

# Supplement to “Simultaneous Inference for High-dimensional Linear Models”

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This supplementary material provides proofs of the main results in the paper as well as some additional numerical results.

## 1 Technical details

We first present two lemmas that will be used in the rest proofs. Define  $\xi_{ij} = \Theta_j^T \tilde{X}_i \epsilon_i$ . Denote by  $c, c', C, C', C_i$  be some generic constants which can be different from line to line.

LEMMA 1.1. *Under Assumptions 2.1-2.3, we have for any  $G \subseteq \{1, 2, \dots, p\}$ ,*

$$\sup_{x \in \mathbb{R}} \left| P \left( \max_{j \in G} \sum_{i=1}^n \xi_{ij} / \sqrt{n} \leq x \right) - P \left( \max_{j \in G} \sum_{i=1}^n z_{ij} / \sqrt{n} \leq x \right) \right| \lesssim n^{-c'}, \quad c' > 0,$$

where  $\{z_i = (z_{i1}, \dots, z_{ip})'\}$  is a sequence of mean zero independent Gaussian vector with  $\mathbb{E}z_i z_i' = \Theta_j^T \Sigma \Theta_j \sigma_\epsilon^2$ .

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*Proof of Lemma 1.1.* We apply Corollary 2.1 of Chernozhukov et al. (2013) to the sequence  $\{\xi_{ij}\}$  by verifying its Condition (E.1). For the sake of clarity, we state the condition below, i.e.

$$c_0 \leq \mathbb{E}\xi_{ij}^2 \leq C_0, \quad \max_{k=1,2} \mathbb{E}|\xi_{ij}|^{2+k}/B^k + \mathbb{E}\exp(|\xi_{ij}|/B) \leq 4, \quad (1)$$

uniformly over  $j$ , where  $c_0, C_0 > 0$ , and  $B$  is some large enough constant. In what follows, we consider two cases for  $\mathbf{X}$ : (i)  $\mathbf{X}$  has i.i.d. sub-Gaussian rows; (ii)  $\mathbf{X}$  is strongly bounded.

(i) By Assumption 2.2,  $\mathbb{E}(\Theta_j^T \tilde{X}_i)^2 = \Theta_j^T \Sigma \Theta_j = \theta_{jj} := 1/\tau_j^2$ , and  $1/c < \Lambda_{\min}^2 \leq \tau_j^2 \leq \Sigma_{j,j} = C$ , for some constants  $c, C > 0$ . Recall that  $\Lambda_{\min}^2$  is the minimal eigenvalue of  $\Sigma$ . Thus we have  $c_1 \sigma_\epsilon^2 \leq \mathbb{E}\xi_{ij}^2 \leq C_1 \sigma_\epsilon^2$ . By the independence between  $\{\tilde{X}_i\}$  and  $\{\epsilon_i\}$ , we have for large enough  $C$  and uniformly for all  $j$ ,

$$\begin{aligned} \mathbb{E}\exp(|\xi_{ij}|/C) &= 1 + \sum_{k=1}^{+\infty} \frac{\mathbb{E}|\xi_{ij}|^k}{C^k k!} = 1 + \sum_{k=1}^{+\infty} \frac{\mathbb{E}|\Theta_j^T \tilde{X}_i|^k \mathbb{E}|\epsilon_i|^k}{C^k k!} \\ &\leq 1 + \sum_{k=1}^{+\infty} \frac{k^k}{(C')^k k!} \leq 1 + \sum_{k=1}^{+\infty} (e/C')^k < \infty, \end{aligned}$$

where we have used the fact that  $k! \geq (k/e)^k$ ,  $\|\Theta_j\|_2 \lesssim \Lambda_{\min}^{-1} = O(1)$  (because  $\|\Theta_j\|_2^2 \Lambda_{\min}^2 \leq c$ ) and  $\mathbb{E}|X|^k \leq (C'')^k k^{k/2}$  with  $C''$  being some positive constant for sub-Gaussian variable  $X$ . Thus we have  $\max_{k=1,2} \mathbb{E}|\xi_{ij}|^{2+k}/B^k + \mathbb{E}\exp(|\xi_{ij}|/B) \leq 4$  uniformly for some large enough constant  $B$ .

(ii) In the strongly bounded case, using the fact that  $\|\Theta_j\|_2^2 \lesssim \Lambda_{\min}^{-2} = O(1)$  and  $\|\Theta_j\|_1 \leq \sqrt{s_j} \|\Theta_j\|_2$ , we have  $|\Theta_j^T \tilde{X}_i| \leq \|\Theta_j\|_1 \|\tilde{X}_i\|_\infty \leq K_n \sqrt{s_j} \|\Theta_j\|_2$ . It is straightforward to verify that  $\max_{k=1,2} \mathbb{E}|\xi_{ij}|^{2+k}/B_n^k + \mathbb{E}\exp(|\xi_{ij}|/B_n) \leq 4$  uniformly with some  $B_n \asymp K_n \max_j \sqrt{s_j}$  and  $B_n^2 (\log(pn))^7 / n \leq C_2 n^{-c_2}$  under part (ii) of Assumption 2.3.  $\diamond$

**REMARK 1.1.** The conclusion in Lemma 1.1 still holds if we assume that (i)  $\max_{i,j} |X_{ij}| \leq K_n$  with  $\max_{1 \leq j \leq p} s_j^2 K_n^4 (\log(pn))^7 / n \leq C_1 n^{-c_1}$  for some constants  $c_1, C_1 > 0$ ; and (ii)  $\{\epsilon_i\}$  are i.i.d with  $\mathbb{E}|\epsilon_i|^4 < \infty$  and  $c' < \sigma_\epsilon^2$  for  $c' > 0$ .

Next we quantify the effect by replacing  $\xi_i$  with  $\hat{\xi}_i$ .

LEMMA 1.2. Suppose Assumptions 2.1-2.3 hold. Assume  $\max_j K_0^2 s_j^2 (\log(pn))^3 (\log(n))^2 / n = o(1)$ . Recall that  $K_0 = 1$  in the sub-Gaussian case and  $K_0 = K_n$  in the strongly bounded case. Then with  $\lambda_j \asymp K_0 \sqrt{\log(p)/n}$  uniformly for  $j$ , there exist  $\zeta_1, \zeta_2 > 0$  such that

$$P \left( \max_{1 \leq j \leq p} \left| \sum_{i=1}^n \widehat{\xi}_{ij} / \sqrt{n} - \sum_{i=1}^n \xi_{ij} / \sqrt{n} \right| \geq \zeta_1 \right) < \zeta_2,$$

where  $\zeta_1 \sqrt{1 \vee \log(p/\zeta_1)} = o(1)$  and  $\zeta_2 = o(1)$ .

