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# Graph Estimation for Matrix-variate Gaussian Data

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*Abstract:* Matrix-variate Gaussian graphical models (GGM) have been widely used for modeling matrix-variate data. Since the support of sparse precision matrix represents the conditional independence graph among matrix entries, conducting support recovery yields valuable information. A commonly used approach is the penalized log-likelihood method. However, due to the complicated structure of precision matrices in the form of Kronecker product, the log-likelihood is non-convex, which presents challenges for both computation and theoretical analysis. In this paper, we propose an alternative approach by formulating the support recovery problem into a multiple testing problem. A new test statistic is developed and based on that, we use the popular Benjamini and Hochberg's procedure to control false discovery rate (FDR) asymptotically. Our method involves only convex optimization, making it computationally attractive. Theoretically, our method allows very weak conditions, i.e., even when the sample size is finite and the dimensions go to infinity, the asymptotic normality of the test statistics and FDR control can still be guaranteed. We further provide the power analysis result. The finite sample performance of the proposed method is illustrated by both simulated and real data analysis.

*Key words and phrases:* Correlated samples, false discovery rate, matrix-variate Gaussian graphical models, multiple tests, support recovery

## 1 Introduction

In the era of big data, matrix-variate observations are becoming prevalent in a wide range of domains, such as biomedical imaging, genomics, financial markets, spatio-temporal environmental data analysis, and more. A typical example is the gene expression data in genomics, in which each observation contains expression levels of  $p$  genes on  $q$  microarrays of the same subject (see, e.g., Efron (2009); Yin and Li (2012)). Another example of such data is the multi-channel electroencephalography (EEG) data for brain imaging studies (see, e.g.,

Bijma et al. (2005)), in which each measurement can be expressed as a matrix with rows corresponding to  $p$  different channels and columns to  $q$  time points. Leng and Tang (2012) provided more interesting examples of matrix-variate data such as the volatility of equality option. Due to the prevalence of matrix-variate observations (especially high-dimensional observations), it is important for us to understand the structural information encoded in these observations.

To study matrix-variate data where each observation  $\mathbf{X}$  is a  $p \times q$  matrix, it is commonly assumed that  $\mathbf{X}$  follows a matrix-variate Gaussian distribution, e.g., Efron (2009); Allen and Tibshirani (2010); Leng and Tang (2012); Yin and Li (2012); Zhou (2014). The matrix-variate Gaussian distribution is a generalization of the familiar multivariate normal distribution for vector-variate data. In particular, let  $\text{vec}(\mathbf{X}) \in \mathbb{R}^{pq \times 1}$  be the vectorization of matrix  $\mathbf{X}$  obtained by stacking the columns of  $\mathbf{X}$  on top of each other. We say that  $\mathbf{X}$  follows a matrix-variate Gaussian distribution  $\mathbf{X} \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma} \otimes \boldsymbol{\Psi})$  with mean matrix  $\boldsymbol{\mu} \in \mathbb{R}^{p \times q}$ , row covariance matrix  $\boldsymbol{\Sigma} \in \mathbb{R}^{p \times p}$  and column covariance matrix  $\boldsymbol{\Psi} \in \mathbb{R}^{q \times q}$  if and only if  $\text{vec}(\mathbf{X}') \sim N(\text{vec}(\boldsymbol{\mu}'), \boldsymbol{\Sigma} \otimes \boldsymbol{\Psi})$ , where  $\mathbf{X}'$  denotes the transpose of  $\mathbf{X}$  and  $\otimes$  is the Kronecker product.

The readers might refer to Dawid (1981) and Gupta and Nagar (1999) for more properties of matrix-variate Gaussian distribution. Similar to the vector-variate Gaussian graphical models (GGMs) in which the conditional independence graph is encoded in the support of the precision matrix, one can analogously define matrix-variate Gaussian graphical models (MGGM) (a.k.a. Gaussian bigraphical models). Let us denote *conditional independence graph* by the undirected graph  $G = (V, E)$ , where  $V = \{V_{ij}\}_{1 \leq i \leq p, 1 \leq j \leq q}$  contains  $p \times q$  nodes and each node corresponds to an entry in the random matrix  $\mathbf{X}$ . We can regard the edge set  $E$  as a  $pq \times pq$  matrix where there is no edge between  $X_{ij}$  and  $X_{kl}$  if and only if  $X_{ij}$  and  $X_{kl}$  are conditionally independent given the rest of the entries. The goal of the *graph estimation* is to estimate the edge set  $E$ , which unveils important structural information on the conditional independence relationship.

The estimation of the conditional independence graph is equivalent to the estimation of *the support of the precision matrix*. In particular, let  $\boldsymbol{\Omega} = \boldsymbol{\Sigma}^{-1} = (\omega_{ik})_{p \times p}$ ,  $\boldsymbol{\Gamma} = \boldsymbol{\Psi}^{-1} = (\gamma_{jl})_{q \times q}$ . The precision matrix of the MGGM is a  $pq \times pq$  matrix  $\boldsymbol{\Omega} \otimes \boldsymbol{\Gamma} = (\boldsymbol{\Sigma} \otimes \boldsymbol{\Psi})^{-1}$ , where  $(\boldsymbol{\Omega} \otimes \boldsymbol{\Gamma})_{q(i-1)+j, q(k-1)+l} = \omega_{ik} \cdot \gamma_{jl}$ . The conditional independence among entries of  $\mathbf{X}$  can be presented by the support of  $\boldsymbol{\Omega} \otimes \boldsymbol{\Gamma}$  (denoted by  $\text{supp}(\boldsymbol{\Omega} \otimes \boldsymbol{\Gamma})$ ), which is equivalent to  $\text{supp}(\boldsymbol{\Omega}) \otimes \text{supp}(\boldsymbol{\Gamma})$ . To see this, we recall the well-known fact that  $X_{ij}$  and  $X_{kl}$  are conditionally independent given the rest of the entries, if and only if  $\varrho_{ij,kl} = 0$ , where  $\varrho_{ij,kl}$

is the partial correlation between  $X_{ij}$  and  $X_{kl}$ :

$$\rho_{ij,kl} = -\frac{\omega_{ik}}{\sqrt{\omega_{ii}\omega_{kk}}} \cdot \frac{\gamma_{jl}}{\sqrt{\omega_{jj}\omega_{ll}}}. \quad (1.1)$$

In other words,  $X_{ij}$  and  $X_{kl}$  are conditionally independent if and only if there is at least one zero in  $\omega_{ik}$  or  $\gamma_{jl}$ . Therefore, to estimate the conditional independence graph, one only needs to estimate  $\text{supp}(\mathbf{\Omega})$  and  $\text{supp}(\mathbf{\Gamma})$ . Their Kronecker product  $\text{supp}(\mathbf{\Omega}) \otimes \text{supp}(\mathbf{\Gamma})$  gives the edge set  $E$ . It is worthwhile to note that for a given matrix-variate Gaussian distribution, multiplying a constant to  $\mathbf{\Omega}$  and dividing  $\mathbf{\Gamma}$  by the same constant will lead to the same distribution. The existing literature usually assumes that  $\omega_{11} = 1$  to make the model identifiable (see, e.g., Leng and Tang (2012)). However, if we are interested in support recovery rather than values of  $\omega_{ik}$  or  $\gamma_{jl}$ , then there is no identifiability issue.

Due to the complicated structure in the precision matrices of MGGMs, research on matrix-variate GGMs (MGGMs) is scarce compared to the large body of literature on vector-variate GGMs. The vector-variate GGM with random vector observations can be viewed as a special case of MGGM with  $p = 1$  or  $q = 1$  and readers may refer to, e.g., Meinshausen and Bühlmann (2006); Yuan and Lin (2007); Rothman et al. (2008); d'Aspremont et al. (2008); Friedman et al. (2008); Yuan (2010); Ravikumar et al. (2011); Cai et al. (2011); Liu et al. (2012); Xue and Zou (2012); Liu (2013); Zhu et al. (2014); Fan and Lv (2016); Ren et al. (2016) for the recent development in vector-variate GGMs. Among these works, our work is closely related to Liu (2013), which conducts graph estimation via false discovery rate (FDR) control for vector-variate GGMs. However, due to the complicated structure of MGGMs, the proposed test statistics are fundamentally different from the ones in Liu (2013) and the theoretical analysis is much more challenging. The details on the comparisons to Liu (2013) are deferred to Section 6.

For estimating sparse precision matrices of matrix-variate Gaussian data, one popular approach is based on the penalized likelihood method. However, since the precision matrices are in the form of a Kronecker product, the negative log-likelihood function is no longer convex, which makes both computation and theoretical analysis significantly more challenging than in the case of classical vector-variate GGMs. A few recent works (Allen and Tibshirani, 2010; Leng and Tang, 2012; Yin and Li, 2012; Kalaitzis et al., 2013; Tsiligkaridis et al., 2013; Ying and Liu, 2013; Huang and Chen, 2015) have focused on developing various penalized likelihood approaches for estimating MGGMs or extensions of MGGMs (e.g., multiple MGGMs in Huang and Chen (2015) and semiparametric extension in Ying and Liu

(2013)). In particular, Leng and Tang (2012) provided pioneering theoretical guarantees on the estimated precision matrices, e.g., rate of convergence under the Frobenius norm and sparsistency. One limitation is that the theoretical results are stated in terms that there *exists* a local minimizer that enjoys good properties. In practice, it might be difficult to determine whether the obtained local minimizer from an optimization solver is a desired local minimizer. In addition, most convergence results require certain conditions on the sample size  $n$  and dimensionality  $p$  and  $q$ , e.g.,  $p$  and  $q$  cannot differ too much from each other and  $n$  should go to infinity at a certain rate. On the other hand, we will show later that  $n \rightarrow \infty$  is not necessary for the control of false discovery rate (FDR) in support recovery for MGGMs. Zhou (2014) developed new penalized methods for estimating  $\Sigma \otimes \Psi$  and  $\Omega \otimes \Gamma$  and established the convergence rate under both the spectral norm and the Frobenius norm. However, the main focus of Zhou (2014) is not the support recovery of  $\Omega \otimes \Gamma$ , and our goal of accurate FDR control cannot be achieved by the method in Zhou (2014) nor other penalized optimization approaches.

