#### **REPRODUCIBLE LEARNING IN**

#### LARGE-SCALE MULTIPLE GRAPHICAL MODELS

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#### Supplementary Material

This Supplementary Material contains four auxiliary lemmas in Section S1 and their proofs in Section S6-S9, as well as the proofs of Lemmas 1-2 in Sections S2-S3 and the proof of Theorems 1-2 in Sections S4-S5. Additionally, two figures about the real data analysis are provided in Section S10. For convenience, in the following, we use C and c to denote some positive constants which can vary from expression to expression.

#### S1 Auxiliary Lemmas

**Lemma S1.1.** For any given node  $a \in (1, ..., p)$ , take any subset  $S \subset [-a]$ . Then  $(\mathcal{X}_{-a}, \mathcal{Y}_{a}) \stackrel{d}{=} ((\mathcal{X}_{-a})_{swap(S)}, \mathcal{Y}_{a})$ . Here,  $(\mathcal{X}_{-a})_{swap(S)}$  is obtained from  $\mathcal{X}_{-a}$  by swapping the  $\mathbf{X}_{j}^{(t)}$  and  $\widetilde{\mathbf{X}}_{j}^{(t)}$  for all  $1 \leq t \leq k$  with  $j \in S$ .

**Lemma S1.2.** For any  $a \in \{1, \ldots, p\}$ , conditional on  $(|W_{a,j}|, j \in [-a])$ , the signs of the null  $W_{a,j}$ ,  $j \in [-a] \setminus NE_a$  are *i.i.d.* coin flips. **Lemma S1.3.** For any target FDR level  $q \in (0,1)$ , the estimated edge set  $\widehat{E}$  obtained by the multiple graphical knockoff filter with the true precision matrices  $\{\Omega^{(t)}\}_{t=1}^k$  satisfies the exact FDR control, that is  $\text{FDR}(\widehat{E}) = \mathbb{E}\left[(|\widehat{E} \cap E^c|)/(|\widehat{E}| \lor 1)\right] \le q$ .

Lemma S1.4. Assume that Conditions 1-2 hold, the smallest eigenvalue of  $2\operatorname{diag}(\mathbf{s}_{a}^{(t)}) - \operatorname{diag}(\mathbf{s}_{a}^{(t)})\mathbf{\Omega}_{-a}^{(t)}\operatorname{diag}(\mathbf{s}_{a}^{(t)})$  is uniformly bounded from below by some positive constant for all  $1 \leq a \leq p, \ 1 \leq t \leq k$ . Let  $\widehat{\boldsymbol{\beta}}_{a}^{\operatorname{aug}}(\theta)$  be the solution of (2.5) with the knockoff matrices constricting based on  $\theta, \lambda =$  $\frac{\xi+1}{\xi-1}\left[\frac{k+2\upsilon\log(p)+2\sqrt{\upsilon k\log(p)}}{n(1-\tau)}\right]^{1/2}, \ \tau^{2} = 8(\upsilon\log(p)+\log(k))/n = o(1), \ and \ \upsilon > 2$ for some constant. Define  $\mathcal{T}_{a} = \{1,\ldots,2p\}\setminus\{a,(a+p)\},\ l_{a} = |NE_{a}|,\ and$  $\boldsymbol{\Theta} = \left\{\{\boldsymbol{\Gamma}_{-a}^{(t)}\}_{1\leq a\leq p,1\leq t\leq k}: \max_{1\leq a\leq p,1\leq t\leq k} \|\boldsymbol{\Gamma}_{-a}^{(t)}-\boldsymbol{\Omega}_{-a}^{(t)}\|_{2}\leq Cb_{n}\right\}.$  If  $l_{m} = o(n/\log(p)),\ then$ 

$$\sup_{\theta \in \Theta} \sum_{j \in \mathcal{T}_a} \|\widehat{\boldsymbol{\beta}}_{a(j)}^{aug}(\theta) - \boldsymbol{\beta}_{a(j)}^{aug}\|_2 = O(l_a\lambda)$$
(S1.1)

holds simultaneously for all  $1 \le a \le p$  with probability at least  $1 - p^{-c_v}$  for some positive constant  $c_v$ , where  $\boldsymbol{\beta}_a^{aug} = \left( (\boldsymbol{\beta}_a^{(1)})^\top, (\mathbf{0})^\top, \dots, (\boldsymbol{\beta}_a^{(k)})^\top, (\mathbf{0})^\top \right)^\top$ .

**Remark 1.** Slightly different from the main body, for convenience, hereafter, we use  $\hat{\beta}_{a(j)}^{\text{aug}}(\theta)$  to uniformly represent the regression coefficients corresponding to the original variables and the knockoff variables. We divide the whole regression coefficient vector  $\hat{\beta}_{a}^{\text{aug}}(\theta)$  into 2(p-1) groups, indexed by  $\mathcal{T}_a = \{1, \dots, 2p\} \setminus \{a, (a+p)\}$ . For  $1 \leq j \leq p$ ,  $\widehat{\boldsymbol{\beta}}_{a(j)}^{\mathrm{aug}}(\theta) = \widehat{\boldsymbol{\beta}}_{a(j)}(\theta)$  and for  $p \leq j \leq 2p$ ,  $\widehat{\boldsymbol{\beta}}_{a(j)}^{\mathrm{aug}}(\theta) = \widetilde{\boldsymbol{\beta}}_{a(j-p)}(\theta)$ , which are defined in (2.6).

## S2 Proof of Lemma 1

In view of (2.6), we can see that the statistic  $W_{a,j}(\theta)$  is only determined by the estimator  $\hat{\beta}_a^{\text{aug}}(\theta)$ . Note that the HGSL solution  $\hat{\beta}_a^{\text{aug}}(\theta)$  is a global minimizer of the objective function (2.5) with the knockoff matrices constricting based on  $\theta$ , which can be equivalently formulated as

$$\begin{aligned} \widehat{\boldsymbol{\beta}}_{a}^{\mathrm{aug}}(\theta) &= \arg_{\mathbf{b}^{\mathrm{aug}} \in \mathbb{R}^{2(p-1)k}} \left\{ \sum_{t=1}^{k} \sqrt{(\ddot{\mathbf{b}}^{(t)'} \mathbf{U}_{-a}^{(t)}(\theta) \ddot{\mathbf{b}}^{(t)} - 2\mathbf{V}_{-a}^{(t)}(\theta) \ddot{\mathbf{b}}^{(t)})} + \lambda \left( \sum_{j \in \mathcal{T}_{a}} \|\mathcal{D}_{a(j)}^{1/2}(\theta) \mathbf{b}_{(j)}^{\mathrm{aug}}\|_{2} \right) \right\} \\ \text{where } \mathcal{T}_{a} &= \{1, \ldots, 2p\} \setminus \{a, (a+p)\}, \mathbf{U}_{-a}^{(t)}(\theta) = [\mathbf{X}_{-a}^{(t)}, \widetilde{\mathbf{X}}_{-a}^{(t)}(\theta)]^{\top} [\mathbf{X}_{-a}^{(t)}, \widetilde{\mathbf{X}}_{-a}^{(t)}(\theta)] / n \\ \text{and } \mathbf{V}_{-a}^{(t)}(\theta) &= [\mathbf{X}_{-a}^{(t)}, \widetilde{\mathbf{X}}_{-a}^{(t)}(\theta)]^{\top} \mathbf{X}_{a}^{(t)} / n. \text{ For simplicity, we use notation } \ddot{\mathbf{b}}^{(t)} \\ \text{denotes } ((\mathbf{b}^{(t)})^{\top}, (\widetilde{\mathbf{b}}^{(t)})^{\top})^{\top} \text{ defined in } (2.5). \text{ For } j \leq p, \mathcal{D}_{a(j)}(\theta) = \mathbf{D}_{a(j)} \\ \text{defined in equation } (2.5), \text{ and for } j > p, \mathcal{D}_{a(j)}(\theta) = \widetilde{\mathbf{D}}_{a(l)}(\theta) \text{ with } l = j - p \\ \text{defined in equation } (2.5). \text{ Note that the the entry of } \mathcal{D}_{a(j)}(\theta) \text{ is equal to } \\ \frac{n}{n^{(t)}} \mathbf{U}_{j}^{(t)}(\theta) \text{ for all } j \in \mathcal{T}_{a}, 1 \leq t \leq k. \text{ Thus, } \mathcal{D}_{a(j)}(\theta) \text{ can be completely represented by } \mathbf{U}_{-a}(\theta) = (\mathbf{U}_{-a}^{(1)}(\theta), \ldots, \mathbf{U}_{-a}^{(k)}(\theta)) \text{ since } n/n^{(t)} \text{ is a fixed positive constant.} \end{aligned}$$

Obviously, we can see that  $\widehat{\boldsymbol{\beta}}_{a}^{\mathrm{aug}}(\theta)$  depends on the data  $(\mathcal{X}_{-a}(\theta), \mathcal{Y}_{a})$ only through  $\mathbf{U}_{-a}(\theta)$  and  $\mathbf{V}_{-a}(\theta) = \left(\mathbf{V}_{-a}^{(1)}(\theta), \dots, \mathbf{V}_{-a}^{(k)}(\theta)\right)$ . Recall that  $\mathbf{H}_{a}(\theta) = (\mathbf{U}_{-a}(\theta), \mathbf{V}_{-a}(\theta)).$  From the above analysis, we can conclude that for the statistic vector  $\mathbf{W}_{a}(\theta)$ , it only depends on  $\mathbf{H}_{a}(\theta)$ . Considering the whole statistics  $\{\mathbf{W}_{a}(\theta), 1 \leq a \leq p\}$ , since the zeros has no influence in the knockoff procedure, we can write the statistics matrix as

$$\left( \begin{array}{ccc} \mathbf{W}_1(\theta) & & & \\ & \mathbf{W}_2(\theta) & & \\ & & \ddots & \\ & & & \ddots & \\ & & & \mathbf{W}_p(\theta) \end{array} \right) = g(\mathbf{H}(\theta)).$$

Further, note that the threshold vector  $\mathbf{T}(\theta)$  is completely determined by the whole statistics  $\{\mathbf{W}_a(\theta), 1 \leq a \leq p\}$ . By the process of obtaining the estimated edge set, it's obvious to see that the estimated  $\widehat{E}(\theta)$  identified by our procedure with the given sequence of precision matrices  $\theta$  depends only on  $\mathbf{H}(\theta)$ . Thus, we have completed the proof of Lemma 1.

#### S3 Proof of Lemma 2

Recall that  $\mathcal{A}_{a}^{*}(\theta)$  is the support of knockoff statistics  $\mathbf{W}_{a}(\theta)$ . Thus, the threshold vector  $\left(\widehat{T}_{1}(\theta), \ldots, \widehat{T}_{p}(\theta)\right)$  depends only on  $\{W_{a,j}(\theta), j \in \mathcal{A}_{a}\}_{a=1}^{p}$ as  $\mathcal{A}_{a}^{*}(\theta) \subset \mathcal{A}_{a}$ . By equation of (2.6), it shows that

$$W_{a,j}(\theta) = \|\widehat{\boldsymbol{\beta}}_{a(j)}(\theta)\|_2 - \|\widetilde{\boldsymbol{\beta}}_{a(j)}(\theta)\|_2,$$

with

$$\widehat{\boldsymbol{\beta}}_{a}^{\mathrm{aug}}(\theta) = \arg\min_{\mathbf{c}\in\mathbb{R}^{2(p-1)k}} \left\{ \sum_{t=1}^{k} Q_{t\theta}(\mathbf{c}^{(t)}) + \lambda\left(\sum_{j\in\mathcal{T}_{a}} \|\mathcal{D}_{a(j)}^{1/2}(\theta)\mathbf{c}_{(j)}\|_{2}\right) \right\}$$
(S3.1)

where

$$Q_{\theta t}(\mathbf{c}^{(t)}) = \frac{\|\mathbf{X}_{a}^{(t)} - [\mathbf{X}_{-a}^{(t)}, \widetilde{\mathbf{X}}_{-a}^{(t)}(\theta)]\mathbf{c}^{(t)}\|_{2}}{\sqrt{n}}.$$

Here, we use the notation  $\mathbf{c}^{(t)}$  denotes the subvector corresponding to the *t*th class and  $\mathbf{c}_{(l)}$  represents its subvector corresponding to the *l*th group. The notation of  $\mathcal{D}_{a(j)}^{1/2}(\theta)$  is the same as that in the proof of Lemma 1.