*Proof of Lemma 1.2.* Let  $\widetilde{K}_0 = \log(np) \log(n)$  in the sub-Gaussian case and  $\widetilde{K}_0 = K_n \log(n)$  in the strongly bounded case. Using Lemma A.1 in Chernozhukov et al. (2013), we deduce that

$$\begin{aligned} \mathbb{E} \left\{ \max_{1 \leq j \leq p} \left| \sum_{i=1}^n X_{ij} \epsilon_i / n \right| \right\} &\lesssim \sigma_\epsilon \sqrt{\max_j \Sigma_{j,j}} \sqrt{\log(p)/n} + \sqrt{\mathbb{E} \max_{i,j} |X_{ij} \epsilon_i|^2 \log(p)/n} \\ &\lesssim \sqrt{\log(p)/n} + \sqrt{\mathbb{E} \max_{i,j} X_{ij}^2} \sqrt{\mathbb{E} \max_i \epsilon_i^2 \log(p)/n} \\ &\lesssim \sqrt{\log(p)/n} + \widetilde{K}_0 \log(p)/n, \end{aligned}$$

where we have used the fact that  $\sqrt{\mathbb{E} \max_i \epsilon_i^2} \lesssim \log(n) \max_{1 \leq i \leq n} \|\epsilon_i\|_{\psi_1} \lesssim \log n$  with  $\psi_1(x) = \exp(x) - 1$  and  $\|\cdot\|_{\psi_1}$  being the corresponding Orlicz norm, and similar result for  $\sqrt{\mathbb{E} \max_{i,j} X_{ij}^2}$  (see Lemma 2.2.2 in van der Vaart and Wellner 1996). Because  $\|\widehat{\Theta}_j - \Theta_j\|_1 = O_P(K_0 s_j \sqrt{\log(p)/n})$  uniformly for  $j$ , we obtain,

$$\begin{aligned} \left| \sum_{i=1}^n \widehat{\xi}_{ij} / \sqrt{n} - \sum_{i=1}^n \xi_{ij} / \sqrt{n} \right| &= \left| (\widehat{\Theta}_j^T - \Theta_j^T) \sum_{i=1}^n \widetilde{X}_i \epsilon_i / \sqrt{n} \right| \leq \|\widehat{\Theta}_j - \Theta_j\|_1 \left\| \sum_{i=1}^n \widetilde{X}_i \epsilon_i / \sqrt{n} \right\|_\infty \\ &= O_P \left( K_0 s_j \sqrt{\log(p)/n} \left\| \sum_{i=1}^n \widetilde{X}_i \epsilon_i / \sqrt{n} \right\|_\infty \right) \\ &= O_P \left( K_0 s_j \log(p) / \sqrt{n} + \sqrt{n} K_0 \widetilde{K}_0 s_j (\log(p)/n)^{3/2} \right) \\ &\leq O_P \left( \max_j s_j K_0 \log(p) / \sqrt{n} \right), \end{aligned}$$

uniformly for all  $j$ . Choosing  $\zeta_1$  such that  $\max_j K_0 s_j \log(p) / (\sqrt{n} \zeta_1) = o(1)$  and  $\zeta_1 \sqrt{1 \vee \log(p/\zeta_1)} =$

$o(1)$  (e.g.  $\zeta_1^2 = O(\max_j K_0 s_j \sqrt{\log(p)/n})$ ), we deduce that

$$P \left( \max_{1 \leq j \leq p} \left| \sum_{i=1}^n \hat{\xi}_{ij} / \sqrt{n} - \sum_{i=1}^n \xi_{ij} / \sqrt{n} \right| \geq \zeta_1 \right) < \zeta_2, \quad \zeta_2 = o(1).$$

◇

**REMARK 1.2.** With a more delicate analysis, one can specify the order of  $\zeta_2$  in Lemma 1.2; see e.g., Theorem 6.1 and Lemma 6.2 of Bühlmann and van de Geer (2011).

*Proof of Theorem 2.2.* Without loss of generality, we set  $G = \{1, 2, \dots, p\}$ . Define

$$T_G = \max_{j \in G} \sqrt{n}(\check{\beta}_j - \beta_j^0), \quad T_{0,G} = \max_{j \in G} \sum_{i=1}^n \xi_{ij} / \sqrt{n}.$$

Let  $\pi(v) = C_2 v^{1/3} (1 \vee \log(p/v))^{2/3}$  with  $C_2 > 0$ , and

$$\Gamma = \max_{1 \leq j, k \leq p} |\hat{\sigma}_\epsilon^2 \hat{\Theta}_j^T \hat{\Sigma} \hat{\Theta}_k - \sigma_\epsilon^2 \Theta_j^T \Sigma \Theta_k|, \quad \hat{\Sigma} = \mathbf{X}^T \mathbf{X} / n.$$

Notice that

$$|T_G - T_{0,G}| \leq \max_{1 \leq j \leq p} \left| \sum_{i=1}^n \hat{\xi}_{ij} / \sqrt{n} - \sum_{i=1}^n \xi_{ij} / \sqrt{n} \right| + \|\Delta\|_\infty.$$

By similar arguments in the proof of Theorem 2.4 of van de Geer et al. (2014) and the results in Theorem 2.1, we have

$$\|\Delta\|_\infty \leq \|\hat{\beta} - \beta^0\|_1 \max_j \sqrt{n} \lambda_j / \hat{\tau}_j^2 = O_P(K_0 \sqrt{\log(p)} \|\hat{\beta} - \beta^0\|_1) = O_P(K_0^2 s_0 \log(p) / \sqrt{n}),$$

where we use the fact that  $\max_j \lambda_j / \hat{\tau}_j^2 = O_P(K_0 \sqrt{\log(p)/n})$  and  $\|\hat{\beta} - \beta^0\|_1 = O_P(s_0 \lambda)$  with  $\lambda = O(K_0 \sqrt{\log(p)/n})$ . Thus by Lemma 1.2 and the assumption that  $K_0^4 s_0^2 (\log(p))^3 / n = o(1)$ , we have

$$P(|T_G - T_{0,G}| > \zeta_1) < \zeta_2,$$

for  $\zeta_1 \sqrt{1 \vee \log(p/\zeta_1)} = o(1)$  and  $\zeta_2 = o(1)$ .

