithm and derive the minimax lower bound. Since the algorithm using the optimal weight depends on the initial estimate $\hat{B}$, in Section 4, we verify the cluster separation condition and stability condition required in Theorem 3.1 for clustering consistency. The practical implementation of the algorithm is discussed in Section 5. The simulation results and real data analysis are shown in Sections 6 and 7. The paper concludes with some discussions in Section 8.

**Notations.** For any $1 \leq a \neq b \leq p$, we write $a \sim_G b$ if $a$ and $b$ are in the same cluster (i.e., $a, b \in G_k$ for some $k$). Otherwise, we write $a \not\sim_G b$. For a matrix $X$, we use the following norms $\|X\|_{\text{max}} = \max_{i,j} |X_{ij}|$, $\|X\|_{\infty} = \max_i \sum_{j=1}^q |X_{ij}|$, $\|X\|_F = \sqrt{\sum_{i,j} X_{ij}^2}$ and $\|X\|_{op}$ denotes the largest singular value of $X$. The largest and smallest eigenvalues are denoted by $\lambda_{\text{max}}(\cdot)$ and $\lambda_{\text{min}}(\cdot)$. We use $X_{j\cdot}$ and $X_{\cdot j}$ to denote the $j$th column and row of $X$. For two positive sequences $a_n$ and $b_n$, we write $a_n \asymp b_n$ if $C \leq a_n / b_n \leq C'$ for some $C, C' > 0$. Similarly, we use $a_n \lesssim b_n$ ($a_n \gtrsim b_n$) to denote $a_n \leq Cb_n$ ($a_n \geq Cb_n$) for some constant $C > 0$. 

4
2 Methodology

2.1 Hierarchical clustering via weighted covariance difference

Recall that the random matrix $X$ follows the model (1.1). In this section, we propose a class of clustering methods for the rows of $X$ based on the weighted covariance matrix $\Sigma_{p,W} = \mathbb{E}(XWXT)$, where $W \in \mathbb{R}^{q \times q}$ is some positive semi-definite matrix to be chosen. We add a subscript $p$ to indicate $\Sigma_{p,W}$ is a $p \times p$ matrix corresponding to the rows. The same type of method can be used to cluster the columns of $X$.

In the following, we first outline how to identify the unknown membership matrix $A$ from the weighted covariance matrix $\Sigma_{p,W}$ on the population level. Under model (1.1), by the independence between $Z$ and $\Gamma$, we obtain that

$$\Sigma_{p,W} = A \mathbb{E}(ZB^T W BZ^T) A^T + \mathbb{E}(\Gamma W^T \Gamma).$$

To recover the membership matrix $A$ from $\Sigma_{p,W}$, one needs to first separate the two matrices $A \mathbb{E}(ZB^T W BZ^T) A^T$ and $\mathbb{E}(\Gamma W^T \Gamma)$. Noting that $\mathbb{E}(\Gamma W^T \Gamma)$ is a diagonal matrix as the errors in $\Gamma$ are mutually independent, we therefore focus on the non-diagonal entries of $\Sigma_{p,W}$, that is $[\Sigma_{p,W}]_{ac} = [A \mathbb{E}(ZB^T W BZ^T) A^T]_{ac}$ for any $1 \leq a \neq c \leq p$. By the definition of the membership matrix $A$, for any $a \in G_k$, $c \in G_\ell$ and $a \neq c$, we have

$$[\Sigma_{p,W}]_{ac} = [A \mathbb{E}(ZB^T W BZ^T) A^T]_{ac} = [\mathbb{E}(ZB^T W BZ^T)]_{k\ell}.$$

In view of (2.2), the within-cluster covariance difference $(\Sigma_{p,W})_{ac} - (\Sigma_{p,W})_{bc}$ with $a \sim \mathcal{G} b$ is always 0 for any $c \neq a, b$. In other words, as long as $(\Sigma_{p,W})_{ac} - (\Sigma_{p,W})_{bc}$ is nonzero for some $c$, it indicates that $a$ and $b$ are not in the same cluster. Thus, the covariance difference is indicative of the clustering structure. Following Bunea et al. (2018), we formally define the covariance difference (COD) as

$$\text{COD}_{\Sigma_{p,W}}(a,b) := \max_{c \neq a,b} |(\Sigma_{p,W})_{ac} - (\Sigma_{p,W})_{bc}|.$$

From the above argument, we have $\text{COD}_{\Sigma_{p,W}}(a,b) = 0$ if $a \sim \mathcal{G} b$. Moreover, if $\text{COD}_{\Sigma_{p,W}}(a,b) > 0$ holds for all $a \not\sim \mathcal{G} b$, we are able to identify all the clusters. Let

$$\text{MCOD}(\Sigma_{p,W}) := \min_{a \not\sim \mathcal{G} b} \text{COD}_{\Sigma_{p,W}}(a,b)$$

denote the minimum COD value over all possible $a \not\sim \mathcal{G} b$. On the population level, provided $\text{MCOD}(\Sigma_{p,W}) > 0$, the membership matrix $A$ (or equivalently $\mathcal{G}^{(r)}$ in (1.2)) is identified from the weighted covariance matrix $\Sigma_{p,W}$ up to column permutation (or equivalently label switching).

Based on the above results on the population level, we will develop a hierarchical clustering algorithm to estimate the membership matrix $A$ (or equivalently $\mathcal{G}^{(r)}$ in (1.2)). Given $n$ i.i.d. samples $X^{(1)}, \ldots, X^{(n)}$, we first estimate $\Sigma_{p,W}$ by

$$\hat{\Sigma}_{p,W} = \frac{1}{n} \sum_{i=1}^n X^{(i)} W X^{(i)T},$$
and then plug this into (2.3) to form a dissimilarity measure $\text{COD}_{\hat{\Sigma}_{p,W}}(a,b)$ for any $1 \leq a, b \leq p$. The hierarchical algorithm starts with every variable representing a singleton cluster. At each step, the closest two clusters are merged into one single cluster based on the following dissimilarity measure between two sets $I$ and $J$

$$\text{COD}_{\hat{\Sigma}_{p,W}}(I,J) = \max_{a \in I, b \in J} \text{COD}_{\hat{\Sigma}_{p,W}}(a,b). \quad (2.5)$$

We refer to Hastie et al. (2009) for alternative definitions of dissimilarity between two clusters and further discussions. Finally, we terminate this process and report the clusters, when the dissimilarity measure $\text{COD}_{\hat{\Sigma}_{p,W}}(I,J)$ exceeds a threshold value $\alpha > 0$. The hierarchical algorithm, summarized in Algorithm 1, improves the existing COD algorithm proposed by Bunea et al. (2018). First, our algorithm satisfies the so-called monotonicity property, which means the merged clusters always have smaller values of $\text{COD}_{\hat{\Sigma}_{p,W}}(I,J)$ than the unmerged ones (Hastie et al., 2009). However, the algorithm in Bunea et al. (2018) may instead merge indices $a$ and $b$ into one cluster even if there exists another index $c$ with $\text{COD}_{\hat{\Sigma}_{p,W}}(a,c)$ smaller than $\text{COD}_{\hat{\Sigma}_{p,W}}(a,b)$. We refer to the Supplementary Appendix A for a toy example. Empirically, we find that our hierarchical algorithm produces more stable clustering results than the algorithm in Bunea et al. (2018). Second, the hierarchical algorithm is more flexible to incorporate side information, such as the number of row clusters $K_1$. While Algorithm 1 does not require the user to know $K_1$, with such information from domain knowledge or existing literature, the algorithm is expected to yield more reliable clustering results.

**Algorithm 1: Hierarchical Algorithm with COD**

- **INPUT**: The estimated covariance $\hat{\Sigma}_{p,W}$ and a threshold $\alpha > 0$.
- Calculate $\text{COD}_{\hat{\Sigma}_{p,W}}(a,b)$ for $1 \leq a, b \leq q$
- Create a hierarchical tree based on the value of $\text{COD}_{\hat{\Sigma}_{p,W}}(I,J)$ in (2.5).
- Use the threshold value $\alpha$ to cut the tree and obtain the estimated clusters $\hat{\mathcal{G}}$. More precisely, we use the following rule to find the clusters. For any two sets of candidate clusters $I$ and $J$ from the hierarchical tree, we merge them into one cluster if and only if $\text{COD}_{\hat{\Sigma}_{p,W}}(I,J) \leq \alpha$.

In the following subsection, we consider the hierarchical algorithm with two instances of $W$. In the first setting, the algorithm is non-iterative and very convenient in practice, but may not be optimal for clustering. In the second setting, the algorithm requires the user to iteratively cluster the rows and columns, leading to optimal clustering results.
2.2 Optimal choice of $W$

While our Algorithm 1 can be applied with any weight matrix $W$ in $\hat{\Sigma}_{p,W}$, the empirical and theoretical performance of the algorithm critically depends on the choice of $W$. In practice, the simplest choice of $W$ could be $W = I_q/q$, where $I_q$ is a $q \times q$ identity matrix. With this choice of $W_I$, the weighted covariance matrix $\Sigma_{p,W_I}$ can be interpreted as the average of the second order moment of the columns of $X$, $\frac{1}{q} \sum_{j=1}^{q} \mathbb{E}(X_jX_j^T)$. However, as shown in the next section, Algorithm 1 with this simple choice $W_I$ is generally not optimal for clustering the rows. Indeed, the performance of the algorithm can be improved, if the clustering structure of the columns is taken into account.

To motivate the development of the optimal choice of $W$, we temporarily assume that the true column cluster structure (i.e., the membership matrix $B$) is known up to label switching. We define $X^* = XB(B^TB)^{-1} \in \mathbb{R}^{p \times K_2}$, which can be interpreted as the average of $X$ over columns in the same column cluster. To see this, let us consider a toy example. Assume that $X$ has $q = 4$ columns with $K_2 = 2$ column clusters, where the first two columns belong to cluster 1 and the last two columns are in cluster 2. In this case, the membership matrix $B$ can be written as

$$B = \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \end{bmatrix} \in \mathbb{R}^{4 \times 2}. \quad \text{Then we have } \quad X^* = \begin{bmatrix} \frac{X_{11}+X_{12}}{2} & \frac{X_{13}+X_{14}}{2} \\ \vdots & \vdots \\ \frac{X_{p1}+X_{p2}}{2} & \frac{X_{p3}+X_{p4}}{2} \end{bmatrix} \in \mathbb{R}^{p \times 2}. $$

Clearly, the two columns of $X^*$ represent the averages of $X$ in the same column cluster. Inspired by the interpretation of $\Sigma_{p,W_I}$, we now compute the average of the second order moment of columns of $X^*$, that is

$$\frac{1}{K_2} \sum_{j=1}^{K_2} \mathbb{E}(X_j^*X_j^{*T}) = \frac{1}{K_2} \mathbb{E}(X^*X^{*T}) = \mathbb{E}(XW_OX^T) = \Sigma_{p,W_O},$$

where we set $W_O = B(B^TB)^{-2}B^T/K_2$ by the definition of $X^*$. This matrix $W_O$ is the optimal weight. Intuitively, the weighted covariance matrix $\Sigma_{p,W_O}$ with $W_O$ is more informative for clustering than $\Sigma_{p,W_I}$, as the random noise in $\Gamma$ is reduced when we construct $X^*$ by aggregating the columns of $X$ in the same column cluster. To better illustrate this point, we consider a special case. Assume that the columns of $X$ have $K_2$ clusters with equal size $q/K_2$. After some algebra, it is shown that

$$\Sigma_{p,W_I} = \frac{1}{K_2} A \mathbb{E}(ZZ^T)A^T + \frac{1}{q} \mathbb{E}(\Gamma \Gamma^T),$$

and

$$\Sigma_{p,W_O} = \frac{1}{K_2} A \mathbb{E}(ZZ^T)A^T + \frac{K_2}{q} \left\{ \frac{1}{q} \mathbb{E}(\Gamma \Gamma^T) \right\}. $$

Clearly, both $\Sigma_{p,W_I}$ and $\Sigma_{p,W_O}$ contain the same amount of row clustering information via the term $\frac{1}{K_2} A \mathbb{E}(ZZ^T)A^T$. However, compared to $\Sigma_{p,W_I}$, the error matrix induced by the covariance of $\Gamma$ is further reduced by a factor of $K_2/q$ in $\Sigma_{p,W_O}$. Therefore, we expect that the clustering algorithm using $\Sigma_{p,W_O}$ would outperform the method using $\Sigma_{p,W_I}$ for recovering the membership matrix $A$, which is indeed the case in simulations; see Section 6.
Since \( W_O = B(B^T B)^{-2}B^T / K_2 \) depends on the unknown membership matrix \( B \), the hierarchical algorithm 1 is not directly applicable. In principle, if an initial estimate of \( B \), say \( \hat{B} \), is available, we can plug in the estimator \( \hat{B} \) and apply Algorithm 1 with \( \hat{W}_O = \hat{B} (\hat{B}^T \hat{B})^{-2} \hat{B}^T / s \) and \( s \) denotes the estimated number of clusters from \( \hat{B} \). Theoretically, in the next section, we will establish a general result on the clustering consistency of Algorithm 1 with a data dependent weight matrix \( \hat{W} \), which covers the case with \( \hat{W}_O \). In practice, we recommend using an iterative hierarchical algorithm to repeatedly cluster the rows and columns of \( X \). The detailed implementation of the algorithm using the optimal weight is discussed in Section 5.

3 Theoretical Guarantees

In this section, we establish the theoretical results for the clustering problem. In Section 3.1, we present a general result on the clustering consistency of Algorithm 1 with a data dependent weight matrix \( \hat{W} \). Subsequently, we develop the minimax lower bound for the matrix clustering problem in Section 3.2. In particular, these results imply that Algorithm 1 with the estimated optimal weight matrix \( \hat{W}_O \) defined in Section 2.2 is minimax optimal for clustering.

3.1 Clustering consistency of our algorithm

To formally study the clustering consistency property, we need to first define a proper notion of cluster separation distance. Recall from the argument in Section 2.1 that \( \text{MCOD}(\Sigma_p, W) > 0 \) implies the identifiability of \( A \) up to column permutations. One may attempt to use \( \text{MCOD}(\Sigma_p, W) \) to measure cluster separation. However, using \( \text{MCOD}(\Sigma_p, W) \) alone is not ideal, as \( \text{MCOD}(\Sigma_p, W) \) is not invariant to the scale of \( W \). To be specific, we have \( \text{MCOD}(\Sigma_p, tW) = t \text{MCOD}(\Sigma_p, W) \) for any \( t > 0 \), implying that the MCOD value can be arbitrarily large by rescaling \( W \).