When we restrict ourselves to a sequence of subset  $\{\mathcal{A}_a(\theta)\}_{a=1}^p$  that satisfies  $\mathcal{A}_a \supset \mathcal{A}_a^*(\theta)$  for all  $1 \leq a \leq p$ , let  $\widehat{\boldsymbol{\beta}}_{a(\mathcal{J}_a)}^{\operatorname{aug}}(\theta)$  be the subvector of  $\widehat{\boldsymbol{\beta}}_a^{\operatorname{aug}}(\theta)$  consists of components indexed by  $\mathcal{J}_a$  with  $\mathcal{J}_a = \mathcal{A}_a \cup \{\mathcal{A}_a + p\}$ . To prove this lemma it's sufficient to prove that  $\widehat{\boldsymbol{\beta}}_{a(\mathcal{J}_a)}^{\operatorname{aug}}(\theta) = \widehat{\boldsymbol{\zeta}}_a^{\operatorname{aug}}(\theta)$  since  $\widehat{\boldsymbol{\beta}}_{a(\mathcal{J}_a^c)}^{\operatorname{aug}}(\theta) = \mathbf{0}$  that doesn't work for the knockoff procedure, where

$$\widehat{\boldsymbol{\zeta}}_{a}^{\mathrm{aug}}(\theta) = \arg\min_{\mathbf{b}\in\mathbb{R}^{2|\mathcal{A}_{a}|k}} \left\{ \sum_{t=1}^{k} Q_{\theta t}^{\mathcal{A}_{a}}(\mathbf{b}^{(t)}) + \lambda \left( \sum_{j\in\mathcal{J}_{a}} \|\mathcal{D}_{a(j)}^{1/2}(\theta)\mathbf{b}_{(j)}\|_{2} \right) \right\},\$$

with the same  $\lambda$  and  $\theta$  as in (S3.1). Here

$$Q_{\theta t}^{\mathcal{A}_a}(\mathbf{b}^{(t)}) = \frac{\|\mathbf{X}_a^{(t)} - [\mathbf{X}_{\mathcal{A}_a}, \widetilde{\mathbf{X}}_{\mathcal{A}_a}(\theta)]\mathbf{b}^{(t)}\|_2}{\sqrt{n}}.$$

We can see that by equation (S3.1) it shows that for any  $\mathbf{b} \in \mathbb{R}^{2(p-1)k}$ 

and  $\mathbf{b} \neq \widehat{\boldsymbol{\beta}}_{a}^{\mathrm{aug}}(\theta),$  $\sum_{t=1}^{k} \frac{\|\mathbf{X}_{a}^{(t)} - [\mathbf{X}_{-a}^{(t)}, \widetilde{\mathbf{X}}_{-a}^{(t)}(\theta)][(\widehat{\boldsymbol{\beta}}_{a}^{(t)}(\theta))^{\top}, (\widetilde{\boldsymbol{\beta}}_{a}^{(t)}(\theta))^{\top}]^{\top}\|_{2}}{\sqrt{n}} + \lambda \left(\sum_{j \in \mathcal{T}_{a}} \|\mathcal{D}_{a(j)}^{1/2}(\theta)\widehat{\boldsymbol{\beta}}_{a(j)}^{\mathrm{aug}}(\theta)\|_{2}\right)$   $< \sum_{t=1}^{k} \frac{\|\mathbf{X}_{a}^{(t)} - [\mathbf{X}_{-a}^{(t)}, \widetilde{\mathbf{X}}_{-a}^{(t)}(\theta)]\mathbf{b}^{(t)}\|_{2}}{\sqrt{n}} + \lambda \left(\sum_{j \in \mathcal{T}_{a}} \|\mathcal{D}_{a(j)}^{1/2}(\theta)\mathbf{b}_{(j)}\|_{2}\right). \quad (S3.2)$ 

Then we claim that for any  $\mathbf{c} \in \mathbb{R}^{|\mathcal{J}_a|k}$ ,

$$\sum_{t=1}^{k} \frac{\|\mathbf{X}_{a}^{(t)} - [\mathbf{X}_{\mathcal{A}_{a}}^{(t)}, \widetilde{\mathbf{X}}_{\mathcal{A}_{a}}^{(t)}(\theta)][(\widehat{\boldsymbol{\beta}}_{a,\mathcal{A}_{a}}^{(t)}(\theta))^{\top}, (\widetilde{\boldsymbol{\beta}}_{a,\mathcal{A}_{a}}^{(t)}(\theta))^{\top}]^{\top}\|_{2}}{\sqrt{n}} + \lambda \left(\sum_{j \in \mathcal{J}_{a}} \|\mathcal{D}_{a(j)}^{1/2}(\theta)\widehat{\boldsymbol{\beta}}_{a(j)}^{\mathrm{aug}}(\theta)\|_{2}\right) \\ < \sum_{t=1}^{k} \frac{\|\mathbf{X}_{a}^{(t)} - [\mathbf{X}_{\mathcal{A}_{a}}^{(t)}, \widetilde{\mathbf{X}}_{\mathcal{A}_{a}}^{(t)}(\theta)]\mathbf{c}^{(t)}\|_{2}}{\sqrt{n}} + \lambda \left(\sum_{j \in \mathcal{J}_{a}} \|\mathcal{D}_{a(j)}^{1/2}(\theta)\mathbf{c}_{(k)}\|_{2}\right),$$

where k is the order of j in  $\mathcal{J}_a$ . Otherwise, if there exists  $\widehat{\mathbf{C}}_{a(\mathcal{J}_a)} \in \mathbb{R}^{|\mathcal{J}_a|k}$ 

$$\sum_{t=1}^{k} \frac{\|\mathbf{X}_{a}^{(t)} - [\mathbf{X}_{-a}^{(t)}, \widetilde{\mathbf{X}}_{-a}^{(t)}(\theta)] \widehat{\mathbf{C}}_{a(\mathcal{J}_{a})}^{(t)}(\theta)\|_{2}}{\sqrt{n}} + \lambda \left( \sum_{j \in \mathcal{J}_{a}} \|\mathcal{D}_{a(j)}^{1/2}(\theta) \widehat{\mathbf{C}}_{a(j)}(\theta)\|_{2} \right)$$
$$< \sum_{t=1}^{k} \frac{\|\mathbf{X}_{a}^{(t)} - [\mathbf{X}_{-a}^{(t)}, \widetilde{\mathbf{X}}_{-a}^{(t)}(\theta)] [(\widehat{\boldsymbol{\beta}}_{a,\mathcal{A}_{a}}^{(t)}(\theta))^{\top}, (\widetilde{\boldsymbol{\beta}}_{a,\mathcal{A}_{a}}^{(t)}(\theta))^{\top}]^{\top}\|_{2}}{\sqrt{n}} + \lambda \left( \sum_{j \in \mathcal{J}_{a}} \|\mathcal{D}_{a(j)}^{1/2}(\theta) \widehat{\boldsymbol{\beta}}_{a(j)}^{\mathrm{aug}}(\theta)\|_{2} \right)$$

Then, let  $\widehat{\mathbf{C}}_{a(\mathcal{T}_a \setminus \mathcal{J}_a)} = \mathbf{0}$  it holds that

$$\sum_{t=1}^{k} \frac{\|\mathbf{X}_{a}^{(t)} - [\mathbf{X}_{-a}^{(t)}, \widetilde{\mathbf{X}}_{-a}^{(t)}(\theta)] \widehat{\mathbf{C}}_{a}^{(t)}(\theta)\|_{2}}{\sqrt{n}} + \lambda \left( \sum_{j \in \mathcal{T}_{a}} \|\mathcal{D}_{a(j)}^{1/2}(\theta) \widehat{\mathbf{C}}_{a(j)}(\theta)\|_{2} \right) \\ < \sum_{t=1}^{k} \frac{\|\mathbf{X}_{a}^{(t)} - [\mathbf{X}_{-a}^{(t)}, \widetilde{\mathbf{X}}_{-a}^{(t)}(\theta)] [(\widehat{\boldsymbol{\beta}}_{a}^{(t)}(\theta))^{\top}, (\widetilde{\boldsymbol{\beta}}_{a}^{(t)}(\theta))^{\top}]^{\top}\|_{2}}{\sqrt{n}} + \lambda \left( \sum_{j \in \mathcal{T}_{a}} \|\mathcal{D}_{a(j)}^{1/2}(\theta) \widehat{\boldsymbol{\beta}}_{a(j)}^{\mathrm{aug}}(\theta)\|_{2} \right),$$

which contradicts equation (S3.2). Thus, we can conclude that  $(\widehat{\boldsymbol{\beta}}_{a(\mathcal{J}_{a})}^{\operatorname{aug}}(\theta)) = \widehat{\boldsymbol{\zeta}}_{a}^{\operatorname{aug}}(\theta)$ . This guarantees that  $E_{\mathcal{F}}(\mathbf{H}(\theta))$  and  $E_{\mathcal{A}}(\mathbf{H}_{\mathcal{A}}(\theta))$  are identical and thus concludes the proof of Lemma 2.

## S4 Proof of Theorem 1

Let  $\mathcal{A}_{a}^{*}(\widehat{\theta})$  be the support of knockoff statistic vector  $\mathbf{W}_{a}(\widehat{\theta})$ . Define set  $\widehat{\mathcal{A}}_{a}(\widehat{\theta}) := \mathcal{A}_{a}^{*}(\widehat{\theta}) \cup \mathcal{A}_{a}^{*}(\theta_{0})$ . It follows from Condition 4 that the cardinality of  $\widehat{\mathcal{A}}_{a}(\widehat{\theta})$  is bounded by d. Hereafter we write  $\widehat{\mathcal{A}}_{a}(\widehat{\theta})$  as  $\widehat{\mathcal{A}}_{a}$  for notational simplicity. Additionally, we use  $\widehat{\mathcal{A}}$  to denote the set of  $\{\widehat{\mathcal{A}}_{a}\}_{a=1}^{p}$ .

Recall the definitions of  $\mathbb{I}_{\mathcal{A}}$  as in (3.14). Define the event

$$\mathcal{E}_{np} = \left\{ \mathbf{H}_{\widehat{\mathcal{A}}}(\widehat{\theta}) \in \mathbb{I}_{\widehat{\mathcal{A}}} \right\} \cap \left\{ \mathbf{H}_{\widehat{\mathcal{A}}}(\theta_0) \in \mathbb{I}_{\widehat{\mathcal{A}}} \right\}.$$

It's obvious that  $\mathbf{H}_{\widehat{\mathcal{A}}}(\theta_0) \in \mathbb{I}_{\widehat{\mathcal{A}}}$ . We only need to prove that with the probability at least  $1 - p^{-c_{\delta}}$ 

$$\max_{1 \le a \le p} \|\mathbf{H}_{\widehat{\mathcal{A}}_a}(\widehat{\theta}) - \mathbf{H}_{\widehat{\mathcal{A}}_a}(\theta_0)\|_2 = o(1),$$
(S4.1)

which entails that  $\mathbb{P}(\mathcal{E}_{np}^{c}) \leq p^{-c_{\delta}}$ . Then, according to Lemma S1.3, we have  $\mathrm{FDR}(\mathbf{H}_{\widehat{\mathcal{A}}}(\theta_{0})) = \mathrm{FDR}(\mathbf{H}) \leq q$ . Combining with the Condition 5, the rest of the proof is similar to the proof of theorem 1 in Fan et al. (2020) with  $\pi_{np} = p^{-c_{\delta}}$ , so we have omitted it.

Now we will focus on the proof of equation (S4.1). For convenience, in the following, we will abbreviate  $\mathbf{H}_{\widehat{\mathcal{A}}_a}(\theta_0)$  to  $\mathbf{H}_{\widehat{\mathcal{A}}_a}, \mathbf{U}_{\widehat{\mathcal{A}}_a}^{(t)}(\theta_0)$  to  $\mathbf{U}_{\widehat{\mathcal{A}}_a}^{(t)}$  and  $\mathbf{V}_{\widehat{\mathcal{A}}_a}^{(t)}(\theta_0)$  to  $\mathbf{V}_{\widehat{\mathcal{A}}_a}^{(t)}$ . Similarly, we abbreviate  $\mathbf{H}_{\widehat{\mathcal{A}}_a}(\widehat{\theta})$  to  $\widehat{\mathbf{H}}_{\widehat{\mathcal{A}}_a}, \mathbf{U}_{\widehat{\mathcal{A}}_a}^{(t)}(\widehat{\theta})$  to  $\widehat{\mathbf{U}}_{\widehat{\mathcal{A}}_a}^{(t)}$  and  $\mathbf{V}_{\widehat{\mathcal{A}}_a}^{(t)}(\widehat{\theta})$  to  $\widehat{\mathbf{V}}_{\widehat{\mathcal{A}}_a}^{(t)}$ . By the definition of  $\mathbf{H}_{\widehat{\mathcal{A}}_a}(\widehat{\theta})$ , we have

$$\max_{1 \le a \le p} \|\widehat{\mathbf{H}}_{\widehat{\mathcal{A}}_{a}} - \mathbf{H}_{\widehat{\mathcal{A}}_{a}}\|_{2} = \max_{1 \le a \le p} \left\| \left( \widehat{\mathbf{U}}_{\widehat{\mathcal{A}}_{a}}^{(1)}, \dots, \widehat{\mathbf{U}}_{\widehat{\mathcal{A}}_{a}}^{(k)}, \widehat{\mathbf{V}}_{\widehat{\mathcal{A}}_{a}}^{(1)}, \dots, \widehat{\mathbf{V}}_{\widehat{\mathcal{A}}_{a}}^{(k)} \right) - \left( \mathbf{U}_{\widehat{\mathcal{A}}_{a}}^{(1)}, \dots, \mathbf{U}_{\widehat{\mathcal{A}}_{a}}^{(k)}, \mathbf{V}_{\widehat{\mathcal{A}}_{a}}^{(1)}, \dots, \mathbf{V}_{\widehat{\mathcal{A}}_{a}}^{(k)} \right) \right\|_{2} \\ \le \max_{1 \le a \le p} \left( \sum_{t=1}^{k} \|\widehat{\mathbf{U}}_{\widehat{\mathcal{A}}_{a}}^{(t)} - \mathbf{U}_{\widehat{\mathcal{A}}_{a}}^{(t)} \|_{2} + \sum_{t=1}^{k} \|\widehat{\mathbf{V}}_{\widehat{\mathcal{A}}_{a}}^{(t)} - \mathbf{V}_{\widehat{\mathcal{A}}_{a}}^{(t)} \|_{2} \right) \\ \le k \left( \max_{1 \le a \le p, 1 \le t \le k} \|\widehat{\mathbf{U}}_{\widehat{\mathcal{A}}_{a}}^{(t)} - \mathbf{U}_{\widehat{\mathcal{A}}_{a}}^{(t)} \|_{2} + \max_{1 \le a \le p, 1 \le t \le k} \|\widehat{\mathbf{V}}_{\widehat{\mathcal{A}}_{a}}^{(t)} - \mathbf{V}_{\widehat{\mathcal{A}}_{a}}^{(t)} \|_{2} \right)$$
(S4.2)