Let  $c_{z,G}(\alpha) = \inf\{t \in \mathbb{R} : P(\max_{j \in G} \sum_{i=1}^n z_{ij} / \sqrt{n} \leq t) \geq 1 - \alpha\}$ , where the sequence  $\{z_{ij}\}$  is

defined in Lemma 1.1. Following the arguments in the proof of Lemma 3.2 in Chernozhukov et al. (2013), we have

$$P(c_G(\alpha) \leq c_{z,G}(\alpha + \pi(v))) \geq 1 - P(\Gamma > v), \quad (2)$$

$$P(c_{z,G}(\alpha) \leq c_G(\alpha + \pi(v))) \geq 1 - P(\Gamma > v). \quad (3)$$

By Lemma 1.1, (2) and (3), we have for every  $v > 0$ ,

$$\begin{aligned} \sup_{\alpha \in (0,1)} |P(T_{0,G} > c_G(\alpha)) - \alpha| &\lesssim \sup_{\alpha \in (0,1)} \left| P \left( \max_{j \in G} \sum_{i=1}^n z_{ij} / \sqrt{n} > c_G(\alpha) \right) - \alpha \right| + n^{-c'} \\ &\lesssim \pi(v) + P(\Gamma > v) + n^{-c'}. \end{aligned}$$

Moreover, by the arguments in the proof of Theorem 3.2 in Chernozhukov et al. (2013), we have

$$\sup_{\alpha \in (0,1)} |P(T_G > c_G(\alpha)) - \alpha| \lesssim \pi(v) + P(\Gamma > v) + n^{-c'} + \zeta_1 \sqrt{1 \vee \log(p/\zeta_1)} + \zeta_2.$$

By Lemma 5.3 and Lemma 5.4 of van de Geer et al. (2014), we have

$$\max_{1 \leq j, k \leq p} |\widehat{\Theta}_j^T \widehat{\Sigma} \widehat{\Theta}_k - \Theta_j^T \Sigma \Theta_k| = O_P(\max_j \lambda_j \sqrt{s_j}).$$

Since  $|\Theta_j^T \Sigma \Theta_k| \leq 1/(\tau_j \tau_k) = O(1)$  uniformly for  $1 \leq j, k \leq p$ , we have

$$\Gamma = O_P \left( |\widehat{\sigma}_\epsilon^2 - \sigma_\epsilon^2| + \max_j \lambda_j \sqrt{s_j} \right).$$

Under Assumption 2.4, choosing  $v = 1/(\alpha_n(\log(p))^2)$ , we deduce that

$$\sup_{\alpha \in (0,1)} \left| P \left( \max_{1 \leq j \leq p} \sqrt{n}(\check{\beta}_j - \beta_j^0) > c_G(\alpha) \right) - \alpha \right| = o(1),$$

which completes the proof. ◇

*Proof of Theorem 2.3.* From the arguments in the proof of Theorem 2.2, we have

$$\Gamma = \max_{1 \leq j, k \leq p} |\hat{\sigma}_\epsilon^2 \hat{\Theta}_j^T \hat{\Sigma} \hat{\Theta}_k - \sigma_\epsilon^2 \Theta_j^T \Sigma \Theta_k| = O_P \left( |\hat{\sigma}_\epsilon^2 - \sigma_\epsilon^2| + \max_j \lambda_j \sqrt{s_j} \right),$$

which implies that  $\max_{1 \leq j \leq p} |\hat{\omega}_{jj} - \omega_{jj}| = O_P \left( |\hat{\sigma}_\epsilon^2 - \sigma_\epsilon^2| + \max_j \lambda_j \sqrt{s_j} \right)$  with  $\omega_{jj} = \sigma_\epsilon^2 \theta_{jj}$ . We then have

$$P(\omega_{jj}/2 < \hat{\omega}_{jj} < 2\omega_{jj} \text{ for all } 1 \leq j \leq p) \rightarrow 1. \quad (4)$$

The fact that  $1/c < \Lambda_{\min}^2 \leq \tau_j^2 = 1/\theta_{jj} \leq \Sigma_{j,j} = C$  implies that  $\omega_{jj}$  is uniformly bounded away from zero and infinity.

Define  $\bar{T}_G = \max_{j \in G} \sqrt{n}(\check{\beta}_j - \beta_j^0)/\sqrt{\hat{\omega}_{jj}}$  and  $\bar{T}_{0,G} = \max_{j \in G} \sum_{i=1}^n \xi_{ij}/\sqrt{n\omega_{jj}}$ . Denote by  $\Delta = (\Delta_1, \dots, \Delta_p)^T$  and  $\bar{\Delta} = (\bar{\Delta}_1, \dots, \bar{\Delta}_p)^T$  with  $\bar{\Delta}_j = \Delta_j/\sqrt{\hat{\omega}_{jj}}$ . Then we have

$$\begin{aligned} & |\bar{T}_G - \bar{T}_{0,G}| \\ & \leq \max_{1 \leq j \leq p} \left| \sum_{i=1}^n \hat{\xi}_{ij}/\sqrt{n\hat{\omega}_{jj}} - \sum_{i=1}^n \xi_{ij}/\sqrt{n\omega_{jj}} \right| + \|\bar{\Delta}\|_\infty \\ & \leq \max_{1 \leq j \leq p} \left| \sum_{i=1}^n \hat{\xi}_{ij}/\sqrt{n\hat{\omega}_{jj}} - \sum_{i=1}^n \hat{\xi}_{ij}/\sqrt{n\omega_{jj}} \right| + \max_{1 \leq j \leq p} \left| \sum_{i=1}^n \hat{\xi}_{ij}/\sqrt{n\omega_{jj}} - \sum_{i=1}^n \xi_{ij}/\sqrt{n\omega_{jj}} \right| + \|\bar{\Delta}\|_\infty \\ & \leq C' \max_{1 \leq j \leq p} \left| \sum_{i=1}^n \hat{\xi}_{ij}/\sqrt{n} \right| \max_{1 \leq j \leq p} \left| \sqrt{\omega_{jj}/\hat{\omega}_{jj}} - 1 \right| + C'' \max_{1 \leq j \leq p} \left| \sum_{i=1}^n (\hat{\xi}_{ij} - \xi_{ij})/\sqrt{n} \right| + \|\bar{\Delta}\|_\infty, \\ & = I_1 + I_2 + I_3, \end{aligned}$$

where  $C', C'' > 0$ .