To measure the cluster separation, we define a quasinorm of \( X \),

\[
\|X\|_W = K_2^{1/2} \max_{1 \leq a \leq p} \|L^T \text{Var}(X_a) L\|_F,
\]

where \( L \) is a matrix satisfying \( LL^T = W \). We note that \( \|X\|_W \) can be interpreted as the amount of the variance of the row vector in \( X \) reweighted by \( L \). From the technical aspect, such a quantity plays a natural role when applying the concentration inequality to control \( \hat{\Sigma}_p, W - \Sigma_p, W \). For convenience, we also include a \( K_2^{1/2} \) factor in \( \|X\|_W \) to rescale the quasinorm to be of constant order. For example, under our model (1.1) and some mild conditions, we show in Supplementary Appendix B that \( \|X\|_W = O(1) \).

In this paper, we define the cluster separation metric as \( \text{MCOD}(\Sigma_p, W)/\|X\|_W \). First, we can view \( \text{MCOD}(\Sigma_p, W)/\|X\|_W \) as a standardized distance, which measures cluster separation per unit “variance” of \( X \). Second, \( \text{MCOD}(\Sigma_p, W)/\|X\|_W \) is invariant to the scale of \( W \) and also the scale of \( X \) (e.g., transform \( X \) to \( tX \) for any \( t \in \mathbb{R} \)). Finally, we note that our cluster separation metric depends on the choice of the weight matrix \( W \), since we use a weighted covariance distance to construct the MCOD in (2.4). Thus, even if we consider the same data generating model (1.1),
the value of the cluster separation metric may differ by the choice of $W$. This has important implications for clustering consistency (see Remark 3.2) and the minimax lower bound (see Section 3.2).

If the weight $W$ is known, we can directly apply our Algorithm 1 with the input $\hat{\Sigma}_{p,W}$. However, if $W$ depends on the unknown parameters (e.g., the optimal weight $W_O$), we need to estimate $W$ and use a data dependent weight in Algorithm 1. To study clustering consistency of the algorithm with a data dependent weight, we assume that there exists an initial estimator $\hat{W}$ of a deterministic weight matrix $W$. To simplify the theoretical analysis, we focus on analyzing Algorithm 1 with sample splitting. Specifically, we randomly divide the data into two folds, $\{X^{(i)} : i \in D_1\}$ and $\{X^{(i)} : i \in D_2\}$, where $D_1 \cap D_2 = \emptyset$ and $D_1 \cup D_2 = \{1, ..., n\}$. The estimator $\hat{W}$ is constructed using the data in $D_1$, and then we apply Algorithm 1 with the input $\hat{\Sigma}_{p,\hat{W}} = \frac{1}{|D_2|} \sum_{i \in D_2} X^{(i)}\hat{W}X^{(i)T}$, where $\hat{\Sigma}_{p,\hat{W}}$ is the weighted sample covariance matrix using the data in $D_2$. By using this simple procedure, we can remove the dependence of $\hat{W}$ and the data in $D_2$.

Let us denote $\Sigma_{p,\hat{W}} = E(X\hat{W}X^T|\hat{W})$, where the expectation is taken with respect to $X$ which is independent of $\hat{W}$. The following main theorem in this section shows the clustering consistency of our algorithm in the non-asymptotic regime.

**Theorem 3.1.** Under model (1.1), assume that vec$(X)$ is multivariate Gaussian, $\log p = o(n)$ and the following two conditions hold:

(A1) Cluster separation condition: $\text{MCOD}(\Sigma_{p,W})/\|X\|_W > c_0 \eta$, where $\eta \geq c_1 \sqrt{\frac{\log p}{nk^2}}$ for some constants $c_0, c_1 > 0$.

(A2) Stability condition: $\{\text{MCOD}(\Sigma_{p,\hat{W}})/\|X\|_{\hat{W}}\}/\{\text{MCOD}(\Sigma_{p,W})/\|X\|_W\} > 4/c_0$, where $c_0$ is defined in (A1).

Then using our Algorithm 1 with $\hat{\Sigma}_{p,\hat{W}}$ and the threshold $\alpha = 2 \eta \cdot \|X\|_{\hat{W}}$, we obtain perfect row cluster recovery (i.e., $\hat{G}^{(r)} = G^{(r)}$) with probability greater than $1 - \frac{c_2}{p}$ for some constant $c_2 > 0$.

In the following, we start from the discussion on the conditions in Theorem 3.1. The Gaussian assumption is imposed in order to derive a sharp bound for $(\hat{\Sigma}_{p,\hat{W}} - \Sigma_{p,\hat{W}})_{jk}$ when applying the Hanson-Wright inequality, as we can decorrelate two dependent Gaussian variables to make them independent. Recently, Adamczak (2015) derived a variant of the Hanson-Wright inequality for dependent data with the so-called convex concentration property. Using this new inequality, we can relax the Gaussian assumption to more general distributions (e.g., sub-Gaussian) with the convex concentration property. The conclusion in Theorem 3.1 remains the same. However, to keep our presentation focused, we impose the Gaussian assumption in this theorem.

The condition $\log p = o(n)$ is standard for high-dimensional data. We further assume two major conditions (A1) and (A2). Recall from the previous discussion that the cluster separation is measured by $\text{MCOD}(\Sigma_{p,W})/\|X\|_W$. The condition (A1) implies that, in the ideal case (i.e., the weight matrix $W$ is known), the clusters must be separated by a factor of $\sqrt{\frac{\log p}{nk^2}}$. For this reason, we call (A1) the cluster separation condition. On top of (A1), we also need condition (A2), because
in some cases the target weight matrix $W$ (e.g., the optimal weight $W_O$) needs to be estimated. The condition (A2) quantifies the stability of the cluster separation metric $\text{MCOD}(\Sigma_{p,W})/\|X\|_W$ with respect to the perturbation of $W$. Essentially, condition (A2) guarantees that $\text{MCOD}(\Sigma_{p,W})/\|X\|_W$ with the estimate $\hat{W}$ is still beyond the order $\sqrt{\frac{\log p}{nK^2}}$. When $W$ does not need to be estimated, we can simply use $\hat{\Sigma}_{p,W}$ in Algorithm 1, and in this case (A2) holds trivially. Finally, we note that (A1) and (A2) are both high-level technical conditions, which will be further explored in Section 4 under additional modeling assumptions.

One important implication of Theorem 3.1 is that the minimum cluster separation for clustering consistency is of order $\sqrt{\frac{\log p}{nK^2}}$, which decreases as the number of column clusters $K$ grows. In other words, clustering the rows of $X$ becomes easier, if the columns of $X$ have more column clusters. Indeed, this phenomenon is reasonable, as the data from two different column clusters show weaker dependence and therefore improve the convergence rate of $(\hat{\Sigma}_{p,W} - \Sigma_{p,W})_{jk}$ in the Hanson-Wright inequality. This result clearly demonstrates the benefit of clustering the matrix $X$ over vector clustering. To be precise, consider the following simple alternative. We just take any column of $X$ and apply our algorithm to cluster this $p \times 1$ vector. This corresponds to a special case of our framework with $q = K = 1$. From Theorem 3.1, we can see that the minimum cluster separation for clustering any column of $X$ is of order $\sqrt{\frac{\log p}{n}}$, which is much stronger than the condition (A1) when $K$ diverges. Finally, we note that in this special case $q = K = 1$, the order of our cluster separation metric matches the existing result for vector clustering in Bunea et al. (2018).

Remark 3.2. The results in Theorem 3.1 are generally applicable to our clustering algorithm with any positive semi-definite matrix $W$, provided (A1) and (A2) hold. Recall that in Section 2.2, we consider two specific weights, $W_I = I_q/q$ and $W_O = B(B^TB)^{-2}B^T/K$, where the latter is called the optimal weight. We can apply our algorithm with either $\hat{\Sigma}_{p,W_I}$ or $\hat{\Sigma}_{p,W_O}$, where $\hat{W}_O$ is an estimate of $W_O$ defined in Section 2.2. In this remark, we will discuss the implication of Theorem 3.1 on our algorithm with these two weights. Since the rate of the cluster separation for consistency is always $\sqrt{\frac{\log p}{nK^2}}$, which does not depend on $W$, one might be tempted to conclude that there is no benefit of using the optimal weight $W_O$ over $W_I$ for clustering consistency. However, this conclusion is imprecise, as the value of the cluster separation metric $\text{MCOD}(\Sigma_{p,W})/\|X\|_W$ depends on $W$ and may differ substantially. To better illustrate this point, we consider a special case where all column clusters have equal size and $\text{Var}(\Gamma_{aj}) = \sigma^2$. By definition, $\text{MCOD}(\Sigma_{p,W})/\|X\|_W$ depends on the noise level $\sigma^2$. After some analysis, we can show that the cluster separation condition (A1) with $W_I$ and $W_O$ holds, provided the noise level satisfies $\sigma^2 = O\left(\frac{1}{\eta}(\frac{q}{K^2})^{1/2}\right)$ and $\sigma^2 = O\left(\frac{q}{\eta K^2}\right)$, respectively. As a result, when $q \gg K$, our algorithm with the optimal weight $W_O$ attains clustering consistency in the presence of a larger noise level $\sigma^2$. This is the benefit of using the optimal weight in our algorithm. We refer to Supplementary Appendix C for the derivation and further discussion.

3.2 Minimax lower bound

In this section, we establish the minimax lower bound for the matrix clustering problem. Since the cluster separation metric $\text{MCOD}(\Sigma_{p,W})/\|X\|_W$ depends on $W$, we specialize the lower bound
results to two cases $W = W_I$ and $W = W_O$.

**Lower bound for clustering with $W = W_I$.**

Assume that $\text{vec}(X) \sim N(0, \Sigma)$, where $\Sigma \in \mathbb{R}^{pq \times pq}$. We define the following parameter space:

$$M_I = M_I(p, q, K_1, K_2, \eta) = \{ \Sigma \in \mathbb{R}^{pq \times pq} | X \text{ satisfies model (1.1), } \text{MCOD}(\Sigma_{p,W_I})/\|X\|_{W_I} \geq \eta \},$$

which consists of all possible configurations of $\Sigma$ under model (1.1) with the cluster separation metric greater than $\eta$. Let $P_\Sigma$ denote the probability under $\text{vec}(X) \sim N(0, \Sigma)$. We establish the minimax lower bound over the parameter space $M_I$ for clustering in the following theorem.

**Theorem 3.3.** For $K_1 \geq 3$, there exists a positive constant $c$ such that, for any $\eta$

$$0 \leq \eta < c \sqrt{\frac{\log p}{n(K_2q)^{1/2}}} ,$$

we have

$$\inf_{\hat{G}} \sup_{\Sigma \in M_I} P_\Sigma(\hat{G} \neq G) \geq \frac{1}{7},$$

where the infimum is taken over all possible estimators of $G$.

Theorem 3.3 shows that it is impossible to attain clustering consistency uniformly over the parameter space $M_I$, when the minimum cluster separation value $\eta$ is below the threshold $(\frac{\log p}{n(K_2q)^{1/2}})^{1/2}$. Since this threshold is of a smaller order than $(\frac{\log p}{nK_2})^{1/2}$ in condition (A1) in Theorem 3.1 for clustering consistency, the optimality of our algorithm using the weight $W_I$ is in doubt. Indeed, we expect that the thresholds for $\eta$ in Theorems 3.1 and 3.3 are sharp, and therefore our algorithm using the weight $W_I$ is expected to be sub-optimal. In simulation studies, we find that the performance of our algorithm using the weight $W_I$ is often worse than some competitors, which is also a sign of the suboptimality of this approach.

**Lower bound for clustering with $W = W_O$.**

Similarly, we define the parameter space as

$$M_O = M_O(p, q, K_1, K_2, \eta) = \{ \Sigma \in \mathbb{R}^{pq \times pq} | X \text{ satisfies model (1.1), } \text{MCOD}(\Sigma_{p,W_O})/\|X\|_{W_O} \geq \eta \},$$

where the cluster separation metric is defined based on $W_O$. Since the two parameter spaces $M_O$ and $M_I$ are different, the lower bound may also differ. The following theorem provides the lower bound for clustering over the parameter space $M_O$.

**Theorem 3.4.** For $K_1 \geq 3$, there exists a positive constant $c$ such that, for any $\eta$

$$0 \leq \eta < c \sqrt{\frac{\log p}{nK_2}} ,$$

we have

$$\inf_{\hat{G}} \sup_{\Sigma \in M_O} P_\Sigma(\hat{G} \neq G) \geq \frac{1}{7},$$

where the infimum is taken over all possible estimators of $G$. 

11
In contrast to the previous Theorem 3.3, the threshold for the minimum cluster separation based on $W_O$ is of order $(\log p/nK_2)^{1/2}$, which matches with the rate of $\eta$ in condition (A1) in Theorem 3.1. Thus, provided the stability condition (A2) in Theorem 3.1 holds, our Algorithm 1 using $\hat{\Sigma}_pW_O$ and $\alpha = 2\eta \cdot \|X\|_W^{-1}$ is minimax optimal for clustering.

4 Applications to Matrix Normal Models

As seen from the previous section, our Algorithm 1 using the weighted covariance matrix $\hat{\Sigma}_pW_O$ is minimax optimal, provided the conditions (A1) and (A2) in Theorem 3.1 hold. In this section, we will verify conditions (A1) and (A2) with $W = \hat{W}_O$. To make the analysis of the cluster separation metric MCOD($\Sigma_pW$)/$\|X\|_W$ tractable, we will make some additional modeling assumptions.

On top of our model (1.1), we further assume that the latent variable $Z$ follows the matrix normal distribution. That is $Z \sim \text{MN}(0, U, V)$, where $U \in \mathbb{R}^{K_1 \times K_1}$ and $V \in \mathbb{R}^{K_2 \times K_2}$ are positive definite matrices. Note that this is equivalent to saying that $\text{vec}(Z) \sim \text{MVN}(\text{vec}(0), V \otimes U)$, which gives us $E(Z_{jk}Z_{j'k'}) = U_{jj'}V_{kk'}$ and $E(Z_{jk}) = 0$ for any $1 \leq j, j' \leq K_1$ and $1 \leq k, k' \leq K_2$.