The main goal of this work is to infer the support of the precision matrix for an MGGM in the high-dimensional setting, which fully characterizes the conditional independence relationship. Our method differs from the common approaches that turn the problem into a joint optimization over  $\Omega$  and  $\Gamma$  as penalized likelihood methods. Instead, we utilize the large-scale testing framework and formulate the problem into multiple testing problems for  $\Omega$  and  $\Gamma$ :

$$H_{0ij}^{\Omega} : \omega_{ij} = 0 \quad \text{vs} \quad H_{0ij}^{\Omega} : \omega_{ij} \neq 0, \quad 1 \leq i < j \leq p \quad (1.2)$$

and

$$H_{0ij}^{\Gamma} : \gamma_{ij} = 0 \quad \text{vs} \quad H_{0ij}^{\Gamma} : \gamma_{ij} \neq 0, \quad 1 \leq i < j \leq q. \quad (1.3)$$

By conducting the multiple testing for (1.2) and (1.3), we obtain the estimates for the support of  $\Omega$  and  $\Gamma$ , denoted by  $\widehat{\text{supp}}(\Omega)$  and  $\widehat{\text{supp}}(\Gamma)$ , respectively. Then, the support of  $\Omega \otimes \Gamma$  can be naturally estimated by  $\widehat{\text{supp}}(\Omega) \otimes \widehat{\text{supp}}(\Gamma)$ . Instead of aiming for perfect support recovery, which will require strong conditions, our goal is to asymptotically control the false discovery rate (FDR). The FDR, originally introduced for multiple testing (Benjamini and Hochberg, 1995), has been considered one of the most important criterion for evaluating the quality of estimated networks (e.g., in the application of genetic data analysis (Schafer and Strimmer, 2005; Ma et al., 2007)). Please refer to (4.25) and (4.28) in Section 4.2 for the definition of FDR in our graph estimation problems.

Although conducting variable selection via multiple testing is not a new idea, how to im-

plement such a high-level idea for MGGMs with a complicated covariance structure requires several innovations in the methodology development. In particular, to conduct the multiple testing in (1.2) and (1.3), it is critical to construct a test statistic with the explicit asymptotic null distribution for each edge. To this end, we propose a new approach that fully utilizes the correlation structures among rows and columns of  $\mathbf{X}$ . In particular, suppose that there are  $n$  *i.i.d.*  $p \times q$  matrix-variate samples  $\mathbf{X}^{(1)}, \dots, \mathbf{X}^{(n)}$ . To conduct the testing in (1.3) and estimate the support of  $q \times q$  matrix  $\mathbf{\Gamma}$ , we treat each row of  $\mathbf{X}^{(k)}$  as a  $q$ -dimensional sample. In such a way, we construct  $n \cdot p$  *correlated* vector-variate samples for the testing problem in (1.3), where the correlation among these “row samples” is characterized by the covariance matrix  $\mathbf{\Sigma}$ . One important advantage of this approach is that it only requires number of row samples  $np \rightarrow \infty$  to control FDR asymptotically and thus allows the finite sample size  $n$  even when  $p$  and  $q$  go to infinity. On the other hand, the correlation structure among row samples also presents a significant challenge to the development of the FDR control approach, and most existing inference techniques for vector-variate GGMs heavily rely on the independence assumption (see, e.g., Liu (2013); van de Geer et al. (2014); Ren et al. (2015)). To address this challenge, we summarize the effect of correlation among “row samples” into a simple quantity depending on  $\mathbf{\Sigma}$ , and based on that, introduce a variance correction technique into the construction of the test statistics (see Section 3.1). It is noteworthy that the testing of the  $\text{supp}(\mathbf{\Omega})$  in (1.2) can be performed in a completely symmetric way with  $nq$  correlated “column samples” from the data.

More specifically, the high-level description of the proposed large-scale testing approach is as follows. Given the “row samples” from the data, the first step is to construct an asymptotically normal test statistic for each  $H_{0ij}^{\mathbf{\Gamma}}$  in (1.3). We utilize a fundamental result from multivariate analysis which relates the partial correlation coefficient to the correlation coefficient of residuals from linear regression. To compute the sample version of the correlation coefficient of the residuals, we first construct an initial estimator for the regression coefficients. With the initial estimator in place, we can directly show that the sample correlation coefficient of the residuals is asymptotically normal under the null. We further apply the aforementioned variance correction technique and obtain the final test statistic for each  $H_{0ij}^{\mathbf{\Gamma}}$ . Combining the developed test statistics with the Benjamini and Hochberg approach (Benjamini and Hochberg, 1995), we show that the resulting procedure asymptotically controls the FDR for both  $\widehat{\text{supp}}(\mathbf{\Gamma})$  and  $\widehat{\text{supp}}(\mathbf{\Omega})$  (and thus  $\widehat{\text{supp}}(\mathbf{\Gamma}) \otimes \widehat{\text{supp}}(\mathbf{\Omega})$ ) under some sparsity conditions of  $\mathbf{\Gamma}$  and  $\mathbf{\Omega}$ .

The proposed method described above is the first to investigate FDR control in MGGMs.



This work greatly generalizes the method on FDR control for *i.i.d.* vector-variate GGMs in Liu (2013) and improves over optimization-based approaches. The main contribution and difference between our results and the existing ones for vector-variate GGMs (e.g., Liu (2013)) are summarized as follows,

1. We propose a novel *test statistic* in Section 3.1. By introducing a new construction of the initial regression coefficients (i.e., setting a particular element in each initial Lasso estimator to zero), our testing approach no longer requires a complicated bias-correlation step as in Eq. (6) in Liu (2013). Furthermore, the limiting null distribution of the sample covariance coefficient between residuals (see  $\hat{r}_{ij}$  in (3.10)) can be easily obtained. In fact, this idea can be used to provide simpler testing procedure for ordinary vector-variate high-dimensional graphical models.
2. Instead of relying on the *i.i.d.* assumption in GGM literature, we propose to extract  $np$  correlated vector-variate “rows samples” (as well  $nq$  correlated “column samples”) from matrix-variate observations. By utilizing correlation structure among rows and columns, our approach allows for finite sample size, which is a very attractive property from both theoretical and practical perspectives. More specifically, even in the case that  $n$  is a constant and  $p \rightarrow \infty$  and  $q \rightarrow \infty$ , our method still guarantees the asymptotic normality of the test statistics and FDR control. This is fundamentally different from the case of vector-variate GGMs, which always requires  $n \rightarrow \infty$  for the support recovery. Therefore, this work greatly generalizes Liu (2013), which only deals with *i.i.d.* vector-variate Gaussian samples, to correlated data.

In this paper, we developed new techniques and theoretical analysis to address the challenges arising from correlated samples. For example, the proposed *variance correlation technique* can be used as a general technique for high-dimensional inference with correlated samples. Moreover, the initial estimator is now based on the Lasso with correlated samples. To this end, we establish the consistency result for the Lasso with correlated samples, which itself is of independent interest for high-dimensional linear regression.

3. Theoretically, by utilizing the Kronecker product structure of the covariance matrix of  $\mathbf{X}$ , the proposed method allows the partial correlation between  $X_{ij}$  and  $X_{kl}$  (i.e.,  $\varrho_{ij,kl}$  in (1.1)) to be of the order of  $\frac{1}{n-1} \sqrt{\frac{\log p \log q}{pq}}$  so that the corresponding edge can be detected (please see the power analysis in Section 4.3 and Theorem 4 for details.)

This is essentially different from any vector-variate GGM estimator (e.g., the one from Liu (2013)) that requires the partial correlation to be at least  $C \frac{1}{\sqrt{n}}$ .

Moreover, in terms of support recovery and computation cost, the proposed method has several advantages as compared to popular penalized likelihood approaches:

1. As we mentioned before, the FDR is a basic performance measure of support recovery of MGGMs. The proposed method provides an accurate control of FDR (see Theorem 3); however, the existing optimization-based approaches remain unclear about how to choose the tuning parameter to control a desired FDR while keeping nontrivial statistical power. In fact, existing support recovery results only guarantee that the estimated positions of zeros are supersets of the positions of true zeros in  $\Omega$  and  $\Gamma$  with probability tending to one when  $n, p, q$  all go to infinity at certain rates. (see, e.g., Leng and Tang (2012); Yin and Li (2012)).
2. In terms of computation, as compared to existing penalized likelihood methods whose objective functions are non-convex, our approach is completely based on convex optimization and thus computationally more attractive. In particular, the main computational cost of our approach is the construction of initial estimates for  $p + q$  regression coefficient vectors, which will directly lead to our test statistics. The corresponding computational problems are completely independent allowing an efficient parallel implementation.
3. Theoretically, our approach allows a wider range of  $p$  and  $q$ . In particular, our result on FDR control holds for  $(p, q)$  such that  $q^{r_2} \leq p \leq q^{r_1}$  for some  $0 < r_2 \leq r_1$ , while in comparison, Leng and Tang (2012) require that  $p \log(p) = o(nq)$  and  $q \log(q) = o(np)$ . As one can see, if  $n$  is a constant or  $n \rightarrow \infty$  but  $n = o(\min(\log p, \log q))$ , such a condition will not hold.

## 2 Notations and Organization of the paper

We introduce some necessary notations. Let  $\mathbf{X}^{(k)} = (X_{ij}^{(k)})_{p \times q}$  for  $k = 1, \dots, n$  be the  $n$  *i.i.d.* matrix-variate observations from  $N_{p,q}(\boldsymbol{\mu}, \boldsymbol{\Sigma} \otimes \boldsymbol{\Psi})$  and let  $\bar{\mathbf{X}} = \frac{1}{n} \sum_{k=1}^n \mathbf{X}^{(k)}$ . Put  $\boldsymbol{\Sigma} = (\sigma_{ij})$  and  $\boldsymbol{\Psi} = (\psi_{ij})$ . For any vector  $\mathbf{x} = (x_1, \dots, x_p)'$ , let  $\mathbf{x}_{-i}$  denote  $p - 1$  dimensional vector by removing  $x_i$  from  $\mathbf{x}$ . Let  $\langle \mathbf{x}, \mathbf{y} \rangle$  be the inner product of two vectors  $\mathbf{x}$  and  $\mathbf{y}$ . For any  $p \times q$  matrix  $\mathbf{A}$ , let  $\mathbf{A}_{i \cdot}$  denote the  $i$ -th row of  $\mathbf{A}$  (or  $\mathbf{A}_i$  when it is clear from the context)



and  $\mathbf{A}_{\cdot,j}$  denote the  $j$ -th column of  $\mathbf{A}$  (or  $\mathbf{A}_j$  when it is clear from the context). Further, let  $\mathbf{A}_{i,-j}$  denote the  $i$ -th row of  $\mathbf{A}$  with its  $j$ -th entry being removed and  $\mathbf{A}_{-i,j}$  denotes the  $j$ -th column of  $\mathbf{A}$  with its  $i$ -th entry being removed.  $\mathbf{A}_{-i,-j}$  denote a  $(p-1) \times (q-1)$  matrix by removing the  $i$ -th row and  $j$ -th column of  $\mathbf{A}$ . Define  $[n] = \{1, \dots, n\}$ ,  $[p] = \{1, \dots, p\}$  and  $[q] = \{1, \dots, q\}$ . For a  $p$ -dimensional vector  $\mathbf{x}$ , let  $\|\mathbf{x}\|_0 = \sum_{j=1}^p I(x_j \neq 0)$ ,  $\|\mathbf{x}\|_1 = \sum_{j=1}^p |x_j|$  and  $\|\mathbf{x}\|_2 = \sqrt{\sum_{j=1}^p x_j^2}$  be the  $\ell_0$ ,  $\ell_1$  and Euclidean norm of  $\mathbf{x}$ , respectively. For a matrix  $\mathbf{A} = (a_{ij}) \in \mathbb{R}^{p \times q}$ , let  $\|\mathbf{A}\|_F = \sqrt{\sum_{i \in [p], j \in [q]} a_{ij}^2}$  be the Frobenius norm of  $\mathbf{A}$ ,  $\|\mathbf{A}\|_\infty = \max_{i \in [p], j \in [q]} |a_{ij}|$  be the element-wise  $\ell_\infty$ -norm of  $\mathbf{A}$  and  $\|\mathbf{A}\|_2 = \sup_{\|\mathbf{x}\|_2 \leq 1} \|\mathbf{A}\mathbf{x}\|_2$  be the spectral norm of  $\mathbf{A}$ . For a square matrix  $\mathbf{A}$ , let  $\text{tr}(\mathbf{A})$  denote the trace of  $\mathbf{A}$ . For a given set  $\mathcal{H}$ , let  $\text{Card}(\mathcal{H})$  be the cardinality of  $\mathcal{H}$ . Throughout the paper, we use  $\mathbf{I}_p$  to denote the  $p \times p$  identity matrix, and use  $C$ ,  $c$ , etc. to denote generic constants whose values might change from place to place.