On the event  $\omega_{jj}/2 < \widehat{\omega}_{jj} < 2\omega_{jj}$  for all  $1 \leq j \leq p$ ,

$$\begin{aligned}
\max_{1 \leq j \leq p} \left| \sqrt{\omega_{jj}/\widehat{\omega}_{jj}} - 1 \right| &\leq \max_{1 \leq j \leq p} \left| \sqrt{\omega_{jj}} - \sqrt{\widehat{\omega}_{jj}} \right| \max_{1 \leq j \leq p} \sqrt{2/\omega_{jj}} \\
&\leq \max_{1 \leq j \leq p} \left| \frac{\omega_{jj} - \widehat{\omega}_{jj}}{\sqrt{\omega_{jj}} + \sqrt{\widehat{\omega}_{jj}}} \right| \max_{1 \leq j \leq p} \sqrt{2/\omega_{jj}} \\
&\leq \max_{1 \leq j \leq p} |\omega_{jj} - \widehat{\omega}_{jj}| \max_{1 \leq j \leq p} 1/\omega_{jj} \\
&= O_P \left( |\widehat{\sigma}_\epsilon^2 - \sigma_\epsilon^2| + \max_j \lambda_j \sqrt{s_j} \right).
\end{aligned}$$

On the other hand,

$$\begin{aligned}
\max_{1 \leq j \leq p} \left| \sum_{i=1}^n \widehat{\xi}_{ij}/\sqrt{n} \right| &\leq \max_{1 \leq j \leq p} \left| \sum_{i=1}^n (\widehat{\xi}_{ij} - \xi_{ij})/\sqrt{n} \right| + \max_{1 \leq j \leq p} \left| \sum_{i=1}^n \xi_{ij}/\sqrt{n} \right| \\
&= O_P(\sqrt{\log(p)} + \max_j \sqrt{s_j} \widetilde{K}_0 \log(p)/\sqrt{n}) = O_P(\sqrt{\log p}),
\end{aligned}$$

where  $\widetilde{K}_0 = \log(np) \log(n)$  in the sub-Gaussian case and  $\widetilde{K}_0 = K_n \log(n)$  in the strongly bounded case. Therefore, on the above event,  $I_1 \leq O_P \left( \sqrt{\log(p)} |\widehat{\sigma}_\epsilon^2 - \sigma_\epsilon^2| + \sqrt{\log(p)} \max_j \lambda_j \sqrt{s_j} \right)$ . Under Assumption 2.4, we can find  $\zeta'_1$  such that  $P(I_1 > \zeta'_1) = o(1)$  and  $\zeta'_1 \sqrt{1 \vee \log(p/\zeta'_1)} = o(1)$ . Using the fact that  $\|\Delta\|_\infty \leq O_P(K_0^2 s_0 \log(p)/\sqrt{n})$ , we can prove the same result for  $\|\bar{\Delta}\|_\infty$  conditional on the event  $\{\omega_{jj}/2 < \widehat{\omega}_{jj} < 2\omega_{jj} \text{ for all } 1 \leq j \leq p\}$ . Thus by Lemma 1.2 and (4), we have

$$P(|\bar{T}_G - \bar{T}_{0,G}| > \zeta_1) \leq P(I_1 + I_2 + I_3 > \zeta_1) < \zeta_2,$$

for  $\zeta_1 \sqrt{1 \vee \log(p/\zeta_1)} = o(1)$  and  $\zeta_2 = o(1)$ .

Let  $\bar{\Gamma} = \max_{1 \leq j, k \leq p} |\widehat{\sigma}_\epsilon^2 \widehat{\Theta}_j^T \widehat{\Sigma} \widehat{\Theta}_k / \sqrt{\widehat{\omega}_{jj} \widehat{\omega}_{kk}} - \sigma_\epsilon^2 \Theta_j^T \Sigma \Theta_k / \sqrt{\omega_{jj} \omega_{kk}}|$ . Note that

$$|\sqrt{\omega_{jj} \omega_{kk}} - \sqrt{\widehat{\omega}_{jj} \widehat{\omega}_{kk}}| = \frac{|\omega_{jj} \omega_{kk} - \widehat{\omega}_{jj} \widehat{\omega}_{kk}|}{\sqrt{\omega_{jj} \omega_{kk}} + \sqrt{\widehat{\omega}_{jj} \widehat{\omega}_{kk}}}.$$

On the event  $\omega_{jj}/2 < \widehat{\omega}_{jj} < 2\omega_{jj}$  for all  $1 \leq j \leq p$ , we have

$$\frac{|\omega_{jj}\omega_{kk} - \widehat{\omega}_{jj}\widehat{\omega}_{kk}|}{\sqrt{\omega_{jj}\omega_{kk}} + \sqrt{\widehat{\omega}_{jj}\widehat{\omega}_{kk}}} \leq \frac{|\omega_{jj}\omega_{kk} - \widehat{\omega}_{jj}\widehat{\omega}_{kk}|}{\sqrt{\omega_{jj}\omega_{kk}} + \sqrt{\omega_{jj}\omega_{kk}/4}} \leq (2/3)|\omega_{jj}\omega_{kk} - \widehat{\omega}_{jj}\widehat{\omega}_{kk}| \max_{1 \leq j \leq p} 1/\omega_{jj},$$

which implies that

$$\begin{aligned} \max_{1 \leq j, k \leq p} \left| \sqrt{\omega_{jj}\omega_{kk}/\widehat{\omega}_{jj}\widehat{\omega}_{kk}} - 1 \right| &\leq \max_{1 \leq j, k \leq p} \left| \sqrt{\omega_{jj}\omega_{kk}} - \sqrt{\widehat{\omega}_{jj}\widehat{\omega}_{kk}} \right| \max_{1 \leq j \leq p} 2/\omega_{jj} \\ &\leq (4/3) \max_{1 \leq j, k \leq p} |\omega_{jj}\omega_{kk} - \widehat{\omega}_{jj}\widehat{\omega}_{kk}| \max_{1 \leq j \leq p} 1/\omega_{jj}^2 \\ &= O_P \left( |\widehat{\sigma}_\epsilon^2 - \sigma_\epsilon^2| + \max_j \lambda_j \sqrt{s_j} \right). \end{aligned}$$

Using similar arguments above, we can show that  $P(\bar{\Gamma} > v) = o(1)$  for  $v = 1/(\alpha_n(\log(p)))^2$ . The rest of the proofs is similar to those in the proof of Theorem 2.2. We skip the details  $\diamond$

