

# Inferring Hub Nodes on Differential Gaussian Graphical Models

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## Abstract

This document contains the supplementary material to the paper “Inferring Hub Nodes on Differential Gaussian Graphical Models”. In Appendix A, we provide the proof of Theorem 4.1 and Lemma 4.2. In Appendix B, we prove Theorem 4.4. Appendix C states some technical lemmas of Appendix A. Appendix D presents additional numeric results for Section 5.1.

Throughout the Appendix, we will use the following Landau symbols. We write  $f(n, d) = O(g(n, d))$  if  $f(n, d) \leq Cg(n, d)$  for some positive constant  $C$  and all sufficiently large  $n$  and  $d$ . The constant  $C$  is independent of the sample size  $n$  and the dimension  $d$ , but may vary from line to line. For simplicity, we also write  $f(n, d) \lesssim g(n, d)$  to indicate  $f(n, d) = O(g(n, d))$ . And we write  $f(n, d) = o(g(n, d))$  if  $f(n, d)/g(n, d) \rightarrow 0$  as  $n \rightarrow \infty$  and  $d \rightarrow \infty$ .

## A Proof of Theorem 4.1 and Lemma 4.2

In this section, we provide the proofs for Theorem 4.1 and Lemma 4.2. To this end, we start with some technical lemmas that will be helpful in the proof. The proofs of the technical lemmas are deferred to Appendix C. The following lemma shows that the term  $\widehat{\Delta}^d - \Delta$  can be rewritten as the summation of a leading term and a remainder term.

**Lemma A.1.** We have  $\widehat{\Delta}^d - \Delta = \text{Leading} + \text{Remainder}$ , where

$$\text{Leading} = (\mathbf{V}_Y - \Delta)(\widehat{\Sigma}_X - \Sigma_X)\mathbf{V}_X^T - \mathbf{V}_Y(\widehat{\Sigma}_Y - \Sigma_Y)(\mathbf{V}_X + \Delta)^T;$$

$$\begin{aligned} \text{Remainder} = & \{(\widehat{\Delta} - \Delta) - \mathbf{V}_Y\widehat{\Sigma}_Y(\widehat{\Delta} - \Delta)(\mathbf{V}_X\widehat{\Sigma}_X)^T\} - \mathbf{V}_Y(\widehat{\Sigma}_Y - \Sigma_Y)\Delta(\widehat{\Sigma}_X - \Sigma_X)\mathbf{V}_X^T \\ & - \mathbf{V}_Y(\widehat{\Sigma}_Y - \Sigma_Y)\Delta(\mathbf{V}_X\Sigma_X - \mathbf{I})^T - (\mathbf{V}_Y\Sigma_Y - \mathbf{I})\Delta(\widehat{\Sigma}_X - \Sigma_X)\mathbf{V}_X^T. \end{aligned}$$

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The next lemma summarizes the estimation rates of the estimators. The results follow directly from Theorem 3 in Zhao et al. (2014), and from Lemma E.5 in Ma et al. (2017). Thus the proof is omitted.

**Lemma A.2.** Assume the conditions in Theorem 4.1. We have with probability at least  $1 - c/d$ ,

$$\|\widehat{\Delta} - \Delta\|_{1,1} = O(s\sqrt{\log d/n}), \quad \|\widehat{\Sigma}_X - \Sigma_X\|_{\max} = O(\sqrt{\log d/n}), \quad \text{and} \quad \|\widehat{\Sigma}_Y - \Sigma_Y\|_{\max} = O(\sqrt{\log d/n}),$$

where  $c$  is a generic constant. Furthermore, we define the event  $\Gamma$  as follows:

$$\Gamma = \{(\mathbb{X}^T, \mathbb{Y}^T) \in \mathbb{R}^{2n \times d} \mid \|\widehat{\Sigma}'_X - \Sigma_X\|_{\max} \leq C\sqrt{\log d/n}, \|\widehat{\Sigma}'_Y - \Sigma_Y\|_{\max} \leq C\sqrt{\log d/n}\}, \quad (\text{A.1})$$

where  $\widehat{\Sigma}'_X, \widehat{\Sigma}'_Y$  are sample covariance matrices obtained from the splitted data  $\mathcal{D}_2$  as suggested in Section 3.1, and  $C$  is a sufficiently large constant. Then we have  $\mathbb{P}(\mathcal{D}_2 \in \Gamma) \geq 1 - 4d^{-1}$ .

The next lemma establishes properties of the bias correction matrices  $\mathbf{V}_X$  and  $\mathbf{V}_Y$  that will be useful for bounding the remainder term.

**Lemma A.3.** Assume the conditions in Theorem 4.1. Let  $\lambda'$  in (34) satisfies  $\lambda' = C'\sqrt{\log d/n}$ , where  $C'$  is a sufficiently large constant. We have with probability at least  $1 - c/d$ ,

$$\|\mathbf{V}_X\|_{\infty} = O(1); \quad \|\mathbf{V}_Y\|_{\infty} = O(1);$$

$$\|\mathbf{V}_X \widehat{\Sigma}_X - \mathbf{I}\|_{\max} = O(\sqrt{\log d/n}); \quad \text{and} \quad \|\mathbf{V}_Y \widehat{\Sigma}_Y - \mathbf{I}\|_{\max} = O(\sqrt{\log d/n}),$$

where  $c$  is a generic constant.

Next, we present a lemma on an upper bound for the remainder term.

**Lemma A.4.** Assume the conditions in Theorem 4.1. We have with probability at least  $1 - c/d$  that  $\|\text{Remainder}\|_{\max} = O(s \log d/n)$ , where  $c$  is a generic constant.

The next lemma provides a lower bound for the asymptotic variance  $\xi_{jk}$  defined in (43).

**Lemma A.5.** Under conditions in Theorem 4.1, we have  $1/\xi_{jk} = O_P(1)$ .

The sixth lemma bounds of the third moment of a random variable, which can lead to the asymptotic normality of the Leading term.

**Lemma A.6.** (Third moment bound) Suppose the conditions of Theorem 4.1 hold, and denote

$$Z_{jk} = (\mathbf{V}_Y - \mathbf{\Delta})_{j\bullet} (\mathbf{X}\mathbf{X}^T - \mathbf{\Sigma}_X) \mathbf{V}_{X,k\bullet}^T - \mathbf{V}_{Y,j\bullet} (\mathbf{Y}\mathbf{Y}^T - \mathbf{\Sigma}_Y) (\mathbf{V}_X + \mathbf{\Delta})_{k\bullet}^T, \quad \forall j, k \in [d].$$

We have  $\forall (\mathbb{X}^T, \mathbb{Y}^T)^T \in \Gamma$ ,  $\rho := \mathbb{E}(|Z_{jk}|^3 | \mathcal{D}_2 = (\mathbb{X}^T, \mathbb{Y}^T)^T) = O(1)$ .

With Lemmas A.1–A.6, we now provide the proof of Theorem 4.1.

### A.1 Proof of Theorem 4.1

*Proof.* From Lemma A.1, we have

$$\sqrt{n}(\widehat{\mathbf{\Delta}}_{jk}^d - \mathbf{\Delta}_{jk})/\xi_{jk} = \sqrt{n}\text{Leading}_{jk}/\xi_{jk} + \sqrt{n}\text{Remainder}_{jk}/\xi_{jk}.$$

From Lemmas A.4–A.5 and the scaling condition  $s \log d/\sqrt{n} = o(1)$ , we have  $\sqrt{n}\text{Remainder}_{jk}/\xi_{jk} = o_P(1)$ . By Slutsky's theorem, it remains to show that  $\sqrt{n}\text{Leading}_{jk}/\xi_{jk} \rightsquigarrow N(0, 1)$ . To this end, let

$$Z_{i,jk} = (\mathbf{V}_Y - \mathbf{\Delta})_{j\bullet} (\mathbf{X}_i \mathbf{X}_i^T - \mathbf{\Sigma}_X) \mathbf{V}_{X,k\bullet}^T - \mathbf{V}_{Y,j\bullet} (\mathbf{Y}_i \mathbf{Y}_i^T - \mathbf{\Sigma}_Y) (\mathbf{V}_X + \mathbf{\Delta})_{k\bullet}^T,$$

$S_n = \sum_{i=1}^n Z_{i,jk} = n \cdot \text{Leading}_{jk}$ , and  $s_n = \sqrt{n}\xi_{jk}$ . Conditioning on  $\mathcal{D}_2$ , we know that  $Z_{1,jk}, \dots, Z_{n,jk}$  are i.i.d., so we can apply the Berry-Esseen Theorem (see Theorem 3.4.17 in Durrett (2019)) by conditioning on  $\mathcal{D}_2$  to obtain an upper bound: there exists a universal constant  $C$  such that for every  $(\mathbb{X}^T, \mathbb{Y}^T)^T \in \Gamma$  in (A.1) and every  $x \in \mathbb{R}$ ,

$$\left| \mathbb{P}\left(\frac{S_n}{s_n} \leq x \mid \mathcal{D}_2 = (\mathbb{X}^T, \mathbb{Y}^T)^T\right) - \Phi(x) \right| \leq \frac{C\rho}{\sqrt{n}\xi_{jk}^3} \leq \frac{C}{\sqrt{n}}, \quad (\text{A.2})$$

where  $\rho$  is the conditional third moment in Lemma A.6 and  $C_2$  is another universal constant. Note that the last inequality holds by an application of Lemmas A.5 and A.6.