Thus, we can see that it is sufficient to deduce the bounds of  $\max_{1 \le a \le p, 1 \le t \le k} \|\widehat{\mathbf{U}}_{\widehat{\mathcal{A}}_a}^{(t)} - \widehat{\mathbf{U}}_{\widehat{\mathcal{A}}_a}^{(t)}\|$  $\mathbf{U}_{\widehat{\mathcal{A}}_a}^{(t)} \|_2 \text{ and } \max_{1 \leq a \leq p, 1 \leq t \leq k} \| \widehat{\mathbf{V}}_{\widehat{\mathcal{A}}_a}^{(t)} - \mathbf{V}_{\widehat{\mathcal{A}}_a}^{(t)} \|_2.$ 

The error bounds of  $\max_{1 \le a \le p, 1 \le t \le k} \| \widehat{\mathbf{U}}_{\widehat{\mathcal{A}}_a}^{(t)} - \mathbf{U}_{\widehat{\mathcal{A}}_a}^{(t)} \|_2$ . Recalling the definition of  $\mathbf{U}_{\widehat{\mathcal{A}}_{a}}^{(t)}$ , we have

$$\begin{split} \left\| \widehat{\mathbf{U}}_{\hat{\mathcal{A}}_{a}}^{(t)} - \mathbf{U}_{\hat{\mathcal{A}}_{a}}^{(t)} \right\|_{2} &= \left\| [\mathbf{X}_{\hat{\mathcal{A}}_{a}}^{(t)}, \widehat{\widetilde{\mathbf{X}}}_{\hat{\mathcal{A}}_{a}}^{(t)}]^{\top} [\mathbf{X}_{\hat{\mathcal{A}}_{a}}^{(t)}, \widehat{\widetilde{\mathbf{X}}}_{\hat{\mathcal{A}}_{a}}^{(t)}] / n - [\mathbf{X}_{\hat{\mathcal{A}}_{a}}^{(t)}, \widetilde{\mathbf{X}}_{\hat{\mathcal{A}}_{a}}^{(t)}]^{\top} [\mathbf{X}_{\hat{\mathcal{A}}_{a}}^{(t)}, \widetilde{\mathbf{X}}_{\hat{\mathcal{A}}_{a}}^{(t)}]^{\top} [\mathbf{X}_{\hat{\mathcal{A}}_{a}}^{(t)}, \widetilde{\mathbf{X}}_{\hat{\mathcal{A}}_{a}}^{(t)}] / n \right\|_{2} \\ &= \left\| \left\| \begin{pmatrix} \mathbf{0} & (\mathbf{X}_{\hat{\mathcal{A}}_{a}}^{(t)})^{\top} (\widehat{\widetilde{\mathbf{X}}}_{\hat{\mathcal{A}}_{a}}^{(t)} - \widetilde{\mathbf{X}}_{\hat{\mathcal{A}}_{a}}^{(t)})^{\top} (\widehat{\widetilde{\mathbf{X}}}_{\hat{\mathcal{A}}_{a}}^{(t)} - \widetilde{\mathbf{X}}_{\hat{\mathcal{A}}_{a}}^{(t)}) / n \\ (\mathbf{X}_{\hat{\mathcal{A}}_{a}}^{(t)})^{\top} (\widehat{\widetilde{\mathbf{X}}}_{\hat{\mathcal{A}}_{a}}^{(t)} - \widetilde{\mathbf{X}}_{\hat{\mathcal{A}}_{a}}^{(t)}) / n \\ (\mathbf{X}_{\hat{\mathcal{A}}_{a}}^{(t)})^{\top} (\widehat{\widetilde{\mathbf{X}}}_{\hat{\mathcal{A}}_{a}}^{(t)} - \widetilde{\mathbf{X}}_{\hat{\mathcal{A}}_{a}}^{(t)})^{\top} \widehat{\mathbf{X}}_{\hat{\mathcal{A}}_{a}}^{(t)} - (\widetilde{\mathbf{X}}_{\hat{\mathcal{A}}_{a}}^{(t)})^{\top} \widetilde{\mathbf{X}}_{\hat{\mathcal{A}}_{a}}^{(t)}] / n \\ \leq 2 \left\| (\mathbf{X}_{\hat{\mathcal{A}}_{a}}^{(t)})^{\top} (\widehat{\widetilde{\mathbf{X}}}_{\hat{\mathcal{A}}_{a}}^{(t)} - \widetilde{\mathbf{X}}_{\hat{\mathcal{A}}_{a}}^{(t)})^{\top} n \right\|_{2} + \left\| [(\widehat{\widetilde{\mathbf{X}}}_{\hat{\mathcal{A}}_{a}}^{(t)})^{\top} \widehat{\mathbf{X}}_{\hat{\mathcal{A}}_{a}}^{(t)} - (\widetilde{\mathbf{X}}_{\hat{\mathcal{A}}_{a}}^{(t)})^{\top} \widetilde{\mathbf{X}}_{\hat{\mathcal{A}}_{a}}^{(t)}] / n \\ = :2A_{at} + B_{at} \end{aligned} \tag{S4.3}$$

where

$$A_{at} = \| (\mathbf{X}_{\widehat{\mathcal{A}}_{a}}^{(t)})^{\top} (\widehat{\widetilde{\mathbf{X}}}_{\widehat{\mathcal{A}}_{a}}^{(t)} - \widetilde{\mathbf{X}}_{\widehat{\mathcal{A}}_{a}}^{(t)}) / n \|_{2}, \text{ and } B_{at} = \left\| \left[ (\widehat{\widetilde{\mathbf{X}}}_{\widehat{\mathcal{A}}_{a}}^{(t)})^{\top} \widehat{\widetilde{\mathbf{X}}}_{\widehat{\mathcal{A}}_{a}}^{(t)} - (\widetilde{\mathbf{X}}_{\widehat{\mathcal{A}}_{a}}^{(t)})^{\top} \widetilde{\mathbf{X}}_{\widehat{\mathcal{A}}_{a}}^{(t)} \right] / n \right\|_{2}.$$
  
Here, the notation  $\widehat{\widetilde{\mathbf{X}}}_{\widehat{\mathcal{X}}}^{(t)}$  is the abbreviation of  $\widehat{\widetilde{\mathbf{X}}}_{\widehat{\mathcal{X}}}^{(t)} (\widehat{\theta}).$ 

 $-\mathcal{A}_a$  $\mathcal{A}_a \setminus$  Recalling the knockoff generation process (2.5), for the original data matrix  $\mathbf{X}_{-a}^{(t)}$ , the ideal knockoff matrix and the approximate knockoff matrix constructed using the estimated precision matrices can be represented as

$$\widetilde{\mathbf{X}}_{-a}^{(t)} = \mathbf{X}_{-a}^{(t)} \mathbf{C}_{a}^{(t)} + \mathbf{Z}_{a}^{(t)} \mathbf{B}_{a}^{(t)} \text{ and } \widetilde{\widetilde{\mathbf{X}}}_{-a}^{(t)} = \mathbf{X}_{-a}^{(t)} \widehat{\mathbf{C}}_{a}^{(t)} + \mathbf{Z}_{a}^{(t)} \widehat{\mathbf{B}}_{a}^{(t)}.$$

respectively, where  $\mathbf{Z}_{a}^{(t)}$  is a random matrix whose rows are i.i.d copies of  $N(\mathbf{0}, \mathbf{I_{p-1}})$  and independent of  $\mathbf{X}_{-a}^{(t)}, \mathbf{C}_{a}^{(t)} = \mathbf{I}_{p-1} - \operatorname{diag}\{\mathbf{s}_{a}^{(t)}\} \mathbf{\Omega}_{-a}^{(t)}$  and  $\widehat{\mathbf{C}}_{a}^{(t)} = \mathbf{I}_{p-1} - \operatorname{diag}\{\mathbf{s}_{a}^{(t)}\} \mathbf{\Omega}_{-a}^{(t)}$ ,  $\mathbf{B}_{a}^{(t)} = \left(2\operatorname{diag}\{\mathbf{s}_{a}^{(t)}\} - \operatorname{diag}\{\mathbf{s}_{a}^{(t)}\} \mathbf{\Omega}_{-a}^{(t)}\operatorname{diag}\{\mathbf{s}_{a}^{(t)}\}\right)^{1/2}$ , and  $\widehat{\mathbf{B}}_{a}^{(t)} = \left(2\operatorname{diag}\{\mathbf{s}_{a}^{(t)}\} - \operatorname{diag}\{\mathbf{s}_{a}^{(t)}\} - \operatorname{diag}\{\mathbf{s}_{a}^{(t)}\}\right)^{1/2}$ .

For convenience, denote by

$$G_{1} = \max_{1 \leq a \leq p, 1 \leq t \leq k} \|\frac{1}{n} (\mathbf{X}_{\widehat{\mathcal{A}}_{a}}^{(t)})^{\top} \mathbf{X}_{\widehat{\mathcal{A}}_{a}}^{(t)} \|_{2}, \qquad G_{2} = \max_{1 \leq a \leq p, 1 \leq t \leq k} \|\widehat{\mathbf{C}}_{a}^{(t)} - \mathbf{C}_{a}^{(t)}\|_{2},$$

$$G_{3} = \max_{1 \leq a \leq p, 1 \leq t \leq k} \|\frac{1}{n} (\mathbf{X}_{\widehat{\mathcal{A}}_{a}}^{(t)})^{\top} \mathbf{Z}_{\widehat{\mathcal{A}}_{a}}^{(t)} \|_{2}, \qquad G_{4} = \max_{1 \leq a \leq p, 1 \leq t \leq k} \|\widehat{\mathbf{B}}_{a}^{(t)} - \mathbf{B}_{a}^{(t)}\|_{2},$$
and 
$$G_{5} = \max_{1 \leq a \leq p, 1 \leq t \leq k} \|\frac{1}{n} (\mathbf{Z}_{\widehat{\mathcal{A}}_{a}}^{(t)})^{\top} \mathbf{Z}_{\widehat{\mathcal{A}}_{a}}^{(t)} \|_{2}. \quad \text{Here } \mathbf{Z}_{\widehat{\mathcal{A}}_{a}}^{(t)} \text{ is the submatrix of } \mathbf{Z}_{a}^{(t)} \text{ with the columns in } \widehat{\mathcal{A}}_{a}. \text{ By a more elaborate derivation, we have}$$

$$\begin{aligned} \max_{1 \le a \le p, 1 \le t \le k} \left\| \frac{1}{n} (\mathbf{X}_{\widehat{\mathcal{A}}_{a}}^{(t)})^{\top} (\widehat{\widetilde{\mathbf{X}}}_{\widehat{\mathcal{A}}_{a}}^{(t)} - \widetilde{\mathbf{X}}_{\widehat{\mathcal{A}}_{a}}^{(t)}) \right\|_{2} \le G_{1}G_{2} + G_{3}G_{4}, \\ \max_{1 \le a \le p, 1 \le t \le k} \frac{1}{n} \left\| (\widehat{\widetilde{\mathbf{X}}}_{\widehat{\mathcal{A}}_{a}}^{(t)})^{\top} \widehat{\widetilde{\mathbf{X}}}_{\widehat{\mathcal{A}}_{a}}^{(t)} - (\widetilde{\mathbf{X}}_{\widehat{\mathcal{A}}_{a}}^{(t)})^{\top} \widetilde{\mathbf{X}}_{\widehat{\mathcal{A}}_{a}}^{(t)} \right\|_{2} \\ \le G_{1}G_{2}^{2} + 2G_{3}G_{2}G_{4} + G_{5}G_{4}^{2} + 2G_{1}G_{2} + 2G_{3}G_{4}, \end{aligned}$$

Combining with formula (S4.3), we can conclude that

$$\max_{1 \le a \le p, 1 \le t \le k} \left\| \widehat{\mathbf{U}}_{\widehat{\mathcal{A}}_a}^{(t)} - \mathbf{U}_{\widehat{\mathcal{A}}_a}^{(t)} \right\|_2 \le 4G_1G_2 + 4G_3G_4 + G_1G_2^2 + G_5G_4^2 + 2G_3G_2G_4.$$

Thus, in the following, we will deduce the upper bounds of  $G_1$ ,  $G_2$ ,  $G_3$ ,  $G_4$ and  $G_5$  respectively.