*Proof of Theorem 2.4.* Define  $\widetilde{T}_G = \max_{j \in G} |\sqrt{n}(\check{\beta}_j - \beta_j^0)/\sqrt{\widehat{\omega}_{jj}}|$  and  $\widetilde{T}_{0,G} = \max_{j \in G} \sum_{i=1}^n |\xi_{ij}/\sqrt{n\omega_{jj}}|$ . Under the assumptions in Theorem 2.3, we can show that  $P(|\widetilde{T}_G - \widetilde{T}_{0,G}| > \zeta_1) < \zeta_2$  for  $\zeta_1 \sqrt{1 \vee \log(p/\zeta_1)} = o(1)$  and  $\zeta_2 = o(1)$ . In another word, the distribution of  $\max_{j \in G} \sqrt{n}|\check{\beta}_j - \beta_j^0|/\sqrt{\widehat{\omega}_{jj}}$  can be approximated by  $\max_{j \in G} |Z_j|$  with  $Z = (Z_1, \dots, Z_p) \sim^d N(0, \widetilde{\Theta})$ . Under Assumption 2.5, by Lemma 6 of Cai et al. (2014), we have for any  $x \in \mathbb{R}$  and as  $|G| \rightarrow +\infty$ ,

$$P \left( \max_{j \in G} |Z_j|^2 - 2 \log(|G|) + \log \log(|G|) \leq x \right) \rightarrow F(x) := \exp \left\{ -\frac{1}{\sqrt{\pi}} \exp \left( -\frac{x}{2} \right) \right\}.$$

It implies that

$$P \left( \max_{j \in G} n|\check{\beta}_j - \beta_j^0|^2/\widehat{\omega}_{jj} \leq 2 \log(|G|) - \log \log(|G|)/2 \right) \rightarrow 1. \quad (5)$$

The bootstrap consistency result implies that

$$|(\bar{c}_G^*(\alpha))^2 - 2 \log(|G|) + \log \log(|G|) - q_\alpha| = o_P(1), \quad (6)$$

where  $q_\alpha$  is the  $100(1 - \alpha)$ th quantile of  $F(x)$ . Consider any  $j^* \in G$  such that  $|\check{\beta}_{j^*} - \beta_{j^*}^0|/\sqrt{\widehat{\omega}_{j^*j^*}} >$



$(\sqrt{2} + \varepsilon_0)\sqrt{(\log |G|)/n}$ . Using the inequality  $2a_1a_2 \leq \delta^{-1}a_1^2 + \delta a_2^2$  for any  $\delta > 0$ , we have

$$n|\tilde{\beta}_{j^*} - \beta_{j^*}^0|^2/\widehat{\omega}_{j^*j^*} \leq (1 + \delta^{-1})n|\check{\beta}_{j^*} - \beta_{j^*}^0|^2/\widehat{\omega}_{j^*j^*} + (1 + \delta)n|\check{\beta}_{j^*} - \tilde{\beta}_{j^*}|^2/\widehat{\omega}_{j^*j^*}, \quad (7)$$

where  $n|\check{\beta}_{j^*} - \beta_{j^*}^0|^2/\widehat{\omega}_{j^*j^*} = o_p(\log |G|)$  as  $j^*$  is fixed and  $|G|$  grows. From the proof of Theorem 2.3, we know the difference between  $n|\tilde{\beta}_{j^*} - \beta_{j^*}^0|^2/\widehat{\omega}_{j^*j^*}$  and  $n|\check{\beta}_{j^*} - \beta_{j^*}^0|^2/\omega_{j^*j^*}$  is asymptotically negligible. Thus by (7) and the fact that  $\beta^0 \in \mathcal{U}_G(\sqrt{2} + \varepsilon_0)$ , we have,

$$\max_{j \in G} n|\check{\beta}_j - \tilde{\beta}_j|^2/\widehat{\omega}_{jj} \geq \frac{1}{1 + \delta} \left\{ (\sqrt{2} + \varepsilon_0)^2(\log |G|) - o_p(\log |G|) \right\}. \quad (8)$$

The conclusion thus follows from (8) and (6) provided that  $\delta$  is small enough.  $\diamond$

*Proof of Proposition 3.1.* Similar to the proof of Theorem 2.4, the distribution of  $\max_{1 \leq j \leq p} \sqrt{n}|\check{\beta}_j - \beta_0|/\sqrt{\widehat{\omega}_{jj}}$  can be approximated by  $\max_{1 \leq j \leq p} |Z_j|$  with  $Z = (Z_1, \dots, Z_p) \stackrel{d}{\sim} N(0, \tilde{\Theta})$ . Under Assumption 2.5, by Lemma 6 of Cai et al. (2014), we have for any  $x \in \mathbb{R}$  and as  $p \rightarrow +\infty$ ,

$$P\left(\max_{1 \leq i \leq p} |Z_i|^2 - 2 \log(p) + \log \log(p) \leq x\right) \rightarrow \exp\left\{-\frac{1}{\sqrt{\pi}} \exp\left(-\frac{x}{2}\right)\right\}.$$

It implies that

$$P\left(\max_{j \in \mathcal{S}_0^c} n|\check{\beta}_j|^2/\widehat{\omega}_{jj} \leq 2 \log(p) - \log \log(p)/2\right) \rightarrow 1. \quad (9)$$

On the other hand, we note that

$$\min_{j \in \mathcal{S}_0} n|\beta_j^0|^2/\widehat{\omega}_{jj} \leq 2 \max_{j \in \mathcal{S}_0} n|\check{\beta}_j - \beta_j^0|^2/\widehat{\omega}_{jj} + 2 \min_{j \in \mathcal{S}_0} n|\check{\beta}_j|^2/\widehat{\omega}_{jj}$$

Because the difference between  $\min_{j \in \mathcal{S}_0} n|\beta_j^0|^2/\widehat{\omega}_{jj}$  and  $\min_{j \in \mathcal{S}_0} n|\beta_j^0|^2/\omega_{jj}$  is asymptotically negligible, and  $P(2 \max_{j \in \mathcal{S}_0} n|\check{\beta}_j - \beta_j^0|^2/\widehat{\omega}_{jj} \leq 4 \log(p) - \log \log(p)) \rightarrow 1$ , we obtain

$$\begin{aligned} & P\left(\min_{j \in \mathcal{S}_0} n|\check{\beta}_j|^2/\widehat{\omega}_{jj} > 2 \log p\right) \\ & \geq P\left(2 \min_{j \in \mathcal{S}_0} n|\check{\beta}_j|^2/\widehat{\omega}_{jj} + 4 \log(p) - \log \log(p) > 8 \log(p)\right) \rightarrow 1. \end{aligned} \quad (10)$$

Hence, (16) follows from (9) and (10).