Define the event  $\mathcal{E} = \{\mathcal{D}_2 \in \Gamma\}$ . Using the law of total probability, we have

$$\begin{aligned} \left| \mathbb{P}\left(\frac{S_n}{s_n} \leq x\right) - \Phi(x) \right| &= \left| \mathbb{P}\left(\frac{S_n}{s_n} \leq x \mid \mathcal{E}\right) \mathbb{P}(\mathcal{E}) + \mathbb{P}\left(\frac{S_n}{s_n} \leq x \mid \mathcal{E}^c\right) \mathbb{P}(\mathcal{E}^c) - \Phi(x) \right| \\ &\leq \left| \mathbb{P}\left(\frac{S_n}{s_n} \leq x \mid \mathcal{E}\right) - \Phi(x) \right| \mathbb{P}(\mathcal{E}) + \left| \mathbb{P}\left(\frac{S_n}{s_n} \leq x \mid \mathcal{E}^c\right) - \Phi(x) \right| \mathbb{P}(\mathcal{E}^c) \quad (\text{A.3}) \\ &\leq \left| \mathbb{P}\left(\frac{S_n}{s_n} \leq x \mid \mathcal{E}\right) - \Phi(x) \right| + 2\mathbb{P}(\mathcal{E}^c). \end{aligned}$$

From (A.2), we have

$$\left| \mathbb{P}\left(\frac{S_n}{s_n} \leq x \mid \mathcal{E}\right) - \Phi(x) \right| = \left| \int \left[ \mathbb{P}\left(\frac{S_n}{s_n} \leq x \mid \mathcal{D}_2 = (\mathbb{X}^T, \mathbb{Y}^T)^T\right) - \Phi(x) \right] d\mathbb{P}(\mathbb{X}^T, \mathbb{Y}^T)^T \right| \leq \frac{C}{\sqrt{n}}.$$

From Lemma A.2, we have  $\mathbb{P}(\mathcal{E}^c) \leq 4d^{-1}$ . From (A.3), we have

$$\left| \mathbb{P}\left(\frac{\sqrt{n}\text{Leading}_{jk}}{\xi_{jk}} \leq x\right) - \Phi(x) \right| = \left| \mathbb{P}\left(\frac{S_n}{s_n} \leq x\right) - \Phi(x) \right| \leq \frac{C}{\sqrt{n}} + \frac{8}{d} = o(1),$$

indicating that  $\sqrt{n}\text{Leading}_{jk}/\xi_{jk} \rightsquigarrow N(0, 1)$ , as desired.  $\square$

## A.2 Proof of Lemma 4.2

*Proof.* It suffices to prove  $|\hat{\xi}_{jk}^2 - \xi_{jk}^2| = O_P(1)$ . Recall from the definition of  $\xi_{jk}$  in (43), we have

$$\begin{aligned} \xi_{jk}^2 &= \underbrace{((\mathbf{V}_Y - \Delta)_{j\bullet} \Sigma_X (\mathbf{V}_Y - \Delta)_{j\bullet}^T) (\mathbf{V}_{X,k\bullet} \Sigma_X \mathbf{V}_{X,k\bullet}^T)}_{I_1} + \underbrace{((\mathbf{V}_Y - \Delta)_{j\bullet} \Sigma_X \mathbf{V}_{X,k\bullet}^T)}_{I_2} \\ &\quad + \underbrace{(\mathbf{V}_{Y,j\bullet} \Sigma_Y \mathbf{V}_{Y,j\bullet}^T) ((\mathbf{V}_X + \Delta)_{k\bullet} \Sigma_Y (\mathbf{V}_X + \Delta)_{k\bullet}^T)}_{I_3} + \underbrace{(\mathbf{V}_{Y,j\bullet} \Sigma_Y (\mathbf{V}_X + \Delta)_{k\bullet}^T)}_{I_4} \end{aligned}$$

Similarly we use the definition of  $\hat{\xi}_{jk}$  in (45) to expand  $\hat{\xi}_{jk}^2 = \hat{I}_1 + \hat{I}_2 + \hat{I}_3 + \hat{I}_4$ . Then  $|\hat{\xi}_{jk}^2 - \xi_{jk}^2| \leq \sum_{t=1}^4 |I_t - \hat{I}_t|$ . We start with showing  $|I_1 - \hat{I}_1| = O_P(1)$ . Note that

$$\begin{aligned} |I_1 - \hat{I}_1| &= |((\mathbf{V}_Y - \Delta)_{j\bullet} \Sigma_X (\mathbf{V}_Y - \Delta)_{j\bullet}^T) (\mathbf{V}_{X,k\bullet} \Sigma_X \mathbf{V}_{X,k\bullet}^T) - ((\mathbf{V}_Y - \hat{\Delta})_{j\bullet} \hat{\Sigma}_X (\mathbf{V}_Y - \hat{\Delta})_{j\bullet}^T) (\mathbf{V}_{X,k\bullet} \hat{\Sigma}_X \mathbf{V}_{X,k\bullet}^T)| \\ &\leq |((\mathbf{V}_Y - \Delta)_{j\bullet} \Sigma_X (\mathbf{V}_Y - \Delta)_{j\bullet}^T - (\mathbf{V}_Y - \hat{\Delta})_{j\bullet} \hat{\Sigma}_X (\mathbf{V}_Y - \hat{\Delta})_{j\bullet}^T) (\mathbf{V}_{X,k\bullet} \Sigma_X \mathbf{V}_{X,k\bullet}^T)| \\ &\quad + |(\mathbf{V}_Y - \hat{\Delta})_{j\bullet} \hat{\Sigma}_X (\mathbf{V}_Y - \hat{\Delta})_{j\bullet}^T \{ \mathbf{V}_{X,k\bullet} (\hat{\Sigma}_X - \Sigma_X) \mathbf{V}_{X,k\bullet}^T \}|. \end{aligned}$$

From Assumption 1, we have  $\|(\mathbf{V}_Y - \Delta)_{j\bullet}\|_1 = O_P(1)$ ,  $\|(\mathbf{V}_Y - \widehat{\Delta})_{j\bullet} - (\mathbf{V}_Y - \Delta)_{j\bullet}\|_1 = O_P(1)$ ,  $\|\mathbf{V}_{k\bullet}^X\|_1 = O_P(1)$ ,  $\|\Sigma_X\|_{\max} = O(1)$ , and  $\|\widehat{\Sigma}_X - \Sigma_X\|_{\max} = O_P(\sqrt{\log d/n})$ . Combining the above with Lemma A.2, we further have

$$|((\mathbf{V}_Y - \widehat{\Delta})_{j\bullet} \widehat{\Sigma}_X (\mathbf{V}_Y - \widehat{\Delta})_{j\bullet}^T) - ((\mathbf{V}_Y - \Delta)_{j\bullet} \Sigma_X (\mathbf{V}_Y - \Delta)_{j\bullet}^T)| = O_P(1); |(\mathbf{V}_{X,k\bullet} \Sigma_X \mathbf{V}_{X,k\bullet}^T)| = O_P(1);$$

$$|(\mathbf{V}_{X,k\bullet} \widehat{\Sigma}_X \mathbf{V}_{X,k\bullet}^T) - (\mathbf{V}_{X,k\bullet} \Sigma_X \mathbf{V}_{X,k\bullet}^T)| = O_P(1); |((\mathbf{V}_Y - \Delta)_{j\bullet} \Sigma_X (\mathbf{V}_Y - \Delta)_{j\bullet}^T)| = O_P(1).$$

Through the use of the inequality  $|\mathbf{u}^T \mathbf{A} \mathbf{v}| \leq \|\mathbf{u}\|_1 \|\mathbf{A}\|_{\max} \|\mathbf{v}\|_1$  that holds for any vector  $\mathbf{u}$ ,  $\mathbf{v}$  and any matrix  $\mathbf{A}$ , we conclude that  $|I_1 - \widehat{I}_1| = O_P(1)$ , as desired.

The other quantities can be derived similarly and are hence omitted from the proof.  $\square$

## B Proof of Theorem 4.4

In this proof, we will use the notation  $T^E$  to indicate the test statistic  $T_E$  and  $T^B$  to indicate  $T_E^B$ . To approximate the statistic  $T^E$  by the multiplier bootstrap process  $T^B$ , we also define two intermediate processes

$$T_0^E := \max_{(j,k) \in E} \frac{1}{\sqrt{n}} \sum_{i=1}^n [(\mathbf{V}_Y - \Delta)_{j\bullet} (\mathbf{X}_i \mathbf{X}_i^T - \Sigma_X) \mathbf{V}_{X,k\bullet}^T - \mathbf{V}_{Y,j\bullet} (\mathbf{Y}_i \mathbf{Y}_i^T - \Sigma_Y) (\mathbf{V}_X + \Delta)_{k\bullet}^T],$$

$$T_0^B := \max_{(j,k) \in E} \frac{1}{\sqrt{n}} \sum_{i=1}^n [(\mathbf{V}_Y - \Delta)_{j\bullet} (\mathbf{X}_i \mathbf{X}_i^T - \Sigma_X) \mathbf{V}_{X,k\bullet}^T - \mathbf{V}_{Y,j\bullet} (\mathbf{Y}_i \mathbf{Y}_i^T - \Sigma_Y) (\mathbf{V}_X + \Delta)_{k\bullet}^T] \xi_i.$$

Since  $T_0^B$  is the multiplier bootstrap process of  $T_0^E$ , we can use  $T_0^B$  to estimate the quantiles of  $T_0^E$ . We will prove that we can utilize  $T_0^E$  and  $T_0^B$  to approximate  $T^E$  and  $T^B$ , respectively. To prove this theorem, it suffices to check three conditions in Corollary 3.1 of Chernozhukov et al. (2013), stated as follows:

1. For some positive constants  $c$  and  $C$ , we have

$$\min_{(j,k) \in E} \mathbb{E}[(\mathbf{V}_Y - \Delta)_{j\bullet} (\mathbf{X} \mathbf{X}^T - \Sigma_X) \mathbf{V}_{X,k\bullet}^T]^2 \geq c, \quad \min_{(j,k) \in E} \mathbb{E}[\mathbf{V}_{Y,j\bullet} (\mathbf{Y} \mathbf{Y}^T - \Sigma_Y) (\mathbf{V}_X + \Delta)_{k\bullet}^T]^2 \geq c;$$

$$\max_{(j,k) \in E} \mathbb{E}[(\mathbf{V}_Y - \Delta)_{j\bullet} (\mathbf{X} \mathbf{X}^T - \Sigma_X) \mathbf{V}_{X,k\bullet}^T]^2 \leq C, \quad \max_{(j,k) \in E} \mathbb{E}[\mathbf{V}_{Y,j\bullet} (\mathbf{Y} \mathbf{Y}^T - \Sigma_Y) (\mathbf{V}_X + \Delta)_{k\bullet}^T]^2 \leq C;$$

$$2. \mathbb{P}(|T^E - T_0^E| > \zeta_1) < \zeta_2;$$

$$3. \text{ And } \mathbb{P}(\mathbb{P}(|T^B - T_0^B| > \zeta_1 | \mathcal{D}_1) > \zeta_2) < \zeta_2 \text{ hold for } \zeta_1 \sqrt{\log d} + \zeta_2 = o(1).$$

Note that since we do not emphasize on the polynomial decaying in our result, we need only  $\zeta_1 \sqrt{\log d} + \zeta_2 = o(1)$  and the scaling condition  $(\log(dn))^7/n = o(1)$ . We choose  $\zeta_1 = C \sqrt{\frac{s^2(\log^3(dn))}{n}}$  and  $\zeta_2 = c/d$  to check these conditions, where  $c$  and  $C$  are two constants. The scaling conditions in Theorem 4.4 imply the aforementioned two scaling conditions.

We start with checking the first condition. The first two inequalities are proven in the proof of Lemma A.5. Moreover, in the proof of Lemma A.6, we have  $\forall j, k \in [d]$ ,

$$\|(\mathbf{V}_Y - \mathbf{\Delta})_{j\bullet}(\mathbf{X}\mathbf{X}^T - \mathbf{\Sigma}_X)\mathbf{V}_{X,k\bullet}^T\|_{\psi_1} = O(1) \text{ and } \|\mathbf{V}_{Y,j\bullet}(\mathbf{Y}\mathbf{Y} - \mathbf{\Sigma}_Y)(\mathbf{V}_X + \mathbf{\Delta})_{k\bullet}^T\|_{\psi_1} = O(1),$$

which imply the two inequalities in the first condition.

Second, we bound the difference between  $T^E$  and  $T_0^E$ . Note that  $T_0^E$  can be rewritten as  $T_0^E = \max_{(j,k) \in E} \sqrt{n} \text{Leading}_{jk}$ . By Lemma A.1, we have

$$|T^E - T_0^E| \leq \sqrt{n} \max_{(j,k) \in E} |\text{Remainder}_{jk}| \leq \sqrt{n} \|\text{Remainder}\|_{\max}.$$

From Lemma A.4, we have  $|T^E - T_0^E| \leq Cs \log d / \sqrt{n}$  with probability at least  $1 - c/d$  for some positive constants  $C$  and  $c$ , implying the second condition.

Finally, to verify the third condition, we bound the difference between  $T^B$  and  $T_0^B$ :

$$\begin{aligned} |T^B - T_0^B| &= \max_{(j,k) \in E} |f(\mathcal{D}_1, \xi)|, \text{ where} \\ f(\mathcal{D}_1, \xi) &= \frac{1}{\sqrt{n}} \sum_{i=1}^n [((\mathbf{V}_Y - \widehat{\mathbf{\Delta}})_{j\bullet}(\mathbf{X}_i\mathbf{X}_i^T - \widehat{\mathbf{\Sigma}}_X)\mathbf{V}_{X,k\bullet}^T - (\mathbf{V}_Y - \mathbf{\Delta})_{j\bullet}(\mathbf{X}_i\mathbf{X}_i^T - \mathbf{\Sigma}_X)\mathbf{V}_{X,k\bullet}^T) \\ &\quad - (\mathbf{V}_{Y,j\bullet}(\mathbf{Y}_i\mathbf{Y}_i^T - \widehat{\mathbf{\Sigma}}_Y)(\mathbf{V}_X + \widehat{\mathbf{\Delta}})_{k\bullet}^T - \mathbf{V}_{Y,j\bullet}(\mathbf{Y}_i\mathbf{Y}_i^T - \mathbf{\Sigma}_Y)(\mathbf{V}_X + \mathbf{\Delta})_{k\bullet}^T)] \xi_i \end{aligned} \quad (\text{B.1})$$

Notice that the right hand side of the above inequality is a suprema of the Gaussian process when conditioning on the data  $\mathcal{D}_1$ , so we need to bound the conditional variance of  $f(\mathcal{D}_1, \xi)$  as  $\sigma_\xi^2$  in the

following inequality.

$$\begin{aligned}
& \frac{1}{n} \max_{(j,k) \in E} \left| \sum_{i=1}^n \left( [(\mathbf{V}_Y - \widehat{\Delta})_{j\bullet} (\mathbf{X}_i \mathbf{X}_i^T - \widehat{\Sigma}_X) \mathbf{V}_{X,k\bullet}^T - (\mathbf{V}_Y - \Delta)_{j\bullet} (\mathbf{X}_i \mathbf{X}_i^T - \Sigma_X) \mathbf{V}_{X,k\bullet}^T] \right. \right. \\
& \quad \left. \left. - (\mathbf{V}_{Y,j\bullet} (\mathbf{Y}_i \mathbf{Y}_i^T - \widehat{\Sigma}_Y) (\mathbf{V}_X + \widehat{\Delta})_{k\bullet}^T - \mathbf{V}_{Y,j\bullet} (\mathbf{Y}_i \mathbf{Y}_i^T - \Sigma_Y) (\mathbf{V}_X + \Delta)_{k\bullet}^T) \right] \right|^2 \\
& \leq \max_{i \in [n]} \max_{(j,k) \in E} \left| [(\mathbf{V}_Y - \widehat{\Delta})_{j\bullet} (\mathbf{X}_i \mathbf{X}_i^T - \widehat{\Sigma}_X) \mathbf{V}_{X,k\bullet}^T - (\mathbf{V}_Y - \Delta)_{j\bullet} (\mathbf{X}_i \mathbf{X}_i^T - \Sigma_X) \mathbf{V}_{X,k\bullet}^T] \right. \\
& \quad \left. - (\mathbf{V}_{Y,j\bullet} (\mathbf{Y}_i \mathbf{Y}_i^T - \widehat{\Sigma}_Y) (\mathbf{V}_X + \widehat{\Delta})_{k\bullet}^T - \mathbf{V}_{Y,j\bullet} (\mathbf{Y}_i \mathbf{Y}_i^T - \Sigma_Y) (\mathbf{V}_X + \Delta)_{k\bullet}^T) \right|^2 \tag{B.2} \\
& \leq 2 \max_{i \in [n]} \max_{(j,k) \in E} \left| [(\mathbf{V}_Y - \widehat{\Delta})_{j\bullet} (\mathbf{X}_i \mathbf{X}_i^T - \widehat{\Sigma}_X) \mathbf{V}_{X,k\bullet}^T - (\mathbf{V}_Y - \Delta)_{j\bullet} (\mathbf{X}_i \mathbf{X}_i^T - \Sigma_X) \mathbf{V}_{X,k\bullet}^T] \right|^2 \\
& \quad + 2 \max_{i \in [n]} \max_{(j,k) \in E} \left| (\mathbf{V}_{Y,j\bullet} (\mathbf{Y}_i \mathbf{Y}_i^T - \widehat{\Sigma}_Y) (\mathbf{V}_X + \widehat{\Delta})_{k\bullet}^T - \mathbf{V}_{Y,j\bullet} (\mathbf{Y}_i \mathbf{Y}_i^T - \Sigma_Y) (\mathbf{V}_X + \Delta)_{k\bullet}^T) \right|^2.
\end{aligned}$$

Denote the right hand side of (B.2) as  $V_M$ . We now bound each term of  $V_M$ . For the first term, we have

$$\begin{aligned}
& (\mathbf{V}_Y - \widehat{\Delta})_{j\bullet} (\mathbf{X}_i \mathbf{X}_i^T - \widehat{\Sigma}_X) \mathbf{V}_{X,k\bullet}^T - (\mathbf{V}_Y - \Delta)_{j\bullet} (\mathbf{X}_i \mathbf{X}_i^T - \Sigma_X) \mathbf{V}_{X,k\bullet}^T \\
& = (\mathbf{V}_Y - \widehat{\Delta})_{j\bullet} (\Sigma_X - \widehat{\Sigma}_X) \mathbf{V}_{X,k\bullet}^T - (\widehat{\Delta} - \Delta)_{j\bullet} (\mathbf{X}_i \mathbf{X}_i^T - \Sigma_X) \mathbf{V}_{X,k\bullet}^T.
\end{aligned}$$