## The upper bounds of $G_1, G_3, G_5$ .

It follows from Cauchy's interlace theorem and Condition 1 that

$$1/M_1 \le \lambda_{\min}(\boldsymbol{\Sigma}^{(t)}) \le \lambda_{\min}(\boldsymbol{\Sigma}_{\widehat{\mathcal{A}}_a,\widehat{\mathcal{A}}_a}^{(t)}) \le \lambda_{\max}(\boldsymbol{\Sigma}_{\widehat{\mathcal{A}}_a,\widehat{\mathcal{A}}_a}^{(t)}) \le \lambda_{\max}(\boldsymbol{\Sigma}^{(t)}) \le M_1$$

holds uniformly for any  $1 \le a \le p, 1 \le t \le k$ . By Remark 5.40 in Vershynin (2010), it yields that with probability at least  $1 - 2pk \exp(-cn)$ 

$$G_{1} = \max_{1 \le a \le p, 1 \le t \le k} \frac{n^{(t)}}{n} \left\| \frac{1}{n^{(t)}} (\mathbf{X}_{\hat{\mathcal{A}}_{a}}^{(t)})^{\top} \mathbf{X}_{\hat{\mathcal{A}}_{a}}^{(t)} \right\|_{2}$$
$$\leq \frac{n^{(t)}}{n} \max_{1 \le a \le p, 1 \le t \le k} \lambda_{\max} (\mathbf{\Sigma}_{\hat{\mathcal{A}}_{a}, \hat{\mathcal{A}}_{a}}^{(t)}) + \frac{n^{(t)}}{n} \max\{\eta_{1}, \eta_{1}^{2}\} \le C \qquad (S4.4)$$

where  $\eta_1 = C_1 \sqrt{d/n^{(t)}} + 1$  with  $C_1$  is a positive constant. Under Condition 4 and Condition 2 that d < n and  $n \asymp n^{(t)}$ , we have  $\eta_1 = O(1)$ , which entails the last inequality.

Correspondingly, with probability at least  $1 - 2pk \exp(-cn)$ 

$$G_{3} = \max_{1 \le a \le p, 1 \le t \le k} \frac{n^{(t)}}{n} \left\| \frac{1}{n^{(t)}} (\mathbf{X}_{\hat{\mathcal{A}}_{a}}^{(t)})^{\top} \mathbf{Z}_{\hat{\mathcal{A}}_{a}}^{(t)} \right\|_{2} \le \frac{n^{(t)}}{n} \max\{\eta_{1}, \eta_{1}^{2}\} \le C \quad (S4.5)$$

since  $\mathbb{E}\left[\frac{1}{n^{(t)}}(\mathbf{X}_{\hat{\mathcal{A}}_a}^{(t)})^{\top}\mathbf{Z}_{\hat{\mathcal{A}}_a}^{(t)}\right] = 0$ . Similarly, with probability at least  $1-2pk \exp(-cn)$ 

$$G_{5} = \max_{1 \le a \le p, 1 \le t \le k} \frac{n^{(t)}}{n} \left\| \frac{1}{n^{(t)}} (\mathbf{Z}_{\hat{\mathcal{A}}_{a}}^{(t)})^{\top} \mathbf{Z}_{\hat{\mathcal{A}}_{a}}^{(t)} \right\|_{2} \le \frac{n^{(t)}}{n} \left( 1 + \max\{\eta_{1}, \eta_{1}^{2}\} \right) \le C,$$
(S4.6)

since  $\mathbb{E}\left[\frac{1}{n^{(t)}} (\mathbf{Z}^{(t)})^{\top} \mathbf{Z}^{(t)}\right] = \mathbf{I}.$ 

The upper bounds of  $G_2$  and  $G_4$ .

Since the vector  $\mathbf{s}_{a}^{(t)}$  is chosen such that  $\Sigma_{-a,-a} - 2^{-1} \operatorname{diag}\{\mathbf{s}_{a}^{(t)}\}$  is positive semidefinite, we have

$$\max_{1 \le a \le p, 1 \le t \le k} \|\mathbf{s}_a^{(t)}\|_{\infty} \le 2 \max_{1 \le a \le p, 1 \le t \le k} \lambda_{\max}(\boldsymbol{\Sigma}_{-a,-a}^{(t)}) \le 2\lambda_{\max}(\boldsymbol{\Sigma}^{(t)}) \le 2M_1$$

where the second inequality follows form Cauchy's interlace theorem and the last inequality is due to Condition 1. Therefore, under Conditions 1 and 3, we have with probability at least  $1 - p^{-\delta}$ 

$$G_{2} = \max_{1 \le a \le p, 1 \le t \le k} \| (\widehat{\mathbf{C}}_{a}^{(t)} - \mathbf{C}_{a}^{(t)}) \|_{2}$$
  
$$\leq \max_{1 \le a \le p, 1 \le t \le k} \| \mathbf{s}_{a}^{(t)} \|_{\infty} \max_{1 \le a \le p, 1 \le t \le k} \| \widehat{\mathbf{\Omega}}_{-a}^{(t)} - \mathbf{\Omega}_{-a}^{(t)} \|_{2} \le Cb_{n}$$
(S4.7)

It follows from the definitions of  $\mathbf{B}_{a}^{(t)}$  and  $\widehat{\mathbf{B}}_{a}^{(t)}$  that  $(\mathbf{B}_{a}^{(t)})^{2} - (\widehat{\mathbf{B}}_{a}^{(t)})^{2} =$ diag $\{\mathbf{s}_{a}^{(t)}\}(\mathbf{\Omega}_{-a}^{(t)} - \widehat{\mathbf{\Omega}}_{-a}^{(t)})$ diag $\{\mathbf{s}_{a}^{(t)}\}$  and thus by Condition 3 it holds that with probability at least  $1 - p^{-\delta}$ 

$$\max_{1 \le a \le p, 1 \le t \le k} \|(\widehat{\mathbf{B}}_{a}^{(t)})^{2} - (\mathbf{B}_{a}^{(t)})^{2}\|_{2}$$
  
$$\leq \max_{1 \le a \le p, 1 \le t \le k} \|\mathbf{s}_{a}^{(t)}\|_{\infty}^{2} \cdot \max_{1 \le a \le p, 1 \le t \le k} \|\mathbf{\Omega}_{-a}^{(t)} - \widehat{\mathbf{\Omega}}_{-a}^{(t)}\|_{2} \le Cb_{n}.$$
(S4.8)

This, together with the fact that  $(\widehat{\mathbf{B}}_a^{(t)})^2 = (\mathbf{B}_a^{(t)})^2 + [(\widehat{\mathbf{B}}_a^{(t)})^2 - (\mathbf{B}_a^{(t)})^2]$ , yields

that

$$\lambda_{\min}\{(\widehat{\mathbf{B}}_{a}^{(t)})^{2}\} \geq \lambda_{\min}\{(\mathbf{B}_{a}^{(t)})^{2}\} + \lambda_{\min}\{(\widehat{\mathbf{B}}_{a}^{(t)})^{2} - (\mathbf{B}_{a}^{(t)})^{2}\}$$
$$\geq \lambda_{\min}\{(\mathbf{B}_{a}^{(t)})^{2}\} - \lambda_{\max}\{(\mathbf{B}_{a}^{(t)})^{2} - (\widehat{\mathbf{B}}_{a}^{(t)})^{2}\} \geq \lambda_{\min}\{(\mathbf{B}_{a}^{(t)})^{2}\} - Cb_{n}$$
(S4.9)

holds uniformly for all  $1 \le a \le p, 1 \le t \le k$ .

Recall that  $(\mathbf{B}_{a}^{(t)})^{2} = 2\operatorname{diag}\{\mathbf{s}_{a}^{(t)}\} - \operatorname{diag}\{\mathbf{s}_{a}^{(t)}\}\mathbf{\Omega}_{-a}^{(t)}\operatorname{diag}\{\mathbf{s}_{a}^{(t)}\}$ . The assumption that  $\lambda_{\min}(2\operatorname{diag}\{\mathbf{s}_{a}^{(t)}\} - \operatorname{diag}\{\mathbf{s}_{a}^{(t)}\}\mathbf{\Omega}_{-a}^{(t)}\operatorname{diag}\{\mathbf{s}_{a}^{(t)}\}) \geq C_{3}$  uniformly for all  $1 \leq a \leq p, 1 \leq t \leq k$  with some constant  $C_{3} > 0$  implies that

$$\lambda_{\min}\{(\mathbf{B}_a^{(t)})^2\} \ge C_3$$

holds uniformly over  $1 \le a \le p$ ,  $1 \le t \le k$ . This, together with (S4.9) and the assumption that  $b_n \to 0$  as  $n \to \infty$ , yields that  $\lambda_{\min}\{(\widehat{\mathbf{B}}_a^{(t)})^2\} \ge C_3/2$ holds uniformly over  $1 \le a \le p$ ,  $1 \le t \le k$  for all n large enough. Thus, it follows from Lemma 2.2 in Schmitt (1992) that with probability at least  $1 - p^{-\delta}$ 

$$G_{4} = \max_{1 \le a \le p, 1 \le t \le k} \|\widehat{\mathbf{B}}_{a}^{(t)} - \mathbf{B}_{a}^{(t)}\|_{2} \le C \max_{1 \le a \le p, 1 \le t \le k} \|(\widehat{\mathbf{B}}_{a}^{(t)})^{2} - (\mathbf{B}_{a}^{(t)})^{2}\|_{2} \le C_{4}b_{n}.$$
(S4.10)

The last inequality is given by (S4.8). Therefore, in view of these results of (S4.4), (S4.5), (S4.6), (S4.7), and (S4.10), we can conclude that with proba-

bility at least  $1 - 6pk \exp(-cn) - 2p^{-\delta}$ 

$$\max_{1 \le a \le p, 1 \le t \le k} \left\| \widehat{\mathbf{U}}_{\widehat{\mathcal{A}}_a}^{(t)} - \mathbf{U}_{\widehat{\mathcal{A}}_a}^{(t)} \right\|_2 \le Cb_n \tag{S4.11}$$

The error bounds of  $\max_{1 \le a \le p, 1 \le t \le k} \| \widehat{\mathbf{V}}_{\widehat{\mathcal{A}}_a}^{(t)} - \mathbf{V}_{\widehat{\mathcal{A}}_a}^{(t)} \|_2$ . Recalling the definition of  $\mathbf{V}_{\widehat{\mathcal{A}}_a}$ , we have that

$$\max_{1 \le a \le p, 1 \le t \le k} \|\widehat{\mathbf{V}}_{\hat{\mathcal{A}}_{a}}^{(t)} - \mathbf{V}_{\hat{\mathcal{A}}_{a}}^{(t)}\|_{2} = \max_{1 \le a \le p, 1 \le t \le k} \left\|\frac{1}{n} [\mathbf{X}_{\hat{\mathcal{A}}_{a}}^{(t)}, \widehat{\widetilde{\mathbf{X}}}_{\hat{\mathcal{A}}_{a}}^{(t)}]^{\mathsf{T}} \mathbf{X}_{a}^{(t)} - \frac{1}{n} [\mathbf{X}_{\hat{\mathcal{A}}_{a}}^{(t)}, \widetilde{\mathbf{X}}_{\hat{\mathcal{A}}_{a}}^{(t)}]^{\mathsf{T}} \mathbf{X}_{a}^{(t)}\right\|_{2} \\
= \max_{1 \le a \le p, 1 \le t \le k} \left\|\frac{1}{n} (\widehat{\widetilde{\mathbf{X}}}_{\hat{\mathcal{A}}_{a}}^{(t)} - \widetilde{\mathbf{X}}_{\hat{\mathcal{A}}_{a}}^{(t)})^{\mathsf{T}} \mathbf{X}_{a}^{(t)}\right\|_{2} \le \max_{1 \le a \le p, 1 \le t \le k} \frac{1}{n} \left\| (\widehat{\widetilde{\mathbf{X}}}_{\hat{\mathcal{A}}_{a}}^{(t)} - \widetilde{\mathbf{X}}_{\hat{\mathcal{A}}_{a}}^{(t)}) \right\|_{2} \left\|\mathbf{X}_{a}^{(t)}\right\|_{2} \\
\le \frac{1}{\sqrt{n}} \max_{1 \le a \le p, 1 \le t \le k} \|\mathbf{X}_{a}^{(t)}\|_{2} \sqrt{G_{1}}G_{2} + \frac{1}{\sqrt{n}} \max_{1 \le a \le p, 1 \le t \le k} \|\mathbf{X}_{a}^{(t)}\|_{2} \sqrt{G_{5}}G_{4}.$$

Since we have already deduced bounds of  $G_1$ ,  $G_2$ ,  $G_4$ , and  $G_5$ , we only need to deduce the bounds of  $\max_{1 \le a \le p, 1 \le t \le k} \frac{1}{\sqrt{n}} \|\mathbf{X}_a^{(t)}\|_2$  in the following.

Under Condition 1, since  $\|\mathbf{X}_{a}^{(t)}\|_{2}/\sigma_{aa} \sim \chi^{2}_{(n^{(t)})}$  for any  $1 \leq a \leq p$ with  $\sigma_{aa}^{(t)}$  denoting the (a, a)th entry of  $\Sigma^{(t)}$ , applying the following tail probability bound with t = 1/2 for the chi-squared distribution with  $n^{(t)}$ degrees of freedom

$$\mathbb{P}\{|\frac{\chi^2_{(n^{(t)})}}{n^{(t)}} - 1| \ge 1/2\} \le 2\exp(-n^{(t)}/32)$$

gives that

$$\sqrt{\frac{1}{2}}\sigma_{aa}^{(t)} \le \|\mathbf{X}_{a}^{(t)}\|_{2}/\sqrt{n^{(t)}} \le \sqrt{\frac{3}{2}}\sigma_{aa}^{(t)}$$

holds with probability at least  $1 - 2 \exp(-n^{(t)}/32)$ .