We next prove the optimality of  $\tau^* = 2$ , i.e., (17). For large enough  $p$ , we can choose a set  $G^*$  such that  $\beta_j = 0$  for  $j \in G^*$ , and  $|G^*| = \lfloor p^{\tau_2} \rfloor$  with  $\tau/2 < \tau_2 < 1$ . Following the above arguments, we know that the distribution of  $\max_{j \in G^*} \sqrt{n} |\check{\beta}_j - \beta_j^0| / \sqrt{\hat{\omega}_{jj}}$  can be approximated by  $\max_{j \in G^*} |Z_j|$  with  $Z = (Z_1, \dots, Z_p) \sim^d N(0, \tilde{\Theta})$ . Then we have

$$P \left( \max_{j \in G^*} n |\check{\beta}_j|^2 / \hat{\omega}_{jj} \geq c \log(p) \right) \rightarrow 1,$$

where  $\tau < c < 2\tau_2 < 2$ . The conclusion thus follows immediately.  $\diamond$

*Proof of Theorem 4.1.* For simplicity, we only prove the result for the one-sided case (the arguments below can be easily modified for the two-sided case). Define  $T_G = \max_{j \in G} \sqrt{n} (\check{\beta}_j - \beta_j^0)$  and  $T_{0,G} = \max_{j \in G} \sum_{i=1}^n \xi_{ij} / \sqrt{n}$ . Let  $\tilde{c}_G(\alpha)$  be the bootstrap critical value for the one-sided test at level  $\alpha$ . We first show that there exist  $\zeta_1, \zeta_2 > 0$  such that

$$P(|T_G - T_{0,G}| \geq \zeta_1) < \zeta_2, \tag{11}$$

where  $\zeta_1 \sqrt{1 \vee \log(p/\zeta_1)} = o(1)$  and  $\zeta_2 = o(1)$ . Notice that

$$|T_G - T_{0,G}| \leq \max_{j \in G} \sqrt{n} |(\Theta_j^T - \hat{\Theta}_j^T) \mathbb{E}_n \dot{L}_{\beta_0}| + \|\Delta\|_\infty + \sqrt{n} \|\hat{\Theta} \mathcal{R}\|.$$

Under the Lipschitz continuity in Assumption 4.1, we have

$$\hat{\Theta}_j^T \mathbb{E}_n \dot{L}_{\hat{\beta}} = \hat{\Theta}_j^T \mathbb{E}_n \dot{L}_{\beta_0} + \hat{\Theta}_j^T \mathbb{E}_n \ddot{L}_{\hat{\beta}} (\hat{\beta} - \beta^0) + \mathcal{R}_j,$$

where  $\mathcal{R}_j = \hat{\Theta}_j^T \mathcal{R} \leq \max_i |\hat{\Theta}_j^T x_i| \cdot \|\mathbf{X}(\hat{\beta} - \beta^0)\|_2^2 / n = O_P(K_n s_0 \lambda^2)$  (see the proof of Theorem 3.1 in van de Geer et al. 2014). It thus implies that  $\sqrt{n} \|\hat{\Theta} \mathcal{R}\|_\infty = O_P(\sqrt{n} K_n s_0 \lambda^2)$ . By Assumptions 4.3-4.4, we have

$$\|\Delta\|_\infty = \|\sqrt{n}(\hat{\Theta} \hat{\Sigma} - I)(\hat{\beta} - \beta_0)\|_\infty \leq \|\hat{\Theta} \hat{\Sigma} - I\|_\infty \sqrt{n} \|\hat{\beta} - \beta_0\|_1 = O_P(\sqrt{n} \lambda \lambda_* s_0)$$

Following the arguments in the proof of Lemma 1.2, it can be shown that under Assumption 4.5

$$\begin{aligned} \max_{j \in G} \sqrt{n} |(\Theta_j^T - \widehat{\Theta}_j^T) \mathbb{E}_n \dot{L}_{\beta_0}| &= \max_{j \in G} \left| \sum_{i=1}^n \widehat{\xi}_{ij} / \sqrt{n} - \sum_{i=1}^n \xi_{ij} / \sqrt{n} \right| \\ &= O_P(K_n \max_j s_j \log(p) / \sqrt{n}) + O_P\left(K_n^2 s_0 \left(\lambda^2 \sqrt{n} \vee \lambda \sqrt{\log(p)}\right)\right) \end{aligned}$$

Thus (11) follows from a proper choice of  $\zeta_1$ .

By Lemma 1.1, we have

$$\sup_{x \in \mathbb{R}} \left| P\left(\max_{j \in G} \sum_{i=1}^n \xi_{ij} / \sqrt{n} \leq x\right) - P\left(\max_{j \in G} \sum_{i=1}^n z_{ij} / \sqrt{n} \leq x\right) \right| \lesssim n^{-c'}, \quad c' > 0,$$

where  $\{z_i = (z_{i1}, \dots, z_{ip})'\}$  is a sequence of mean zero independent Gaussian vector with  $\mathbb{E} z_i z_i' = \Theta_j^T \Sigma_{\beta_0} \Theta_j$ . By the arguments in the proof of Theorem 3.2 in Chernozhukov et al. (2013), we have

$$\sup_{\alpha \in (0,1)} |P(T_G > \widetilde{c}_G^*(\alpha)) - \alpha| \lesssim \pi(v) + P(\widetilde{\Gamma} > v) + n^{-c'} + \zeta_1 \sqrt{1 \vee \log(p/\zeta_1)} + \zeta_2, \quad (12)$$

where  $\pi(v) = C_2 v^{1/3} (1 \vee \log(p/v))^{2/3}$ . The conclusion follows by choosing  $v = 1/(\alpha_n (\log(p))^2)$  in (12).  $\diamond$

## 2 Additional numerical results

We consider the linear models where the rows of  $\mathbf{X}$  are fixed i.i.d realizations from  $N_p(0, \Sigma)$  with  $\Sigma = (\Sigma_{i,j})_{i,j=1}^p$  under two scenarios: (i) Toeplitz:  $\Sigma_{i,j} = 0.9^{|i-j|}$ ; (ii) Exchangeable/Compound symmetric:  $\Sigma_{i,i} = 1$  and  $\Sigma_{i,j} = 0.8$  for  $i \neq j$ . The active set is  $\mathcal{S}_0 = \{1, 2, \dots, s_0\}$  with  $s_0 = 3$  or 15. To obtain the main Lasso estimator, we implemented the scaled Lasso with the tuning parameter  $\lambda_0 = \sqrt{2} \widetilde{L}_n(k_0/p)$  with  $\widetilde{L}_n(t) = n^{-1/2} \Phi^{-1}(1-t)$ , where  $\Phi$  is the cumulative distribution function for  $N(0, 1)$ , and  $k_0$  is the solution to  $k = \widetilde{L}_1^4(k/p) + 2\widetilde{L}_1^2(k/p)$ . We estimate the noise level  $\sigma^2$  using the modified variance estimator.