The rest of the paper is organized as follows. In Section 3, we introduce our test statistics and then describe the FDR control procedure for MGGM estimation. Theoretical results on asymptotic normality of our test statistic and FDR control are given in Section 4. Simulations and real data analysis are given in Section 5. In Section 6, we provide further discussions on the proposed method and also point out some interesting future work. All of the technical proofs and some additional experimental results are relegated to the supplementary material.

### 3 Methodology

Recall the definition of false discover proportion (FDP) as the proportion of false discoveries among total rejections. Note that, if  $\widehat{\text{supp}}(\mathbf{\Omega})$  and  $\widehat{\text{supp}}(\mathbf{\Gamma})$  are the estimators of  $\text{supp}(\mathbf{\Omega})$  and  $\text{supp}(\mathbf{\Gamma})$ , respectively, under the control of FDP at level  $\alpha \in [0, 1]$ , it is clear that the FDP of  $\widehat{\text{supp}}(\mathbf{\Omega}) \otimes \widehat{\text{supp}}(\mathbf{\Gamma})$  as an estimator of  $\text{supp}(\mathbf{\Omega} \otimes \mathbf{\Gamma})$  will be controlled at some level  $\alpha'$ . Here, the level  $\alpha'$  (explicitly given later in (4.32)) is a monotonically increasing function in  $\alpha$ . Therefore, we reduce our task to design an estimator of  $\text{supp}(\mathbf{\Gamma})$  under the FDP level  $\alpha$  and the estimator of  $\text{supp}(\mathbf{\Omega})$  can be constructed in a completely symmetric way. We propose to estimate  $\text{supp}(\mathbf{\Gamma})$  by implementing the following large-scale multiple tests:

$$H_{0ij} : \gamma_{ij} = 0 \quad \text{vs.} \quad H_{1ij} : \gamma_{ij} \neq 0, \quad 1 \leq i < j \leq q. \quad (3.4)$$

### 3.1 Construction of test statistics

In this section, we propose our test statistic for each  $H_{0ij}$  in (3.4) constructed from  $n$  *i.i.d.*  $p \times q$  matrix-variate samples  $\mathbf{X}^{(1)}, \dots, \mathbf{X}^{(n)}$  with the population distribution  $\mathbf{X} \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma} \otimes \boldsymbol{\Psi})$ . Let us denote the partial correlation matrix associated with  $\boldsymbol{\Gamma}$  by  $\boldsymbol{\rho}^{\boldsymbol{\Gamma}} = (\rho_{ij}^{\boldsymbol{\Gamma}})_{q \times q}$ , where each  $\rho_{ij}^{\boldsymbol{\Gamma}} = -\frac{\gamma_{ij}}{\sqrt{\gamma_{ii}\gamma_{jj}}}$  is the partial correlation coefficient between  $X_{li}$  and  $X_{lj}$  for any  $1 \leq l \leq p$ . The following well-known result relates the partial correlation coefficient  $\rho_{ij}^{\boldsymbol{\Gamma}}$  to regression problems. In particular, for  $1 \leq i < j \leq q$  and any  $1 \leq l \leq p$ , let us define the population regression coefficients:

$$(\alpha_i, \boldsymbol{\beta}_i) = \arg \min_{a \in \mathbb{R}, \mathbf{b} \in \mathbb{R}^{q-1}} \mathbb{E}(X_{li} - a - \mathbf{X}_{l,-i} \mathbf{b})^2, (\alpha_j, \boldsymbol{\beta}_j) = \arg \min_{a \in \mathbb{R}, \mathbf{b} \in \mathbb{R}^{q-1}} \mathbb{E}(X_{lj} - a - \mathbf{X}_{l,-j} \mathbf{b})^2. \quad (3.5)$$

The standard linear regression result shows that

$$\boldsymbol{\beta}_i = -\gamma_{ii}^{-1} \boldsymbol{\Gamma}_{-i,i}; \quad \boldsymbol{\beta}_j = -\gamma_{jj}^{-1} \boldsymbol{\Gamma}_{-j,j}. \quad (3.6)$$

For such defined  $\boldsymbol{\beta}_i$  and  $\boldsymbol{\beta}_j$ , the corresponding residuals  $\epsilon_{li}$  and  $\epsilon_{lj}$  take the following form,

$$\epsilon_{li} = X_{li} - \alpha_i - \mathbf{X}_{l,-i} \boldsymbol{\beta}_i; \quad \epsilon_{lj} = X_{lj} - \alpha_j - \mathbf{X}_{l,-j} \boldsymbol{\beta}_j. \quad (3.7)$$

It is known that  $\mathbb{E}(\epsilon_{li}) = \mathbb{E}(\epsilon_{lj}) = 0$ . Moreover, the correlation between  $\epsilon_{li}$  and  $\epsilon_{lj}$  is  $\text{Corr}(\epsilon_{li}, \epsilon_{lj}) = -\rho_{ij}^{\boldsymbol{\Gamma}} = \frac{\gamma_{ij}}{\sqrt{\gamma_{ii}\gamma_{jj}}}$ . To see this, let  $\boldsymbol{\gamma}_i$  be the  $i$ -th column of  $\boldsymbol{\Gamma}$  for  $1 \leq i \leq q$ . By (3.6) and (3.7), we can equivalently write  $\epsilon_{li} = -\alpha_i + \gamma_{ii}^{-1} \mathbf{X}_{l,\cdot} \boldsymbol{\gamma}_i$  and  $\epsilon_{lj} = -\alpha_j + \gamma_{jj}^{-1} \mathbf{X}_{l,\cdot} \boldsymbol{\gamma}_j$ . Since the covariance of  $\mathbf{X}_{l,\cdot}$ ,  $\text{Cov}(\mathbf{X}_{l,\cdot})$ , is  $\sigma_u \boldsymbol{\Psi} = \sigma_u \boldsymbol{\Gamma}^{-1}$ , we have

$$\text{Cov}(\epsilon_{li}, \epsilon_{lj}) = \gamma_{ii}^{-1} \gamma_{jj}^{-1} \boldsymbol{\gamma}_i^T \text{Cov}(\mathbf{X}_{l,\cdot}) \boldsymbol{\gamma}_j = \sigma_u \gamma_{ii}^{-1} \gamma_{jj}^{-1} (\boldsymbol{\gamma}_i^T \boldsymbol{\Gamma}^{-1}) \boldsymbol{\gamma}_j = \sigma_u \gamma_{ii}^{-1} \gamma_{jj}^{-1} \gamma_{ij}, \quad (3.8)$$

where the last equality is because  $\boldsymbol{\gamma}_i^T \boldsymbol{\Gamma}^{-1} = \mathbf{e}_i^T$  and  $\mathbf{e}_i$  denotes the  $i$ -th canonical vector. Similarly, we obtain that  $\text{Var}(\epsilon_{li}) = \sigma_u \gamma_{ii}^{-1}$  and  $\text{Var}(\epsilon_{lj}) = \sigma_u \gamma_{jj}^{-1}$ , which together with (3.8) imply that  $\text{Corr}(\epsilon_{li}, \epsilon_{lj}) = \frac{\gamma_{ij}}{\sqrt{\gamma_{ii}\gamma_{jj}}}$ . Therefore, testing whether  $\gamma_{ij} = 0$  (or  $\rho_{ij}^{\boldsymbol{\Gamma}} = 0$ ) is equivalent to testing whether  $\text{Corr}(\epsilon_{li}, \epsilon_{lj}) = 0$ . We will build our test statistics based on this key equivalence relationship.

To implement the aforementioned idea, one needs to construct an initial estimator for each  $\boldsymbol{\beta}_j$  so that the distribution of sample correlation coefficient of residuals can be deduced

easily. To construct the initial estimator, we first let  $\widehat{\boldsymbol{\beta}}_j = (\widehat{\beta}_{1,j}, \dots, \widehat{\beta}_{q-1,j})'$  be any estimator for  $\boldsymbol{\beta}_j$ , which satisfies

$$\max_{1 \leq j \leq q} |\widehat{\boldsymbol{\beta}}_j - \boldsymbol{\beta}_j|_1 = O_{\mathbb{P}}(a_{n1}), \quad \text{and} \quad \max_{1 \leq j \leq q} |\widehat{\boldsymbol{\beta}}_j - \boldsymbol{\beta}_j|_2 = O_{\mathbb{P}}(a_{n2}), \quad (3.9)$$

where  $a_{n1} \rightarrow 0$  and  $a_{n2} \rightarrow 0$  at some rate that will be specified later. The Lasso (Tibshirani, 1996), Dantzig selector (Candès and Tao, 2007), or other sparse regression approaches can be adopted provided that (3.9) is satisfied (see Section 3.2 for details). Under the null  $H_{0ij}$ :  $\gamma_{ij} = 0$ , according to (3.6), the  $i$ -th element in  $\boldsymbol{\beta}_j$ , which corresponds to the covariate  $X_{li}$  in (3.7), is zero; and the  $(j-1)$ -th element in  $\boldsymbol{\beta}_i$  which corresponds to the covariate  $X_{lj}$  in (3.7), is also zero. Hence, for each pair  $i < j$ , we construct the initial estimators  $\widehat{\boldsymbol{\beta}}_{j,\setminus i} = (\widehat{\beta}_{1,j}, \dots, \widehat{\beta}_{i-1,j}, 0, \widehat{\beta}_{i+1,j}, \dots, \widehat{\beta}_{q-1,j})'$  and  $\widehat{\boldsymbol{\beta}}_{i,\setminus j} = (\widehat{\beta}_{1,i}, \dots, \widehat{\beta}_{j-2,i}, 0, \widehat{\beta}_{j,i}, \dots, \widehat{\beta}_{q-1,i})'$  for  $\boldsymbol{\beta}_j$  and  $\boldsymbol{\beta}_i$ , respectively. For notation brevity, we let  $\widehat{\boldsymbol{\beta}}_{j,\setminus j} = \widehat{\boldsymbol{\beta}}_j$  so that the ‘‘sample residual’’  $\widehat{\varepsilon}_{ljj}^{(k)}$  introduced in the below is also well-defined (see (3.10)).