By Condition 1 that the eigenvalues of  $\Sigma^{(t)}$  are within the interval  $[1/M_1, M_1]$ , we have  $1/M_1 \leq \sigma_{aa}^{(t)} \leq M_1$  for any  $1 \leq a \leq p$ . Since  $n = O(n^{(t)})$  by Condition 2, it follows that for sufficiently large n, with probability at least  $1 - 2 \exp(-n/32)$ ,

$$\frac{\|\mathbf{X}_{a}^{(t)}\|_{2}}{\sqrt{n}} = \frac{\|\mathbf{X}_{a}^{(t)}\|_{2}}{\sqrt{n^{(t)}}} \sqrt{\frac{n^{(t)}}{n}} \le \sqrt{\frac{n^{(t)}}{n}} \sqrt{\frac{3}{2}} \sigma_{aa}^{(t)} \le C.$$

Thus, we conclude that with the probability at least  $1 - 2pk \exp(-n/32)$ 

$$\max_{1 \le a \le p, 1 \le t \le k} \frac{\|\mathbf{X}_a^{(t)}\|_2}{\sqrt{n}} \le C.$$
 (S4.12)

Combining these results (S4.4), (S4.6), (S4.7), (S4.10), and (S4.12), we can deduce that with the probability at least  $1 - 4pk \exp(-cn) - 2p^{-\delta} - 2pk \exp(-n/32)$ 

$$\max_{1 \le a \le p, 1 \le t \le k} \|\widehat{\mathbf{V}}_{\widehat{\mathcal{A}}_a}^{(t)} - \mathbf{V}_{\widehat{\mathcal{A}}_a}^{(t)}\|_2 \le Cb_n.$$
(S4.13)

By (S4.2), (S4.11) and (S4.13), we can conclude that with probability at least  $1 - 10pk \exp(-cn) - 4p^{-\delta} - 2pk \exp(-n/32)$ 

$$\max_{1 \le a \le p} \|\widehat{\mathbf{H}}_{\widehat{\mathcal{A}}_a} - \mathbf{H}_{\widehat{\mathcal{A}}_a}\|_2 \le Ckb_n,$$

for some positive constants C. Since  $\log(p) = o(n)$ , there exits some positive constant  $c_{\delta}$  such that  $p^{-c_{\delta}} > 10pk \exp(-cn) + 4p^{-\delta} + 2pk \exp(-n/32)$ . Further, as  $kb_n = o(1)$  assumed in the theorem, it holds that with the probability at least  $1 - p^{-c_{\delta}}$ 

$$\max_{1 \le a \le p} \|\widehat{\mathbf{H}}_{\widehat{\mathcal{A}}_a} - \mathbf{H}_{\widehat{\mathcal{A}}_a}\|_2 = o(1),$$

which completes the proof of Theorem 1.

#### S5 Proof of Theorem 2

By Lemma S1.4, we have that with the probability at least  $1 - p^{-c_v}$ 

$$\sup_{\theta \in \Theta} \sum_{j \in \mathcal{T}_a} \|\widehat{\boldsymbol{\beta}}_{a(j)}^{\mathrm{aug}}(\theta) - \boldsymbol{\beta}_{a(j)}^{\mathrm{aug}}\|_2 \le C_l l_a \lambda, \tag{S5.1}$$

holds simultaneously for all  $1 \leq a \leq p$ , where  $\lambda = C_{\lambda} \left[\frac{k+\log(p)}{n}\right]^{1/2}$  with  $C_{\lambda} > 0$  some constant and  $C_{l}$  is some positive constant. For the notational simplicity, hereafter we write  $W_{a,j}(\theta)$  which are constructed based on  $\widehat{\boldsymbol{\beta}}_{a}^{\mathrm{aug}}(\theta)$  as  $\check{W}_{a,j}$ .

Let  $|\check{W}_{a,(1)}| \geq \ldots \geq |\check{W}_{a,(p-1)}|$  be the ordered knockoff statistics according to magnitude. Denote by  $j^*$  the index such that  $|\check{W}_{a,(j^*)}| = T_a(\theta)$ . Then, by the definition of  $T_a(\theta)$ , it holds that  $-T_a(\theta) < \check{W}_{a,(j^*+1)} \leq 0$ . As in the proof of Theorem 3 in Fan et al. (2020), it's sufficient to consider the two case of  $\check{W}_{a,(j^*+1)} = 0$  and  $-T_a(\theta) < \check{W}_{a,(j^*+1)} < 0$  separately.

**Case 1.** Consider the case of  $-T_a(\theta) < \check{W}_{a,(j^*+1)} < 0$ . In this case, from the definition of threshold  $T_a(\theta)$ , we have

$$\frac{\gamma+1+|\{j\in\{1,\ldots,p\}, \check{W}_{a,j}\leq -T_a(\theta)\}|}{|\widehat{E}(\theta)|\vee 1} > \frac{q}{c_{\gamma}p}$$

Using the same argument as in Lemma 6 of Fan et al. (2020) together with Lemma S1.4, we can prove from Condition 7 that  $|\hat{E}(\theta)| \geq M_4 |E|$ with asymptotic probability one. This leads to  $|\{j \in \{1, \ldots, p\}, \check{W}_{a,j} \leq -T_a(\theta)\}| > (M_4 |E|q)/(c_{\gamma}p) - \gamma - 1$  with the same probability. Moreover, when  $\check{W}_{a,j} \leq -T_a(\theta)$ , we have  $\|\widehat{\boldsymbol{\beta}}_{a(j)}^{\mathrm{aug}}(\theta)\|_2 - \|\widehat{\boldsymbol{\beta}}_{a(j+p)}^{\mathrm{aug}}(\theta)\|_2 \leq -T_a(\theta)$ , and  $\|\widehat{\boldsymbol{\beta}}_{a(j+p)}^{\mathrm{aug}}(\theta)\|_2 \geq T_a(\theta)$ . Using equation (S5.1), we obtain

$$\begin{split} C_l l_a \lambda &\geq \sum_{j \in \mathcal{T}_a} \|\widehat{\boldsymbol{\beta}}_{a(j)}^{\mathrm{aug}}(\theta) - \boldsymbol{\beta}_{a(j)}^{\mathrm{aug}}\|_2 \geq \sum_{\{j: \breve{W}_{a,j} \leq -T_a\}} \|\widehat{\boldsymbol{\beta}}_{a(j+p)}^{\mathrm{aug}}(\theta)\|_2 \\ &\geq T_a |\{j: \breve{W}_{a,j} \leq -T_a(\theta)\}|. \end{split}$$

Combining these results leads to  $C_l l_a \lambda \ge T_a(\theta)((qM_4|E|)/(c_{\gamma}p) - 1 - \gamma).$ According to Condition 8 that  $|E| \ge \alpha p l_m$ , we have

$$T_{a}(\theta) \leq \frac{C_{l}l_{a}\lambda c_{\gamma}p}{qM_{4}|E| - pc_{\gamma} - p\gamma c_{\gamma}} \leq \frac{C_{l}l_{m}\lambda c_{\gamma}}{qM_{4}\alpha l_{m} - c_{\gamma} - \gamma c_{\gamma}} \leq \nu_{n}\lambda/(2C_{\lambda})$$
(S5.2)

for large enough n since  $\nu_n \to \infty$  as  $n \to \infty$ .

In light of Equation (S5.1), we derive

$$C_{l}l_{a}\lambda \geq \sum_{j\in\mathcal{T}_{a}} \|\widehat{\boldsymbol{\beta}}_{a(j)}^{\mathrm{aug}}(\theta) - \boldsymbol{\beta}_{a(j)}^{\mathrm{aug}}\|_{2} = \sum_{j\in[-a]} \left[ \|\widehat{\boldsymbol{\beta}}_{a(j)}^{\mathrm{aug}}(\theta) - \boldsymbol{\beta}_{a(j)}^{\mathrm{aug}}\|_{2} + \|\widehat{\boldsymbol{\beta}}_{a(j+p)}^{\mathrm{aug}}(\theta)\|_{2} \right]$$
$$\geq \sum_{j\in\mathrm{NE}_{a}\cap(\widehat{\mathrm{NE}}_{a}(\theta))^{c}} \left[ \|\widehat{\boldsymbol{\beta}}_{a(j)}^{\mathrm{aug}}(\theta) - \boldsymbol{\beta}_{a(j)}^{\mathrm{aug}}\|_{2} + \|\widehat{\boldsymbol{\beta}}_{a(j+p)}^{\mathrm{aug}}(\theta)\|_{2} \right]$$
$$\geq \sum_{j\in\mathrm{NE}_{a}\cap(\widehat{\mathrm{NE}}_{a}(\theta))^{c}} \left[ \|\widehat{\boldsymbol{\beta}}_{a(j)}^{\mathrm{aug}}(\theta) - \boldsymbol{\beta}_{a(j)}^{\mathrm{aug}}\|_{2} + \|\widehat{\boldsymbol{\beta}}_{a(j)}^{\mathrm{aug}}(\theta)\|_{2} - T_{a}(\theta) \right]$$

since  $\|\widehat{\boldsymbol{\beta}}_{a(j+p)}^{\mathrm{aug}}(\theta)\|_{2} \geq \|\widehat{\boldsymbol{\beta}}_{a(j)}^{\mathrm{aug}}(\theta)\|_{2} - T_{a}(\theta)$  when  $j \in (\widehat{\mathrm{NE}}_{a}(\theta))^{c}$ . Using the triangle inequality and noting that  $\|\boldsymbol{\beta}_{a(j)}^{\mathrm{aug}}\|_{2} \geq \nu_{n}\lambda/C_{\lambda}$  for  $j \in \mathrm{NE}_{a}$ , we can conclude that

$$C_l l_a \lambda \ge \sum_{j \in \operatorname{NE}_a \cap (\widehat{\operatorname{NE}}_a(\theta))^c} (\|\beta_{a(j)}^{\operatorname{aug}}\|_2 - T_a(\theta)) \ge (\nu_n \lambda / C_\lambda - T_a(\theta)) |\operatorname{NE}_a \cap (\widehat{\operatorname{NE}}_a(\theta))^c|.$$

Thus, it follows that

$$\frac{|\mathrm{NE}_a \cap \widehat{\mathrm{NE}}_a(\theta)|}{l_a} = 1 - \frac{|\mathrm{NE}_a \cap (\widehat{\mathrm{NE}}_a(\theta))^c|}{l_a} \ge 1 - \frac{C_l \lambda}{\lambda \nu_n / C_\lambda - T_a(\theta)} \ge 1 - \frac{2C_l}{\nu_n C_\lambda}$$

uniformly over all  $\theta \in \Theta$  since  $T_a(\theta) \leq \nu_n \lambda/(2C_\lambda)$ 

**Case 2.** Consider the case of  $\breve{W}_{a,(j*+1)} = 0$ . In this case, by the definition of  $T_a(\theta)$ 

$$\frac{\gamma + |j : \check{W}_{a,j} < 0|}{\widehat{E}(\theta)} \le q/c_{\gamma}p.$$

If  $|j: \check{W}_{a,j} < 0| > 2C_l C_{\lambda} c_{\gamma} l_a \nu_n^{-1}$ , then using the same argument as in (S5.2), we can also obtain that  $T_a(\theta) \leq \nu_n \lambda/(2C_{\lambda})$ , and the rest proof is the same as in Case 1. On the other hand, if  $|j: \check{W}_{a,j} < 0| \leq 2C_l C_{\lambda} c_{\gamma} l_a \nu_n^{-1}$  we have

$$|\widehat{\operatorname{NE}}_{a}(\theta) \cap \operatorname{NE}_{a}| = |\operatorname{supp}(\breve{\mathbf{W}}_{a}) \cap \operatorname{NE}_{a}| - |\{j : \breve{W}_{a,j} < 0\} \cap \operatorname{NE}_{a}|$$
$$\geq |\operatorname{supp}(\breve{\mathbf{W}}_{a}) \cap \operatorname{NE}_{a}| - 2C_{l}C_{\lambda}c_{\gamma}l_{a}\nu_{n}^{-1} \quad (S5.3)$$

since  $\widehat{\operatorname{NE}}_{a}(\theta) = \operatorname{supp}(\breve{\mathbf{W}}_{a}) \setminus \{j : \breve{W}_{a,j} < 0\}$ . Let us now focus on  $|\operatorname{supp}(\breve{\mathbf{W}}_{a}) \cap \operatorname{NE}_{a}|$ . We observe that

$$\operatorname{supp}(\check{\mathbf{W}}_a) \supset \{1, \dots, p\} \setminus \mathcal{L}_a$$
 (S5.4)

where  $\mathcal{L}_a = \{1 \leq j \leq p : \widehat{\boldsymbol{\beta}}_{a(j)}^{\text{aug}}(\theta) = 0\}$ . Meanwhile, note that in view of Equation (S5.1) we have with probability at least  $1 - p^{-c_v}$ 

$$C_{l}l_{a}\lambda \geq \sup_{\theta \in \Theta} \sum_{j \in \mathcal{T}_{a}} \|\widehat{\boldsymbol{\beta}}_{a(j)}^{\mathrm{aug}}(\theta) - \boldsymbol{\beta}_{a(j)}^{\mathrm{aug}}\|_{2} \geq \sup_{\theta \in \Theta} \sum_{j \in \mathcal{L}_{a} \cap \mathrm{NE}_{a}} \|\widehat{\boldsymbol{\beta}}_{a(j)}^{\mathrm{aug}}(\theta) - \boldsymbol{\beta}_{a(j)}^{\mathrm{aug}}\|_{2}$$
$$= \sum_{j \in \mathcal{L}_{a} \cap \mathrm{NE}_{a}} \|\boldsymbol{\beta}_{a(j)}^{\mathrm{aug}}\|_{2} \geq |\mathcal{L}_{a} \cap \mathrm{NE}_{a}| \min_{j \in \mathrm{NE}_{a}} \|\boldsymbol{\beta}_{a(j)}^{\mathrm{aug}}\|_{2}.$$

By Condition 6, we can further deduce from the above inequality that

$$|\mathcal{L}_a \cap \mathrm{NE}_a| \le C_l C_\lambda \nu_n^{-1} l_a,$$

which together with  $|NE_a| = l_a$  entails that

$$|(\{1,\ldots,p\}\setminus\mathcal{L}_a)\cap \mathrm{NE}_a| \ge (1-C_lC_\lambda\nu_n^{-1})l_a.$$

Combining this result with Equations (S5.4) yields

$$|\operatorname{supp}(\breve{\mathbf{W}}_a) \cap \operatorname{NE}_a| \ge |(\{1,\ldots,p\} \setminus \mathcal{L}_a) \cap \operatorname{NE}_a| \ge (1 - C_l C_\lambda \nu_n^{-1}) l_a.$$
 (S5.5)

Thus, in view of inequalities Equations (S5.3) and (S5.5), with probability at least  $1 - p^{-c_v}$  it holds uniformly over all  $1 \le a \le p$  that

$$\frac{|\tilde{\mathrm{NE}}_{a}(\theta) \cap \mathrm{NE}_{a}|}{l_{a}} \ge 1 - C_{l}C_{\lambda}\nu_{n}^{-1} - 2C_{l}C_{\lambda}c_{\gamma}\nu_{n}^{-1}$$

for all  $\theta \in \Theta$ .