Recall that $\hat{W}_O = \hat{B}(\hat{B}^T\hat{B})^{-2}\hat{B}^T/s$, where $\hat{B}$ is an initial estimator of the column membership matrix $B$ and $s$ is the estimated number of clusters. To facilitate the analysis, we use $\mathcal{G}^{(c)} = \{G_1^{(c)}, \ldots, G_{K_2}^{(c)}\}$ and $\hat{\mathcal{G}}^{(c)} = \{\hat{G}_1^{(c)}, \ldots, \hat{G}_s^{(c)}\}$ to denote the true column cluster structure and the estimated column structure, respectively. We define a $K_2 \times s$ matrix $G$ that carries information about the clustering accuracy of the initial estimator $\hat{B}$:

$$G = B^T\hat{B}(\hat{B}^T\hat{B})^{-1} = \begin{bmatrix} |G_1^{(c)}| & |G_1^{(c)} \cap \hat{G}_1^{(c)}| & \ldots & |G_1^{(c)} \cap \hat{G}_s^{(c)}| \\ |G_2^{(c)}| & |G_2^{(c)} \cap \hat{G}_1^{(c)}| & \ldots & |G_2^{(c)} \cap \hat{G}_s^{(c)}| \\ \vdots & \vdots & \ddots & \vdots \\ |G_{K_2}^{(c)}| & |G_{K_2}^{(c)} \cap \hat{G}_1^{(c)}| & \ldots & |G_{K_2}^{(c)} \cap \hat{G}_s^{(c)}| \end{bmatrix}.$$  

Note that the columns of $G$ sum to 1, and in the ideal case of $\mathcal{G}^{(c)} = \hat{\mathcal{G}}^{(c)}$, we have that $G = I_{K_2}$.

Denote by

$$C_K = \max_{1 \leq a \leq p} \frac{1}{K_2} \sum_{t=1}^{K_2} \left( \frac{\sum_{j \in [t]} \sigma_{aj}^2}{\|t\|^4} \right)^2$$  

(4.1)

the maximum weighted average of the error variances over $K_2$ column clusters, where $[t]$ denotes the $t$-th cluster. Similarly, we define

$$C_s = \max_{1 \leq a \leq p} \frac{1}{s} \sum_{t=1}^{s} \left( \frac{\sum_{j \in [\widehat{t}]} \sigma_{aj}^2}{\|\widehat{t}\|^4} \right)^2$$  

(4.2)

where $[\widehat{t}]$ denotes the estimated $t$-th cluster.

The following proposition shows the conditions under which (A1) and (A2) in Theorem 3.1 hold in the matrix normal model. The proof can be found in Supplementary Appendix E.3.

**Proposition 4.1.** Under model (1.1) and the above matrix normal model assumptions, assume:
(P0) All the eigenvalues of the column covariance matrix $V$ are bounded between two positive constants $C_{\text{min}}$ and $C_{\text{max}}$.

(P1) (Cluster Separation) For any $1 \leq j \neq k \leq K_1$, there exists an index $1 \leq l \leq K_1$ such that

$$|U_{jl} - U_{kl}| > c_1^* \sqrt{\frac{\log(p)}{nK_2}} \cdot \frac{K_2}{\text{tr}(V)} \cdot \left\{ \|\text{diag}(U)\|_{\text{max}} \cdot C_{\text{max}} + C_{K}^{1/2} \right\}$$

holds for some positive constant $c_1^*$, where $\|\text{diag}(U)\|_{\text{max}} = \max_{1 \leq j \leq K_1} U_{jj}$.

(P2) (Stability)

(i) \[ \frac{1}{\lambda_{\text{min}}(GG^T)} \leq \frac{c_0}{8} \cdot \sqrt{\frac{C_K}{C_s}} \cdot \sqrt{\frac{K_2}{s}}, \]

(ii) \[ \frac{\lambda_{\text{max}}(GG^T)}{\lambda_{\text{min}}(GG^T)} \leq \frac{c_0}{8} \cdot \frac{C_{\text{min}}}{C_{\text{max}}} \cdot \frac{\|\text{diag}(U)\|_{\text{min}}}{\|\text{diag}(U)\|_{\text{max}}} \cdot \sqrt{\frac{K_2}{\min(s,K_2^2)}}, \]

where $c_0$ is the constant defined in Theorem 3.1, $C_K$ and $C_s$ are defined in (4.1) and (4.2), and $\|\text{diag}(U)\|_{\text{min}} = \min_{1 \leq j \leq K_1} U_{jj}$.

Then the conditions (A1) and (A2) in Theorem 3.1 hold.

The assumption (P0) is standard and commonly used in the high-dimensional statistics literature (Basu and Michailidis, 2015; Cai et al., 2010; Bai and Silverstein, 2010). For (P1), it says that any two rows of the row covariance matrix $U$ (excluding the diagonal terms) cannot be nearly identical, otherwise, the corresponding two clusters are not identifiable. When the error variances are not too large (e.g., $\sum_{j \in \mathcal{I}_t} \sigma_{aj}^2 \lesssim |\mathcal{I}_t|^2$), then $C_K$ behaves as a constant. If we further assume $\|\text{diag}(U)\|_{\text{max}} = O(1)$, then the cluster separation reduces to $|U_{jl} - U_{kl}| \gtrsim \sqrt{\frac{\log(p)}{nK_2}}$, which decreases with $n$ and $K_2$ as we have discussed before. Finally, (P2) requires the estimated cluster structure to be close enough to the true cluster structure. When the initial estimator $\hat{B}$ is reasonably accurate, we would expect that $C_K$ and $C_s$ are similar or at least of the same order. When $K_2 \asymp s$ and $\|\text{diag}(U)\|_{\text{max}} \asymp \|\text{diag}(U)\|_{\text{min}}$, (P2) reduces to the condition that the smallest (nonzero) eigenvalue of $GG^T$ is bounded from below by a constant and its condition number is bounded from above by a constant. Recall that when $\hat{B}$ is more accurate, $G$ would be closer to an identity matrix and therefore (P2) would be more likely to hold. Thus, (P2) essentially gives a sharp characterization of the “contraction region” in which the algorithm with the imperfect initial estimator $\hat{B}$ still leads to clustering consistency.

5 Some Practical Considerations

In this section, we discuss the practical implementation of our algorithm using the optimal weight. The detailed algorithm is shown in Algorithm 2. In the algorithm, we first apply our hierarchical Algorithm 1 to cluster the columns, which yields an initial estimator $\hat{B}$. Then we estimate $W_O$ by plugging in $\hat{B}$ and applying Algorithm 1 using the estimated optimal weight to obtain the final row clusters. We call this algorithm as one-step hierarchical algorithm with the optimal weight.
Intuitively, we can further repeat steps 2-4 in Algorithm 2 to iteratively cluster the rows and columns of $X$, leading to a multi-step algorithm. In the simulation, we compare our one-step algorithm with a two-step algorithm, which is summarized in Supplementary Appendix D.

We note that, to facilitate the theoretical analysis of our algorithm, we split the data into two folds. Such a data splitting procedure is feasible in practice when $n$ is relatively large. However, in practice, when we apply our algorithm to the data with very small $n$ (e.g., $n = 10$), data splitting tends to yield unstable clustering results. In this case, we choose to implement steps 2-4 in Algorithm 2 on the entire dataset.

In practice, the feature matrix $X$ may have different variability. While the theoretical guarantees of our algorithm in Section 3.1 remains valid, the concentration bound for $(\hat{\Sigma}_{p,W} - \Sigma_{p,W})_{jk}$ via the Hanson-Wright inequality will be dominated by the variables with large variance. To tighten this upper bound, we recommend applying our algorithm to standardized data. That is, every element in $X$ has mean 0 and variance 1. Empirically, we observe that the clustering accuracy can be significantly improved when the algorithm is applied to the standardized data.

Finally, we note that, in steps 2 and 4 in Algorithm 2, we need to choose the threshold value $\alpha$ in our hierarchical algorithm. In Supplementary Appendix D, we present a cross-validation approach to choose the optimal threshold value $\alpha$.

Algorithm 2: One-step Hierarchical Algorithm with Optimal Weight

1. Split the data into two folds: $D_1$, $D_2$.

2. On data $D_1$, apply Algorithm 1 with the sample covariance matrix
   \[ \hat{\Sigma}_q = \frac{1}{p|D_1|} \sum_{i \in D_1} X^{(i)T} X^{(i)} \]
   to cluster the columns of $X$ and find an initial estimator $\hat{B}$.

3. Compute the estimate of the optimal weight $\hat{W}_O = \hat{B} (\hat{B}^T \hat{B})^{-2} \hat{B}^T / s$, where $s$ denotes the estimated number of clusters.

4. On data $D_2$, apply Algorithm 1 with $\hat{\Sigma}_{p,W} = \frac{1}{|D_2|} \sum_{i \in D_2} X^{(i)} \hat{W}_O X^{(i)T}$ to cluster the rows of $X$. Obtain the resulting cluster $\hat{G}^{(r)}$ or equivalently the membership matrix $\hat{A}$.

6 Simulation Results

We consider the following data generating process. We fix $p = q = 100$, $K_1 = K_2 = 10$ and a moderately unbalanced row and column cluster size structure (both having cluster sizes of 3, 6, 6, 8, 10, 12, 12, 14, 19, respectively). This gives us the membership matrices $A$ and $B$. The latent variable $Z$ is generated from the matrix normal distribution $MN(0_{K_1 \times K_2}, U_{K_1 \times K_1}, V_{K_2 \times K_2})$, where $U_{jk} = (-0.4)^{j-k}$ and $V_{jk} = 0.3^{j-k}$. We further generate $\Gamma_{ij} \sim N(0, \sigma^2_{ij})$, where we consider the following three settings for the noise variance.

1. Homogeneous noise variances $\sigma^2_{ij} = 15$. 

14
2. Heterogeneous noise variances proportional to the corresponding row and column cluster sizes:

\[ \sigma^2_{ij} = 15pq \cdot v_{ij}, \quad v_{ij} = \frac{m_p^{(i)} \cdot m_q^{(j)}}{\sqrt{pqK_1K_2}}, \]

where \( m_p^{(i)} \) and \( m_q^{(j)} \) are the size of the row cluster and column cluster which \( X_{ij} \) belongs to.

3. Heterogeneous noise variances randomly generated from the Uniform distribution:

\[ \sigma^2_{ij} = 15pq \cdot u^h_{ij}, \quad u_{ij} \sim \text{Unif}(0,1), \]

where \( h \) determines the level of heterogeneity.

Recall that in Section 3.1, the noise variances play an important role on the clustering consistency of our algorithm. We design these three settings to test the performance of our algorithm under different patterns of noise variances. We keep the mean noise variance to be 15 for all three cases. For the third setting, we set \( h = 0.87 \) because it gives us a similar level of heterogeneity as the second setting. In both the second and third settings, the standard deviation of the noise variances is around 7.95. Finally, we generate \( X \) from the model (1.1). We vary the sample size \( n \) in the simulations. The simulations are repeated 30 times.

We consider the following clustering methods: (1) the sparse biclustering method (Tan and Witten, 2014) implemented via the R package sparseBC (sparseBC); (2) our hierarchical clustering Algorithm 1 using \( W_I \) (Naive COD); (3) our one-step Algorithm 2 using the optimal weight (1-step COD); and (4) our two-step algorithm shown in the Supplementary Appendix (2-step COD). We refer to Section 5 for the implementation of our algorithm. As mentioned in the introduction, there are many other biclustering methods such as convex clustering. Similar to sparseBC, these methods cluster the data matrix \( X \) based on the model of \( \mathbb{E}(X) \). However, under our data generating process, we always have \( \mathbb{E}(X) = 0 \). So, the existing methods are not appropriate for clustering in our simulation setting. For clarity, we only report the results from sparseBC.

To measure the clustering accuracy, we consider the following quantities: the adjusted rand index (ARI) (Hubert and Arabie, 1985), sensitivity (true positive rate), and specificity (false positive rate) (Parikh et al., 2008). To compute sensitivity and specificity, we follow the pairwise approach in Wiwie et al. (2015). The formal definitions are shown in Supplementary Appendix G. Note that an ARI value of 1 implies a perfect match between the true and estimated cluster partitions.

In Figure 1, we plot the average ARI values from the four methods against the sample size \( n \) \( (n = 6, 12, 18, 24, 30) \), where the tuning parameters in our algorithms are chosen by the cross-validation procedure in the Supplementary Appendix D. As expected, sparseBC is not informative for clustering in our setting. In most cases, our iterative algorithms 1-step COD and 2-step COD improve the performance of the Naive COD, which is consistent with our theoretical analysis. In particular, 1-step COD and 2-step COD can achieve an ARI value close to 1 when \( n = 18 \), whereas the Naive COD may require \( n \) much larger than 30 to attain the same level of accuracy. The phenomenon holds for both the row clustering and the column clustering. We also find that when
is moderate (e.g., \( n \geq 18 \)), 1-step COD and 2-step COD have very similar performances. Due to the extra computational cost of the 2-step COD, we generally recommend 1-step COD for practical use if \( n \) is moderate or large. However if \( n \) is small, 2-step COD may outperform the 1-step COD.

The ROC curves of these four methods are shown in Figure 2. To plot the ROC curve, we vary the tuning parameter \( \alpha \) in a grid, instead of choosing the optimal one via cross-validation. We set \( n = 40 \). In all cases, 1-step COD and 2-step COD have similar performances and are both superior to the other algorithms.

We conduct additional simulation studies to evaluate how \( K_2 \) affects the performance of our clustering algorithm for the rows. As expected from Theorem 3.1, we find that a larger value of \( K_2 \) may indeed improve the performance of our algorithm. We also consider the simulation settings with an unbalanced structure with \( p = 300 \) and \( q = 30 \). The detailed results are deferred to Supplementary Appendix F.

7 Genomic Data Analysis

We apply our method to the atlas of gene expression in the mouse aging project dataset (Zahn et al., 2007), which contains gene expression values of 8932 genes in 16 tissues for 40 mice. Similar to Ning and Liu (2013) and Yin and Li (2012), we only focus on a subset of 37 genes belonging to the mouse vascular endothelial growth factor signaling pathway. In order to maximize our usage of the tissue data, we drop 4 samples that have missing data for the tissues. So, in the end, our data is a \( 37 \times 12 \times 36 \) array that corresponds to \( p = 37 \) genes, \( q = 12 \) tissues, and \( n = 36 \) mice.