Given the initial estimators under the null, we construct the ‘‘sample residuals’’ by treating each row  $l \in [p]$  of a matrix-variate observation  $\mathbf{X}^{(k)}$  for  $k \in [n]$  as a ‘‘row sample’’, i.e.,  $\mathbf{X}_l^{(k)} = (X_{l1}^{(k)}, \dots, X_{lq}^{(k)})$ . The ‘‘sample residuals’’ corresponding to  $\epsilon_{li}$  and  $\epsilon_{lj}$  in (3.7) are defined as follows:

$$\widehat{\varepsilon}_{lij}^{(k)} = X_{li}^{(k)} - \bar{X}_{li} - (\mathbf{X}_{l,-i}^{(k)} - \bar{\mathbf{X}}_{l,-i}) \widehat{\boldsymbol{\beta}}_{i,\setminus j}, \quad \widehat{\varepsilon}_{lji}^{(k)} = X_{lj}^{(k)} - \bar{X}_{lj} - (\mathbf{X}_{l,-j}^{(k)} - \bar{\mathbf{X}}_{l,-j}) \widehat{\boldsymbol{\beta}}_{j,\setminus i}, \quad (3.10)$$

where  $\bar{X}_{li} = \frac{1}{n} \sum_{k=1}^n X_{li}^{(k)}$  and  $\bar{\mathbf{X}}_{l,-i} = \frac{1}{n} \sum_{k=1}^n \mathbf{X}_{l,-i}^{(k)}$ . Further let  $\widehat{r}_{ij}$  be the sample covariance coefficient between constructed residuals,

$$\widehat{r}_{ij} = \frac{1}{(n-1)p} \sum_{k=1}^n \sum_{l=1}^p \widehat{\varepsilon}_{lij}^{(k)} \widehat{\varepsilon}_{lji}^{(k)}, \quad (3.11)$$

and  $\frac{\widehat{r}_{ij}}{\sqrt{\widehat{r}_{ii}\widehat{r}_{jj}}}$  be the corresponding sample correlation coefficient of residuals.

The proposed construction of the sample correlation of residuals has twofold benefits. First, under the null  $H_{0ij}$ , incorporating the fact that  $\gamma_{ij} = 0$  into the regression coefficients enables us to derive the asymptotic null distribution of the sample correlation coefficients. In particular, later in Proposition 1, we show that under the null,

$$\sqrt{\frac{(n-1)p}{A_p}} \frac{\widehat{r}_{ij}}{\sqrt{\widehat{r}_{ii}\widehat{r}_{jj}}} \Rightarrow N(0, 1), \quad (3.12)$$

where

$$A_p = \frac{p \|\boldsymbol{\Sigma}\|_F^2}{(\text{tr}(\boldsymbol{\Sigma}))^2}. \quad (3.13)$$

Here,  $A_p$  is the asymptotic variance of  $\sqrt{(n-1)p} \frac{\hat{r}_{ij}}{\sqrt{\hat{r}_{ii}\hat{r}_{jj}}}$  under the null. It is noteworthy that the term  $A_p$  is critical since it plays the role of *variance correction* when treating rows of matrix-variate data as correlated samples. The second merit of the proposed construction is that, although the sample correlation coefficients are constructed under the null, we can show that  $\frac{\hat{r}_{ij}}{\sqrt{\hat{r}_{ii}\hat{r}_{jj}}}$  converges to  $(1 - \gamma_{ij}\psi_{ij})\rho_{ij}^\Gamma$  in probability as  $np \rightarrow \infty$  under both the null and alternative (see Proposition 2). This result indicates that the test statistic based on  $\frac{\hat{r}_{ij}}{\sqrt{\hat{r}_{ii}\hat{r}_{jj}}}$  can properly reject the null when the magnitude of partial correlation coefficient  $|\rho_{ij}^\Gamma|$  is away from zero. It is worth noting that for many widely studied covariance structures of  $\boldsymbol{\Psi}$  and  $\boldsymbol{\Gamma} = \boldsymbol{\Psi}^{-1}$ , the quantity  $\psi_{ij}\gamma_{ij}$  is often non-positive, which makes the signal strength  $(1 - \gamma_{ij}\psi_{ij})\rho_{ij}^\Gamma$  even larger than the partial correlation coefficient and thus leads to good statistical power. For example, for two variables which are directly positively/negatively correlated, they will often be positively/negatively conditional correlated.

It is worthwhile to note that the variance correction quantity  $A_p \in \mathbb{R}$  in (3.12) is unknown as it involves  $\boldsymbol{\Sigma}$ . In the next subsection, we will propose a ratio consistent estimator  $\hat{A}_p$  such that  $\hat{A}_p/A_p \rightarrow 1$  in probability as  $nq \rightarrow \infty$ . Using the estimator  $\hat{A}_p$ , we construct the final test statistic for  $H_{0ij}$ :

$$\hat{T}_{ij} = \sqrt{\frac{(n-1)p}{\hat{A}_p} \frac{\hat{r}_{ij}}{\sqrt{\hat{r}_{ii}\hat{r}_{jj}}}}, \quad (3.14)$$

which is asymptotically normal given (3.12) and the ratio consistency of  $\hat{A}_p$ .

### 3.1.1 Estimator for $A_p$

We propose an estimator  $\hat{A}_p$  of  $A_p$  based on a thresholding estimator of  $\boldsymbol{\Sigma}$ . We first construct an initial estimator of  $\boldsymbol{\Sigma}$  based on  $nq$  ‘‘column samples’’, where each column of  $\mathbf{X}^{(k)}$  for  $k \in [n]$  is treated as a  $p$ -dimensional sample. In particular, let  $\bar{\mathbf{X}} = \frac{1}{n} \sum_{k=1}^n \mathbf{X}^{(k)}$ , each centered column sample  $\mathbf{Y}_{kj} = \mathbf{X}_{\cdot,j}^{(k)} - \bar{\mathbf{X}}_{\cdot,j} \in \mathbb{R}^{p \times 1}$  for  $k \in [n]$  and  $j \in [q]$ . Moreover, let us define  $\hat{\boldsymbol{\Sigma}} = (\hat{\sigma}_{ij})_{p \times p} := \frac{1}{(n-1)q} \sum_{k=1}^n \sum_{j=1}^q (\mathbf{Y}_{kj})(\mathbf{Y}_{kj})'$ . In a more succinct notation, let  $\mathbf{Y} = [\mathbf{X}^{(1)} - \bar{\mathbf{X}}, \dots, \mathbf{X}^{(n)} - \bar{\mathbf{X}}] \in \mathbb{R}^{p \times (nq)}$  and  $\hat{\boldsymbol{\Sigma}} = \frac{1}{(n-1)q} \mathbf{Y}\mathbf{Y}'$ . Then, we threshold the elements

of  $\widehat{\Sigma}$  as follows:

$$\widehat{\sigma}_{ij,\lambda} = \widehat{\sigma}_{ij} I \left\{ |\widehat{\sigma}_{ij}| \geq \lambda \sqrt{\frac{\log \max(p, nq)}{nq}} \right\} \quad \text{for } i \neq j; \quad (3.15)$$

and  $\widehat{\sigma}_{ii,\lambda} = \widehat{\sigma}_{ii}$  for  $i \in [p]$ . Set  $\widehat{\Sigma}_\lambda = (\widehat{\sigma}_{ij,\lambda})_{p \times p}$  and define the plug-in estimator of  $A_p$ :

$$\widehat{A}_p = \frac{p \|\widehat{\Sigma}_\lambda\|_F^2}{(\text{tr}(\widehat{\Sigma}_\lambda))^2}. \quad (3.16)$$

In Proposition 3 in Section 4, we show that  $\widehat{A}_p/A_p \rightarrow 1$  in probability as  $nq \rightarrow \infty$  for a properly chosen  $\lambda$  (a data-driven approach for the choice of  $\lambda$  will be discussed later in Section 3.2). Therefore, by (3.12), we have the desired asymptotic normality of  $\widehat{T}_{ij}$  under the null:  $\widehat{T}_{ij} \Rightarrow N(0, 1)$  as  $np \rightarrow \infty$ .

We further note that when the columns of  $\mathbf{X}$  are *i.i.d.* (i.e.,  $\Psi = \mathbf{I}_q$ ), consistency under the spectral norm  $\|\widehat{\Sigma}_\lambda - \Sigma\|_2$  has been established if the sparsity condition of  $\Sigma$  satisfies the row sparsity level  $s_0(p) = O(\sqrt{nq/\log p})$  (see, e.g., Bickel and Levina (2008); Cai and Liu (2011) and references therein). We do not need such a strong consistency result of  $\widehat{\Sigma}_\lambda$  in the spectral norm to establish the consistency of  $\widehat{A}_p$ . In fact, since  $A_p$  only involves  $\|\Sigma\|_F$  rather than  $\Sigma$  itself, the sparsity condition on  $s_0(p)$  is no longer necessary; see Proposition 3 and its proof for more details. It is also noteworthy that some other estimators of  $\|\Sigma\|_F$  have been proposed (e.g., by Chen and Qin (2010)). However, those approaches heavily rely on the *i.i.d.* assumption on the columns of  $\mathbf{X}$ , which is not valid in our setting.

### 3.2 Initial estimators of regression coefficients

In the construction of the test statistic  $\widehat{T}_{ij}$ , we need the estimate  $\widehat{\beta}_j$  that satisfies the condition in (3.9). Here, we choose to construct  $\widehat{\beta}_j$  using Lasso for the presentation simplicity, however other approaches such as the Dantzig selector can also be used. In particular, let  $\mathbf{Z} = [(\mathbf{X}^{(1)})' - \bar{\mathbf{X}}', \dots, (\mathbf{X}^{(n)})' - \bar{\mathbf{X}}'] \in \mathbb{R}^{q \times (np)}$  be  $np$   $q$ -dimensional samples extracted from the data, and  $\widehat{\Psi} = \frac{1}{(n-1)p} \mathbf{Z}\mathbf{Z}' =: (\widehat{\psi}_{ij})_{q \times q}$ . For  $1 \leq j \leq q$ , define the scaling/normalizing vector  $\mathbf{D}_j = \text{diag}(\widehat{\Psi}_{-j,-j}) \in \mathbb{R}^{(q-1) \times (q-1)}$ . The coefficients  $\beta_j$  can be estimated by Lasso as follows:

$$\widehat{\beta}_j(\delta) = \mathbf{D}_j^{-1/2} \widehat{\alpha}_j(\delta), \quad (3.17)$$

where

$$\widehat{\boldsymbol{\alpha}}_j(\delta) = \arg \min_{\boldsymbol{\alpha} \in \mathbb{R}^{q-1}} \left\{ \frac{1}{2np} \sum_{k=1}^n \sum_{l=1}^p (X_{lj}^{(k)} - \bar{X}_{lj} - (\mathbf{X}_{l,-j}^{(k)} - \bar{\mathbf{X}}_{l,-j}) \mathbf{D}_j^{-1/2} \boldsymbol{\alpha})^2 + \theta_{nj}(\delta) |\boldsymbol{\alpha}|_1 \right\} \quad (3.18)$$

and

$$\theta_{nj}(\delta) = \delta \sqrt{\frac{\widehat{\psi}_{jj} \log \max(q, np)}{np}}. \quad (3.19)$$

In the Lasso estimate in (3.18), the  $np$  covariates-response pairs  $(\mathbf{X}_{l,-j}^{(k)} - \bar{\mathbf{X}}_{l,-j}, X_{lj}^{(k)} - \bar{X}_{lj})$  for  $k \in [n]$  and  $j \in [p]$  are not *i.i.d.* and thus the standard consistency result of Lasso cannot be applied here. By exploring the correlation structure among rows of  $\mathbf{X}$ , we managed to derive the rate of convergence of the Lasso estimator in the  $\ell_1$  and the  $\ell_2$  norms. This result (see Proposition 4 and its proof) might be of independent interest for dealing with high-dimensional correlated data. For the choice of tuning parameters, our theoretical results will hold for any large enough constants  $\lambda$  in (3.15) for estimating  $\widehat{A}_p$  (see Proposition 3) and  $\delta > 0$  in (3.19) for  $\widehat{\boldsymbol{\beta}}_j(\delta)$  (see Proposition 4). In our experiment, we will adopt a data-driven parameter-tuning strategy from Liu (2013).