Moreover, with probability at least  $1 - c/d$ , we have

$$\begin{aligned}
& \max_{(j,k) \in E} |(\mathbf{V}_Y - \widehat{\Delta})_{j\bullet}|_1 \leq \|\mathbf{V}_Y\|_\infty + \|\Delta\|_\infty + \|\widehat{\Delta} - \Delta\|_\infty = O(1), \\
& \|\Sigma_X - \widehat{\Sigma}_X\|_{\max} = O(\sqrt{\log d/n}), \text{ and } \max_{(j,k) \in E} |\mathbf{V}_{X,k\bullet}|_1 \leq \|\mathbf{V}_X\|_\infty = O(1).
\end{aligned}$$

Thus, we have with probability at least  $1 - c/d$ ,

$$\begin{aligned}
& \max_{i \in [n]} \max_{(j,k) \in E} |(\mathbf{V}_Y - \widehat{\Delta})_{j\bullet} (\Sigma_X - \widehat{\Sigma}_X) \mathbf{V}_{X,k\bullet}^T| \\
& \leq \max_{(j,k) \in E} |(\mathbf{V}_Y - \widehat{\Delta})_{j\bullet}|_1 \|\Sigma_X - \widehat{\Sigma}_X\|_{\max} \max_{(j,k) \in E} |\mathbf{V}_{X,k\bullet}|_1 = O(\sqrt{\log d/n}). \tag{B.3}
\end{aligned}$$

From Lemma A.2, we have with probability at least  $1 - (dn)^{-1}$ ,  $\|\mathbf{X}_i \mathbf{X}_i^T - \Sigma_X\|_{\max} = O(\log(dn))$ .

This implies that with probability at least  $1 - 1/d$ ,  $\max_{i \in [n]} \|\mathbf{X}_i \mathbf{X}_i^T - \Sigma_X\|_{\max} = O(\log(dn))$ . In addition, we have with probability no smaller than  $1 - c/d$ ,

$$|(\widehat{\Delta} - \Delta)_{j\bullet}|_1 \leq \|\widehat{\Delta} - \Delta\|_\infty = O(s\sqrt{\log d/n}), \text{ and } \max_{(j,k) \in E} |\mathbf{V}_{X,k\bullet}|_1 \leq \|\mathbf{V}_X\|_\infty = O(1),$$

Therefore, we have with probability no smaller than  $1 - c/d$ ,

$$\begin{aligned} & \max_{i \in [n]} \max_{(j,k) \in E} |(\widehat{\Delta} - \Delta)_{j\bullet} (\mathbf{X}_i \mathbf{X}_i^T - \Sigma_X) \mathbf{V}_{X,k\bullet}^T| \\ & \leq |(\widehat{\Delta} - \Delta)_{j\bullet}|_1 \max_{i \in [n]} \|\mathbf{X}_i \mathbf{X}_i^T - \Sigma_X\|_{\max} \max_{(j,k) \in E} |\mathbf{V}_{X,k\bullet}|_1 = O\left(\frac{s \log(dn)}{\sqrt{n}}\right). \end{aligned} \quad (\text{B.4})$$

The second term in (B.2) can be bounded using a similar argument.

Next, we define the event  $\mathcal{E}$  about  $V_M$  as  $\mathcal{E} = \{V_M \leq C \frac{s^2(\log^2(dn))}{n}\}$  where  $C$  is a constant. From (B.2), (B.3) and (B.4), we have  $\mathbb{P}(\mathcal{E}^c) \leq \frac{c}{d}$ , where  $c$  is a constant related to  $C$ . By Lemma A.1 in Chernozhukov et al. (2013), under the event  $\mathcal{E}$ , recall that  $f(\mathcal{D}_1, \xi)$  is defined in (B.1) and we have

$$E_M := \mathbb{E}\left[\max_{(j,k) \in E} f(\mathcal{D}_1, \xi) \middle| \mathcal{D}_1\right] \lesssim \sqrt{n V_M} \sqrt{\log d/n} = O\left(\sqrt{\frac{s^2(\log^3(dn))}{n}}\right). \quad (\text{B.5})$$

Applying Borell's inequality (see Proposition A.2.1 in Van Der Vaart and Wellner (1996)), we have  $\forall t > 0$ ,

$$\mathbb{P}\left(\max_{(j,k) \in E} |f(\mathcal{D}_1, \xi) - E_M| > t \middle| \mathcal{D}_1\right) \leq 2 \exp\left(-\frac{t^2}{2\sigma_\xi^2}\right),$$

where the conditional variance  $\sigma_\xi^2$  is the left side in (B.2). From (B.2) and (B.5), setting  $t = \sqrt{c \log(2d) \sigma_\xi^2}$ , we have under the event  $\mathcal{E}$ ,

$$\mathbb{P}\left(\max_{(j,k) \in E} f(\mathcal{D}_1, \xi) > C \sqrt{\frac{s^2(\log^3(dn))}{n}} \middle| \mathcal{D}_1\right) \leq \frac{c}{d}.$$

From (B.1), we have

$$\mathbb{P}\left(\mathbb{P}\left(|T^B - T_0^B| > C \sqrt{\frac{s^2(\log^3(dn))}{n}} \middle| \mathcal{D}_1\right) > \frac{c}{d}\right) \leq \mathbb{P}(\mathcal{E}^c) \leq \frac{c}{d},$$

as desired. Therefore, by Corollary 3.1 of Chernozhukov et al. (2013), we have

$$\lim_{n \rightarrow \infty} |\mathbb{P}(T^E > c(\alpha, E)) - \alpha| = 0,$$

as desired.



## C Proof of Lemmas A.1–A.6

In this section, we provide proofs for Lemmas A.1–A.6 provided in Section A. We start with a lemma on the the basic property of the fourth order moments of a multivariate Gaussian random variables.

**Lemma C.1.** For a random vector  $\mathbf{X} \sim N(\mathbf{0}, \boldsymbol{\Sigma})$  and four matrices  $\mathbf{A}, \mathbf{B}, \mathbf{C}, \mathbf{D}$ , we have

$$\mathbb{E}[(\mathbf{A}\mathbf{X})(\mathbf{B}\mathbf{X})^T(\mathbf{C}\mathbf{X})(\mathbf{D}\mathbf{X})^T] = (\mathbf{A}\boldsymbol{\Sigma}\mathbf{B}^T)(\mathbf{C}\boldsymbol{\Sigma}\mathbf{D}^T) + (\mathbf{A}\boldsymbol{\Sigma}\mathbf{C}^T)(\mathbf{B}\boldsymbol{\Sigma}\mathbf{D}^T) + \text{tr}(\mathbf{B}\boldsymbol{\Sigma}\mathbf{C}^T)(\mathbf{A}\boldsymbol{\Sigma}\mathbf{D}^T).$$

*Proof.* The proof can be found in Isserlis (1916). □

### C.1 Proof of Lemma A.1

*Proof.* Using the equality  $\boldsymbol{\Sigma}_Y \boldsymbol{\Delta} \boldsymbol{\Sigma}_X - (\boldsymbol{\Sigma}_X - \boldsymbol{\Sigma}_Y) = \mathbf{0}$ , from (31), we have

$$\widehat{\boldsymbol{\Delta}}^d - \boldsymbol{\Delta} = -\mathbf{V}_Y(\widehat{\boldsymbol{\Sigma}}_Y \widehat{\boldsymbol{\Delta}} \widehat{\boldsymbol{\Sigma}}_X - (\widehat{\boldsymbol{\Sigma}}_X - \widehat{\boldsymbol{\Sigma}}_Y))\mathbf{V}_X^T + (\widehat{\boldsymbol{\Delta}} - \boldsymbol{\Delta}) + \mathbf{V}_Y(\boldsymbol{\Sigma}_Y \boldsymbol{\Delta} \boldsymbol{\Sigma}_X - (\boldsymbol{\Sigma}_X - \boldsymbol{\Sigma}_Y))\mathbf{V}_X^T.$$

Note that  $\widehat{\boldsymbol{\Sigma}}_Y \widehat{\boldsymbol{\Delta}} \widehat{\boldsymbol{\Sigma}}_X = \widehat{\boldsymbol{\Sigma}}_Y(\widehat{\boldsymbol{\Delta}} - \boldsymbol{\Delta})\widehat{\boldsymbol{\Sigma}}_X + \widehat{\boldsymbol{\Sigma}}_Y \boldsymbol{\Delta} \widehat{\boldsymbol{\Sigma}}_X$ . Thus, we have

$$\widehat{\boldsymbol{\Sigma}}_Y \boldsymbol{\Delta} \widehat{\boldsymbol{\Sigma}}_X - \boldsymbol{\Sigma}_Y \boldsymbol{\Delta} \boldsymbol{\Sigma}_X = (\widehat{\boldsymbol{\Sigma}}_Y - \boldsymbol{\Sigma}_Y)\boldsymbol{\Delta}(\widehat{\boldsymbol{\Sigma}}_X - \boldsymbol{\Sigma}_X) + (\widehat{\boldsymbol{\Sigma}}_Y - \boldsymbol{\Sigma}_Y)\boldsymbol{\Delta}\boldsymbol{\Sigma}_X + \boldsymbol{\Sigma}_Y\boldsymbol{\Delta}(\widehat{\boldsymbol{\Sigma}}_X - \boldsymbol{\Sigma}_X).$$

The result in Lemma A.1 can then be obtained after some algebraic manipulation. □