Figure 3 shows the gene clusters and tissue clusters obtained from our 2-step hierarchical algorithm with data-driven tuning parameters. Disregarding the singletons - clusters with only one element - the estimated number of gene clusters is 4 and the estimated number of tissue clusters is 3. In Zahn et al. (2007), the authors group the tissues through hierarchical clustering, but they group genes that are similarly age-regulated through empirical meta analysis. Our method, on the other hand, can conveniently be applied to both the genes and the tissues at the same time. Interestingly, the tissue clustering result from our method agrees with the tissue clustering result in Zahn et al. (2007). Zahn et al. (2007) classifies tissues into 3 groups - vascular, neural, and steroid responsive. The cerebrum, cerebellum, and hippocampus are all neural tissues that are a part of the brain, and they are all clustered into one tissue cluster by our algorithm. Also, adrenal and thymus tissues are steroid responsive tissues, and the lung and kidney tissues are vascular tissues. The respective pairs appear in our clustering result as well. As for the gene clustering, it is known in the biology community that the O03Rik gene inhibits the Nfat5 gene. More specifically, O03Rik acts as a negative regulator of the calcineurin/NFAT signaling pathway and it inhibits NFAT nuclear translocation and transcriptional activity by suppressing the calcium-dependent calcineurin phosphatase activity (OriGene, 2020). It is then reasonable that the two genes are clustered together, because they would be highly negatively correlated. Also, calcineurin (Ppp3) is a serine/threonine protein phosphatase that is dependent on calcium and calcium modulated proteins (Hogan et al., 2003). It activates nuclear factor of activated T cell cytoplasmic (Nfatec), a transcription factor, by dephosphorylating
Figure 1: ARI of sparse biclustering (sparseBC), our hierarchical clustering Algorithm 1 using $W_I$ (Naive COD), one-step Algorithm 2 using the optimal weight (1-step COD) and two-step Algorithm 3 (2-step COD) under three different noise variance settings. The two columns correspond to the row clustering and column clustering.
Figure 2: ROC curves of sparse biclustering (sparseBC), our hierarchical clustering Algorithm 1 using $W_1$ (Naive COD), one-step Algorithm 2 using the optimal weight (1-step COD) and two-step Algorithm 3 (2-step COD) under three different noise variance settings. The two columns correspond to the row clustering and column clustering.
This Nfatc happens to be encoded in part by the Nfatc4 gene. On the other hand, there are three isozymes of the catalytic subunit of calcineurin and this is encoded in part by the Ppp3r1 gene (Liu et al., 2005). Thus, the Ppp3r1 and Nfatc4 genes are both related to calcineurin - one having to do with how it is generated, and one having to do with something it activates. This reasonably explains the highly correlated results obtained from our clustering algorithm. Another possible explanation is given in Heit et al. (2006) which postulates that calcineurin/NFAT signaling is critical in β-cell growth in the pancreas. All this external evidence suggests that our clustering results are biologically meaningful.

8 Discussion

In this paper, we study the variable clustering problem for matrix valued data $X$ under the latent variable model (1.1). A class of hierarchical clustering algorithms based on the weighted covariance difference is proposed. The theoretical and empirical performance of the algorithm heavily depends on the weight matrix $W$. Theoretically, we show that, under mild conditions, our algorithm with a large class of weight matrices $W$ can attain clustering consistency with high probability. To further characterize the effect of the weight matrix $W$ on the theoretical performance of our algorithm, we establish the minimax lower bound under the latent variable model (1.1), from which we prove that our algorithm using the weight matrix $W_O$ is minimax optimal for variable clustering. Empirically, we develop one-step and two-step algorithms based on the weight matrix $W_O$, which outperform the other methods.

In this paper, we focused on the clustering of the random matrix $X$. We believe our latent variable model (1.1) and the hierarchical clustering algorithm can be extended to a more general tensor setting. Another interesting extension is to generalize our method to the overlapping clustering setting (Bing et al., 2020), where the rows and columns may simultaneously belong to multiple row and column clusters. For now, however, we leave them for future studies.
Acknowledgment

Ning is supported in part by National Science Foundation (NSF) CAREER award DMS-1941945 and NSF award DMS-1854637.

Supplementary Material

The supplement consists of additional technical details, proofs and additional numerical results.

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Supplementary Material

We use the following notation: \( [t] \) denotes the t-th column cluster (a set), and \( m_q^{(t)} = |[t]| \) denotes the cardinality of the t-th column cluster. Likewise, \( m_p^{(t)} \) denotes the cardinality of the t-th row cluster. In addition, \( M_q = \max_{1 \leq t \leq K_2} |[t]| \) denotes the maximum column cluster size and \( m_q = \min_{1 \leq t \leq K_2} |[t]| \) denotes the minimum column cluster size.

A  Comparison of Hierarchical Algorithm with Bunea et al. (2018)

Like shown in Figure 4, if C,D,E have not been clustered yet and A and B are considered first, because of the greedy nature of COD in Bunea et al. (2018), since the distance between C and A is less than \( \alpha \), C will be clustered with A and B even though C,D,E are closer to each other. If we implement a hierarchical approach, the distances between all the pairs of points will be considered at the same time, and a tree structure will naturally be constructed. The two groups of \{A,B\} and \{C,D,E\} will be formed in the “lower” part of the tree first, and even if the same \( \alpha \) threshold value is used, the two groups will not be merged together.

![Figure 4](image)

Figure 4: (a) Due to the greedy nature of COD from Bunea et al. (2018), A and B are closest together and thus will be clustered before C,D,E are considered. Then, since the distance between A and C is below the threshold value \( \alpha \), C will be incorrectly clustered with A and B. (b) With the hierarchical algorithm, the distances between all the points are considered at the same time and thus C will be correctly clustered with D and E.

B  Upper Bound for the quasinorm of \( X \)

In this section, we provide an upper bound for the quasinorm \( \|X\|_W \). We first study the case with \( W_I = I_q/q \). The goal is to show that

\[
\|X\|_{W_I} \leq \sqrt{\frac{K_2 M_q^2}{q^2}} \max_k \|\text{Var}(Z_k)\|_F + \max_a \sqrt{\frac{K_2 1}{q} \sum_{j=1}^{q} \sigma_{aj}^4}, \tag{B.1}
\]
where $M_q$ is the maximum column cluster size and $\sigma_{aj}^2 = \Var(\Gamma_{aj})$. By definition, it suffices to upper bound $\max_k \| \Var(X_k) \|_F$ as follows

$$
\max_a \| \Var(X_a) \|_F \leq \max_k \| B \Var(Z_k)B^T \|_F + \max_a \| \Var(\Gamma_a) \|_F
\leq M_q \max_k \| \Var(Z_k) \|_F + \max_a \sqrt{q \sum_{j=1}^q \sigma_{aj}^4}.
$$

With $W = I_q/q$ (or equivalently, $L = I_q/\sqrt{q}$), we can obtain (B.1). Note that if $K_2M_q/q = O(1)$ (balanced cluster sizes), and if we further assume $\frac{1}{q} \sum_{j=1}^q \sigma_{aj}^4 \leq CM_q$ and $\| \Var(Z_k) \|_{op} \leq C$ for some constant $C$, then (B.1) implies $\| X \|_{W_I} = O(1)$.

Similarly, if we choose the optimal weight $W_O = B(B^T B)^{-2}B^T/K_2$ (i.e., set $L = B(B^T B)^{-1}/\sqrt{K_2}$), then

$$
\max_a \| \Var(X_a L) \|_F \leq \frac{1}{K_2} \max_k \| \Var(Z_k) \|_F + \max_a \| \Var(\Gamma_a L) \|_F
= \frac{1}{K_2} \max_k \| \Var(Z_k) \|_F + \frac{1}{K_2} \max_a \left( \frac{1}{K_2} \sum_{t=1}^{K_2} \left( \sum_{j \in [t]} \sigma_{aj}^2 \right)^2 / \| [t] \|_4 \right),
$$

where $[t]$ denotes the $t$th cluster and $\| [t] \|$ denotes its cardinality. Thus

$$
\| X \|_{W_O} \leq \sqrt{\frac{1}{K_2} \max_k \| \Var(Z_k) \|_F} + \max_a \sqrt{\frac{1}{K_2} \sum_{t=1}^{K_2} \left( \sum_{j \in [t]} \sigma_{aj}^2 \right)^2 / \| [t] \|_4}.
$$

(B.2)

If we further assume $\frac{1}{K_2} \sum_{t=1}^{K_2} \left( \sum_{j \in [t]} \sigma_{aj}^2 \right)^2 / \| [t] \|_4 \leq C$ and $\| \Var(Z_k) \|_{op} \leq C$ for some constant $C$, then we can show that $\| X \|_{W_O} = O(1)$.

Finally, we note that when the column cluster has equal size (i.e., $K_2M_q = q$) and $\sigma_{aj}^2 = \sigma^2$, we have

$$
\| X \|_{W_I} \leq \sqrt{\frac{1}{K_2} \max_k \| \Var(Z_k) \|_F} + \sqrt{\frac{K_2}{q} \sigma^2},
$$

(B.3)

$$
\| X \|_{W_O} \leq \sqrt{\frac{1}{K_2} \max_k \| \Var(Z_k) \|_F} + \sqrt{\frac{2}{q} \sigma^2}.
$$

(B.4)

Thus, to show $\| X \|_W = O(1)$, the conditions on $\sigma^2$ are $\sqrt{\frac{K_2}{q}} \sigma^2 = O(1)$ and $\frac{K_2}{q} \sigma^2 = O(1)$, respectively. Clearly, the latter one is weaker.

**C Derivation for Remark 3.2**

We consider the setting where the column cluster has equal size (i.e., $K_2M_q = q$) and $\sigma_{aj}^2 = \sigma^2$.

First, we have shown in Section 2.2 that the off diagonal entries of $\Sigma_{p,W_I}$ and $\Sigma_{p,W_O}$ are the same, that is $(\Sigma_{p,W_I})_{jk} = (\Sigma_{p,W_O})_{jk}, j \neq k$. Then we have $\text{MCOD}(\Sigma_{p,W_I}) = \text{MCOD}(\Sigma_{p,W_O}) := \text{MCOD}$. 


For $W_I$, we can show that
\[
\frac{\text{MCOD}(\Sigma_{p,W_I})}{\|X\|_{W_I}} \geq \frac{\text{MCOD}}{\sqrt{\frac{1}{K_2} \max_k \|\text{Var}(Z_k)\|_F}} + \sqrt{\frac{K_2}{q} \sigma^2} \\
\geq C \min \left( \frac{\text{MCOD}}{\sqrt{\frac{1}{K_2} \max_k \|\text{Var}(Z_k)\|_F}}, \frac{\text{MCOD}}{\sqrt{\frac{K_2}{q} \sigma^2}} \right),
\]
where $C$ is a constant and the first step is from (B.3). Hence, the cluster separation condition (A1) for $W_I$ is implied by
\[
\frac{\text{MCOD}}{\sqrt{\frac{1}{K_2} \max_k \|\text{Var}(Z_k)\|_F}} \geq \frac{c_0}{C \eta}, \quad \frac{\text{MCOD}}{\sqrt{\frac{K_2}{q} \sigma^2}} \geq \frac{c_0}{C \eta}.
\]

Similarly, the cluster separation condition (A1) for $W_O$ is implied by
\[
\frac{\text{MCOD}}{\sqrt{\frac{1}{K_2} \max_k \|\text{Var}(Z_k)\|_F}} \geq \frac{c_0}{C \eta}, \quad \frac{\text{MCOD}}{\frac{K_2}{q} \sigma^2} \geq \frac{c_0}{C \eta}.
\]

In terms of the noise level $\sigma^2$, the condition for $W_I$ is $\sigma^2 = O\left(\frac{\text{MCOD} \sqrt{q}}{\eta K_2}\right)$, whereas the condition for $W_O$ is $\sigma^2 = O\left(\frac{\text{MCOD} \cdot q}{\eta K_2}\right)$ which is much weaker.

### D Supplementary Material for Section 5

The two-step algorithm is shown in Algorithm 3. In this algorithm, we ignore the data splitting step for simplicity.

In the following, we describe a data-driven selection method for $\alpha$. To fix the notation, we consider our Algorithm 1 with some sample covariance matrix $\hat{\Sigma}_p$. We assume the data are standardized. The method can be similarly applied to the one-step or two-step algorithm with the optimal weight. The steps are outlined in Algorithm 4.

We first split the data into two, $D_1$, $D_2$, calculate $\hat{\Sigma}_p^{(1)}$, $\hat{\Sigma}_p^{(2)}$. For each tuning parameter $\alpha_l$ in the grid, we perform our algorithm on $\hat{\Sigma}_p^{(1)}$ to get a cluster structure $G_l$. Then we take the average of all the non-diagonal elements in the cluster blocks of $\hat{\Sigma}_p^{(1)}$ via the smoothing operator $\Upsilon(\hat{\Sigma}_p^{(1)}, G_l)$. Finally we calculate the Frobenius loss of $\Upsilon(\Sigma_p^{(1)}, G_l)$ and $\Sigma_p^{(2)}$, and choose $\alpha_l$ that yields the smallest value.

### E Proofs

#### E.1 Clustering consistency

First, we state the Hanson-Wright inequality, which is instrumental in the proof.
Algorithm 3: Two-step Hierarchical Algorithm with Optimal Weight

1. Apply Algorithm 1 with the sample covariance matrix $\hat{\Sigma}_q = \frac{1}{pn} \sum_{i=1}^{n} X^{(i)} X^{(i)^T}$ to cluster the columns of $X$ and find an initial estimator $\hat{B}_1$.

2. Compute the estimate of the optimal weight $\hat{W}_{O_1} = \hat{B}_1 (\hat{B}_1^T \hat{B}_1)^{-1} \hat{B}_1^T / s_1$, where $s_1$ denotes the estimated number of column clusters.

3. Apply Algorithm 1 with $\hat{\Sigma}_p, \hat{W}_{O_1} = \frac{1}{n} \sum_{i=1}^{n} X^{(i)} \hat{W}_{O_1} X^{(i)^T}$ to cluster the rows of $X$. Obtain the estimator $\hat{A}_1$.

4. Apply Algorithm 1 with $\hat{\Sigma}_q = \frac{1}{n} \sum_{i=1}^{n} X^{(i)} \hat{M} X^{(i)}$ to cluster the columns of $X$ and find the estimator $\hat{B}_2$, where $\hat{M} = \hat{A}_1 (\hat{A}_1^T \hat{A}_1)^{-1} \hat{A}_1^T / t$ is the optimal weight for clustering the columns and $t$ is the estimated number of row clusters in $\hat{A}_1$.

5. Compute the estimate of the optimal weight $\hat{W}_{O_2} = \hat{B}_2 (\hat{B}_2^T \hat{B}_2)^{-1} \hat{B}_2^T / s_2$, where $s_2$ denotes the estimated number of column clusters.