### 3.3 FDR control procedure

Given the constructed test statistic  $\widehat{T}_{ij}$ , we can carry out  $(q^2 - q)/2$  tests in (3.4) simultaneously using the popular Benjamini and Hochberg (BH) method (Benjamini and Hochberg, 1995). Let the  $p$ -values  $p_{ij} = 2 - 2\Phi(|\widehat{T}_{ij}|)$  for  $1 \leq i < j \leq q$ . We sort these  $m = (q^2 - q)/2$   $p$ -values such that  $p_{(1)} < \dots < p_{(m)}$ . For a given  $0 < \alpha < 1$ , define

$$\widehat{k} = \max\{0 \leq k \leq m : p_{(k)} \leq \alpha k/m\}.$$

For  $1 \leq i \neq j \leq q$ , we reject  $H_{0ij}$  if  $p_{ij} \leq p_{(\widehat{k})}$  and the estimated support of  $\boldsymbol{\Gamma}$  is

$$\widehat{\text{supp}}(\boldsymbol{\Gamma}) = \{(i, j) : p_{ij} \leq p_{(\widehat{k})}, 1 \leq i \neq j \leq q\} \cup \{(i, i) : 1 \leq i \leq q\}. \quad (3.20)$$

Note that we set  $\widehat{T}_{ji} = \widehat{T}_{ij}$  for  $1 \leq i < j \leq q$  in (3.20).

Note that the original results from Benjamini and Hochberg (1995) cannot be directly applied to obtain the guarantee of FDR control since the test statistics (and thus the  $p$ -



values) are correlated with each other. By utilizing some proof techniques developed by Liu (2013), we manage to prove that this procedure controls the FDR/FDP asymptotically in  $\widehat{\text{supp}}(\mathbf{\Gamma})$  (see Section 4.2 for details).

**Estimation of  $\text{supp}(\mathbf{\Omega})$ .** The estimation of  $\text{supp}(\mathbf{\Omega})$  can be done with a completely symmetric procedure. In particular, we only need to consider the transpose of each matrix-variate observation  $\mathbf{X}^{(k)}$ , i.e.,  $(\mathbf{X}^{(1)})', \dots, (\mathbf{X}^{(n)})'$  and change some necessary notations (e.g.,  $p$  to  $q$  and  $q$  to  $p$ ).

**Estimation of  $\text{supp}(\mathbf{\Omega} \otimes \mathbf{\Gamma})$ .** Let  $\widehat{\text{supp}}(\mathbf{\Omega})$  and  $\widehat{\text{supp}}(\mathbf{\Gamma})$  be the estimators of  $\text{supp}(\mathbf{\Omega})$  and  $\text{supp}(\mathbf{\Gamma})$ , respectively, under the control of FDR at level  $\alpha$ . The support of  $\mathbf{\Omega} \otimes \mathbf{\Gamma}$  can then be estimated by  $\widehat{\text{supp}}(\mathbf{\Omega}) \otimes \widehat{\text{supp}}(\mathbf{\Gamma})$ . In Theorem 3, we will show that the FDR/FDP of this estimator is controlled at level

$$\alpha' = \frac{\alpha((2 - \alpha)ab + aq + bp)}{\max(ab + aq + pb, 1)} \quad (3.21)$$

asymptotically, where  $a$  and  $b$  are the numbers of total discoveries in  $\widehat{\text{supp}}(\mathbf{\Omega})$  and  $\widehat{\text{supp}}(\mathbf{\Gamma})$ , respectively, excluding the diagonal entries. We also note that when the FDR/FDP level  $\alpha'$  for the joint support estimation is given, to determine the FDR level  $\alpha$  for the estimation of  $\text{supp}(\mathbf{\Omega})$  and  $\text{supp}(\mathbf{\Gamma})$ , one can try a sequence of  $\alpha$ 's from a small value to a large value. For each candidate  $\alpha$ , we obtain the value  $a$  and  $b$  by estimating  $\text{supp}(\mathbf{\Omega})$  and  $\text{supp}(\mathbf{\Gamma})$  and plug the obtained values into (3.21). Finally, we will choose the value  $\alpha$  for the separate estimation that leads to the closest value to the pre-given  $\alpha'$ .

**Remark 1.** One natural approach that for solving our problem is the de-correlation method. More precisely, if  $\mathbf{\Sigma}$  is known, the data matrix can be transformed as  $\mathbf{\Sigma}^{-1/2}\mathbf{X} \sim N(\mathbf{\Sigma}^{-1/2}\boldsymbol{\mu}, \mathbf{I}_{p \times p} \otimes \mathbf{\Psi})$ , based on which the method from Liu (2013) can be applied. Therefore, a natural two-stage approach is to first obtain a consistent estimator of  $\mathbf{\Sigma}^{-1/2}$  (e.g., Cai et al. (2011)) and then apply the FDR control approach of Liu (2013) to  $\widehat{\mathbf{\Sigma}}^{-1/2}\mathbf{X}^{(i)}$  for  $1 \leq i \leq n$ . However, this “de-correlation” approach is not applicable under our problem setup. In fact, to ensure the estimation error between  $\widehat{\mathbf{\Sigma}}^{-1/2}$  and  $\mathbf{\Sigma}^{-1/2}$  is negligible for the FDR control, by some elementary calculations, we can find that we need the condition

$$\frac{nq}{(ps^2(p))^{1/(1-\tau)}} \rightarrow \infty \quad (3.22)$$

to replace  $\mathbf{\Sigma}^{-1/2}$  by  $\widehat{\mathbf{\Sigma}}^{-1/2}$ . (This condition means that we need a large sample number  $nq$

to estimate  $\Sigma^{-1/2}$  accurately.) Similarly, to replace  $\Psi^{-1/2}$  by  $\widehat{\Psi}^{-1/2}$ , we need the condition

$$\frac{np}{(qs^2(q))^{1/(1-\tau)}} \rightarrow \infty. \quad (3.23)$$

Hence, to get  $\widehat{\text{supp}}(\Sigma^{-1}) \otimes \widehat{\text{supp}}(\Psi^{-1})$ , we need (3.22) and (3.23) simultaneously. However, when  $n$  is fixed or small, (3.22) and (3.23) are contrary. Hence, it is impossible to do the de-correlation for rows and columns of  $\mathbf{X}$  simultaneously.

## 4 Theoretical Results

In this section, we provide the properties of the developed test statistic in (3.14), the guarantee of FDR control, power analysis and convergence rate of the initial estimator. All the proofs are relegated to the supplement.

Let  $\lambda_{\min}(\Sigma) = \lambda_1^{(1)} \leq \dots \leq \lambda_p^{(1)} = \lambda_{\max}(\Sigma)$  be eigenvalues of  $\Sigma$  and  $\lambda_{\min}(\Psi) = \lambda_1^{(2)} \leq \dots \leq \lambda_q^{(2)} = \lambda_{\max}(\Psi)$  be eigenvalues of  $\Psi$ . We make the following typical assumption on eigenvalues throughout this section:

**(C1).** We assume that  $c^{-1} \leq \lambda_1^{(1)} \leq \dots \leq \lambda_p^{(1)} \leq c$  and  $c^{-1} \leq \lambda_1^{(2)} \leq \dots \leq \lambda_q^{(2)} \leq c$  for some constant  $c > 0$ .

The condition (C1) is a standard eigenvalue assumption in high-dimensional covariance estimation literature (see the survey Cai et al. (2016) and references therein). This assumption is natural for many important classes of covariance matrices, e.g., bandable, Toeplitz, and sparse covariance matrices. It is worthwhile to note that the assumption (C1) implies that  $1/c' \leq A_p \leq c'$  (see  $A_p$  in (3.13)) for some constant  $c' > 0$ . We first provide some key results on the properties of the test statistic and the estimator  $\widehat{A}_p$  of  $A_p$  in the next subsection.

### 4.1 Asymptotic normality and convergence results of the proposed test statistics

The first result gives the asymptotic normality for the test statistic  $\sqrt{\frac{(n-1)p}{A_p}} \frac{\widehat{r}_{ij}}{\sqrt{\widehat{r}_{ii}\widehat{r}_{jj}}}$  in (3.12) under the null.

**Proposition 1.** *Assume that, as  $np \rightarrow \infty$ ,  $\log \max(q, np) = o(np)$ , and the estimator  $\widehat{\beta}_j$*

for  $j \in [q]$  satisfies (3.9) with

$$a_{n1} = o(1/\sqrt{\log \max(q, np)}) \quad \text{and} \quad a_{n2} = o((np)^{-1/4}). \quad (4.24)$$

Under the null  $H_{0ij} : \gamma_{ij} = 0$ , we have, as  $np \rightarrow \infty$ ,

$$\sqrt{\frac{(n-1)p}{A_p}} \frac{\widehat{r}_{ij}}{\sqrt{\widehat{r}_{ii}\widehat{r}_{jj}}} \Rightarrow N(0, 1)$$

in distribution, where  $\widehat{r}_{ii}$  and  $A_p$  are defined in (3.11) and (3.13), respectively.

The next proposition shows that under alternatives,  $\frac{\widehat{r}_{ij}}{\sqrt{\widehat{r}_{ii}\widehat{r}_{jj}}}$  will converge to a nonzero number, which indicates that our test statistics will lead to a non-trivial power. Recall that  $\rho_{ij}^\Gamma$  is the partial correlation coefficient between  $X_{li}$  and  $X_{lj}$  (for any  $1 \leq l \leq p$ ).