### C.2 Proof of Lemma A.3

*Proof.* We first show that  $\boldsymbol{\Theta}_X$  and  $\boldsymbol{\Theta}_Y$  are feasible solutions for the optimization problems in (34), respectively. For two matrices  $\mathbf{A}$  and  $\mathbf{B}$ , we have  $\|\mathbf{A}\mathbf{B}\|_{\max} \leq \|\mathbf{A}^T\|_1 \|\mathbf{B}\|_{\max}$  and  $\|\mathbf{A}\mathbf{B}\|_{\max} \leq \|\mathbf{A}\|_{\infty} \|\mathbf{B}\|_{\max}$ . By the aforementioned inequality, Lemma A.2, and the fact that  $\boldsymbol{\Theta}_X$  is symmetric, we have

$$\|\boldsymbol{\Theta}_X \widehat{\boldsymbol{\Sigma}}'_X - \mathbf{I}\|_{\max} = \|\boldsymbol{\Theta}_X(\widehat{\boldsymbol{\Sigma}}'_X - \boldsymbol{\Sigma}_X)\|_{\max} \leq \|\boldsymbol{\Theta}_X\|_1 \|\widehat{\boldsymbol{\Sigma}}'_X - \boldsymbol{\Sigma}_X\|_{\max} = O(\sqrt{\log d/n}),$$

with probability at least  $1 - c/d$  where  $c$  is some positive constant. Since we select  $\lambda' = C' \sqrt{\log d/n}$ , where  $C'$  is a sufficiently large constant, we know that  $\Theta_X$  and  $\Theta_Y$  are feasible solutions for optimization problem (34) with probability at least  $1 - c/d$ .

Since  $\mathbf{V}_X$  and  $\mathbf{V}_Y$  are minimizers of the optimization problem (34) and by Assumption 1, we have with probability at least  $1 - c/d$  that  $\|\mathbf{V}_X\|_\infty \leq \|\Theta_X\|_\infty = \|\Theta_X\|_1 = O(1)$ ,  $\|\mathbf{V}_Y\|_\infty = O(1)$ , and  $\|\mathbf{V}\|_\infty = \|\mathbf{V}_X\|_\infty \|\mathbf{V}_Y\|_\infty = O(1)$ , where  $\mathbf{V} = \mathbf{V}_X \otimes \mathbf{V}_Y$ .

Finally, by the triangle inequality and Lemma A.2, we have with probability at least  $1 - c/d$  that

$$\|\mathbf{V}_X \widehat{\Sigma}_X - \mathbf{I}\|_{\max} \leq \|\mathbf{V}_X \widehat{\Sigma}'_X - \mathbf{I}\|_{\max} + \|\mathbf{V}_X (\widehat{\Sigma}'_X - \Sigma_X)\|_{\max} + \|\mathbf{V}_X (\widehat{\Sigma}_X - \Sigma_X)\|_{\max} = O(\sqrt{\log d/n}),$$

where we use the inequality  $\|\mathbf{V}_X (\widehat{\Sigma}_X - \Sigma_X)\|_{\max} \leq \|\mathbf{V}_X\|_\infty \|\widehat{\Sigma}_X - \Sigma_X\|_{\max}$ .  $\square$

### C.3 Proof of Lemma A.4

*Proof.* Throughout the proof, for simplicity, we will use the notation  $O_P(\cdot)$  to indicate that an event occurs with probability at least  $1 - c/d$ . The remainder term in (33) is

$$\begin{aligned} \text{Remainder} = & \underbrace{[(\widehat{\Delta} - \Delta) - \mathbf{V}_Y \widehat{\Sigma}_Y (\widehat{\Delta} - \Delta) (\mathbf{V}_X \widehat{\Sigma}_X)^T]}_{I_1} - \underbrace{\mathbf{V}_Y (\widehat{\Sigma}_Y - \Sigma_Y) \Delta (\widehat{\Sigma}_X - \Sigma_X) \mathbf{V}_X^T}_{I_2} \\ & - \underbrace{\mathbf{V}_Y (\widehat{\Sigma}_Y - \Sigma_Y) \Delta (\mathbf{V}_X \Sigma_X - \mathbf{I})^T}_{I_3} - \underbrace{(\mathbf{V}_Y \Sigma_Y - \mathbf{I}) \Delta (\widehat{\Sigma}_X - \Sigma_X) \mathbf{V}_X^T}_{I_4}. \end{aligned}$$

We will provide upper bounds for  $I_1$ ,  $I_2$ ,  $I_3$ , and  $I_4$  under the max norm, respectively.

We start with obtaining an upper bound for  $\|I_1\|_{\max}$ . First, note that

$$\begin{aligned} \|I_1\|_{\max} &= \|(\widehat{\Delta} - \Delta) - \mathbf{V}_Y \widehat{\Sigma}_Y (\widehat{\Delta} - \Delta) (\mathbf{V}_X \widehat{\Sigma}_X)^T\|_{\max} \\ &= \|\{\mathbf{I} - \mathbf{V}(\widehat{\Sigma}_X \otimes \widehat{\Sigma}_Y)\} \text{vec}(\widehat{\Delta} - \Delta)\|_\infty \\ &\leq \|\mathbf{I} - \mathbf{V}(\widehat{\Sigma}_X \otimes \widehat{\Sigma}_Y)\|_{\max} \cdot \|\text{vec}(\widehat{\Delta} - \Delta)\|_1, \end{aligned}$$

where the second equality holds by vectorizing the product of matrices. It suffices to obtain upper bounds for  $\|\mathbf{I} - \mathbf{V}(\widehat{\Sigma}_X \otimes \widehat{\Sigma}_Y)\|_{\max}$  and  $\|\text{vec}(\widehat{\Delta} - \Delta)\|_1$ . By Lemma A.2,  $\|\text{vec}(\widehat{\Delta} - \Delta)\|_1 = O_P(s\sqrt{\log d/n})$ . Next, we bound the term  $\|\mathbf{I} - \mathbf{V}(\widehat{\Sigma}_X \otimes \widehat{\Sigma}_Y)\|_{\max}$ .

By the triangle inequality, we have

$$\begin{aligned} \|\mathbf{V}(\widehat{\boldsymbol{\Sigma}}_X \otimes \widehat{\boldsymbol{\Sigma}}_Y) - \mathbf{I}\|_{\max} &= \|\mathbf{V}\{(\widehat{\boldsymbol{\Sigma}}_X \otimes \widehat{\boldsymbol{\Sigma}}_Y) - (\boldsymbol{\Sigma}_X \otimes \boldsymbol{\Sigma}_Y)\}\|_{\max} + \|\mathbf{V}\{(\boldsymbol{\Sigma}_X \otimes \boldsymbol{\Sigma}_Y) - (\widehat{\boldsymbol{\Sigma}}'_X \otimes \widehat{\boldsymbol{\Sigma}}'_Y)\}\|_{\max} \\ &\quad + \|\mathbf{V}(\widehat{\boldsymbol{\Sigma}}'_X \otimes \widehat{\boldsymbol{\Sigma}}'_Y) - \mathbf{I}\|_{\max}. \end{aligned}$$

To bound the above term, we start with some intermediate results obtained from Lemma A.2 and Assumption 1:

$$\begin{aligned} \|(\widehat{\boldsymbol{\Sigma}}_X - \boldsymbol{\Sigma}_X) \otimes \boldsymbol{\Sigma}_Y\|_{\max} &= O_P(\sqrt{\log d/n}); \\ \|\boldsymbol{\Sigma}_X \otimes (\widehat{\boldsymbol{\Sigma}}_Y - \boldsymbol{\Sigma}_Y)\|_{\max} &= O_P(\sqrt{\log d/n}); \\ \|(\widehat{\boldsymbol{\Sigma}}_X - \boldsymbol{\Sigma}_X) \otimes (\widehat{\boldsymbol{\Sigma}}_Y - \boldsymbol{\Sigma}_Y)\|_{\max} &= O_P(\log d/n). \end{aligned}$$

Moreover, it can be shown that

$$\|\widehat{\boldsymbol{\Sigma}}_X \otimes \widehat{\boldsymbol{\Sigma}}_Y - \boldsymbol{\Sigma}_X \otimes \boldsymbol{\Sigma}_Y\|_{\max} = O_P(\sqrt{\log d/n}); \quad \|\widehat{\boldsymbol{\Sigma}}'_X \otimes \widehat{\boldsymbol{\Sigma}}'_Y - \boldsymbol{\Sigma}_X \otimes \boldsymbol{\Sigma}_Y\|_{\max} = O_P(\sqrt{\log d/n}).$$

The first term can then be upper bounded as

$$\|\mathbf{V}(\widehat{\boldsymbol{\Sigma}}_X \otimes \widehat{\boldsymbol{\Sigma}}_Y - \boldsymbol{\Sigma}_X \otimes \boldsymbol{\Sigma}_Y)\|_{\max} \leq \|\mathbf{V}\|_{\infty} \|(\widehat{\boldsymbol{\Sigma}}_X \otimes \widehat{\boldsymbol{\Sigma}}_Y) - (\boldsymbol{\Sigma}_X \otimes \boldsymbol{\Sigma}_Y)\|_{\max} = O_P(\sqrt{\log d/n}).$$

The second term can be proven similarly. Finally, since  $\lambda' = C' \sqrt{\log d/n}$  for some sufficient large constant  $C'$ , from (34), we have  $\|((\mathbf{V}_X \widehat{\boldsymbol{\Sigma}}'_X) \otimes (\mathbf{V}_Y \widehat{\boldsymbol{\Sigma}}'_Y)) - \mathbf{I} \otimes \mathbf{I}\|_{\max} = O_P(\sqrt{\log d/n})$ , which implies  $\|\mathbf{V}(\widehat{\boldsymbol{\Sigma}}'_X \otimes \widehat{\boldsymbol{\Sigma}}'_Y) - \mathbf{I}\|_{\max} = O_P(\sqrt{\log d/n})$ . Combining the above, we have  $\|I_1\|_{\max} = O_P(s \log d/n)$ .