6. Apply Algorithm 1 with $\hat{\Sigma}_p, \hat{W}_{O_2} = \frac{1}{n} \sum_{i=1}^{n} X^{(i)} \hat{W}_{O_2} X^{(i)^T}$ to cluster the rows of $X$. Obtain the final estimator $\hat{A}_2$.

Lemma E.1. (Hanson-Wright) There exist positive constants $c, c'$ such that for all $n \times n$ matrices $H$, if $\xi = (\xi_1, ..., \xi_n)^T$ is a vector of independent mean 0 sub-Gaussian random variables with $||\xi||_{\psi_2} \leq L$ for some $L > 0$, then for all $t$, the following holds:

$$\mathbb{P} \left[ \xi^T H \xi - \mathbb{E}(\xi^T H \xi) > cL^2(||H||_F \sqrt{t} + c'||H||_{op} t) \right] \leq e^{-t}.$$

E.1.1 Proof of Theorem 3.1

Proof. Denote $\hat{L} \hat{L}^T = \hat{W}$ and $\hat{X}^{(i)} = X^{(i)} \hat{L}$. So, $\hat{\Sigma}_{p,\hat{W}} = \frac{1}{|D_2|} \sum_{i \in D_2} \hat{X}^{(i)} \hat{X}^{(i)^T}$. For simplicity, we assume $|D_2| = n/2$, and the summation is from 1 to $n/2$. Furthermore, denote $H_{k,m}^+ = \text{Var}(\hat{X}_k + \hat{X}_m), |\hat{W}|)$ and $H_{k,m}^- = \text{Var}(\hat{X}_k - \hat{X}_m, |\hat{W}|)$. Denote $\hat{X}_{k,m}^+ = (H_{k,m}^+)^{-1/2}(\hat{X}_k^T + \hat{X}_m^T)$. Since $\hat{X}_{k,m}^+$ has mean 0 variance 1 given $\hat{W}$ and $X$ is Gaussian, $\hat{X}_{k,m}^+$ is a vector of independent Gaussian random variables given $\hat{W}$.
Algorithm 4: A Data-Driven Tuning Parameter Selection Process

1. Split the data into two: $D_1$ and $D_2$

2. Using $D_1$, calculate $\hat{\Sigma}_p^{(1)}$.

3. Using $D_2$, calculate $\hat{\Sigma}_p^{(2)}$.

4. For $r > 1$ and each value $\alpha_l$ on a grid ($l = 1, ..., r$), perform Algorithm 1 with $\hat{\Sigma}_p^{(1)}$ to get a row cluster structure $G^{(r)}_l$.

5. Perform the smoothing operator $\Upsilon(\hat{\Sigma}_p^{(1)}, G^{(r)}_l)$ where $\Upsilon$ is defined as the following:

$$\left[\Upsilon(\hat{\Sigma}_p^{(1)}, G^{(r)}_l)\right]_{ab} = \begin{cases} 
|G^{(r)}_k|^{-1} \left( \left| G^{(r)}_k \right| - 1 \right)^{-1} \sum_{i,j \in G_k, \ i \neq j} [\hat{\Sigma}_p]_{ij} & \text{if } a \neq b, \text{ and } k = k' \\
|G^{(r)}_k|^{-1} \left| G^{(r)}_{k'} \right|^{-1} \sum_{i \in G_k, \ j \in G_{k'}} [\hat{\Sigma}_p]_{ij} & \text{if } a \neq b, \text{ and } k \neq k' \\
1 & \text{if } a = b.
\end{cases}$$

6. Our data dependent tuning parameter for the threshold is:

$$\hat{\alpha} = \arg\min_{\alpha_l} L \left( \Upsilon(\hat{\Sigma}_p^{(1)}, G^{(r)}_l), \hat{\Sigma}_p^{(2)} \right),$$

where $L(A, B) := ||A - B||_F$ is the Frobenius loss.
Denote
\[
\bar{X}_{k,m}^+ = \begin{bmatrix}
(H_{k,m}^+)^{-1/2} & \cdots & \cdots & \cdots & \cdots & \cdots & (H_{k,m}^+)^{-1/2}
\end{bmatrix},
\bar{X}_{k,m}^- = \begin{bmatrix}
(H_{k,m}^-)^{-1/2} & \cdots & \cdots & \cdots & \cdots & \cdots & (H_{k,m}^-)^{-1/2}
\end{bmatrix},
\]
and
\[
\mathbb{H}_{k,m}^+ = \begin{bmatrix}
(H_{k,m}^+)^{-1/2} & \cdots & \cdots & \cdots & \cdots & \cdots & (H_{k,m}^+)^{-1/2}
\end{bmatrix}, \quad \mathbb{H}_{k,m}^- = \begin{bmatrix}
(H_{k,m}^-)^{-1/2} & \cdots & \cdots & \cdots & \cdots & \cdots & (H_{k,m}^-)^{-1/2}
\end{bmatrix},
\]
where \(\mathbb{H}_{k,m}^+\) and \(\mathbb{H}_{k,m}^-\) each have \(n/2\) blocks on the diagonal. Note that the quadratic forms can be used to get the sum of the products. The following calculation holds for one observation:
\[
(\bar{X}_{k,m}^+)^T H_{k,m}^+ \bar{X}_{k,m}^+ - (\bar{X}_{k,m}^-)^T H_{k,m}^- \bar{X}_{k,m}^- = \sum_{j=1}^q (\bar{X}_{kj}^2 + 2 \bar{X}_{kj} \bar{X}_{mj} + \bar{X}_{mj}^2) - \sum_{j=1}^q (\bar{X}_{kj}^2 - 2 \bar{X}_{kj} \bar{X}_{mj} + \bar{X}_{mj}^2)
= 4 \sum_{j=1}^q \bar{X}_{kj} \bar{X}_{mj}.
\]
We can extend this to \(n/2\) observations by using block matrix notation from above.
\[
(\bar{X}_{k,m}^+)^T \mathbb{H}_{k,m}^+ \bar{X}_{k,m}^+ - (\bar{X}_{k,m}^-)^T \mathbb{H}_{k,m}^- \bar{X}_{k,m}^-
= \sum_{i=1}^{n/2} \sum_{j=1}^q (\bar{X}_{ij}^2 + 2 \bar{X}_{kj} \bar{X}_{mj} + \bar{X}_{mj}^2) - \sum_{i=1}^{n/2} \sum_{j=1}^q (\bar{X}_{ij}^2 - 2 \bar{X}_{kj} \bar{X}_{mj} + \bar{X}_{mj}^2)
= 4 \sum_{i=1}^{n/2} \sum_{j=1}^q \bar{X}_{ij} \bar{X}_{mj}.
\]
Thus, we have
\[
\left\| \tilde{\Sigma}_p \hat{W} - \Sigma_{p, \hat{W}} \right\|_{\max} = \max_{k,m} \frac{2}{n} \sum_{i=1}^{n/2} \sum_{j=1}^q \bar{X}_{ij} \bar{X}_{mj} - \sum_{j=1}^q \mathbb{E}(\bar{X}_{kj} \bar{X}_{mj} \hat{W})
\leq \max_{k,m} \frac{1}{2n} \left( \mathbb{E}(\bar{X}_{k,m}^+ \mathbb{H}_{k,m}^+ \bar{X}_{k,m}^+) - \mathbb{E}(\bar{X}_{k,m}^- \mathbb{H}_{k,m}^- \bar{X}_{k,m}^-) \right) \leq c \left( \left\| H_{k,m}^+ \right\| \sqrt{t} + c' \left\| \mathbb{H}_{k,m}^+ \right\|_{\text{op}} \cdot t \right).
\]
Similarly, conditioned on \( \hat{W} \) with probability greater than \( 1 - e^{-t} \),
\[
\left\| (\hat{x}_{k,m}^-, \hat{x}_{k,m}^-) \hat{W} \hat{x}_{k,m}^- - \mathbb{E}( (\hat{x}_{k,m}^-)^T \hat{W} \hat{x}_{k,m}^- \mid \hat{W}) \right\| \leq c'' \left( \left\| \hat{W} \right\| \cdot \frac{1}{n} \max_{k,m} \left( \sqrt{1 + ||\hat{H}_{k,m}^+||_F^2} \cdot nt + \left| \hat{H}_{k,m}^+ \right| \right) + \frac{1}{n} \max_{k,m} \left( \sqrt{1 + ||\hat{H}_{k,m}^-||_F^2} \cdot nt + \left| \hat{H}_{k,m}^- \right| \right) \right).
\]
By the definition of \( \hat{W} \), we know \( ||\hat{W}||_F^2 = n||H_{k,m}^+||_F^2/2 \) and \( ||\hat{W}||_\text{op} = ||H_{k,m}^+||_\text{op} \). Thus, with a union bound over \( k, m \), we get the following concentration inequality:
\[
\left| \left| \sum_{p} \hat{W} - \sum_{p} \hat{W} \right| \right| \leq \frac{1}{n} \max_{k,m} \left( \sqrt{1 + ||H_{k,m}^+||_F^2} \cdot nt + \left| H_{k,m}^+ \right| \right) + \frac{1}{n} \max_{k,m} \left( \sqrt{1 + ||H_{k,m}^-||_F^2} \cdot nt + \left| H_{k,m}^- \right| \right) \tag{E.1}
\]
conditioned on \( \hat{W} \) with probability greater than \( 1 - \frac{p(p-1)}{2}e^{-t} \), and setting \( t = 3 \log p \), we know the inequality (E.1) holds with conditional probability greater than \( 1 - \frac{1}{2p} \). By taking another expectation with \( \hat{W} \), the inequality (E.1) holds with probability greater than \( 1 - \frac{1}{2p} \) unconditionally.

Because \( \| \cdot \|_F \geq \| \cdot \|_\text{op} \) holds in general, the Frobenius term dominates in the regime of \( \frac{\log p}{n} = \Theta(1) \), so all that is left to do is to bound \( ||H_{k,m}^+||_F^2 \). An identical argument can be made for \( ||H_{k,m}^-||_F^2 \), and we know the following upper bound holds for both terms,
\[
||H_{k,m}^+||_F \leq \| \text{Var}(\hat{X}_k, \hat{W}) \|_F + \| \text{Var}(\hat{X}_m, \hat{W}) \|_F + 2 \cdot || \text{Cov}(\hat{X}_k, \hat{X}_m, \hat{W}) \|_F \leq C_1 \max_k \| \text{Var}(\hat{X}_k, \hat{W}) \|_F.
\]
This holds for all pairs \((k, m)\), and so it also holds for the maximum over the pairs:
\[
\max_{k,m} ||H_{k,m}^+||_F \leq C_1 \max_k \| \text{Var}(\hat{X}_k, \hat{W}) \|_F = C_1 \max_k \| \hat{L}^T \text{Var}(X_k) \hat{L} \|_F = C_1 K_{-1/2} \| X \|_{\hat{W}} \tag{E.2}
\]
Thus, with probability greater than \( 1 - \frac{1}{2p} \),
\[
\left| \left| \sum_{p} \hat{W} - \sum_{p} \hat{W} \right| \right| \leq C_1 \sqrt{\frac{\log p}{nK_{-1/2}}} \| X \|_{\hat{W}} \leq \eta \| X \|_{\hat{W}}. \tag{E.3}
\]
for some constant \( C_1 \), where the last step is from condition (A1).

Note that conditions (A1) and (A2) together imply that
\[
\text{MCOD}(\hat{W}, X) / \| X \|_{\hat{W}} \geq 4\eta. \tag{E.4}
\]
In the following, we show how perfect clustering is achieved under the event that the inequality (E.3) holds. For simplicity, we drop the subscript \( \hat{W} \) in \( \hat{W}, \hat{W}, \sum_{p} \hat{W}, \sum_{p} \hat{W} \) and \( \| X \|_{\hat{W}} \) and just write \( \hat{W}, \sum_{p} \hat{W}, \sum_{p} \hat{W} \) and \( \| X \|_{\hat{W}} \). Also, for simplicity, in the following derivation, we will denote the \((i, j)\)-th element of \( \sum_{p} \hat{W} \) as \( \sum_{p, ij} \). Define the following quantity
\[
\tau := \max_{a,b,c} \left| \sum_{p, ac} - \sum_{p, bc} - (\sum_{p, ac} - \sum_{p, bc}) \right|.
\]
Then we have:

\[
\tau = \max_{a,b,c} \left| \widehat{\Sigma}_{p,ac} - \Sigma_{p,ac} - (\widehat{\Sigma}_{p,bc} - \Sigma_{p,bc}) \right|
\]

\[
\leq \max_{a,b,c} \left| \widehat{\Sigma}_{p,ac} - \Sigma_{p,ac} \right| + \max_{a,b,c} \left| \widehat{\Sigma}_{p,bc} - \Sigma_{p,bc} \right|
\]

\[
\leq 2 \cdot ||\widehat{\Sigma}_{p} - \Sigma_{p}||_{\text{max}}
\]

\[
\leq 2\eta \cdot ||X||,
\]

where the last step is from (E.3). We now want to show the following inequality:

\[
\text{COD}_{\hat{\Sigma}_{p}}(a, b) - \tau \leq \text{COD}_{\Sigma_{p}}(a, b) \leq \text{COD}_{\hat{\Sigma}_{p}}(a, b) + \tau. \tag{E.5}
\]

The inequality on the left holds because of the following:

\[
\text{COD}_{\hat{\Sigma}_{p}}(a, b) = \max_{c \neq a,b} |\hat{\Sigma}_{p,ac} - \hat{\Sigma}_{p,bc}|
\]

\[
= \max_{c \neq a,b} |\hat{\Sigma}_{p,ac} - \hat{\Sigma}_{p,bc} - (\Sigma_{p,ac} - \Sigma_{p,bc}) + (\Sigma_{p,ac} - \Sigma_{p,bc})|
\]

\[
\leq \max_{c \neq a,b} |\Sigma_{p,ac} - \Sigma_{p,bc}| + \max_{c \neq a,b} |\hat{\Sigma}_{p,ac} - \hat{\Sigma}_{p,bc} - (\Sigma_{p,ac} - \Sigma_{p,bc})|
\]

\[
\leq \text{COD}_{\Sigma_{p}}(a, b) + \tau. \tag{E.6}
\]

With a similar technique, we can get the inequality on the right as well. Now, for any two sets \(A\) and \(B\), if \(A\) and \(B\) indeed belong to the same cluster (i.e., \(a, b \in G_k\) for some \(k\) and for any \(a \in A\) and \(b \in B\)), we have \(\text{COD}_{\Sigma_{p}}(a, b) = 0\) and therefore by (E.5)

\[
\text{COD}_{\widehat{\Sigma}_{p}}(A, B) = \max_{a \in A, b \in B} \text{COD}_{\widehat{\Sigma}_{p}}(a, b) \leq \tau \leq 2\eta \cdot ||X||.
\]

If \(A\) and \(B\) are not the same clusters, there must exist \(a \in A\) and \(b \in B\) with \(a \in G_k\) and \(b \in G_j\) for some \(k \neq j\). Then

\[
\text{COD}_{\widehat{\Sigma}_{p}}(A, B) \geq \text{COD}_{\widehat{\Sigma}_{p}}(a, b) \geq \text{COD}_{\Sigma_{p}}(a, b) - \tau \geq \text{MCOD}(\Sigma_{p}) - \tau \geq \text{MCOD}(\Sigma_{p}) - 2\eta \cdot ||X||,
\]

where the first inequality is from the definition of \(\text{COD}_{\widehat{\Sigma}_{p}}(A, B)\), the second one is from (E.5), the third one is from the definition of MCOD, and finally the last one is from (E.6).