**Proposition 2.** *Suppose that conditions in Proposition 1 hold. We have, for  $1 \leq i < j \leq q$ ,*

$$\frac{\widehat{r}_{ij}}{\sqrt{\widehat{r}_{ii}\widehat{r}_{jj}}} - (1 - \gamma_{ij}\psi_{ij})\rho_{ij}^\Gamma \rightarrow 0$$

in probability as  $np \rightarrow \infty$ .

Also note that the condition in (4.24) will be established later in Proposition 4. It is interesting to see that in Propositions 1 and 2, we only require  $np \rightarrow \infty$ , which means that the sample size  $n$  can be a constant. This is a significant difference between the estimation of MGGMs and that of vector-variate GGMs. In the latter problem, to establish the asymptotic consistency or normality, the sample size is usually required to go to infinity in the existing literature (see, e.g., Rothman et al. (2008); Lam and Fan (2009); Liu (2013); Ren et al. (2015)).

We next establish the convergence rate for the estimator of  $A_p$ . To this end, we need an additional condition on  $\Sigma$ .

**(C2).** For some  $0 < \tau < 2$ , assume that  $\sum_{j=1}^p |\sigma_{ij}|^\tau \leq C s(p)$  with  $s(p) = \frac{1}{(\log q)^2} \left( \sqrt{\frac{nq}{\log \max(p, nq)}} \right)^{(2-\tau) \wedge 1}$  uniformly in  $1 \leq i \leq p$ .

Note that when  $0 < \tau < 1$ , this assumption becomes the typical weak sparsity assumption in high-dimensional covariance estimation (Bühlmann and van de Geer, 2011).

**Proposition 3.** *Let  $\widetilde{\lambda} = \lambda \sqrt{\frac{\log \max(p, nq)}{nq}}$  with  $\lambda$  being sufficiently large. Suppose that (C2) holds. We have  $\widehat{A}_p/A_p = 1 + O_{\mathbb{P}}(\widetilde{\lambda}^{(2-\tau) \wedge 1} s(p))$  as  $nq \rightarrow \infty$ .*

Combining Propositions 1 and 3, we have the asymptotic normality under the null for our final test statistic  $\widehat{T}_{ij} = \sqrt{\frac{(n-1)p}{\widehat{A}_p}} \frac{\widehat{r}_{ij}}{\sqrt{\widehat{r}_{ii}\widehat{r}_{jj}}}$  in (3.14).

## 4.2 Guarantees on FDP/FDR control

We next show that the FDP and FDR of  $\widehat{\text{supp}}(\widehat{\Omega}) \otimes \widehat{\text{supp}}(\widehat{\Gamma})$  can be controlled asymptotically. To this end, we discuss the FDP and FDR of the estimation of  $\text{supp}(\Gamma)$  and  $\text{supp}(\Omega)$  separately. For the estimation of  $\text{supp}(\Gamma)$ , recall the definition of FDP and FDR:

$$\text{FDP}_1 = \frac{\sum_{(i,j) \in \mathcal{H}_0} I\{(i,j) \in \widehat{\text{supp}}(\Gamma)\}}{\max(\sum_{1 \leq i < j \leq q} I\{(i,j) \in \widehat{\text{supp}}(\Gamma)\}, 1)}, \quad \text{FDR}_1 = \mathbb{E}(\text{FDP}_1), \quad (4.25)$$

where  $\mathcal{H}_0 = \{(i,j) : \gamma_{ij} = 0, \quad 1 \leq i < j \leq q\}$ . Let  $\mathcal{H}_1 = \{(i,j) : \gamma_{ij} \neq 0, \quad 1 \leq i < j \leq q\}$ . Further define  $\varpi_0 = \text{Card}(\mathcal{H}_0)$  as the total number of true nulls,  $\varpi_1 = \text{card}(\mathcal{H}_1)$  as the number of true alternatives, and  $\varpi = (q^2 - q)/2$  as the total number of hypotheses. For a constant  $\gamma > 0$  and  $1 \leq i \leq q$ , define  $\mathcal{A}_i(\gamma) = \{j : 1 \leq j \leq q, j \neq i, |\gamma_{ij}| \geq (\log q)^{-2-\gamma}\}$ . Theorem 1 shows that our procedure controls FDP and FDR at a given level  $\alpha$  asymptotically.

**Theorem 1.** *Let the dimension  $(p, q)$  satisfy  $q \leq (np)^r$  for some  $r > 0$ . Suppose that*

$$\text{Card}\left\{(i,j) : 1 \leq i < j \leq q, \quad |(1 - \gamma_{ij}\psi_{ij})\rho_{ij}^\Gamma| \geq 4\sqrt{\frac{A_p \log q}{(n-1)p}}\right\} \geq \sqrt{\log \log q}, \quad (4.26)$$

where  $A_p$  is defined in (3.13). Assume that  $\varpi_1 \leq c\varpi$  for some  $c < 1$  and  $\{\widehat{\beta}_i\}_{i \in [q]}$  satisfy (3.9) with

$$a_{n1} = o(1/\log \max(q, np)) \quad \text{and} \quad a_{n2} = o((np \log q)^{-1/4}). \quad (4.27)$$

Under (C1), (C2), and  $\max_{1 \leq i \leq q} \text{Card}(\mathcal{A}_i(\gamma)) = O(q^\vartheta)$  for some  $\vartheta < 1/2$  and  $\gamma > 0$ , we have  $\lim_{np, q \rightarrow \infty} \frac{\text{FDR}_1}{\alpha \varpi_0 / \varpi} = 1$  and  $\frac{\text{FDP}_1}{\alpha \varpi_0 / \varpi} \rightarrow 1$  in probability as  $np, q \rightarrow \infty$ .

Condition (4.26) requires the number of true alternatives is at least  $\sqrt{\log \log q}$ . This condition is very mild and in fact, is a nearly necessary condition for the FDP control. Proposition 2.1 in Liu and Shao (2014) shows that, in large-scale multiple testing problems, if the number of true alternatives is fixed, then it is impossible for the Benjamini and Hochberg method (Benjamini and Hochberg, 1995) to control the FDP with probability tending to one

at any desired level. Note that (4.26) is only slightly stronger than the condition that the number of true alternatives goes to infinity. The condition on  $Card(\mathcal{A}_i(\gamma))$  is a sparsity condition for  $\mathbf{\Gamma}$ . This condition is also quite weak. For the estimation of vector-variate GGMs, the existing literature often requires the row sparsity level of precision matrix to be less than  $O(\sqrt{n})$ . Note that when the dimension  $q$  is much larger than  $n$ , our condition on  $Card(\mathcal{A}_i(\gamma))$  in Theorem 1 is clearly much weaker. It should be noted that in Theorem 1, the sample size  $n$  can be a fixed constant as long as the dimension  $p, q \rightarrow \infty$ .

As in Theorem 1, we have the similar FDP and FDR control result for the estimation of  $\text{supp}(\mathbf{\Omega})$ . Let  $\mathcal{H}'_0 = \{(i, j) : \omega_{ij} = 0, 1 \leq i < j \leq p\}$  and  $\mathcal{H}'_1 = \{(i, j) : \omega_{ij} \neq 0, 1 \leq i < j \leq p\}$ . Further, let  $\kappa_0 = Card(\mathcal{H}'_0)$ ,  $\kappa_1 = Card(\mathcal{H}'_1)$  and  $\kappa = (p^2 - p)/2$ . Recall the definition of FDP and FDR of the estimation of  $\text{supp}(\mathbf{\Omega})$ :

$$\text{FDP}_2 = \frac{\sum_{(i,j) \in \mathcal{H}'_0} I\{(i, j) \in \widehat{\text{supp}}(\mathbf{\Omega})\}}{\max(\sum_{1 \leq i < j \leq p} I\{(i, j) \in \widehat{\text{supp}}(\mathbf{\Omega})\}, 1)}, \quad \text{FDR}_2 = \mathbb{E}(\text{FDP}_2). \quad (4.28)$$

For a constant  $\gamma > 0$  and  $1 \leq i \leq p$ , define  $\mathcal{B}_i(\gamma) = \{j : 1 \leq j \leq p, j \neq i, |\omega_{ij}| \geq (\log p)^{-2-\gamma}\}$ . Let  $B_q = q\|\mathbf{\Psi}\|_{\text{F}}^2/(\text{tr}(\mathbf{\Psi}))^2$  and the partial correlation associated with  $\mathbf{\Omega}$  be  $\rho_{ij}^{\mathbf{\Omega}} = -\frac{\omega_{ij}}{\sqrt{\omega_{jj}\omega_{ii}}}$  for  $1 \leq i < j \leq p$ . As (C2), we assume the following condition on  $\mathbf{\Psi} = (\psi_{ij})_{p \times p}$ ,

**(C3).** For some  $0 < \tau < 2$ , assume that  $\sum_{j=1}^q |\psi_{ij}|^{\tau} \leq Cs(q)$  with  $s(q) = \frac{1}{(\log p)^2} \left( \sqrt{\frac{np}{\log \max(q, np)}} \right)^{(2-\tau) \wedge 1}$  uniformly in  $1 \leq i \leq q$ .

**Theorem 2.** Let the dimension  $(p, q)$  satisfy  $p \leq (nq)^r$  for some  $r > 0$ . Suppose that

$$Card\left\{(i, j) : 1 \leq i < j \leq p, |(1 - \omega_{ij}\sigma_{ij})\rho_{ij}^{\mathbf{\Omega}}| \geq 4\sqrt{\frac{B_q \log p}{(n-1)q}}\right\} \geq \sqrt{\log \log p}. \quad (4.29)$$

Assume that  $\kappa_1 \leq c\kappa$  for some  $c < 1$  and  $\{\widehat{\beta}_i\}_{i \in [p]}$  satisfies (3.9) with

$$a_{n1} = o(1/\log \max(p, nq)) \quad \text{and} \quad a_{n2} = o((nq \log p)^{-1/4}). \quad (4.30)$$

Under (C1), (C3), and  $\max_{1 \leq i \leq p} Card(\mathcal{B}_i(\gamma)) = O(p^{\vartheta})$  for some  $\vartheta < 1/2$  and  $\gamma > 0$ , we have  $\lim_{nq, p \rightarrow \infty} \frac{\text{FDR}_2}{\alpha\kappa_0/\kappa} = 1$  and  $\frac{\text{FDP}_2}{\alpha\kappa_0/\kappa} \rightarrow 1$  in probability as  $nq, p \rightarrow \infty$ .