Combining the above two scenarios, we have shown that with asymptotic probability one, uniformly over all  $1 \le a \le p$  it holds that with probability at least  $1 - p^{-c_v}$ ,

$$\frac{|\widehat{\mathrm{NE}}_a(\theta) \cap \mathrm{NE}_a|}{l_a} \ge 1 - C\nu_n^{-1}$$

for all  $\theta \in \Theta$ , where C is some positive constant. Since

$$|\widehat{E}(\theta) \cap E| \ge \frac{1}{2} \sum_{a=1}^{p} |\operatorname{NE}_a \cap \widehat{\operatorname{NE}}_a(\theta)| \quad \text{and} \quad |E| = \frac{1}{2} \sum_{a=1}^{p} |\operatorname{NE}_a|,$$

then it entails that with probability at least  $1-p^{-c_\upsilon}$ 

$$\frac{|\widehat{E}(\theta) \cap E|}{|E|} \ge \frac{\sum_{a=1}^{p} |\operatorname{NE}_{a} \cap \widehat{\operatorname{NE}}_{a}(\theta)|}{\sum_{a=1}^{p} |\operatorname{NE}_{a}|} \ge \frac{\sum_{a=1}^{p} l_{a}(1 - C/\nu_{n})}{\sum_{a=1}^{p} l_{a}} \ge 1 - \frac{2C}{\nu_{n}}.$$

This along with the assumption  $\mathbb{P}\{\widehat{\theta} \in \Theta\} \ge 1 - p^{-\delta}$  in Condition 3 gives that

$$\operatorname{Power}(\widehat{E}(\widehat{\theta})) = \mathbb{E}\left[\frac{E \cap \widehat{E}(\widehat{\theta})}{|E|}\right] \ge \mathbb{E}\left[\frac{E \cap \widehat{E}(\widehat{\theta})}{|E|}|\widehat{\theta} \in \Theta\right] \mathbb{P}\{\widehat{\theta} \in \Theta\}$$
$$\ge \left[1 - C\nu_n^{-1}\right](1 - p^{-c_v})(1 - p^{-\delta}) \ge 1 - C\nu_n^{-1} - p^{-\tilde{c}_{\delta}} + o(\nu_n^{-1}) \to 1$$

for some positive constant  $\tilde{c}_{\delta}$ , which concludes the proof of Theorem 2.

# S6 Proof of Lemma S1.1

Recalling the expressions of  $\mathcal{X}_{-a}$  and  $\mathcal{Y}_{a}$ , it yields that

$$(\mathcal{X}_{-a}, \mathcal{Y}_{a}) = \begin{pmatrix} \mathbf{X}_{-a}^{(1)} & \widetilde{\mathbf{X}}_{-a}^{(1)} & & \mathbf{X}_{a}^{(1)} \\ & \mathbf{X}_{-a}^{(2)} & \widetilde{\mathbf{X}}_{-a}^{(2)} & & \mathbf{X}_{a}^{(2)} \\ & & \ddots & \ddots & & \vdots \\ & & & \mathbf{X}_{-a}^{(k)} & \widetilde{\mathbf{X}}_{-a}^{(k)} & \mathbf{X}_{a}^{(k)} \end{pmatrix},$$

and

$$((\mathcal{X}_{-a})_{\mathrm{swap}(S)}, \mathcal{Y}_{a}) = \begin{pmatrix} [\mathbf{X}_{-a}^{(1)}, \widetilde{\mathbf{X}}_{-a}^{(1)}]_{\mathrm{swap}(S)} & \mathbf{X}_{a}^{(1)} \\ & [\mathbf{X}_{-a}^{(2)}, \widetilde{\mathbf{X}}_{-a}^{(2)}]_{\mathrm{swap}(S)} & \mathbf{X}_{a}^{(2)} \\ & \ddots & \vdots \\ & & [\mathbf{X}_{-a}^{(k)}, \widetilde{\mathbf{X}}_{-a}^{(k)}]_{\mathrm{swap}(S)} & \mathbf{X}_{a}^{(k)} \end{pmatrix}$$

Since  $\mathbf{X}^{(1)}, \ldots, \mathbf{X}^{(k)}$  are independent, it implies that  $\left( [\mathbf{X}_{-a}^{(t)}, \widetilde{\mathbf{X}}_{-a}^{(t)}], \mathbf{X}_{a}^{(t)} \right)$  are independent over t from 1 to k. Thus, to prove the claim, it suffices to show that  $\left( [\mathbf{X}_{-a}^{(t)}, \widetilde{\mathbf{X}}_{-a}^{(t)}], \mathbf{X}_{a}^{(t)} \right) \stackrel{d}{=} \left( [\mathbf{X}_{-a}^{(t)}, \widetilde{\mathbf{X}}_{-a}^{(t)}]_{\mathrm{swap}(S)}, \mathbf{X}_{a}^{(t)} \right)$ , which trivially follows from the proof of Lemma 3.2 in Candès et al. (2018). Thus, we omitted it here.

#### S7 Proof of Lemma S1.2

For any given  $a \in (1, ..., p)$ , we can write the statistics  $\mathbf{W}_a = f(\mathcal{X}_{-a}, \mathcal{Y}_a)$ for some function f. Let  $\boldsymbol{\epsilon} = (\epsilon_1, ..., \epsilon_p)$  be a sequence of independent random variables such that  $\epsilon_j = \pm 1$  with probability 1/2 if  $j \in [-a] \setminus NE_a$ , and  $\epsilon_j = 1$  otherwise. To prove the claim, it suffices to establish that

$$\mathbf{W}_a \stackrel{d}{=} \boldsymbol{\epsilon} \odot \mathbf{W}_a$$

where  $\odot$  denotes pointwise multiplication, i.e.  $\boldsymbol{\epsilon} \odot \mathbf{W}_a = (\epsilon_1 W_{a,1}, \ldots, \epsilon_p W_{a,p}).$ 

Now, let  $S = \{j : \epsilon_j = -1\}$ . Obviously,  $S \subset [-a] \setminus NE_a$ . In view of (2.6), it's easy to see the statistic  $W_{a,j}$  satisfies the flip-sign property, that

is, when we swap the columns  $\mathbf{X}_{j}^{(t)}$  and  $\widetilde{\mathbf{X}}_{j}^{(t)}$  for all  $1 \leq t \leq k$  simultaneously in the matrix  $\mathcal{X}_{-a}$ , the sign of  $W_{a,j}$  will switch. Then we have

$$\boldsymbol{\epsilon} \odot \mathbf{W}_a = f\left( (\mathcal{X}_{-a})_{\mathrm{swap}(S)}, \mathcal{Y}_a \right).$$

According to Lemma S1.1, it implies that

$$\mathbf{W}_{a} = f\left(\mathcal{X}_{-a}, \mathcal{Y}_{a}\right) \stackrel{d}{=} f\left(\left(\mathcal{X}_{-a}\right)_{\mathrm{swap}(S)}, \mathcal{Y}_{a}\right) = \boldsymbol{\epsilon} \odot \mathbf{W}_{a},$$

which completes the proof of Lemma S1.2.

#### S8 Proof of Lemma S1.3

It follows from our Lemma S1.2 that  $\mathbf{W}_a = (W_{a,j}, j \in [-a])$  enjoys the sign-flip property on  $NE_a^c$  for each  $a \in \{1, \ldots, p\}$ . Thus, we can use Lemma C.4 in Li and Maathuis (2021) to prove these pairs of  $(\gamma, c_{\gamma}) = (1, 1.93)$  and  $(\gamma, c_{\gamma}) = (0.01, 102)$  satisfying

$$\mathbb{E}\left[\frac{\#\{j\notin \mathrm{NE}_{a}, W_{a,j} \ge \widehat{T}_{a}\}}{\gamma + \#\{j\notin \mathrm{NE}_{a}, W_{a,j} \le -\widehat{T}_{a}\}}\right] \le c_{\gamma}.$$
(S8.1)

In addition, note that the global thresholds is obtained by solving the formula (2.8). If feasible thresholds do not exist, we set  $\widehat{\mathbf{T}} = (+\infty, \dots, +\infty)$ . Then the FDR is 0 because no edges can be selected. Thus the inequality  $\mathrm{FDR} \leq q$  holds. If feasible thresholds exist, we have

$$\begin{aligned} \operatorname{FDR} &= \mathbb{E}\left[\frac{|\widehat{E} \cap E^{c}|}{|\widehat{E}| \vee 1}\right] \leq \mathbb{E}\left[\frac{\sum_{a=1}^{p} \#\{j \notin \operatorname{NE}_{a}, W_{a,j} \geq \widehat{T}_{a}\}}{|\widehat{E}| \vee 1}\right] \\ &= \sum_{a=1}^{p} \mathbb{E}\left[\frac{\gamma + \#\{j \in [-a], W_{a,j} \leq -\widehat{T}_{a}\}}{|\widehat{E}| \vee 1} \frac{\#\{j \notin \operatorname{NE}_{a}, W_{a,j} \geq \widehat{T}_{a}\}}{\gamma + \#\{j \in [-a], W_{a,j} \leq -\widehat{T}_{a}\}} \right] \\ &\leq \sum_{a=1}^{p} \mathbb{E}\left[\frac{\gamma + \#\{j \in [-a], W_{a,j} \leq -\widehat{T}_{a}\}}{|\widehat{E}| \vee 1} \frac{\#\{j \notin \operatorname{NE}_{a}, W_{a,j} \geq \widehat{T}_{a}\}}{\gamma + \#\{j \notin \operatorname{NE}_{a}, W_{a,j} \leq -\widehat{T}_{a}\}} \right] \\ &\leq \frac{q}{c_{\gamma}p} \sum_{a=1}^{p} \mathbb{E}\left[\frac{\#\{j \notin \operatorname{NE}_{a}, W_{a,j} \geq \widehat{T}_{a}\}}{\gamma + \#\{j \notin \operatorname{NE}_{a}, W_{a,j} \leq -\widehat{T}_{a}\}}\right] \overset{(\operatorname{S8.1})}{\leq} q, \end{aligned}$$

where the penultimate inequality follows from the property of the threshold vector and the last inequality is due to (S8.1). Therefore, the FDR of our procedure is controlled, which completes the proof of Lemma S1.3.

# S9 Proof of Lemma S1.4

Recalling equation (2.5), the estimated regression coefficient by HGSL with the knockoff matrix based on  $\theta$  can be written as

$$\widehat{\boldsymbol{\beta}}_{a}^{\mathrm{aug}}(\theta) = \arg\min_{\mathbf{c}\in\mathbb{R}^{2(p-1)k}} \left\{ \sum_{t=1}^{k} Q_{t\theta}(\mathbf{c}^{(t)}) + \lambda\left(\sum_{j\in\mathcal{T}_{a}} \|\mathcal{D}_{a(j)}^{1/2}(\theta)\mathbf{c}_{(j)}\|_{2}\right) \right\}$$

where

$$Q_{\theta t}(\mathbf{c}^{(t)}) = \frac{\|\mathbf{X}_{a}^{(t)} - [\mathbf{X}_{-a}^{(t)}, \widetilde{\mathbf{X}}_{-a}^{(t)}(\theta)]\mathbf{c}^{(t)}\|_{2}}{\sqrt{n}}.$$

Before proving (S1.1), we first define an event  $\mathcal{B}_a$ , that

$$\mathcal{B}_{a} = \left\{ \frac{\max_{j \in \mathcal{T}_{a}} \|\mathbf{D}_{Ea}^{-1/2} \mathcal{D}_{a(j)}^{-1/2}(\theta) \mathcal{X}_{(j)}^{\top}(\theta) \mathbf{E}_{a}\|_{2}}{\sqrt{n}} \leq \lambda \frac{\xi - 1}{\xi + 1} \right\},$$

where  $\mathcal{T}_a = \{1, \ldots, 2p\} \setminus \{a, (a + p)\}, \mathbf{D}_{Ea}$  be the  $k \times k$  diagonal matrix with th diagonal entry the squared  $l_2$  norm of the error vector  $\mathbf{E}_a^{(t)}$  for  $1 \leq t \leq k$ , and  $\mathcal{X}_{(j)}(\theta)$  is an  $N \times k$  submatrix of  $\mathcal{X}_{-a}(\theta)$  given by columns corresponding to the *j*th group.