For  $I_2$ , using a similar argument as the upper bound for  $I_1$ , we have

$$\begin{aligned} \|\mathbf{V}_Y(\widehat{\boldsymbol{\Sigma}}_Y - \boldsymbol{\Sigma}_Y) \boldsymbol{\Delta} (\widehat{\boldsymbol{\Sigma}}_X - \boldsymbol{\Sigma}_X) \mathbf{V}_X^T\|_{\max} &= \|\mathbf{V}[(\widehat{\boldsymbol{\Sigma}}_X - \boldsymbol{\Sigma}_X) \otimes (\widehat{\boldsymbol{\Sigma}}_Y - \boldsymbol{\Sigma}_Y)] \text{vec}(\boldsymbol{\Delta})\|_{\infty} \\ &\leq \|\mathbf{V}[(\widehat{\boldsymbol{\Sigma}}_X - \boldsymbol{\Sigma}_X) \otimes (\widehat{\boldsymbol{\Sigma}}_Y - \boldsymbol{\Sigma}_Y)]\|_{\max} \|\text{vec}(\boldsymbol{\Delta})\|_1 \\ &\leq sM \cdot \|\mathbf{V}[(\widehat{\boldsymbol{\Sigma}}_X - \boldsymbol{\Sigma}_X) \otimes (\widehat{\boldsymbol{\Sigma}}_Y - \boldsymbol{\Sigma}_Y)]\|_{\max} \\ &= O_P(s \log d/n), \end{aligned}$$

where the second inequality holds under the family of true differential graphs defined in (41).

For  $I_3$ , similar to the proof of Lemma A.3, we have  $\|\mathbf{V}_X \boldsymbol{\Sigma}_X - \mathbf{I}\|_{\max} = O_P(\sqrt{\log d/n})$ . Moreover,

$\|\mathbf{V}_Y(\widehat{\boldsymbol{\Sigma}}_Y - \boldsymbol{\Sigma}_Y)\|_{\max} \leq \|\mathbf{V}_Y\|_{\infty} \|\widehat{\boldsymbol{\Sigma}}_Y - \boldsymbol{\Sigma}_Y\|_{\max} = O_P(\sqrt{\log d/n})$ . Coupling the above with the fact that  $\|\boldsymbol{\Delta}\|_{1,1} \leq sM = O(s)$  under the condition in (41), we obtain

$$\|I_3\|_{\max} \leq \|\mathbf{V}_Y(\widehat{\boldsymbol{\Sigma}}_Y - \boldsymbol{\Sigma}_Y)\|_{\max} \|\boldsymbol{\Delta}\|_{1,1} \|\mathbf{V}_X \boldsymbol{\Sigma}_X - \mathbf{I}\|_{\max} = O_P(s \log d/n).$$

The upper bound for  $I_4$  can be derived using the same argument as the above and is omitted.

Putting the upper bounds for  $I_1$ ,  $I_2$ ,  $I_3$ , and  $I_4$  together, we obtain the desired result.  $\square$

#### C.4 Proof of Lemma A.5

*Proof.* We first show that conditional on  $\mathcal{D}_2$ ,  $\text{Var}(\sqrt{n}\text{Leading}_{jk}) = \xi_{jk}^2$  for all  $j, k \in [d]$ . From the definition in (32), it can be shown that  $\mathbb{E}(\sqrt{n}\text{Leading}_{jk}) = 0$ . From the fact that conditional on  $\mathcal{D}_2$ ,  $\mathbf{X}_1, \dots, \mathbf{X}_n$  are i.i.d. samples and  $\mathbf{Y}_1, \dots, \mathbf{Y}_n$  are i.i.d. samples, after some algebraic manipulation, we have

$$\text{Var}(\sqrt{n}\text{Leading}_{jk}) = \underbrace{\text{Var}(\mathbf{e}_j^T \mathbf{V}_Y (\mathbf{Y}\mathbf{Y}^T - \boldsymbol{\Sigma}_Y) (\mathbf{V}_X + \boldsymbol{\Delta})^T \mathbf{e}_k)}_{I_1} + \underbrace{\text{Var}(\mathbf{e}_j^T (\mathbf{V}_Y - \boldsymbol{\Delta}) (\mathbf{X}\mathbf{X}^T - \boldsymbol{\Sigma}_X) \mathbf{V}_X^T \mathbf{e}_k)}_{I_2}.$$

The term  $I_1$  can be computed as

$$\begin{aligned} I_1 &= \mathbb{E}(\mathbf{e}_j^T \mathbf{V}_Y (\mathbf{Y}\mathbf{Y}^T - \boldsymbol{\Sigma}_Y) (\mathbf{V}_X + \boldsymbol{\Delta})^T \mathbf{e}_k \mathbf{e}_j^T \mathbf{V}_Y (\mathbf{Y}\mathbf{Y}^T - \boldsymbol{\Sigma}_Y) (\mathbf{V}_X + \boldsymbol{\Delta})^T \mathbf{e}_k) \\ &= I_{11} - (\mathbf{e}_j^T \mathbf{V}_Y \boldsymbol{\Sigma}_Y (\mathbf{V}_X + \boldsymbol{\Delta})^T \mathbf{e}_k \mathbf{e}_j^T \mathbf{V}_Y \boldsymbol{\Sigma}_Y (\mathbf{V}_X + \boldsymbol{\Delta})^T \mathbf{e}_k), \end{aligned}$$

where  $I_{11} = \mathbb{E}((\mathbf{e}_j^T \mathbf{V}_Y \mathbf{Y}) (\mathbf{e}_k^T (\mathbf{V}_X + \boldsymbol{\Delta}) \mathbf{Y})^T (\mathbf{e}_j^T \mathbf{V}_Y \mathbf{Y}) (\mathbf{e}_k^T (\mathbf{V}_X + \boldsymbol{\Delta}) \mathbf{Y})^T)$ . Applying Lemma C.1 to  $I_{11}$ , we obtain

$$I_1 = (\mathbf{V}_{Y,j\bullet} \boldsymbol{\Sigma}_Y \mathbf{V}_{Y,j\bullet}^T) ((\mathbf{V}_X + \boldsymbol{\Delta})_{k\bullet} \boldsymbol{\Sigma}_Y (\mathbf{V}_X + \boldsymbol{\Delta})_{k\bullet}^T) + (\mathbf{V}_{Y,j\bullet} \boldsymbol{\Sigma}_Y (\mathbf{V}_X + \boldsymbol{\Delta})_{k\bullet}^T)^2.$$

The term  $I_2$  can be computed similarly, and thus conditional on  $\mathcal{D}_2$ ,  $\text{Var}(\sqrt{n}\text{Leading}_{jk}) = \xi_{jk}^2$ .

Next, we show that  $1/\xi_{jk} = O_P(1)$ . Similar to the proof of A.3, we have with probability at least  $1 - c/d$  for a universal constant  $c$ ,  $\|\mathbf{V}_X \boldsymbol{\Sigma}_X - \mathbf{I}\|_{\max} = O(\sqrt{\log d/n})$ . And under the conditions

in Lemma A.5, we then know with probability at least  $1 - c/d$ ,

$$\|\mathbf{V}_X - \Theta_X\|_{\max} = \|(\mathbf{V}_X \Sigma_X - \mathbf{I})\Theta_X\|_{\max} \leq \|\mathbf{V}_X \Sigma_X - \mathbf{I}\|_{\max} \|\Theta_X\|_1 = O(\sqrt{\log d/n}).$$

And we have  $\min_{s \in [d]} \{\Theta_{X,ss}\} \geq \lambda_{\min}\{\Theta_X\} = 1/\lambda_{\max}\{\Sigma_X\} = 1/\|\Theta_X\|_2$ . Therefore, with probability at least  $1 - c/d$ , there exists  $K > 0$ , such that

$$\min_{s \in [d]} \|\mathbf{V}_{X,s\bullet}\|_2 \geq \min_{s \in [d]} \{|\mathbf{V}_{X,ss}|\} \geq \min_{s \in [d]} \{\Theta_{X,ss}\} - \|\mathbf{V}_X - \Theta_X\|_{\max} \geq K.$$

Similarly, we have  $\|\mathbf{V}_Y - \Delta - \Theta_X\|_{\max} = \|\mathbf{V}_Y - \Theta_Y\|_{\max} = O_P(\sqrt{\log d/n})$ . Combining the above with Assumption 1, with probability at least  $1 - c/d$ , there exists  $K > 0$ , such that

$$\min_{s \in [d]} \|(\mathbf{V}_Y - \Delta)_{s\bullet}\|_2 \geq \min_{s \in [d]} \{|\mathbf{V}_{Y,ss}|\} \geq \min_{s \in [d]} \{\Theta_{X,ss}\} - \|\mathbf{V}_Y - \Delta - \Theta_X\|_{\max} \geq K.$$