## 2.1 Modified variance estimator

Figure S.1 provides boxplots of  $\hat{\sigma}/\sigma$  for the variance estimator delivered by the scaled Lasso (denoted by “SLasso”) and for the modified variance estimator in (24) of the paper (denoted by “SLasso\*”). Clearly, the modified variance estimator corrects the noise underestimation issue and thus is preferable.

## 2.2 Impact of the remainder term

We discuss the impact of the (normalized) remainder term  $\Delta$  on the coverage accuracy. Recall the linear expansion  $\sqrt{n}(\check{\beta} - \beta^0) = \hat{\Theta}\mathbf{X}^T\epsilon/\sqrt{n} + \Delta$ , where  $\Delta = (\Delta_1, \dots, \Delta_p)^T = -\sqrt{n}(\hat{\Theta}\hat{\Sigma} - I)(\hat{\beta} - \beta^0)$  with  $\hat{\Sigma}$  being the Gram matrix and  $\hat{\beta}$  being the Lasso estimator. The studentized maximum type test statistic can be written as

$$\max_{1 \leq j \leq p} \frac{\sqrt{n}|\check{\beta}_j - \beta_j^0|}{\sqrt{\hat{\omega}_{jj}}} = \max_{1 \leq j \leq p} \left| \frac{\sum_{i=1}^n \hat{\xi}_{ij}}{\sqrt{n\hat{\omega}_{jj}}} + \frac{\Delta_j}{\sqrt{\hat{\omega}_{jj}}} \right|. \quad (13)$$

Thus the coverage accuracy can be greatly affected by the term  $\Delta_j^* := \frac{\Delta_j}{\sqrt{\hat{\omega}_{jj}}}$ . Note that this (normalized) remainder term is determined by  $\hat{\Theta}$ . We now consider three different methods in estimating  $\Theta$ : (i) nodewise Lasso with  $\lambda_j$ s chosen by 10-fold cross validation; (ii) nodewise Lasso with  $\lambda_j = 0.01$ ; (iii) the method in Javanmard and Montanari (2014) with the tuning parameters chosen automatically by their algorithm. To empirically evaluate  $\Delta^* := (\Delta_1^*, \dots, \Delta_p^*)^T$ , we consider the linear models with  $t(4)/\sqrt{2}$  errors,  $n = 100$  and  $p = 500$ . Define  $\Delta_{ac}^* = (\Delta_j^*)_{j \in \mathcal{S}_0}$  and  $\Delta_{in}^* = (\Delta_j^*)_{j \in \mathcal{S}_0^c}$ . Figure S.2 presents the boxplots for  $\|\Delta_{ac}^*\|_\infty$  and  $\|\Delta_{in}^*\|_\infty$ . The nodewise Lasso clearly outperforms the method in Javanmard and Montanari (2014), and the choice of  $\lambda_j = 0.01$  yields the smallest  $\|\Delta_{ac}^*\|_\infty$  in all cases. In addition,  $\|\Delta_{ac}^*\|_\infty$  is relatively large when  $\Sigma$  is exchangeable,  $s_0 = 15$  and  $p = 500$ , which explains the lack of performance/undercoverage in this case. We observe that the maximum norms of  $\Delta_{ac}^*$  and  $\Delta_{in}^*$  generally increase with  $s_0$ . Overall, the above discussions support our observations in Tables 1-2 of the paper in the sense that the lower the (normalized) remainder term is, the more accurate the coverage is.

## References

- [1] JAVANMARD, A. AND MONTANARI, A. (2014). Confidence intervals and hypothesis testing for high-dimensional regression. arXiv:1306.3171.