By Theorems 1 and 2, we can obtain the FDP and FDR result of the estimator  $\widehat{\text{supp}}(\mathbf{\Omega}) \otimes \widehat{\text{supp}}(\mathbf{\Gamma})$ . In particular, let  $a_0$  and  $a$  be the number of false discoveries and total discoveries

in  $\widehat{\text{supp}}(\mathbf{\Omega})$ , excluding the diagonal entries. Similarly, let  $b_0$  and  $b$  be the number of false discoveries and total discoveries in  $\widehat{\text{supp}}(\mathbf{\Gamma})$ , excluding the diagonal entries. It is then easy to calculate that the number of false discoveries in  $\widehat{\text{supp}}(\mathbf{\Omega}) \otimes \widehat{\text{supp}}(\mathbf{\Gamma})$  is  $a_0(q+b) + (a-a_0)b_0 + pb_0$ , and the number of total discoveries in  $\widehat{\text{supp}}(\mathbf{\Omega}) \otimes \widehat{\text{supp}}(\mathbf{\Gamma})$  is  $pb + a(q+b)$  (excluding the diagonal entries). We have the following formulas for FDP and FDR of  $\widehat{\text{supp}}(\mathbf{\Omega}) \otimes \widehat{\text{supp}}(\mathbf{\Gamma})$ :

$$\text{FDP} = \frac{a_0(q+b) + (a-a_0)b_0 + pb_0}{\max(pb + a(q+b), 1)}, \quad \text{FDR} = \mathbb{E}(\text{FDP}). \quad (4.31)$$

The true FDP in (4.31) cannot be computed in practice since the number of false discoveries  $a_0$  and  $b_0$  are unknown. One straightforward estimator for FDP is to replace the unknown quantities  $a_0$  and  $b_0$  with  $\alpha a$  and  $\alpha b$ , respectively, which leads to the following FDP estimator  $\alpha'$ :

$$\alpha' = \frac{\alpha((2-\alpha)ab + aq + bp)}{\max(ab + aq + bp, 1)}. \quad (4.32)$$

Note that the values of  $a$  and  $b$  in (4.32) are known, which represent the number of total discoveries in  $\widehat{\text{supp}}(\mathbf{\Omega})$  and  $\widehat{\text{supp}}(\mathbf{\Gamma})$ , respectively. The FDP estimator  $\alpha'$  takes the value in  $[0, 1]$  and is monotonically increasing as a function of  $\alpha$ . In the next theorem, we show that  $\text{FDP}/\alpha' \rightarrow 1$  in probability as  $p, q \rightarrow \infty$ .

**Theorem 3.** *Under the conditions of Theorems 1 and 2 with the sparsity condition  $\omega_1 = o(\omega)$  and  $\kappa_1 = o(\kappa)$ , we have  $\frac{\text{FDP}}{\alpha'} \rightarrow 1$  in probability as  $p, q \rightarrow \infty$ .*

Theorem 3 shows that the FDP of the proposed estimator  $\widehat{\text{supp}}(\mathbf{\Omega}) \otimes \widehat{\text{supp}}(\mathbf{\Gamma})$  can be estimated consistently by  $\alpha'$ . Note that by Theorems 1 and 2, the sparsity conditions  $\omega_1 = o(\omega)$  and  $\kappa_1 = o(\kappa)$  imply that  $\frac{\text{FDP}_1}{\alpha} \rightarrow 1$  and  $\frac{\text{FDP}_2}{\alpha} \rightarrow 1$  in probability when  $p, q \rightarrow \infty$ . Therefore, one can replace  $a_0$  and  $b_0$  in FDP in (4.31) by  $\alpha a$  and  $\alpha b$ , respectively, and achieve the result in Theorem 3. In fact, we can still obtain the guarantee of FDP of  $\widehat{\text{supp}}(\mathbf{\Omega}) \otimes \widehat{\text{supp}}(\mathbf{\Gamma})$  even without the sparsity conditions  $\omega_1 = o(\omega)$  and  $\kappa_1 = o(\kappa)$ . For any  $\varepsilon > 0$ , Theorems 1 and 2 show that  $\mathbb{P}(\text{FDP}_1 \leq \alpha(1+\varepsilon)) \rightarrow 1$  and  $\mathbb{P}(\text{FDP}_2 \leq \alpha(1+\varepsilon)) \rightarrow 1$  as  $p, q \rightarrow \infty$  regardless of the sparsity conditions. This further implies the following guarantee on the FDP of  $\widehat{\text{supp}}(\mathbf{\Omega}) \otimes \widehat{\text{supp}}(\mathbf{\Gamma})$  for any  $\varepsilon > 0$ :

$$\mathbb{P}\left(\frac{\text{FDP}}{\alpha\{(2ab + aq + bp)/\max(ab + aq + bp, 1)\}} \leq 1 + \varepsilon\right) \rightarrow 1, \text{ as } p, q \rightarrow \infty.$$



### 4.3 Power analysis

We next study the statistical power of the proposed method by considering the following class of alternatives. We assume that for some  $c > 4$ ,

$$|\rho_{ij}^{\Gamma}| = c \sqrt{\frac{A_p \log q}{(n-1)p}} \quad \text{and} \quad |\rho_{kl}^{\Omega}| = c \sqrt{\frac{B_q \log p}{(n-1)q}}, \quad (i, j) \in \mathcal{H}_1, (k, l) \in \mathcal{H}'_1. \quad (4.33)$$

We will show in the next theorem that the power of the support estimators will converge to 1 as  $p, q \rightarrow \infty$ .

**Theorem 4.** *Let the dimension  $(p, q)$  satisfy  $p \leq (nq)^r$  and  $q \leq (np)^r$  for some  $r > 0$ . Assume that (C1)-(C3), (4.27) and (4.30) hold. We have  $\text{supp}(\Gamma) \subseteq \widehat{\text{supp}}(\Gamma)$ ,  $\text{supp}(\Omega) \subseteq \widehat{\text{supp}}(\Omega)$  and  $\text{supp}(\Omega \otimes \Gamma) \subseteq \widehat{\text{supp}}(\Omega) \otimes \widehat{\text{supp}}(\Gamma)$  with probability tending to one as  $p, q \rightarrow \infty$ .*

Recall that the power is defined by the ratio between the number of true discoveries in  $\widehat{\text{supp}}(\Omega) \otimes \widehat{\text{supp}}(\Gamma)$  and the total number of non-zero off-diagonals in  $\text{supp}(\Omega \otimes \Gamma)$ . Thus, Theorem 4 shows that the power converges to 1 as  $p, q \rightarrow \infty$ . In addition, Theorem 4 shows that to detect the edge between  $X_{ij}$  and  $X_{kl}$ , the corresponding partial correlation  $\varrho_{ij,kl} = \rho_{ij}^{\Gamma} \cdot \rho_{kl}^{\Omega}$  can be as small as  $C \frac{1}{n-1} \sqrt{\frac{\log p \log q}{pq}}$  (note that  $A_p$  and  $B_q$  are bounded, see assumption (C1)). This is essentially different from the estimation of vector-variate GGMs. Actually, if we apply the method of estimation of vector-variate GGMs to  $\text{vec}(\mathbf{X})$  directly (e.g., the method from Ren et al. (2015)), even for an individual test (detecting a single edge), the magnitude of the partial correlation  $\varrho_{ij,kl}$  needs to be  $C \frac{1}{\sqrt{n}}$ .

### 4.4 Convergence rate of the initial estimators of regression coefficients

Finally, we present the next proposition, which shows that the convergence rate condition of  $\widehat{\beta}_j$  in (4.24) and (4.27) can be satisfied under some regular conditions. The convergence rate condition in (4.30) can be established similarly. This result establishes the consistency of Lasso for correlated samples, which in itself can yield a separate interesting result.

**Proposition 4.** *Let  $\delta$  in (3.19) be large enough. Suppose that (C1) holds and  $\max_{1 \leq j \leq q} |\beta_j|_0 = o\left(\frac{\sqrt{np}}{(\log \max(q, np))^{3/2}}\right)$ . We have  $\widehat{\beta}_j(\delta)$  for  $1 \leq j \leq q$  are consistent in both  $\ell_1$  and  $\ell_2$  norms with the rate in (4.27).*

## 5 Numerical Results

In this section, we present numerical results on both simulated and real data to investigate the performance of the proposed method on support recovery of matrix-variate data. In our experiment, we adopt the data-driven parameter-tuning approach from Liu (2013) to tune the parameters (see Section E in the supplement for details). Due to space constraints, some simulated experimental results and real data analysis are provided in Section E of the supplement.

### 5.1 Simulated experiments

In the simulated study, we construct  $\mathbf{\Omega}$  and  $\mathbf{\Gamma}$  based on combinations of following graph structures used in Liu (2013).

1. Hub graph (“hub” for short). There are  $p/10$  rows with sparsity 11. The rest of the rows have sparsity 2. In particular, we let  $\mathbf{\Omega}_1 = (\omega_{ij}), \omega_{ij} = \omega_{ji} = 0.5$  for  $i = 10(k-1) + 1$  and  $10(k-1) + 2 \leq j \leq 10(k-1) + 10, 1 \leq k \leq p/10$ . The diagonal  $\omega_{ii} = 1$  and other entries are zero. We also let  $\mathbf{\Omega} = \mathbf{\Omega}_1 + (|\min(\lambda_{\min})| + 0.05)\mathbf{I}_p$  to make the matrix be positive definite.
2. Band graph (“band” for short).  $\mathbf{\Omega} = (\omega_{ij})$ , where  $\omega_{ii} = 1, \omega_{i,i+1} = \omega_{i+1,i} = 0.6, \omega_{i,i+2} = \omega_{i+2,i} = 0.3, \omega_{ij} = 0$  for  $|i-j| \geq 3$ .
3. Erdős-Rényi random graph (“random” for short). There is an edge between each pair of nodes with probability  $\min(0.05, 5/p)$  independently. Let  $\mathbf{\Omega}_1 = (\omega_{ij}), \omega_{ii} = 1$  and  $\omega_{ij} = u_{ij} * \delta_{ij}$  for  $i \neq j$ , where  $u_{ij} \sim U(0.4, 0.8)$  is the uniform random variable and  $\delta_{ij}$  is the Bernoulli random variable with success probability  $\min(0.05, 5/p)$ .  $u_{ij}$  and  $\delta_{ij}$  are independent. We also let  $\mathbf{\Omega} = \mathbf{\Omega}_1 + (|\min(\lambda_{\min})| + 0.05)\mathbf{I}_p$  so that the matrix is positive definite.

The matrix  $\mathbf{\Gamma}$  is also constructed from one of the above three graph structures.

For each combination of  $\mathbf{\Omega}$  and  $\mathbf{\Gamma}$ , we generate  $n$  ( $n = 20$  or  $n = 100$ ) samples  $(\mathbf{X}^{(k)})_{k=1}^n$ , where each  $\mathbf{X}^{(k)} \sim N_{p,q}(\mathbf{0}, \mathbf{\Sigma} \otimes \mathbf{\Psi})$  with  $\mathbf{\Sigma} = \mathbf{\Omega}^{-1}$  and  $\mathbf{\Psi} = \mathbf{\Gamma}^{-1}$ . We consider different settings of  $p$  and  $q$ , i.e.,  $(p, q) = (100, 100), (p, q) = (200, 50), (p, q) = (200, 200)$  and  $(p, q) = (400, 400)$ . The FDR level  $\alpha$  for the support recovery of  $\mathbf{\Gamma}$  and  $\mathbf{\Omega}$  are set to 0.1 (the observations for other  $\alpha$ s are similar and thus omitted for space considerations). The

Table 1: Averaged empirical FDP, the estimated FDP/FDR level  $\alpha'$  in (4.32) and power.