Under Assumption 1, there exists  $\lambda_0 > 0$ , such that  $\lambda_{\min}(\Sigma_X) = 1/\|\Theta_X\|_2 > \lambda_0$ . Therefore, we know that with probability at least  $1 - c/d$ , there exists  $K_1 > 0$ , such that

$$((\mathbf{V}_Y - \Delta)_{j\bullet} \Sigma_X (\mathbf{V}_Y - \Delta)_{j\bullet}^T) (\mathbf{V}_{X,k\bullet} \Sigma_X \mathbf{V}_{X,k\bullet}^T) > K_1.$$

Similarly, with probability at least  $1 - c/d$ , there exists  $K_2 > 0$ , such that  $(\mathbf{V}_{Y,j\bullet} \Sigma_Y \mathbf{V}_{Y,j\bullet}^T) ((\mathbf{V}_X + \Delta)_{k\bullet} \Sigma_Y (\mathbf{V}_X + \Delta)_{k\bullet}^T) > K_2$ . The lemma then follows from these two inequalities.  $\square$

## C.5 Proof of Lemma A.6

*Proof.* Define  $I_{jk} = (\mathbf{V}_Y - \Delta)_{j\bullet} (\mathbf{X} \mathbf{X}^T - \Sigma_X) \mathbf{V}_{X,k\bullet}^T$ ,  $J_{jk} = -\mathbf{V}_{Y,j\bullet} (\mathbf{Y} \mathbf{Y}^T - \Sigma_Y) (\mathbf{V}_X + \Delta)_{k\bullet}^T$ . Since  $|Z_{jk}|^3 \leq 4(|I_{jk}|^3 + |J_{jk}|^3)$ , it suffices to prove

$$\mathbb{E}(|I_{jk}|^3 | \mathcal{D}_2 = (\mathbb{X}^T, \mathbb{Y}^T)^T) = O(1), \text{ and } \mathbb{E}(|J_{jk}|^3 | \mathcal{D}_2 = (\mathbb{X}^T, \mathbb{Y}^T)^T) = O(1).$$

In the following, we will show that  $\mathbb{E}(|I_{jk}|^3 | \mathcal{D}_2 = (\mathbb{X}^T, \mathbb{Y}^T)^T) = O(1)$ . A similar proof technique can be employed to prove  $\mathbb{E}(|J_{jk}|^3 | \mathcal{D}_2 = (\mathbb{X}^T, \mathbb{Y}^T)^T) = O(1)$ . Conditioned on  $\mathcal{D}_2 = (\mathbb{X}^T, \mathbb{Y}^T)^T$ ,

from Lemma A.3 and Assumption 1, we have

$$\|\mathbf{V}_{X,k\bullet}\|_1 \leq \|\mathbf{V}_X\|_\infty \leq \|\Theta_X\|_\infty = O(1), \text{ and } \|\mathbf{V}_{Y,j\bullet}\|_1 = O(1).$$

By Assumption 1, we obtain  $\|\mathbf{V}_Y - \Delta\|_1 = O(1)$ , and  $\|\mathbf{V}_X + \Delta\|_1 = O(1)$ . We define  $I_{jk,1} = (\mathbf{V}_Y - \Delta)_{j\bullet} \mathbf{X}$ , and  $I_{jk,2} = \mathbf{V}_{X,k\bullet} \mathbf{X}$ . Then  $I_{jk,1} \sim N(0, (\mathbf{V}_Y - \Delta)_{j\bullet} \Sigma_X (\mathbf{V}_Y - \Delta)_{j\bullet}^T)$ , and  $I_{jk,2} \sim N(\mathbf{V}_{X,k\bullet} \Sigma_X \mathbf{V}_{X,k\bullet}^T)$ . From Condition 1, we have  $\|\Sigma_X\|_2 = O(1)$ . We also have  $\|(\mathbf{V}_Y - \Delta)_{j\bullet}\|_2 \leq \|(\mathbf{V}_Y - \Delta)_{j\bullet}\|_1 = O(1)$ , and  $\|\mathbf{V}_{X,k\bullet}\|_2 \leq \|\mathbf{V}_{X,k\bullet}\|_1 = O(1)$ . Therefore, both the variance of  $I_{jk,1}$  and that of  $I_{jk,2}$  are  $O(1)$ , which means that  $\|I_{jk,1}\|_{\psi_2} = O(1)$  and  $\|I_{jk,2}\|_{\psi_2} = O(1)$ . Then from the centering property of the sub-exponential norm and the inequality  $\|XY\|_{\psi_1} \leq 2\|X\|_{\psi_2}\|Y\|_{\psi_2}$  which can be found in the proof of Lemma 23 in Javanmard and Montanari (2014), we know that  $I_{jk} = I_{jk,1}I_{jk,2} - \mathbb{E}(I_{jk,1}I_{jk,2})$  satisfies  $\|I_{jk}\|_{\psi_1} = O(1)$ , which implies  $\mathbb{E}(|I_{jk}|^3 | \mathcal{D}_2 = (\mathbb{X}^T, \mathbb{Y}^T)^T) = O(1)$  based on the definition of  $\psi_1$ -norm, as desired.  $\square$

## D Additional numeric results for Section 5.1

Tables 1–4 present the numerical results for Section 5.1, when  $n = \{400, 600, 800\}$ ,  $p = \{1600, 3600\}$ , and  $\text{SP} = \{0.005, 0.01, 0.015, 0.02, 0.025\}$  under the sparse and dense models respectively. We see from Table 1 and 3, only our proposed estimator is able to control the type I error at around  $\alpha = 0.05$  with minimal type II error. To evaluate SP, as it increases from 0.005 to 0.025, both type I error and type II error for three methods would increase. When the model switches from sparse to dense, the type I error of the naive method increases from around 0.08 to around 0.12 for various  $n$  and  $p$ , in which this influence is much more heavy than the other two methods. For the cross-fitting method, although it has smaller type II error, its type I error is always larger than our proposed algorithm. As our algorithm controls the type I error at around  $\alpha = 0.05$ , the cross-fitting method, however, could not provide this guarantee and lead to higher type I errors such as 0.640 in Table 3 even when the sample size is 800. For our proposed method, it not only is able to control the type I error, but also ensures the type II error approaching zero as  $n$  is increased. In addition, we see from Table 2 and 4, the average length of confidence interval over  $\mathcal{S}$  and  $\mathcal{S}^c$  will also increase as SP increases. Although the naive method and the cross-fitting method provides narrower confidence

intervals, these intervals are not valid for the given confidence, since the naive method assumes that both the network  $\Theta_X$  and  $\Theta_Y$  are sparse while our constructed models violate this assumption, and the cross-fitting method considers two dependent debiased estimator as independent.

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Table 1: Type I errors and Type II errors for three methods, averaged over 100 replications, under the sparse model.

$p$	$n$	method	SP=0.005		SP=0.01		SP=0.015		SP=0.02		SP=0.025	
			Type I	Type II	Type I	Type II	Type I	Type II	Type I	Type II	Type I	Type II
1600	400	Proposed	0.0502	0.0500	0.0520	0.1010	0.0532	0.1062	0.0540	0.1125	0.0546	0.1482
		Naive	0.0747	0.0075	0.0751	0.0060	0.0744	0.0142	0.0720	0.0144	0.0749	0.0210
	600	Cross-fitting	0.0557	0.0000	0.0595	0.0000	0.0611	0.0025	0.0637	0.0003	0.0649	0.0013
		Proposed	0.0555	0.0000	0.0519	0.0130	0.0569	0.0054	0.0542	0.0283	0.0531	0.0522
	800	Naive	0.0677	0.0000	0.0682	0.0000	0.0676	0.0000	0.0677	0.0006	0.0670	0.0020
		Cross-fitting	0.0539	0.0000	0.0561	0.0000	0.0577	0.0000	0.0604	0.0000	0.0617	0.0000
3600	400	Proposed	0.0506	0.0000	0.0521	0.0035	0.0515	0.0050	0.0540	0.0072	0.0523	0.0132
		Naive	0.0644	0.0000	0.0648	0.0000	0.0649	0.0000	0.0644	0.0000	0.0642	0.0010
	600	Cross-fitting	0.0530	0.0000	0.0568	0.0000	0.0554	0.0000	0.0588	0.0000	0.0595	0.0000
		Proposed	0.0520	0.0450	0.0522	0.1808	0.0579	0.0898	0.0539	0.2152	0.0555	0.2160
	800	Naive	0.0844	0.0267	0.0855	0.0317	0.0863	0.0383	0.0865	0.0500	0.0853	0.0480
		Cross-fitting	0.0546	0.0022	0.0587	0.0017	0.0625	0.0054	0.0641	0.0056	0.0680	0.0076
3600	600	Proposed	0.0496	0.0372	0.0516	0.0581	0.0530	0.0688	0.0535	0.0837	0.0543	0.0948
		Naive	0.0743	0.0011	0.0746	0.0033	0.0741	0.0050	0.0745	0.0068	0.0740	0.0102
	800	Cross-fitting	0.0519	0.0000	0.0557	0.0000	0.0586	0.0000	0.0616	0.0003	0.0639	0.0009
		Proposed	0.0498	0.0089	0.0505	0.0233	0.0510	0.0262	0.0554	0.0074	0.0544	0.0346
	3600	Naive	0.0685	0.0000	0.0679	0.0006	0.0685	0.0013	0.0691	0.0006	0.0681	0.0015
		Cross-fitting	0.0521	0.0000	0.0536	0.0000	0.0566	0.0000	0.0586	0.0000	0.0606	0.0003



Table 2: The average length of the confidence intervals over  $\mathcal{S}$  and  $\mathcal{S}^c$  for three methods, averaged over 100 replications, under the sparse model.