Note that combined with knockoff matrices, there are 2(p-1) group in  $\mathcal{X}_{-a}(\theta)$ . For convenience, we index them by  $\mathcal{T}_{a} = \{1, \ldots, 2p\} \setminus \{a, (a+p)\}$  according to the corresponding index of variables and knockoff variables. Specifically, for the index  $1 \leq j \leq p$ , it corresponds to the original variable  $X_{j}$ . For the index  $j \in (p+1, \ldots, 2p)$ , it corresponds to the knockoff variable  $\widetilde{X}_{j-p}$ . Thus, for  $j \leq p$ ,  $\mathcal{D}_{a(j)}(\theta) = \mathbf{D}_{a(j)}$ , and for j > p,  $\mathcal{D}_{a(j)}(\theta) = \widetilde{\mathbf{D}}_{a(l)}(\theta)$  with l = j - p, as defined in equation (2.5).

Using the same proof technique as Lemma D.6 in Ren et al. (2019), we can prove that this event  $\mathcal{B}_a$  holds with probability at least  $1 - 3p^{1-\nu}$ . Conditional on the events  $\{\bigcap_{1 \leq a \leq p} \mathcal{B}_a\}$  and  $\theta \in \Theta$ , the proof of Lemma S1.4 is similar to that of Theorem 3.1 in Ren et al. (2019). We will simplify the same parts as that in the proof of Theorem 3.1 in Ren et al. (2019), and emphasize the additional proof techniques and steps that needed to deal with the barriers causing by the estimated precision matrices.

Refer to the proof of Theorem 3.1 in Ren et al. (2019). Denote by  $\bar{\boldsymbol{\beta}}_{a}^{\text{aug}} = \mathcal{D}_{a}^{1/2}(\theta)\boldsymbol{\beta}_{a}^{\text{aug}}, \, \hat{\bar{\boldsymbol{\beta}}}_{a}^{\text{aug}}(\theta) = \mathcal{D}_{a}^{1/2}(\theta)\hat{\boldsymbol{\beta}}_{a}^{\text{aug}}(\theta), \text{ and } \bar{\boldsymbol{\Delta}}_{a} = \hat{\bar{\boldsymbol{\beta}}}_{a}^{\text{aug}}(\theta) - \bar{\boldsymbol{\beta}}_{a}^{\text{aug}}.$  In what follows, we establish all results in terms of  $\overline{\Delta}_a$ . As pointed in Ren et al. (2019) this does not affect our result much since our Condition 1 and the fact of  $(\mathbf{X}_l^{(t)})^{\top} \mathbf{X}_l^{(t)} / (\mathbf{\Sigma}_0^{(t)})_{l,l} \sim \chi^2(n^{(t)})$  and  $(\widetilde{\mathbf{X}}_l^{(t)})^{\top} \widetilde{\mathbf{X}}_l^{(t)} / (\mathbf{\Sigma}_0^{(t)})_{l,l} \sim \chi^2(n^{(t)})$ , together with an application of Lemma E.1 of Ren et al. (2019) and the union bound, entail that with probability at least  $1 - 2pk \exp(-n/32)$ ,

$$M_1/2 \le (\mathbf{X}_l^{(t)})^{\top} \mathbf{X}_l^{(t)} / n^{(t)} \le 3M_1/2 \text{ and } M_1/2 \le (\widetilde{\mathbf{X}}_l^{(t)})^{\top} \widetilde{\mathbf{X}}_l^{(t)} / n^{(t)} \le 3M_1/2$$

holds simultaneously for all  $1 \le l \le p, 1 \le t \le k$ .

Recalling the knockoff generation process (2.3), for the original data matrix  $\mathbf{X}_{-a}^{(t)}$ , the ideal knockoff matrix and the approximate knockoff matrix constructed using some given precision matrices  $\theta$  can be represented as

$$\widetilde{\mathbf{X}}_{-a}^{(t)} = \mathbf{X}_{-a}^{(t)} \mathbf{C}_{a}^{(t)} + \mathbf{Z}_{a}^{(t)} \mathbf{B}_{a}^{(t)} \text{ and } \widetilde{\mathbf{X}}_{-a}^{(t)}(\theta) = \mathbf{X}_{-a}^{(t)} \mathbf{C}_{a}^{(t)}(\theta) + \mathbf{Z}_{a}^{(t)} \mathbf{B}_{a}^{(t)}(\theta)$$

respectively, where  $\mathbf{Z}_{a}^{(t)}$  is a random matrix whose rows are i.i.d copies of  $N(\mathbf{0}, \mathbf{I_{p-1}})$  and independent of  $\mathbf{X}_{-a}^{(t)}$ ,  $\mathbf{C}_{a}^{(t)} = \mathbf{I}_{p-1} - \operatorname{diag}\{\mathbf{s}_{a}^{(t)}\}\mathbf{\Omega}_{-a}^{(t)}$  and  $\mathbf{C}_{a}^{(t)}(\theta) = \mathbf{I}_{p-1} - \operatorname{diag}\{\mathbf{s}_{a}^{(t)}\}\mathbf{\Gamma}_{-a}^{(t)}, \mathbf{B}_{a}^{(t)} = \left(2\operatorname{diag}\{\mathbf{s}_{a}^{(t)}\} - \operatorname{diag}\{\mathbf{s}_{a}^{(t)}\}\mathbf{\Omega}_{-a}^{(t)}\operatorname{diag}\{\mathbf{s}_{a}^{(t)}\}\right)^{1/2}$ , and  $\mathbf{B}_{a}^{(t)}(\theta) = \left(2\operatorname{diag}\{\mathbf{s}_{a}^{(t)}\} - \operatorname{diag}\{\mathbf{s}_{a}^{(t)}\}\mathbf{\Gamma}_{-a}^{(t)}\operatorname{diag}\{\mathbf{s}_{a}^{(t)}\}\right)^{1/2}$ .

According to Lemma B.1 in Kaul et al. (2019), we have with the probability at least  $1 - p^{-c}$  for some positive constant c

$$\max_{1 \le a \le p, 1 \le t \le k} \| (\mathbf{C}_{a}^{(t)}(\theta) - \mathbf{C}_{a}^{(t)})^{\top} (\mathbf{X}_{-a}^{(t)})^{\top} \mathbf{X}_{-a}^{(t)} (\mathbf{C}_{a}^{(t)}(\theta) - \mathbf{C}_{a}^{(t)}) / n^{(t)} \|_{\infty}$$
  
$$\leq \max_{1 \le a \le p, 1 \le t \le k} \| (\mathbf{C}_{a}^{(t)}(\theta) - \mathbf{C}_{a}^{(t)})^{\top} \boldsymbol{\Sigma}_{-a,-a} (\mathbf{C}_{a}^{(t)}(\theta) - \mathbf{C}_{a}^{(t)}) \|_{\infty} + C \sqrt{\log(p) / n^{(t)}}$$

Since  $\theta \in \Theta$ , by Condition 1 and equations (S4.7), we have

$$\max_{1 \le a \le p, 1 \le t \le k} \| (\mathbf{C}_a^{(t)}(\theta) - \mathbf{C}_a^{(t)})^\top \mathbf{\Sigma}_{-a,-a} (\mathbf{C}_a^{(t)}(\theta) - \mathbf{C}_a^{(t)}) \|_{\infty}$$
$$\leq \max_{1 \le a \le p, 1 \le t \le k} \| \mathbf{C}_a^{(t)}(\theta) - \mathbf{C}_a^{(t)} \|_2^2 \| \mathbf{\Sigma} \|_2 \le C b_n,$$

which shows that with the probability at least  $1-p^{-c}$ 

$$\max_{1 \le a \le p, 1 \le t \le k} \| (\mathbf{C}_{a}^{(t)}(\theta) - \mathbf{C}_{a}^{(t)})^{\top} (\mathbf{X}_{-a}^{(t)})^{\top} \mathbf{X}_{-a}^{(t)} (\mathbf{C}_{a}^{(t)}(\theta) - \mathbf{C}_{a}^{(t)}) / n^{(t)} \|_{\infty} = O(b_{n} + d_{n}),$$
  
where  $d_{n} = \sqrt{\log(p)/n^{(t)}}.$ 

Using the same technique, combining with the result of (S4.10), we can prove that with the probability at least  $1 - p^{-c}$ 

$$\max_{1 \le a \le p, 1 \le t \le k} \| (\mathbf{C}_a^{(t)}(\theta) - \mathbf{C}_a^{(t)})^\top (\mathbf{X}_{-a}^{(t)})^\top \mathbf{Z}_{-a}^{(t)} (\mathbf{B}_a^{(t)}(\theta) - \mathbf{B}_a^{(t)}) / n^{(t)} \|_{\infty} = O(d_n),$$

and with the probability at least  $1-p^{-c}$ 

$$\max_{1 \le a \le p, 1 \le t \le k} \| (\mathbf{B}_{a}^{(t)}(\theta) - \mathbf{B}_{a}^{(t)})^{\top} (\mathbf{Z}_{-a}^{(t)})^{\top} \mathbf{Z}_{-a}^{(t)} (\mathbf{B}_{a}^{(t)}(\theta) - \mathbf{B}_{a}^{(t)}) / n^{(t)} \|_{\infty} = O(b_{n} + d_{n}).$$

By the expression of triangle inequality, we can derive

$$\max_{1 \le a \le p, 1 \le t \le k} \| (\widetilde{\mathbf{X}}_{-a}^{(t)}(\theta))^{\top} \widetilde{\mathbf{X}}_{-a}^{(t)}(\theta) / n^{(t)} - (\widetilde{\mathbf{X}}_{-a}^{(t)})^{\top} \widetilde{\mathbf{X}}_{-a}^{(t)} / n^{(t)} \|_{\infty} 
\le \max_{1 \le a \le p, 1 \le t \le k} \| (\mathbf{C}_{a}^{(t)}(\theta) - \mathbf{C}_{a}^{(t)})^{\top} (\mathbf{X}_{-a}^{(t)})^{\top} \mathbf{X}_{-a}^{(t)} (\mathbf{C}_{a}^{(t)}(\theta) - \mathbf{C}_{a}^{(t)}) / n^{(t)} \|_{\infty} 
+ 2 \max_{1 \le a \le p, 1 \le t \le k} \| (\mathbf{C}_{a}^{(t)}(\theta) - \mathbf{C}_{a}^{(t)})^{\top} (\mathbf{X}_{-a}^{(t)})^{\top} \mathbf{Z}_{-a}^{(t)}(\theta) - \mathbf{B}_{a}^{(t)}) / n^{(t)} \|_{\infty} 
+ \max_{1 \le a \le p, 1 \le t \le k} \| (\mathbf{B}_{a}^{(t)}(\theta) - \mathbf{B}_{a}^{(t)})^{\top} (\mathbf{Z}_{-a}^{(t)})^{\top} \mathbf{Z}_{-a}^{(t)} (\mathbf{B}_{a}^{(t)}(\theta) - \mathbf{B}_{a}^{(t)}) / n^{(t)} \|_{\infty}$$

Then, we can conclude that

l

$$\max_{1 \le l \le p, 1 \le t \le k} |(\widetilde{\mathbf{X}}_l^{(t)}(\theta))^\top \widetilde{\mathbf{X}}_l^{(t)}(\theta) / n^{(t)} - (\widetilde{\mathbf{X}}_l^{(t)})^\top \widetilde{\mathbf{X}}_l^{(t)} / n^{(t)}| = O(b_n + \sqrt{\log(p)/n^{(t)}})$$

holds with probability at least  $1 - 3p^{-c}$ . It entails that for sufficiently large n there is a positive constant  $\widetilde{M}_1$  that

$$\widetilde{M}_1/2 \le (\widetilde{\mathbf{X}}_l^{(t)}(\theta))^\top \widetilde{\mathbf{X}}_l^{(t)}(\theta)/n^{(t)} \le 3\widetilde{M}_1/2$$
(S9.1)

holds uniformly over  $1 \leq l \leq p, 1 \leq t \leq k$  with probability at least  $1 - 3p^{-c} - 2pk \exp(-n/32)$  since  $b_n = o(1)$  and  $\log(p) = o(n)$ . Therefore,  $\triangle$  and  $\overline{\triangle}$  are of the same order componentwise and globally.