Together with (E.4), finally we show that \(\text{COD}_{\widehat{\Sigma}_{p}}(A, B) \geq 2\eta \cdot ||X||\), if \(A\) and \(B\) are not the same clusters. By taking the threshold value \(\alpha = 2\eta \cdot ||X||\), we attain perfect clustering using our hierarchical algorithm. This completes the proof.

\[E.2 \quad \text{Minimax Lower Bound}\]

The following lemma is Birge’s Lemma applied to our specific setting, similar to Lemma C.1 in Bunea et al. (2018). Define \(M_I(p, q, K_1, K_2, \eta)\) and \(M_O(p, q, K_1, K_2, \eta)\) as in Section 3.2. Since the same lemma is true for both \(M_I\) and \(M_O\), for ease of notation, we will simply use \(M\).
Lemma E.2. For any partition estimator $\hat{G}$, and for any collection of distinct covariance matrices $\Sigma^{(j)} \in M(p, q, K_1, K_2, \eta)$,
\[
\sup_{\Sigma \in M(p, q, K_1, K_2, \eta)} P(\Sigma \notin \Sigma^*) \geq \max_{j=1, \ldots, N} P(\Sigma^{(j)} \notin \Sigma^{(j)}) \geq \frac{1}{2e + 1} \wedge \left(1 - \max_{j \geq 2} \frac{\text{KL}(\Sigma^{(j)}, \Sigma^{(1)})}{\log(N)}\right).
\]

E.2.1 Proof of Theorem 3.3

Similar to the construction in Bunea et al. (2018), set our collection of covariance matrices as follows:

\[K_1 = 3, m_p^{(1)} = m_p^{(2)} = m_p^{(3)} = \frac{p}{3} \text{ (equal row cluster size)}, \quad X = AZB^T + \Gamma,\]

where $\Gamma_{ij} \sim \text{iid } N(0, \sigma_t^2)$ where $\sigma_t^2$ denotes the noise variance of elements in column cluster $t$. Note that for this construction, we assume the same noise variance within the same column cluster. In addition, we set

\[
Z = \begin{bmatrix} Z_{11} & \ldots & Z_{1K_2} \\ Z_{21} & \ldots & Z_{2K_2} \\ Z_{31} & \ldots & Z_{3K_2} \end{bmatrix} = \begin{bmatrix} Z_1 & \ldots & Z_{K_2} \end{bmatrix}, \quad Z_1, \ldots, Z_{K_2} \sim \text{iid } N(0, C(\epsilon)),
\]

where $C(\epsilon) = \begin{bmatrix} \epsilon & \epsilon - \epsilon^2 & -\epsilon \\ \epsilon - \epsilon^2 & \epsilon & \epsilon \\ -\epsilon & \epsilon & 2 \end{bmatrix}$, and $A = \begin{bmatrix} 1 \\ \vdots \\ 1 \\ 1 \end{bmatrix}$, $B = \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}$, $p \times 3$, $B = \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}$, $q \times K_2$

where $0 < \epsilon < 1$ is a quantity to be specified later. We will consider $N = (\frac{p}{3})^2 + 1$ many covariance matrices that are obtained by switching one of the rows in the first third of the rows in $A$ and one of the rows in the second third of the rows in $A$ (and also counting the original matrix $A$ as well).
It follows that \( \text{Var(\text{vec}(Z))} = I_{K_2} \otimes C(\epsilon) \) and that

\[
\Sigma \in \mathbb{R}^{pq \times pq} = \text{Var(\text{vec}(X))} = (B \otimes A)(\text{Var(\text{vec}(Z))))(B \otimes A)^T + \text{Var(\text{vec}(\Gamma))} = (B \otimes A)(I_{K_2} \otimes C(\epsilon))(B \otimes A)^T + \text{Var(\text{vec}(\Gamma))} = \{BB^T \otimes AC(\epsilon)A^T\} + \text{Var(\text{vec}(\Gamma))}
\]

\[
= \begin{bmatrix}
1_{m_q^{(1)}}1^T_{m_q^{(1)}} \otimes AC(\epsilon)A^T \\
... \\
1_{m_q^{(K_2)}}1^T_{m_q^{(K_2)}} \otimes AC(\epsilon)A^T
\end{bmatrix} + \begin{bmatrix}
\sigma^2_1I_{pm_q^{(1)}} \\
... \\
\sigma^2_{(K_2)}I_{pm_q^{(K_2)}}
\end{bmatrix}.
\]

So we can set \( \tilde{\Sigma}^{(t)} = \{1_{m_q^{(t)}}1^T_{m_q^{(t)}} \otimes AC(\epsilon)A^T\} + \sigma^2_{(t)}I_{pm_q^{(t)}} \) as one of the \((pm_q^{(t)} \times pm_q^{(t)})\) blocks in the block diagonal matrix \( \Sigma \in \mathbb{R}^{pq \times pq} \).

Note that the Kullback-Leibler Divergence for \( n \) i.i.d multivariate normal observations in \( \mathbb{R}^d \) with mean 0 is \( KL(\Sigma', \Sigma) = \frac{n}{2} \left[ \text{tr}(\Sigma^{-1}\Sigma' - I_d) - \log \text{det}(\Sigma^{-1}\Sigma') \right] \), where \( \Sigma \) and \( \Sigma' \) are two covariance matrices constructed as above. Thus, since \( \Sigma \) is a block diagonal matrix with blocks \( \tilde{\Sigma}^{(t)} \), we have the relationship \( KL(\Sigma', \Sigma) = \sum_{t=1}^{K_2} KL(\tilde{\Sigma}^{(t)'}, \tilde{\Sigma}^{(t)}) \), and it suffices to just calculate \( KL(\tilde{\Sigma}^{(t)'}, \tilde{\Sigma}^{(t)}) \) in order to calculate \( KL(\Sigma', \Sigma) \).

Denote the eigenvalues and eigenvectors of \( C(\epsilon) \) as \( \lambda_1, \lambda_2, \lambda_3 \) and \( u_1, u_2, u_3 \), respectively. Also, define the \( pm_q^{(t)} \times 1 \) vector \( v_k^{(t)} \) as \( v_k^{(t)} = \frac{1}{\sqrt{m_p m_q^{(t)}}} (1_{m_q^{(t)}} \otimes Au_k) \).

\[
\tilde{\Sigma}^{(t)} = \{1_{m_q^{(t)}}1^T_{m_q^{(t)}} \otimes AC(\epsilon)A^T\} + \sigma^2_{(t)}I_{pm_q^{(t)}} = \sigma^2_{(t)} \left[ \sum_{k=1}^{2} \frac{\lambda_k m_p m_q^{(t)}}{\sigma^2_{(t)}} \cdot v_k^{(t)} v_k^{(t)T} + I_{pm_q^{(t)}} \right],
\]

where we note that \( \lambda_3 = 0 \). Therefore,

\[
(\tilde{\Sigma}^{(t)})^{-1} = \frac{1}{\sigma^2_{(t)}} \left[ \sum_{k=1}^{2} \frac{\lambda_k m_p m_q^{(t)}}{\lambda_k m_p m_q^{(t)} + \sigma^2_{(t)}} \cdot v_k^{(t)} v_k^{(t)T} + I_{pm_q^{(t)}} \right].
\]

Let \( Q_{p \times p} \) denote a \( p \times p \) perturbation matrix switching one row in the first third of the rows in \( A \) and one row in the second third of the rows in \( A \). Define \( \tilde{Q}^{(t)} = I_{m_q^{(t)}} \otimes Q_{p \times p} \). Then \( \tilde{Q}^{(t)}(\tilde{Q}^{(t)})^T = I_{pm_q^{(t)}} \)
holds. Now, set \( \tilde{Q}(t) v_k(t) = v_k(t) + \Delta_k^{(t)} \). It follows that

\[
\Delta_k^{(t)} = \frac{1}{\sqrt{m_p m_q^{(t)}}} \cdot (1_{m_q^{(t)}} \otimes \tilde{\Sigma}^{(t)} + \lambda^{(t)} \sigma \tilde{\Sigma}^{(t)}) v_k(t) + T^{(t)} v_k(t) = I^{(t)} - I^{(t)} = \sum_{k=1}^{p} \lambda_k m_p m_q^{(t)} (\tilde{Q}(t) v_k(t) v_k(t)^T v_k(t)) + \tilde{Q}(t) v_k(t) - I_{pm_q^{(t)}},
\]

where the last equality holds because \( \Delta_1 = 0 \). Now we compute \((\tilde{\Sigma}^{(t)})^{-1} \tilde{\Sigma}'^{(t)}\) in the following way:

\[
(\tilde{\Sigma}^{(t)})^{-1} \tilde{\Sigma}'^{(t)} = I + (\tilde{\Sigma}^{(t)})^{-1} (\tilde{\Sigma}'^{(t)} - \tilde{\Sigma}^{(t)}) = I + \frac{2}{\sigma^{(t)}} \left[ \sum_{k=1}^{p} \lambda_k m_p m_q^{(t)} (\tilde{Q}(t) v_k(t) v_k(t)^T - v_k(t) v_k(t)) \right] = I + \frac{2}{\sigma^{(t)}} \left[ \sum_{k=1}^{p} \lambda_k m_p m_q^{(t)} (\tilde{Q}(t) v_k(t) v_k(t)^T - v_k(t) v_k(t)) \right]
\]

where the second to third line holds because \( v_1(t)^T v_1(t) \Delta_2 = v_1(t)^T v_1(t) v_2(t) = 0 \). Now we compute \((\tilde{\Sigma}^{(t)})^{-1} \tilde{\Sigma}'^{(t)}\) in the following way:

\[
(\tilde{\Sigma}^{(t)})^{-1} \tilde{\Sigma}'^{(t)} = I + \frac{2}{\sigma^{(t)}} \left[ \sum_{k=1}^{p} \lambda_k m_p m_q^{(t)} (\tilde{Q}(t) v_k(t) v_k(t)^T - v_k(t) v_k(t)) \right] = I + \frac{2}{\sigma^{(t)}} \left[ \sum_{k=1}^{p} \lambda_k m_p m_q^{(t)} (\tilde{Q}(t) v_k(t) v_k(t)^T - v_k(t) v_k(t)) \right]
\]
where \( \tilde{\rho}(t) = \frac{\lambda_2 m_p m_q^{(t)}}{\lambda_2 m_p m_q^{(t)} + \sigma^2_{(t)}} \) and \( s(t) = \Delta_2^{(t)} v_2^{(t)} \). Note that the two non-zero eigenvalues of \( F(t) \), which are \( \mu_1^{(t)} \) and \( \mu_2^{(t)} \), satisfy \( \mu_1^{(t)} + \mu_2^{(t)} = -\tilde{\rho}(t) s(t)(2 + s(t)) \) and \( \mu_1^{(t)} \mu_2^{(t)} = (1 - \tilde{\rho}(t)) s(t)(2 + s(t)) \). Using these facts, we can finally calculate the KL divergence

\[
KL(\tilde{\Sigma}^{(t)'} , \tilde{\Sigma}^{(t)}) = \frac{n}{2} \left[ \text{tr}(\tilde{\Sigma}^{(t)'} - I_{p m_q^{(t)}}) - \log det(\tilde{\Sigma}^{(t)'} - I_{p m_q^{(t)}}) \right]
\]

\[
= \frac{n}{2} \left[ \text{tr}(\lambda_2 m_p m_q^{(t)} + \sigma^2_{(t)}) F(t) - \log det(I_{p m_q^{(t)}} + \lambda_2 m_p m_q^{(t)} + \sigma^2_{(t)}) F(t)) \right]
\]

\[
= \frac{n}{2} \left[ \frac{\lambda_2 m_p m_q^{(t)}}{\sigma^2_{(t)}} (-\tilde{\rho}(t) s(t)(2 + s(t))) \right.
\]

\[
\left. - \log \left\{ 1 + \frac{\lambda_2 m_p m_q^{(t)}}{\sigma^2_{(t)}} (-\tilde{\rho}(t) s(t)(2 + s(t))) + \left( \frac{\lambda_2 m_p m_q^{(t)}}{\sigma^2_{(t)}} \right)^2 (1 - \tilde{\rho}(t)) s(t)(2 + s(t)) \right\} \right]
\]

\[
= \frac{n}{2} \left[ \frac{\lambda_2 m_p m_q^{(t)}}{\sigma^2_{(t)}} (-\tilde{\rho}(t) s(t)(2 + s(t))) \right].
\]

where the last equality holds because \( (1 - \tilde{\rho}(t)) \cdot \frac{\lambda_2 m_p m_q^{(t)}}{\sigma^2_{(t)}} = \tilde{\rho}(t) \). Now, plugging in \( s(t) = -\frac{2\epsilon^2}{m_p(2 + \epsilon^2)} \), we get:

\[
KL(\tilde{\Sigma}^{(t)'} , \tilde{\Sigma}) = 2n\tilde{\rho}(t) \cdot \frac{m_q^{(t)} \lambda_2}{\sigma^2_{(t)}} \frac{\epsilon^2}{2 + \epsilon^2} \left( 1 - \frac{\epsilon^2}{m_p(2 + \epsilon^2)} \right) \leq 2n\epsilon^2 m_q^{(t)} \frac{\lambda_2}{\sigma^2_{(t)}},
\]

where we use the fact that \( \lambda_2 = 2 + \epsilon^2 \). Thus,

\[
KL(\tilde{\Sigma}', \tilde{\Sigma}) \leq 2n\epsilon^2 \sum_{t=1}^{K_2} \frac{m_q^{(t)}}{\sigma^2_{(t)}}. \tag{E.7}
\]

In the following, we will show an upper bound for the rate of \( \frac{MCOD(\Sigma, W_t)}{||X||W_t} \). We will first compute
\[
\text{MCOD}(\Sigma_{p,W_I}), \\
\Sigma_{p,W_I} = \frac{1}{q} \mathbb{E}(X X^T) = \frac{1}{q} \mathbb{E}[(A Z B^T + \Gamma)(B Z A^T + \Gamma^T)] \\
= \frac{1}{q} [A \mathbb{E}(Z B^T B Z A^T + \Gamma \Gamma^T)] \\
= \frac{1}{q} [A \mathbb{E} \left[ \sum_{t=1}^{K_2} ||[t]|| Z_{1t}, \sum_{t=1}^{K_2} ||[t]|| Z_{2t}, \sum_{t=1}^{K_2} ||[t]|| Z_{3t} \right] A^T + \frac{1}{q} \mathbb{E}(\Gamma \Gamma^T)] \\
= \frac{1}{q} \left[ \sum_{t=1}^{K_2} ||[t]|| C(\epsilon)_1, \sum_{t=1}^{K_2} ||[t]|| C(\epsilon)_2, \sum_{t=1}^{K_2} ||[t]|| C(\epsilon)_3 \right] A^T + \frac{1}{q} \mathbb{E}(\Gamma \Gamma^T) \\
= \frac{1}{q} \left( \sum_{t=1}^{K_2} ||[t]|| \right) A C(\epsilon) A^T + \frac{1}{q} \mathbb{E}(\Gamma \Gamma^T) \\
= A C(\epsilon) A^T + \frac{1}{q} \mathbb{E}(\Gamma \Gamma^T)
\]

and from the definition of \( C(\epsilon) \), it is apparent that the minimum of the maximum difference between rows is \( 2\epsilon \), that is

\[
\text{MCOD}(\Sigma_{p,W_I}) = 2\epsilon. \quad (E.8)
\]

Now, we need to look at the quantity \( ||X||_{W_I} \). Recall that \( ||X||_{W_I} = \frac{\sqrt{K_2}}{q} \cdot \max_{1 \leq k \leq p} \| \text{Var}(X_k) \|_F \).