$p$	$n$	method	SP=0.005		SP=0.01		SP=0.015		SP=0.02		SP=0.025	
			Avglen $_{\mathcal{S}}$	Avglen $_{\mathcal{S}^c}$	Avglen $_{\mathcal{S}}$	Avglen $_{\mathcal{S}^c}$	Avglen $_{\mathcal{S}}$	Avglen $_{\mathcal{S}^c}$	Avglen $_{\mathcal{S}}$	Avglen $_{\mathcal{S}^c}$	Avglen $_{\mathcal{S}}$	Avglen $_{\mathcal{S}^c}$
1600	400	Proposed	1.1034	1.1254	1.2323	1.2529	1.2709	1.2953	1.2926	1.3105	1.4076	1.4241
		Naive	0.8692	0.8618	0.9519	0.9460	0.9812	0.9763	0.9922	0.9864	1.0654	1.0624
	600	Cross-fitting	0.5225	0.5546	0.5861	0.6202	0.6114	0.6408	0.6193	0.6446	0.6772	0.7063
		Proposed	0.6401	0.6723	0.9693	0.9883	0.7440	0.7766	1.0175	1.0327	1.1042	1.1221
	800	Naive	0.6958	0.6881	0.7601	0.7553	0.7841	0.7793	0.7920	0.7875	0.8496	0.8480
		Cross-fitting	0.4570	0.4793	0.5107	0.5348	0.5320	0.5537	0.5388	0.5570	0.5846	0.6078
3600	400	Proposed	0.7447	0.7639	0.8320	0.8459	0.8650	0.8747	0.8721	0.8832	0.9422	0.9583
		Naive	0.5960	0.5901	0.6521	0.6475	0.6727	0.6681	0.6793	0.6751	0.7302	0.7269
	600	Cross-fitting	0.4125	0.4294	0.4600	0.4785	0.4786	0.4951	0.4843	0.4984	0.5265	0.5435
		Proposed	0.8573	0.8859	1.4971	1.5139	0.9412	0.9692	1.5821	1.5894	1.6117	1.6198
	800	Naive	1.0815	1.0708	1.1354	1.1297	1.1600	1.1537	1.1837	1.1782	1.2023	1.1978
		Cross-fitting	0.6136	0.6323	0.6567	0.6753	0.6706	0.6912	0.6915	0.7076	0.7075	0.7193
4000	600	Proposed	1.0961	1.1034	1.1621	1.1738	1.1936	1.2015	1.2233	1.2308	1.2496	1.2539
		Naive	0.8481	0.8418	0.8935	0.8879	0.9121	0.9067	0.9307	0.9260	0.9459	0.9413
	800	Cross-fitting	0.5362	0.5511	0.5742	0.5880	0.5871	0.6020	0.6033	0.6155	0.6165	0.6256
		Proposed	0.9312	0.9354	0.9884	0.9935	1.0118	1.0180	0.7676	0.7795	1.0567	1.0603
	1000	Naive	0.7236	0.7168	0.7607	0.7560	0.7762	0.7721	0.7926	0.7884	0.8054	0.8014
		Cross-fitting	0.4859	0.4961	0.5178	0.5284	0.5293	0.5417	0.5444	0.5535	0.5554	0.5626

Table 3: Type I errors and Type II errors for three methods, averaged over 100 replications, under the dense model.

$p$	$n$	method	SP=0.005		SP=0.01		SP=0.015		SP=0.02		SP=0.025	
			Type I	Type II	Type I	Type II	Type I	Type II	Type I	Type II	Type I	Type II
1600	400	Proposed	0.0468	0.1388	0.0503	0.1745	0.0497	0.1779	0.0519	0.2367	0.0534	0.2778
		Naive	0.1258	0.0000	0.1484	0.0020	0.1502	0.0037	0.1643	0.0050	0.1703	0.0115
	600	Cross-fitting	0.0506	0.0000	0.0565	0.0025	0.0570	0.0042	0.0622	0.0067	0.0647	0.0122
		Proposed	0.0482	0.0037	0.0509	0.0215	0.0505	0.0579	0.0511	0.0908	0.0579	0.0532
	800	Naive	0.1060	0.0000	0.1284	0.0000	0.1319	0.0000	0.1420	0.0006	0.1508	0.0018
		Cross-fitting	0.0496	0.0000	0.0534	0.0000	0.0553	0.0000	0.0593	0.0000	0.0620	0.0010
3600	400	Proposed	0.0481	0.0000	0.0519	0.0055	0.0495	0.0192	0.0534	0.0092	0.0572	0.0205
		Naive	0.0959	0.0000	0.1177	0.0000	0.1200	0.0000	0.1287	0.0000	0.1373	0.0000
	600	Cross-fitting	0.0481	0.0000	0.0518	0.0000	0.0531	0.0000	0.0584	0.0000	0.0609	0.0005
		Proposed	0.0491	0.1089	0.0546	0.1839	0.0523	0.3250	0.0539	0.3169	0.0607	0.2050
	800	Naive	0.1368	0.0011	0.1542	0.0158	0.1621	0.0206	0.1693	0.0177	0.1755	0.0219
		Cross-fitting	0.0521	0.0061	0.0575	0.0189	0.0608	0.0323	0.0643	0.0261	0.0680	0.0294
3600	600	Proposed	0.0495	0.0206	0.0539	0.0750	0.0522	0.1621	0.0574	0.0771	0.0590	0.0877
		Naive	0.1163	0.0000	0.1376	0.0011	0.1435	0.0040	0.1520	0.0013	0.1572	0.0049
	800	Cross-fitting	0.0521	0.0061	0.0575	0.0189	0.0608	0.0323	0.0643	0.0261	0.0680	0.0294
		Proposed	0.0490	0.0111	0.0509	0.0683	0.0523	0.0742	0.0555	0.0310	0.0575	0.0331
	3600	Naive	0.1054	0.0000	0.1246	0.0000	0.1354	0.0004	0.1411	0.0000	0.1479	0.0003
		Cross-fitting	0.0506	0.0000	0.0553	0.0006	0.0578	0.0008	0.0606	0.0003	0.0640	0.0006

Table 4: The average length of the confidence intervals over  $\mathcal{S}$  and  $\mathcal{S}^c$  for three methods, averaged over 100 replications, under the dense model.

$p$	$n$	method	SP=0.005		SP=0.01		SP=0.015		SP=0.02		SP=0.025	
			Avglen $_{\mathcal{S}}$	Avglen $_{\mathcal{S}^c}$	Avglen $_{\mathcal{S}}$	Avglen $_{\mathcal{S}^c}$	Avglen $_{\mathcal{S}}$	Avglen $_{\mathcal{S}^c}$	Avglen $_{\mathcal{S}}$	Avglen $_{\mathcal{S}^c}$	Avglen $_{\mathcal{S}}$	Avglen $_{\mathcal{S}^c}$
1600	400	Proposed	1.3266	1.3428	1.4720	1.4889	1.4792	1.4990	1.5747	1.5876	1.6793	1.6945
		Naive	0.4262	0.4653	0.5019	0.5333	0.5073	0.5344	0.5424	0.5693	0.5893	0.6199
	600	Cross-fitting	0.6051	0.6359	0.6833	0.7146	0.6908	0.7180	0.7365	0.7627	0.7953	0.8234
		Proposed	0.7491	0.7748	0.8410	0.8671	1.1714	1.1816	1.2350	1.2483	0.9662	0.9958
	800	Naive	0.3903	0.4216	0.4560	0.4823	0.4595	0.4838	0.4902	0.5151	0.5322	0.5598
		Cross-fitting	0.5339	0.5519	0.5970	0.6183	0.6027	0.6220	0.6378	0.6588	0.6879	0.7100
3600	400	Proposed	0.6772	0.6974	0.7562	0.7792	0.9951	1.0073	0.8036	0.8294	0.8677	0.8933
		Naive	0.3643	0.3895	0.4206	0.4443	0.4251	0.4458	0.4523	0.4745	0.4908	0.5151
	600	Cross-fitting	0.4836	0.4964	0.5374	0.5541	0.5425	0.5578	0.5737	0.5903	0.6175	0.6354
		Proposed	0.9945	1.0413	1.1077	1.1451	1.8902	1.8959	1.8827	1.8959	1.1315	1.1506
	800	Naive	0.5124	0.5384	0.5820	0.6031	0.5960	0.6145	0.5947	0.6082	0.5938	0.6029
		Cross-fitting	0.7132	0.7417	0.7926	0.8161	0.8070	0.8297	0.8048	0.8243	0.8067	0.8202
4000	600	Proposed	0.8760	0.9088	0.9653	0.9968	1.4613	1.4733	0.9838	1.0074	0.9882	1.0044
		Naive	0.4647	0.4895	0.5259	0.5468	0.5381	0.5572	0.5375	0.5518	0.5372	0.5472
	800	Cross-fitting	0.6258	0.6475	0.6906	0.7100	0.7019	0.7220	0.7018	0.7176	0.7043	0.7157
		Proposed	0.7931	0.8225	1.2210	1.2264	1.2397	1.2462	0.8910	0.9098	0.8923	0.9073
	1000	Naive	0.4300	0.4528	0.4844	0.5041	0.4958	0.5138	0.4954	0.5091	0.4950	0.5052
		Cross-fitting	0.5656	0.5842	0.6220	0.6385	0.6324	0.6491	0.6322	0.6460	0.6339	0.6442