Using the same techniques as the *Step 1* of the proof of Theorem 3.1 in Ren et al. (2019), we can obtain that for all  $1 \le a \le p$ ,

$$\sum_{l \in \mathcal{T}_a/\mathrm{NE}_a} \|\bar{\Delta}_{a(l)}\|_2 \le \xi \sum_{l \in \mathrm{NE}_a} \|\bar{\Delta}_{a(l)}\|_2.$$
(S9.2)

Further, under Conditions 1-2 and the fact that  $\mathbf{X}_{a}^{(t)'}\mathbf{X}_{a}^{(t)}/(\mathbf{\Sigma}_{0}^{(t)})_{a,a} \sim \chi^{2}(n^{(t)})$ and  $\mathbf{E}_{a}^{(t)'}\mathbf{E}_{a}^{(t)}/\omega_{aa}^{(t)} \sim \chi^{2}(n^{(t)})$ , by Lemma D.7 in Ren et al. (2019) it holds that with the probability at least  $1 - 4k \exp(-n/32)$ ,

$$\sum_{t=1}^{k} \frac{\|\bar{\mathcal{X}}_{-a}^{(t)}(\theta)\bar{\bigtriangleup}_{a}^{(t)}\|^{2}}{n\zeta_{t}} \ge \frac{1}{\sqrt{6M_{1}M_{2}}} \sum_{t=1}^{k} \frac{\|\bar{\mathcal{X}}_{-a}^{(t)}(\theta)\bar{\bigtriangleup}_{a}^{(t)}\|^{2}}{n}$$
(S9.3)

where  $\bar{\mathcal{X}}_{-a}^{(t)}(\theta) = \mathcal{X}_{-a}^{(t)}(\theta)(\mathcal{D}_{a}^{(t)}(\theta))^{-1/2}$  and  $\zeta_{t} = Q_{t}\left(\hat{\bar{\beta}}_{a}^{\operatorname{aug}(t)}(\theta)\right) + Q_{t}\left(\bar{\beta}_{a}^{\operatorname{aug}(t)}\right)$ .

In addition, since the facts of (A.27), (A.28), and (A.30) in the supplementary materials of Ren et al. (2019) all hold here, using the same techniques of (A.31) in the supplementary materials of Ren et al. (2019), we can prove that

$$\sum_{t=1}^{k} \frac{\|\bar{\mathcal{X}}_{-a}^{(t)}(\theta)\bar{\bigtriangleup}_{a}^{(t)}\|^{2}}{n\zeta_{t}} \leq \lambda \left(\frac{3\xi-1}{\xi+1} + \xi\frac{(\xi-3)_{+}}{\xi+1}\right) \sum_{l\in\mathbb{N}E_{a}} \|\bar{\bigtriangleup}_{a(l)}\|_{2}, \quad (S9.4)$$

Combining with the result of (S9.3), we can conclude that

$$\sum_{t=1}^{k} \frac{\|\bar{\mathcal{X}}_{-a}^{(t)}(\theta)\bar{\bigtriangleup}_{a}^{(t)}\|^{2}}{n} \leq \frac{\lambda}{\sqrt{6M_{1}M_{2}}} \left(\frac{3\xi-1}{\xi+1} + \xi\frac{(\xi-3)_{+}}{\xi+1}\right) \sum_{l\in\mathbb{N}E_{a}} \|\bar{\bigtriangleup}_{a(l)}\|_{2}$$
(S9.5)

holds with the probability at least  $1 - 4k \exp(-n/32)$ .

For convenience, let

$$C_{\xi} = \frac{1}{\sqrt{6M_1M_2}} \left( \frac{3\xi - 1}{\xi + 1} + \xi \frac{(\xi - 3)_+}{\xi + 1} \right).$$

which is shown in equation (S9.4). The inequality (S9.5) implies that with the probability at least  $1 - 4k \exp(-n/32)$ 

$$\sum_{t=1}^{k} \frac{(\bar{\Delta}_{a}^{(t)})^{\top} (\bar{\mathcal{X}}_{-a}^{(t)}(\theta))^{\top} \bar{\mathcal{X}}_{-a}^{(t)}(\theta) \bar{\Delta}_{a}^{(t)}}{n} \le C_{\xi} \lambda \sum_{l \in \mathrm{NE}_{a}} \|\bar{\Delta}_{a(l)}\|_{2}.$$
 (S9.6)

Following the same definition as that in Ren et al. (2019), let

$$\kappa(\xi, \mathrm{NE}_a) = \inf_{\mathbf{u}\neq\mathbf{0}} \left\{ \frac{\sqrt{|\mathrm{NE}_a|} \|\bar{\mathcal{X}}_{-a}(\theta)\mathbf{u}\|_2}{\sqrt{n}\sum_{j\in\mathrm{NE}_a} \|\mathbf{u}_{(j)}\|_2} : \mathbf{u}\in\Psi(\xi, \mathrm{NE}_a) \right\},\,$$

where  $\Psi(\xi, NE_a) = \{ \mathbf{u} \in \mathbb{R}^{2(p-1)k} : \sum_{j \in \mathcal{T}_a/NE_a} \| \mathbf{u}_{(j)} \|_2 \le \xi \sum_{j \in NE_a} \| \mathbf{u}_{(j)} \|_2 \}.$ 

Since  $\overline{\Delta}_a \in \Phi(\xi, NE_a)$  by (S9.2), we have

$$\sum_{t=1}^{k} \frac{(\bar{\bigtriangleup}_{a}^{(t)})^{\top} (\bar{\mathcal{X}}_{-a}^{(t)}(\theta))^{\top} \bar{\mathcal{X}}_{-a}^{(t)}(\theta) \bar{\bigtriangleup}_{a}^{(t)}}{n} \geq \frac{\kappa^{2}(\xi, \operatorname{NE}_{a}) \left(\sum_{j \in \operatorname{NE}_{a}} \|\bar{\bigtriangleup}_{a(j)}\|_{2}\right)^{2}}{|\operatorname{NE}_{a}|}$$
(S9.7)

Recall that for each given  $\theta$ , the rows of  $\mathcal{X}_{-a}^{(t)}(\theta)$  follow the Gaussian distribution  $N(\mathbf{0}, \mathcal{G}(\theta))$ , where

$$\mathcal{G}_{a}(\theta) \left( \begin{array}{ccc} \boldsymbol{\Sigma}_{-a,-a}^{(t)} & \mathbf{C}_{a}^{(t)}(\theta)\boldsymbol{\Sigma}_{-a,-a}^{(t)} \\ \mathbf{C}_{a}^{(t)}(\theta)\boldsymbol{\Sigma}_{-a,-a}^{(t)} & \mathbf{C}_{a}^{(t)}(\theta)\boldsymbol{\Sigma}_{-a,-a}^{(t)}\mathbf{C}_{a}^{(t)}(\theta) + \mathbf{B}_{a}^{(t)}(\theta) \end{array} \right)$$

According to Condition 1 and the assumption in the theorem that the smallest eigenvalue of  $2\operatorname{diag}\{\mathbf{s}_{a}^{(t)}\}-\operatorname{diag}\{\mathbf{s}_{a}^{(t)}\}\mathbf{\Omega}_{-a}^{(t)}\operatorname{diag}\{\mathbf{s}_{a}^{(t)}\}\$  is uniformly bounded from below by some positive constant for all  $1 \leq a \leq p, 1 \leq t \leq k$ , we have

$$1/M_6 \leq \lambda_{\min}(\mathcal{G}_a^{(t)}(\theta_0)) \leq \lambda_{\max}(\mathcal{G}_a^{(t)}(\theta_0)) \leq M_6$$

holds uniformly over  $1 \le a \le p$ ,  $1 \le t \le k$  for some constant  $M_6 > 1$ .

Moreover, by the triangle inequality we have

$$\lambda_{\min}(\mathcal{G}_{a}^{(t)}(\theta)) \geq \lambda_{\min}(\mathcal{G}_{a}^{(t)}(\theta_{0})) + \lambda_{\min}(\mathcal{G}_{a}^{(t)}(\theta) - \mathcal{G}_{a}^{(t)}(\theta_{0}))$$
$$\geq \lambda_{\min}(\mathcal{G}_{a}^{(t)}(\theta_{0})) - \lambda_{\max}(\mathcal{G}_{a}^{(t)}(\theta) - \mathcal{G}_{a}^{(t)}(\theta_{0})).$$

Since  $\theta \in \Theta$ , according to the equation (S4.7) and (S4.10), we have  $\lambda_{\max}(\mathcal{G}_a^{(t)}(\theta) - \mathcal{G}_a^{(t)}(\theta_0)) \leq Cb_n$  holds uniformly over  $1 \leq a \leq p, 1 \leq t \leq k$ . Then for sufficiently large n, we can conclude that there exist some positive constant  $\widetilde{M}_6$  that

$$1/\widetilde{M}_6 \le \lambda_{\min}(\mathcal{G}_a^{(t)}(\theta)) \le \lambda_{\max}(\mathcal{G}_a^{(t)}(\theta)) \le \widetilde{M}_6.$$

Thus, according to the Lemma D.5 in Ren et al. (2019) shows that

$$\kappa(\xi, \mathrm{NE}_{a}) > \min_{l,t} \left\{ \left( \frac{n^{(t)}}{(\mathbf{X}_{l}^{(t)}(\theta))^{\top} \mathbf{X}_{l}^{(t)}(\theta)} \right)^{1/2} \land \left( \frac{n^{(t)}}{(\widetilde{\mathbf{X}}_{l}^{(t)}(\theta)^{\top} \widetilde{\mathbf{X}}_{l}^{(t)}(\theta)} \right)^{1/2} \right\} / (2\widetilde{M}_{6})^{1/2}$$

holds with probability at least  $1 - 2k \exp(-cn)$ . Combining with result of (S9.1), yields that with the probability at least  $1 - 2pk \exp(-n/32) - 2k \exp(-cn) - 3p^{-c}$ ,  $\kappa(\xi, NE_a) > C_{\kappa}$ , where  $C_{\kappa}$  is some positive constant. This together with (S9.6) and (S9.7) yields that with the probability at least  $1 - 2pk \exp(-n/32) - 2k \exp(-cn) - 4k \exp(-n/32) - 3p^{-c}$ 

$$\frac{\left(\sum_{j\in \mathrm{NE}_{a}}\|\bar{\bigtriangleup}_{a(j)}\|_{2}\right)^{2}}{|\mathrm{NE}_{a}|} \leq C\lambda \sum_{l\in \mathrm{NE}_{a}}\|\bar{\bigtriangleup}_{a(l)}\|_{2}$$
(S9.8)

Thus it holds simultaneously for all  $1 \le a \le p$  that

$$\sup_{\theta \in \mathbf{\Theta}} \sum_{j \in \mathrm{NE}_a} \|\bar{\triangle}_{a(j)}\|_2 = O(l_a \lambda)$$

with the probability at least  $1-2pk \exp(-n/32)-2k \exp(-cn)-4k \exp(-n/32)-3p^{-c}$ . This together with (S9.1) and (S9.2) yields that

$$\sup_{\theta \in \Theta} \sum_{j \in \mathcal{T}_a} \| \Delta_{a(j)} \|_2 \le C \sup_{\theta \in \Theta} \sum_{j \in \mathcal{T}_a} \| \bar{\Delta}_{a(j)} \| \\ \le (1+\xi)C \sup_{\theta \in \Theta} \sum_{j \in NE_a} \| \bar{\Delta}_{a(j)} \| = O(l_a\lambda)$$

holds simultaneously over  $1 \le a \le p$  with the probability at least  $1 - 2pk \exp(-n/32) - 2k \exp(-cn) - 4k \exp(-n/32) - 3p^{-c}$ .

Note that the above analysis is conditional on the event  $\bigcap_{1 \le a \le p} \mathcal{B}_a$ .

Since we have proven that  $\mathbb{P}(\mathcal{B}_a) > 1 - 3p^{-\nu+1}$ , it easy to prove that

$$\mathbb{P}(\bigcap_{1 \le a \le p} \mathcal{B}_a) \ge 1 - 3pp^{1-\nu} \ge 1 - p^{2-\nu}$$

Then, we can conclude that with probability at least  $1-2pk\exp(-n/32)-$ 

$$2k\exp(-cn) - 4k\exp(-n/32) - p^{2-\nu} - 3p^{-\nu}$$

$$\sup_{\boldsymbol{\theta}\in\boldsymbol{\Theta}}\sum_{j\in\mathcal{T}_a}\|\Delta_{a(j)}\|_2=O(l_a\lambda),$$

holds simultaneously for all  $1 \le a \le p$ . Since  $\log(p) = O(n)$ , and v > 2defined in the lemma, then there exits some positive constant  $c_v$  such that  $p^{-c_v} > 2pk \exp(-n/32) + 2k \exp(-cn) + 4k \exp(-n/32) + p^{2-v} + 3p^{-c}$ , which completes the proof of Lemma S1.4.

# S10 The figures of real data analysis

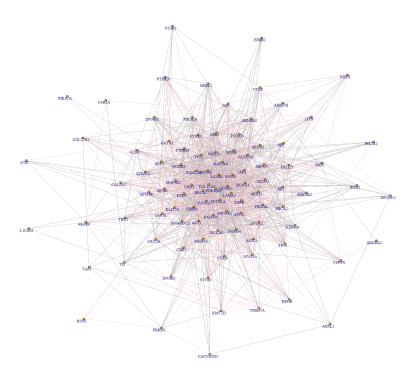


Figure 1: Network structure of genes recovered by our method. The pink lines are the edges identified by both our method and GFC method. Grey lines are identified only by our method.

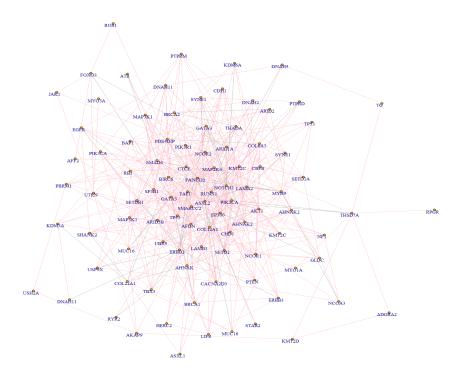


Figure 2: Network structure of genes recovered by GFC method. The pink lines are the edges identified by both GFC method and our method. Grey lines are identified only by GFC method.

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