After some tedious calculation, we have

\[
||X||_{W_I} = \frac{\sqrt{K_2}}{q} \sqrt{\sum_{t=1}^{K_2} m_q(t) (2 + \sigma^2(t))^2 + \sum_{t=1}^{K_2} m_q(t) (m_q(t) - 1) \cdot 4} \\
= \frac{\sqrt{K_2}}{q} \sqrt{\left[ 4 \sum_{t=1}^{K_2} (m_q(t))^2 + \sum_{t=1}^{K_2} m_q(t) \sigma^4(t) + 4 \sum_{t=1}^{K_2} m_q(t) \sigma^2(t) \right]} \quad (E.9)
\]

Let us choose

\[
\epsilon = \sqrt{\left( \frac{\log(p)}{n} \right) \cdot \left( \frac{1}{\sum_{t=1}^{K_2} m_q(t) \sigma^2(t)} \right) \cdot \left( \frac{2e}{2e + 1} \right)}. \quad (E.10)
\]

The choice of \( \epsilon \) will be explained later. Using (E.8) and (E.9), for \( \epsilon \) in (E.10) and \( m_q(t) = \frac{q}{K_2} \).
\[ \sigma(t) = \sigma \] we have
\[
\frac{\text{MCOD}(\Sigma_{p,W_I})}{\|X\|_{W_I}} = \frac{2\epsilon}{\sqrt{K_2(4\sum_{t=1}^{K_2}(m_{(t)}^2) + \sum_{t=1}^{K_2} m_{(t)}^4 \sigma_{(t)}^4 + 4\sum_{t=1}^{K_2} m_{(t)}^2 \sigma_{(t)}^2)}} \leq \frac{1}{\sqrt{n(K_2q)^{1/2}}}
\]

for some universal constants \( c, c' > 0 \). This implies that \( \Sigma \) belongs to the parameter space \( M_I(p,q,K_1,K_2,\eta) \) for some \( \eta \).

Finally, we are ready to invoke Lemma E.2. Recall that \( KL(\Sigma', \Sigma) \) is upper bounded in (E.7). Since we choose \( \epsilon \) in (E.10), we obtain
\[
1 - \frac{KL(\Sigma', \Sigma)}{\log((p/3)^2)} \geq 1 - \frac{2\epsilon \sum_{t=1}^{K_2} \frac{m_{(t)}^2}{\sigma_{(t)}^2}}{\log((p/3)^2)} = \frac{1}{2\epsilon + 1}.
\]
As a result, Lemma E.2 implies
\[
\sup_{\Sigma \in M_I(p,q,K_1,K_2,\eta)} \Pr(\widehat{G} \neq G^*) \geq \frac{1}{2\epsilon + 1},
\]
for any \( \widehat{G} \), which completes the proof of Theorem 3.3.

E.2.2 Proof of Theorem 3.4

We use the same construction from the proof of Theorem 3.3. The only difference here is that our model class is defined with respect to \( \Sigma_{p,W_c} \) instead of \( \Sigma_{p,W_I} \). However, by the below reasoning, this also doesn’t make a difference. Recall that for any index \( u \) of rows of \( X \), we use \( r(u) \) to denote the row cluster label. It can be shown that
\[
\text{COD}_{\Sigma_{p,W_I}}(u,v) = \max_{w \neq u,v} \frac{1}{2} \left[ \text{AE}(ZB'ZT)A^T + \mathbb{E}(\Gamma T) \right]_{uw} - \left[ \text{AE}(ZB'ZT)A^T + \mathbb{E}(\Gamma T) \right]_{vw}
\]
\[
= \max_{w \neq u,v} \frac{1}{2} \sum_{t=1}^{K_2} \mathbb{E} \left\{ (Z_{r(u)t} - Z_{r(v)t})Z_{r(w)t} \epsilon \|t\| \right\}
\]
\[
= \max\{ (Z_{r(u)1} - Z_{r(v)1})Z_{r(w)1} \}
\]
\[
= \max\{ (Z_{r(u)1} - Z_{r(v)1})Z_{r(w)1} \}
\]

36
where the fourth equality holds because the columns of $Z$ are iid. Similar, we get

$$
\text{COD}_{\Sigma, W_O}(u, v) = \max_{w \neq u, v} \frac{1}{K_2} \left| \left[ AE(ZZ^T)A^T + \mathbb{E}(\Gamma B(B^T B)^{-2}B^T \Gamma^T) \right]_{uw} 
+ \left[ AE(ZZ^T)A^T + \mathbb{E}(\Gamma B(B^T B)^{-2}B^T \Gamma^T) \right]_{vw} \right|
$$

$$
= \max_{w \neq u, v} \frac{1}{K_2} \left| \left[ AE(ZZ^T)A^T \right]_{uw} - \left[ AE(ZZ^T)A^T \right]_{vw} \right|
$$

$$(\mathbb{E}(\Gamma B(B^T B)^{-2}B^T \Gamma^T) \text{ is diagonal})$$

$$
= \max_{w \neq u, v} \left| \mathbb{E}\left\{ (Z_{r(u)t} - Z_{r(v)t})Z_{r(u)t} \right\} \right|
$$

$$
= \max_{w \neq u, v} \left| \mathbb{E}\left\{ (Z_{r(u)1} - Z_{r(v)1})Z_{r(u)1} \right\} \right|
$$

Thus, in the minimax construction, $\text{MCOD}(\Sigma_{p, W_I}) = \text{MCOD}(\Sigma_{p, W_O}) = 2\epsilon$. Furthermore, we can show that

$$
||X||_{p, W_O} = \frac{1}{\sqrt{K_2}} \cdot \sqrt{4K_2 + \sum_{t=1}^{K_2} \left[ \frac{4\epsilon^2(t)}{\|\|t\|\|} + \frac{\sigma^4(t)}{\|\|t\|\|^2} \right]}
$$

So, getting rid of the term $\frac{4\epsilon^2(t)}{\|\|t\|\|}$, and using $\epsilon$ in (E.10) and $m_q^{(t)} = \frac{q}{K_2}$, $\sigma(t) = \sigma$, we get the following inequalities:

$$
\frac{\text{MCOD}(\Sigma_{p, W_O})}{||X||_{p, W_O}} \leq \sqrt{K_2} \cdot \sqrt{2\epsilon \sqrt{4K_2 + \sum_{t=1}^{K_2} \frac{\sigma^4(t)}{(m_q^{(t)})^2}}}
$$

$$
\leq \sqrt{K_2} \cdot \sqrt{\left( \frac{\log(p/3)}{n} \right) \left( \frac{2\epsilon}{2\epsilon + 1} \right) \left( \frac{1}{(\sum_{t=1}^{K_2} \frac{m_q^{(t)}}{\sigma(t)}) (4K_2 + \sum_{t=1}^{K_2} \frac{\sigma^4(t)}{(m_q^{(t)})^2})} \right)}
$$

$$
\leq \frac{c \sqrt{\log(p/3)}}{nK_2},
$$

where we use the simple inequality $a^2 + b^2 \geq 2ab$ in the last step. The rest of the proof is identical to the proof of Theorem 3.3 and therefore is omitted.
E.3 Proof of Proposition 4.1

Proof. For any rows $w, x$ of $\Sigma_{p,W_O}$, without loss of generality, we can assume they belong to clusters $i, h$. Then

$$\text{COD}_{\Sigma_{p,W_O}}(w, x) = \max_{1 \leq c \leq K_1} \frac{1}{K_2} \sum_{l=1}^{K_2} \mathbb{E}\{(Z_{il} - Z_{hl})Z_{cl}\}$$

$$= \max_{1 \leq c \leq K_1} \frac{1}{K_2} \sum_{l=1}^{K_2} (U_{ic} - U_{hc})V_{ll}$$

$$= \max_{1 \leq c \leq K_1} \frac{1}{K_2} |U_{ic} - U_{hc}| \sum_{l=1}^{K_2} V_{ll}$$

Looking at the cluster separation condition first, we need this COD value to be greater than $c^* \sqrt{\frac{\log p}{nK_2}} ||X||_{W_O}$ for all $w, x$. We know that $||X||_{W_O} \leq \sqrt{\frac{1}{K_2} \max_a ||\text{Var}(Z_{r(a)})||_F + \sqrt{K_2} \max_a ||\text{Var}(\Gamma_a L)||_F}$ from the definition of $||X||_{W_O}$. In the matrix normal setting, we have

$$\text{Var}(Z_{r(a)}) = \begin{bmatrix} U_{r(a)r(a)} \cdot V_{11} & U_{r(a)r(a)} \cdot V_{12} & \ldots & \vdots \\ U_{r(a)r(a)} \cdot V_{21} & U_{r(a)r(a)} \cdot V_{22} & \ldots & \vdots \\ \vdots & \vdots & \ddots & \vdots \end{bmatrix} = U_{r(a)r(a)} \cdot V$$

and so, $||\text{Var}(Z_{r(a)})||_F = U_{r(a)r(a)} \cdot ||V||_F$ and we have

$$\max_a ||\text{Var}(Z_{r(a)})||_F = ||\text{diag}(U)||_{\max} \cdot ||V||_F \leq ||\text{diag}(U)||_{\max} K_2^{1/2} C_{\max}.$$ 

It is also easily shown that

$$\max_a ||\text{Var}(\Gamma_a L)||_F = \max_a \frac{1}{K_2} \sum_{t=1}^{K_2} \left( \sum_{j \in [t]} \sigma_{aj}^2 \right)^2 / ||t||^4 \leq C_{K}^{1/2} / K_2^{1/2}.$$ 

Rearranging with algebra gives us the cluster separation condition.

Now, let’s consider the stability condition. Again, we need only consider rows in different row clusters when looking at the MCOD value. That is why we assume $i \neq h$. Now for $\text{MCOD}(\Sigma_{p,W_O})$, we have

$$\text{MCOD}_{\Sigma_{p,W_O}}(w, x) = \max_{1 \leq c \leq K_1} \frac{1}{K_2} \sum_{l=1}^{K_2} \mathbb{E}\{(Z_{il} - Z_{hl})Z_{cl}\}$$

$$= \max_{1 \leq c \leq K_1} \frac{1}{K_2} \sum_{l=1}^{K_2} (U_{ic} - U_{hc})V_{ll}$$

$$= \max_{1 \leq c \leq K_1} \frac{1}{K_2} |U_{ic} - U_{hc}| \sum_{l=1}^{K_2} V_{ll}$$

Looking at the cluster separation condition, we need this COD value to be greater than $c^* \sqrt{\frac{\log p}{nK_2}} ||X||_{W_O}$ for all $w, x$. We know that $||X||_{W_O} \leq \sqrt{\frac{1}{K_2} \max_a ||\text{Var}(Z_{r(a)})||_F + \sqrt{K_2} \max_a ||\text{Var}(\Gamma_a L)||_F}$ from the definition of $||X||_{W_O}$. In the matrix normal setting, we have

$$\text{Var}(Z_{r(a)}) = \begin{bmatrix} U_{r(a)r(a)} \cdot V_{11} & U_{r(a)r(a)} \cdot V_{12} & \ldots & \vdots \\ U_{r(a)r(a)} \cdot V_{21} & U_{r(a)r(a)} \cdot V_{22} & \ldots & \vdots \\ \vdots & \vdots & \ddots & \vdots \end{bmatrix} = U_{r(a)r(a)} \cdot V$$

and so, $||\text{Var}(Z_{r(a)})||_F = U_{r(a)r(a)} \cdot ||V||_F$ and we have

$$\max_a ||\text{Var}(Z_{r(a)})||_F = ||\text{diag}(U)||_{\max} \cdot ||V||_F \leq ||\text{diag}(U)||_{\max} K_2^{1/2} C_{\max}.$$ 

It is also easily shown that

$$\max_a ||\text{Var}(\Gamma_a L)||_F = \max_a \frac{1}{K_2} \sum_{t=1}^{K_2} \left( \sum_{j \in [t]} \sigma_{aj}^2 \right)^2 / ||t||^4 \leq C_{K}^{1/2} / K_2^{1/2}.$$ 

Rearranging with algebra gives us the cluster separation condition.
we would need to look at the following equivalent expressions:

\[
\text{COD}_{\Sigma_p, W_O}(w, x) = \max_{1 \leq s \leq K_1} \frac{1}{s} \left| \mathbb{E} \left( \sum_{l=1}^{K_2} (Z_{zl} - Z_{hl}) Z_d \left( \sum_{j=1}^{s} \frac{|G_l \cap \hat{G}_j|^2}{|\hat{G}_j|^2} \right) \right) \right|
\]

\[
+ \mathbb{E} \left( \sum_{l' \neq l''}^{K_2} (Z_{zl'} - Z_{h(l''}) Z_d \left( \sum_{j=1}^{s} \frac{|G_{l'} \cap \hat{G}_j|}{|\hat{G}_j|} \cdot \frac{|G_{l''} \cap \hat{G}_j|}{|\hat{G}_j|} \right) \right)
\]

\[
= \max_{1 \leq s \leq K_1} \frac{1}{s} \left| (U_{ic} - U_{hc}) V_l(l) \left( \sum_{j=1}^{s} \frac{|G_l \cap \hat{G}_j|^2}{|\hat{G}_j|^2} \right) \right|
\]

\[
+ \sum_{l' \neq l''}^{K_2} (U_{ic} - U_{hc}) V_l(\sum_{j=1}^{s} \frac{|G_{l'} \cap \hat{G}_j|}{|\hat{G}_j|} \cdot \frac{|G_{l''} \cap \hat{G}_j|}{|\hat{G}_j|} \right)
\]

\[
= \max_{1 \leq s \leq K_1} \frac{1}{s} \left| U_{ic} - U_{hc} \right| \left( \sum_{l=1}^{K_2} V_l(l) \left( \sum_{j=1}^{s} \frac{|G_l \cap \hat{G}_j|^2}{|\hat{G}_j|^2} \right) \right)
\]

\[
+ \sum_{l' \neq l''}^{K_2} V_l(l') \left( \sum_{j=1}^{s} \frac{|G_{l'} \cap \hat{G}_j|}{|\hat{G}_j|} \cdot \frac{|G_{l''} \cap \hat{G}_j|}{|\hat{G}_j|} \right)
\]

\[
= \max_{1 \leq s \leq K_1} \frac{1}{s} \left| U_{ic} - U_{hc} \right| \left| \text{tr}(V^T GG^T) \right|
\]

where for simplicity we drop the superscript (c) in \(G_l\) and \(\hat{G}_j\).