$p$	$q$	$\Omega$	$\Gamma$	$n = 20$		$n = 100$	
				FDP ( $\alpha'$ )	Power	FDP ( $\alpha'$ )	Power
100	100	hub	hub	0.192 (0.146)	1.000	0.155 (0.145)	1.000
			band	0.158 (0.152)	1.000	0.146 (0.152)	1.000
			random	0.188 (0.154)	0.916	0.156 (0.154)	1.000
			band	0.138 (0.161)	1.000	0.154 (0.162)	1.000
			band	0.152 (0.164)	0.998	0.127 (0.163)	1.000
			random	0.161 (0.164)	0.834	0.104 (0.165)	0.999
200	200	hub	hub	0.183 (0.146)	1.000	0.145 (0.145)	1.000
			band	0.149 (0.152)	1.000	0.144 (0.152)	1.000
			random	0.167 (0.154)	0.981	0.153 (0.154)	1.000
			band	0.138 (0.162)	1.000	0.148 (0.162)	1.000
			band	0.158 (0.164)	1.000	0.134 (0.163)	1.000
			random	0.171 (0.166)	0.980	0.134 (0.166)	1.000
200	50	hub	hub	0.166 (0.145)	1.000	0.154 (0.145)	1.000
			band	0.159 (0.152)	1.000	0.151 (0.152)	1.000
			random	0.138 (0.154)	0.991	0.134 (0.153)	1.000
			band	0.127 (0.161)	1.000	0.146 (0.161)	1.000
			band	0.200 (0.163)	0.894	0.120 (0.163)	0.992
			random	0.194 (0.162)	0.714	0.141 (0.165)	0.980
400	400	hub	hub	0.160 (0.145)	1.000	0.141 (0.145)	1.000
			band	0.146 (0.152)	1.000	0.144 (0.152)	1.000
			random	0.172 (0.154)	0.999	0.151 (0.154)	1.000
			band	0.169 (0.162)	1.000	0.148 (0.162)	1.000
			band	0.159 (0.164)	1.000	0.142 (0.164)	1.000
			random	0.180 (0.166)	1.000	0.147 (0.166)	1.000

parameters  $\lambda$  and  $\delta$  are tuned using the data-driven approach in (23). All the simulation results are based on 100 independent replications.

In Table 1, we report the averaged true FDP in (4.31), the FDP estimator  $\alpha'$  in (4.32) and the power for estimating  $\text{supp}(\Omega \otimes \Gamma)$  over 100 replications. On the one hand, according to Theorem 3, it will be desirable that the true FDP is close to  $\alpha'$ . On the other hand, we are aiming for a large power. In particular, the power of the estimator  $\widehat{\text{supp}}(\Omega) \otimes \widehat{\text{supp}}(\Gamma)$  can be calculated using the following simple formula. Let  $A$  and  $B$  be the number of nonzero off-diagonals in  $\Omega$  and  $\Gamma$ . Recall the definition of  $a_0$ ,  $a$ ,  $b_0$ ,  $b$  in (4.31) and we have

$$\text{Power} = \frac{(pb + a(q + b)) - (a_0(q + b) + (a - a_0)b_0 + pb_0)}{pB + A(q + B)} = \frac{p(b - b_0) + (a - a_0)(q + b - b_0)}{pB + A(q + B)}, \quad (5.34)$$

where the numerator is the number of true discoveries in  $\widehat{\text{supp}}(\mathbf{\Omega}) \otimes \widehat{\text{supp}}(\mathbf{\Gamma})$  and the denominator is the total number of nonzero off-diagonals in  $\text{supp}(\mathbf{\Omega} \otimes \mathbf{\Gamma})$ . From Table 1, in all settings with  $n = 100$ , the true FDPs are close to their estimates  $\alpha'$  and the powers are all very close to 1. For  $n = 20$ , which is a more challenging case due to the small sample size, the true FDPs are still controlled by their estimates  $\alpha'$  for most graphs. When  $\mathbf{\Omega}$  and  $\mathbf{\Gamma}$  are both hub or random graphs, the true FDPs are slightly larger than the corresponding estimates. In terms of power with  $n = 20$ , when  $\mathbf{\Omega}$  and  $\mathbf{\Gamma}$  are both generated from random graphs and either  $p$  or  $q$  is small (e.g.,  $p = q = 100$  or  $p = 200, q = 50$ ) the powers could be away from 1 (but still above 0.7); while for all other cases, the powers are still close to 1. We examined the cases in which the power is much less than one and found that our FDP procedure generates overly sparse estimators, which leads to lower powers. In fact, a lower power for a small  $n$  and  $p$  (or  $q$ ) is expected since we essentially use  $np$  correlated samples to estimate  $\text{supp}(\mathbf{\Gamma})$  and  $nq$  correlated samples to estimate  $\text{supp}(\mathbf{\Omega})$ .

Due to space constraints, we relegate the following simulation studies to the supplement:

1. In Section E.1 of the supplement, we present the boxplots of FDPs over 100 replications. The plots show that FDPs are well concentrated, which suggests that the performance of the proposed estimator is quite stable.
2. In Section E.2 of the supplement, we provide experimental results on the estimation of  $\widehat{A}_p$ , which empirically verify our theoretical result in Proposition 3.
3. In Section E.3 of the supplement, we compare our procedure with the penalized likelihood approach in Leng and Tang (2012). We observe that when  $p, q$  are small as compared to  $n$ , the penalized likelihood approach still achieves good support recovery performance (e.g., the case  $n = 100, p = q = 20$  as reported in Leng and Tang (2012)). When  $p, q$  are comparable to or larger than  $n$ , our testing based method achieves better support recovery performance.
4. In Section E.4 of the supplement, we provide some empirical evidences to show that the de-correlation approach in Remark 1 cannot control FDP well.
5. In Section E.5 of the supplement, we further present simulation studies when the covariance matrix does not follow the form of a Kronecker product.

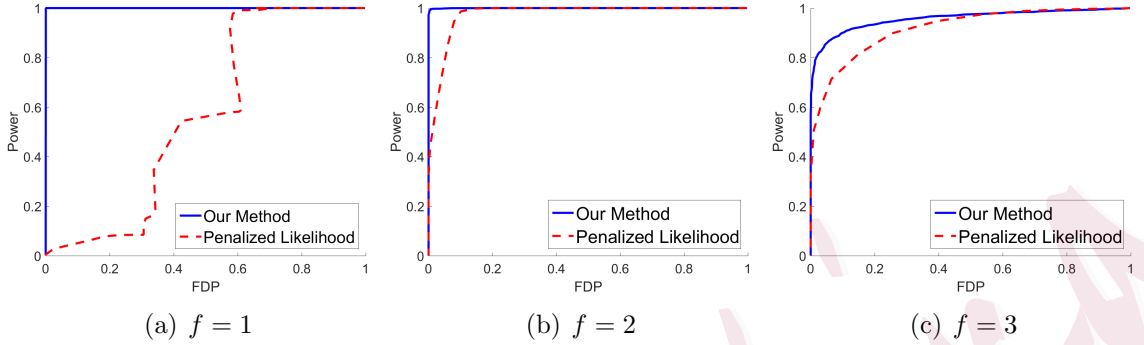


Figure 1: ROC curves for different signal strength when  $\Omega$  and  $\Gamma$  are bandable matrices.

### 5.1.1 ROC curves

In this study, we present comparisons between our method and the penalized likelihood approach in Leng and Tang (2012) (with the SCAD penalty) in terms of the ROC curve. We construct the precision matrices  $\Omega$  and  $\Gamma$  using the graph structures in Section 5.1 but introducing an additional factor  $f$  to tune the signal strength. In particular, for hub graph, we set  $\Omega_1 = (\omega_{ij})$  with  $\omega_{ij} = \omega_{ji} = 0.5/f$ ; for band graph, we set  $\omega_{i,i+1} = \omega_{i+1,i} = 0.6/f$  and  $\omega_{i,i+2} = \omega_{i+2,i} = 0.3/f$ ; and for random graph, we choose  $u_{ij} \sim U(0.4/f, 0.8/f)$ . When  $f = 1$ , the construction of  $\Omega$  and  $\Gamma$  is the same as that in Section 5.1. The higher the value of  $f$  is, the weaker the signal strength is. Due to space constraints, we only report the comparison when  $n = 20$ ,  $p = q = 100$  and observations are similar for other settings of  $n$ ,  $p$ , and  $q$ .

We first compare the support recovery performance for different signal strengths by varying  $f = 1, 2, 3$  and fix  $\Omega$  and  $\Gamma$  to be bandable matrices. We note that the usual ROC curve for binary classification is based on false positive rate (a.k.a.  $1 - \text{specificity}$ ) vs true positive rate (a.k.a. sensitivity or power). However, our problem is essentially a highly unbalanced classification and thus the standard ROC curve is not suitable. In other words, in our high-dimensional setting,  $\Omega \otimes \Gamma$  is a highly sparse matrix and thus the false positive rate will be extremely small for any reasonable choice of  $\alpha$  or regularization parameter that give a small number of discoveries. Therefore, we choose to report the ROC curve in terms of FDP vs power, from which, one can easily compare powers for different methods under the same level of FDP. As one can see from Figure 1, our method achieves better performance than the method in Leng and Tang (2012) for different signal strengths. When the factor

$f = 3$ , the ROC curve of our method is still almost vertical. In Section E.6 in the supplement, we fix the factor  $f = 3$  and consider different types of  $\Omega$  and  $\Gamma$ . For most cases, our method still achieves better performance.

## 5.2 Real data analysis

For the real data analysis, we investigate the performance of the proposed method on two real datasets, the U.S. agricultural export data from Leng and Tang (2012) and the climatological data from Lozano et al. (2009). Due to space constraints, the details of real data analysis are provided in Section E.7 in the supplement.

## 6 Discussions and future work

In this paper, we propose new test statistics with FDR control guarantees for graph estimation from matrix-variate Gaussian data. To handle the correlation structure among “row samples” and “column samples”, we develop the *variance correlation technique*. The proposed variance correlation technique can be directly extended to address the problem of learning high-dimensional GGMs with correlated samples, which has not been studied in the existing literature but finds many important applications in practice. We leave this extension as a future work.

To establish the FDR control result, the correlation among “row samples” makes the theoretical analysis significantly more challenging than the *i.i.d.* case and all the analysis in the *i.i.d.* case must be carefully tailored. For example, we need to establish the consistency for Lasso estimators from correlated samples. We also need a few new large deviation bounds on sample covariance matrices with correlated samples (see Section A in the supplement).

There are several future directions of this work. First, although our paper mainly focuses on the support recovery and graph estimation, it is also interesting to estimate the Kronecker product precision matrix based on the multiple testing framework. Moreover, our work relies on the the Kronecker product structure, it is interesting to consider other forms of the covariance matrices, e.g., the true covariance matrix does not exactly follow Kronecker product structure but close to that structure.

## Supplementary Materials

The supplementary material consists of several technical lemmas and the proofs of our



propositions and theorems. Moreover, it includes additional simulation studies and real data analysis.

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