Note that both \(\text{COD}_{\Sigma_p, W_O}(w, x)\) and \(\text{COD}_{\Sigma_p, W_O}(w, x)\) are influenced by \(i\) and \(h\) \((i \neq h)\) only through the common \(|U_{ic} - U_{hc}|\) term, and so the \((i, h)\) pair that gives the minimum of the two COD expressions is the same. Thus, the following holds:

\[
\frac{\text{MCOD}(\Sigma p, W_O)}{\text{MCOD}(\Sigma p, W_O)} = \frac{|\text{tr}(V^T GG^T)|}{|\text{tr}(V)|} \cdot \frac{K_2}{s}
\]

Thus,

\[
\begin{align*}
\left\{ \frac{\text{MCOD}(\Sigma p, W_O)}{||X||_{W_O}} \right\} & \leq \left\{ \frac{\text{MCOD}(\Sigma p, W_O)}{||X||_{W_O}} \right\} = \frac{|\text{tr}(V^T GG^T)|}{|\text{tr}(V)|} \cdot \frac{K_2}{s} \cdot \frac{||X||_{W_O}}{||X||_{W_O}} > \frac{4}{c_0}
\end{align*}
\]

needs to hold. By Von Neumann’s trace inequality, we have \(|\text{tr}(V^T GG^T)| \geq |\text{tr}(V) \cdot \lambda_{\text{min}}(GG^T)|\), and so it suffices to have:

\[
|\lambda_{\text{min}}(GG^T)| \cdot \frac{K_2}{s} \cdot \frac{||X||_{W_O}}{||X||_{W_O}} > \frac{4}{c_0}
\]

To show the above inequality, we need to further lower bound \(||X||_{W_O} \)

\[
= \max \frac{1}{K_2} \text{Var}(Z_{r(a)},) + \text{Var}(\Gamma a, L) ||F
\]

\[
\max \frac{1}{s} \text{Var}(Z_{\rho(a)}, G) + \text{Var}(\Gamma a, L) ||F
\]

\[
\geq \max \frac{1}{s} \sqrt{\frac{1}{K_2} \left( \text{Var}(Z_{r(a)},) \right)} ||F + \text{Var}(\Gamma a, L) ||F
\]

\[
\max \frac{1}{s} \text{Var}(Z_{\rho(a)}, G) ||F + \text{Var}(\Gamma a, L) ||F
\]

39
For the term $\|G^T \text{Var}(Z_{r(a)\cdot})G\|_F^2$ in the denominator, we have

$$\|G^T \text{Var}(Z_{r(a)\cdot})G\|_F^2 = \sum_{i=1}^{K_2} \lambda_i \{(G^T \text{Var}(Z_{r(a)\cdot})G)^T(G^T \text{Var}(Z_{r(a)\cdot})G)\}$$  \hspace{1cm} (E.11)

$$\leq \min(s, K_2) \cdot \|G^T \text{Var}(Z_{r(a)\cdot})G\|_{op}$$  \hspace{1cm} (E.12)

where (E.11) holds from the fact that there can be at most $\min(s, K_2)$ non-zero eigenvalues of $A^T A = \text{tr}(A^T A)$, and (E.12) holds from the fact there can be at most $\min(s, K_2)$ non-zero eigenvalues of $G^T \text{Var}(Z_{r(a)\cdot})G$ because $\text{rank}(G^T \text{Var}(Z_{r(a)\cdot})G) \leq \min\{\text{rank}(G), \text{rank}(\text{Var}(Z_{r(a)\cdot}))\}$ and $\text{rank}(G) \leq \min(s, K_2)$. Using the similar argument, we also show that

$$\|\text{Var}(Z_{r(a)\cdot})\|_F^2 \geq \|\text{diag}(U)\|_F^2 \geq 2 \min(s, K_2) \|\text{diag}(U)\|_{min}.$$  

Finally, noting that $\|G\|_{op}^2 = \lambda_{max}(GG^T)$, and

$$\max_a \|\text{Var}(\Gamma_a L)\|_F = C_{s,K}^{1/2}/K_2^{1/2}, \quad \max_a \|\text{Var}(\Gamma_a \tilde{L})\|_F = C_{s,K}^{1/2}/s^{1/2},$$

we have

$$\frac{\|X\|_{W_0}}{\|X\|_{\tilde{M}_0}} \geq \frac{\max_a 1/2 \sqrt{\min(s, K_2) \cdot |\lambda_{max}(GG^T)| \cdot \|\text{Var}(Z_{r(a)\cdot})\|_{op}} + C_{s,K}^{1/2}/s^{1/2}}{\frac{1}{s} \sqrt{\min(s, K_2) \cdot |\lambda_{max}(GG^T)| \cdot \|\text{diag}(U)\|_{max} \cdot C_{max} + C_{s,K}^{1/2}/s^{1/2}}}.$$  

So, combining with the above inequality, we need to show the following condition:

$$\frac{K_2^{1/2} |\lambda_{min}(GG^T)| \sqrt{C_{min}^2 \cdot \|\text{diag}(U)\|_{min}^2 + C_K}}{\sqrt{\min(s, K_2) \cdot |\lambda_{max}(GG^T)| \cdot \|\text{diag}(U)\|_{max} \cdot C_{max} + s^{1/2}C_s^{1/2}}} \geq \frac{4}{c_0}.$$  \hspace{1cm} (E.13)

To show (E.13), let’s consider the following two cases. If $\sqrt{\min(s, K_2) \cdot |\lambda_{max}(GG^T)| \cdot \|\text{diag}(U)\|_{max} \cdot C_{max}} \leq C_s^{1/2}/s^{1/2}$ hold, then

$$\frac{K_2^{1/2} |\lambda_{min}(GG^T)| \sqrt{C_{min}^2 \cdot \|\text{diag}(U)\|_{min}^2 + C_K}}{\sqrt{\min(s, K_2) \cdot |\lambda_{max}(GG^T)| \cdot \|\text{diag}(U)\|_{max} \cdot C_{max} + s^{1/2}C_s^{1/2}}} \geq \frac{4}{c_0},$$

when $\frac{1}{\lambda_{min}(GG^T)} \leq \frac{ca_{0}C_K^{1/2}K_2^{1/2}}{8C_s^{1/2}/s^{1/2}}$. In the second case $\sqrt{\min(s, K_2) \cdot |\lambda_{max}(GG^T)| \cdot \|\text{diag}(U)\|_{max} \cdot C_{max}} > C_s^{1/2}/s^{1/2}$, we can similarly show that

$$\frac{K_2^{1/2} |\lambda_{min}(GG^T)| \sqrt{C_{min}^2 \cdot \|\text{diag}(U)\|_{min}^2 + C_K}}{\sqrt{\min(s, K_2) \cdot |\lambda_{max}(GG^T)| \cdot \|\text{diag}(U)\|_{max} \cdot C_{max} + s^{1/2}C_s^{1/2}}} \geq \frac{4}{c_0},$$
when \( \frac{\lambda_{\max}(GG^T)}{\lambda_{\min}(GG^T)} \leq \frac{\sqrt{\log(p)} ||\text{diag}(U)||_{\min}}{\sqrt{\log(n)}} \frac{\sqrt{K_2}}{\min(s,K_2)} \). This completes the proof.

\( \square \)

### F Additional Simulations

Additional simulations were done in two different settings.

#### F.1 Smaller \( K_2 \)

Since the threshold for the cluster separation depend on \( \sqrt{\log(p) n K_2} \), we can compare the performance of row clustering by varying the value of \( K_2 \). Keeping everything else the same (\( p = q = 100, K_1 = 10, \) row cluster sizes = (3, 6, 6, 8, 10, 10, 12, 12, 14, 19)), we halved the number of column clusters to be \( K_2 = 5 \) instead of \( K_2 = 10 \), and changed the column cluster sizes to be (6, 12, 20, 28, 34) instead of (3, 6, 6, 8, 10, 10, 12, 12, 14, 19). The ARI values are shown in Figure 5.

When compared to the graphs in Section 6, the ARI values are generally smaller, especially for \( n = 12 \). Since the rate of \( \sqrt{\log(p) n K_2} \) increases as \( K_2 \) decreases, the condition (A1) becomes more restrictive, and thus clustering consistency is harder to attain.

#### F.2 Unbalanced \( p \) and \( q \)

To see how the performance changes when \( p \) and \( q \) have very different values, we set \( p = 300, q = 30, K_1 = 20, K_2 = 5 \) and the row and column cluster sizes to be (4, 4, 4, 4, 4, 8, 8, 8, 8, 12, 12, 12, 12, 12, 15, 15, 18, 20, 112) and (3, 3, 5, 6, 13), respectively. Simulations were done with 30 repetitions in each setting.

The ARI values are shown in Figure 6. It is apparent that clustering the columns is easier in this case due to the high value of \( p = 300 \) and \( K_1 = 20 \) and the relatively low value of \( q = 30 \) and \( K_2 = 5 \). This is again consistent with our theoretical results on the rate of the cluster separation metric. When we assume the random noise variance setting, 2-STEP COD and 1-STEP COD are both significantly better than Naive COD. This is apparent in the more difficult row clustering situation.

### G Cluster Evaluation Metrics

For this section, the true row cluster partition will be denoted simply as \( \mathcal{G} = \{G_1, ..., G_{K_1}\} \), where \( G_k = \{a : A_{ak} = 1\} \), while the estimated row cluster partition will be denoted as \( \hat{\mathcal{G}} = \{\hat{G}_1, ..., \hat{G}_s\} \), where \( \hat{G}_k = \{a : \hat{A}_{ak} = 1\} \).
Figure 5: ARI values when $K_2 = 5$
Figure 6: ARI values when \( p = 300, q = 30, K_1 = 20, K_2 = 5 \).
G.1 Sensitivity and Specificity

Then, for any pair $1 \leq j < k \leq p$, we can define

$$TP_{jk} = 1 \{j, k \in G_a \text{ and } j, k \in \hat{G}_b \text{ for some } 1 \leq a \leq K_1, 1 \leq b \leq s\}$$

$$TN_{jk} = 1 \{j, k \notin G_a \text{ and } j, k \notin \hat{G}_b \text{ for some } 1 \leq a \leq K_1, 1 \leq b \leq s\}$$

$$FP_{jk} = 1 \{j, k \notin G_a \text{ and } j, k \in \hat{G}_b \text{ for some } 1 \leq a \leq K_1, 1 \leq b \leq s\}$$

$$FN_{jk} = 1 \{j, k \in G_a \text{ and } j, k \notin \hat{G}_b \text{ for some } 1 \leq a \leq K_1, 1 \leq b \leq s\}$$

and define

$$TP = \sum_{1 \leq j < k \leq p} TP_{jk}, \quad TN = \sum_{1 \leq j < k \leq p} TN_{jk}$$

$$FP = \sum_{1 \leq j < k \leq p} FP_{jk}, \quad FN = \sum_{1 \leq j < k \leq p} FN_{jk}$$

Sensitivity (SN) and specificity (SP) can then be defined as follows:

$$SN = \frac{TP}{TP + FN} \quad SP = \frac{TN}{TN + FP}$$

G.2 Adjusted Rand Index (ARI)

The following is a cross tabulation of two cluster partitions (the true partition and the estimated partition).

|        | $\hat{G}_1$ | $\hat{G}_2$ | ... | $\hat{G}_s$ | Sum |
|--------|-------------|-------------|-----|-------------|-----|
| $G_1$  | $n_{11}$    | $n_{12}$    | ... | $n_{1s}$    | $|G_1|$ |
| $G_2$  | $n_{21}$    | $n_{22}$    | ... | $n_{2s}$    | $|G_2|$ |
| ...    | ...         | ...         | ... | ...         |     |
| $G_{K_1}$ | $n_{K_11}$ | $n_{K_12}$ | ... | $n_{K_1s}$ | $|G_{K_1}|$ |
| Sum    | $|\hat{G}_1|$ | $|\hat{G}_2|$ | ... | $|\hat{G}_s|$ | $p$ |

The ARI is then defined as follows:

$$ARI = \frac{\sum_{i,j} \binom{n_{ij}}{2} - \left[ \sum_i \binom{|G_i|}{2} \sum_j \binom{|\hat{G}_j|}{2} \right] / \binom{p}{2}}{\frac{1}{2} \left[ \sum_i \binom{|G_i|}{2} + \sum_j \binom{|\hat{G}_j|}{2} \right] - \left[ \sum_i \binom{|G_i|}{2} \sum_j \binom{|\hat{G}_j|}{2} \right] / \binom{p}{2}}$$

Note that this is the corrected-for-chance version of the Rand index (Rand, 1971). An ARI value of 1 implies a perfect match between the two cluster partitions.