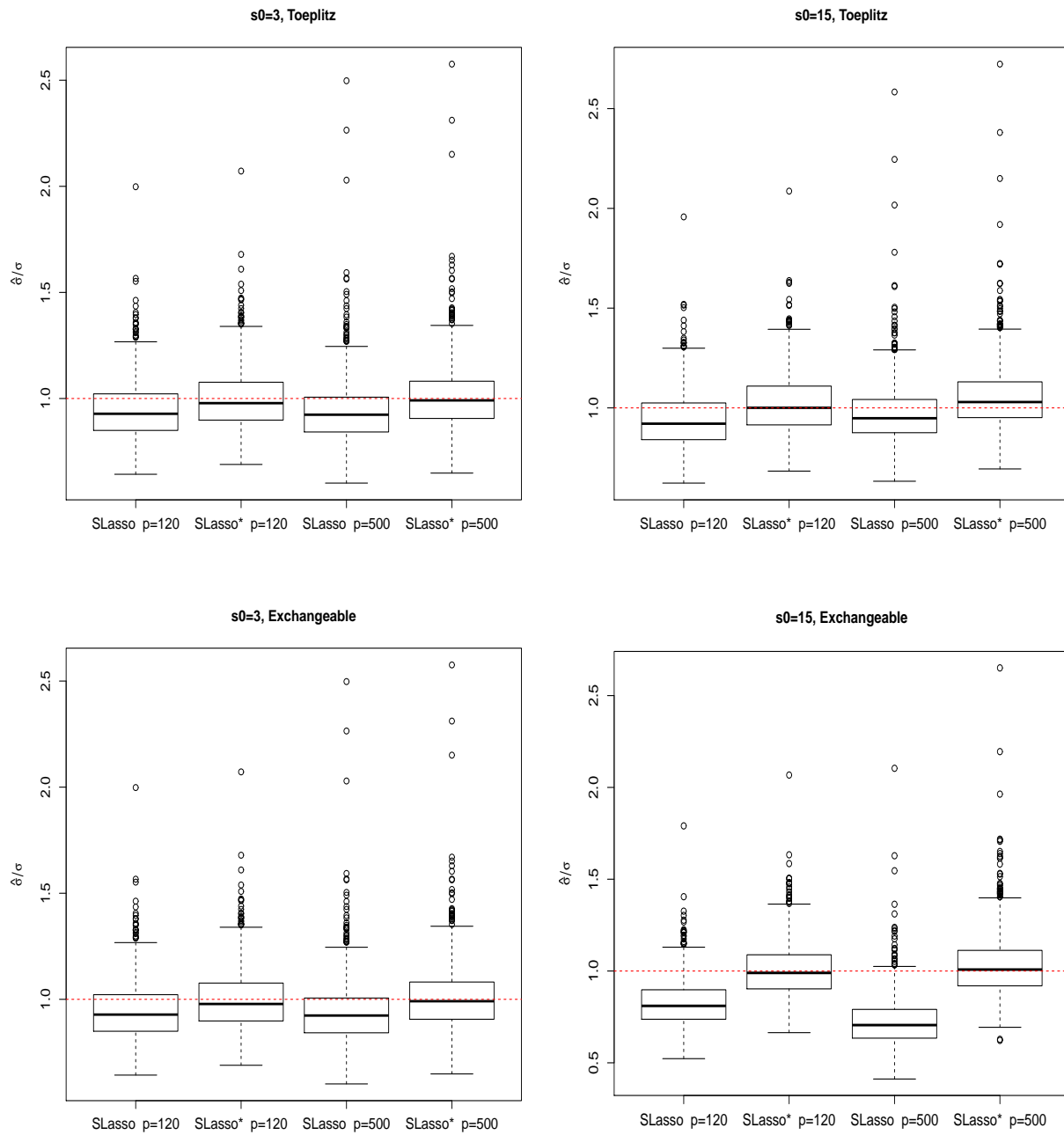


Figure S.1: Boxplots for  $\hat{\sigma}/\sigma$ , where  $s_0 = 3$  or  $15$ ,  $\Sigma$  is Toeplitz or exchangeable, and the errors are generated from the studentized  $t(4)$  distribution. Here “SLasso” corresponds to the variance estimator delivered by the scaled Lasso and “SLasso\*” corresponds to the modified variance estimator.

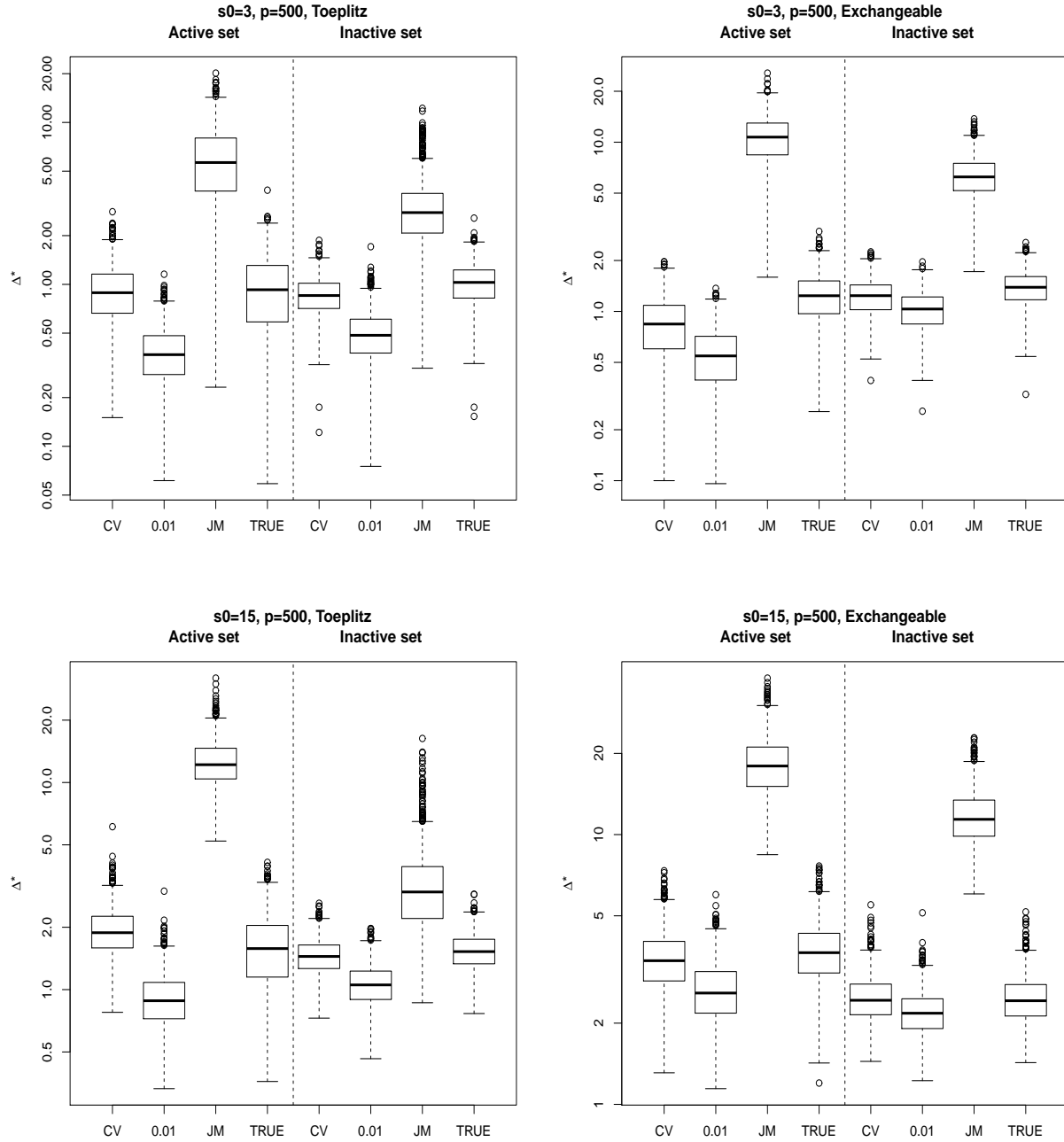


Figure S.2: Boxplots for  $\|\Delta_{ac}^*\|_\infty$  and  $\|\Delta_{in}^*\|_\infty$ , where  $s_0 = 3$  or  $15$ ,  $p = 500$ ,  $\Sigma$  is Toeplitz or exchangeable, and the errors are  $t(4)/\sqrt{2}$ . Here “CV”, “0.01”, “JM” and “TRUE” denote the nodewise Lasso with  $\lambda_j$ s chosen by 10-fold cross validation and  $\lambda_j = 0.01$ , the method in Javanmard and Montanari (2014) and the method with the true  $\Theta$  respectively. Note that the  $y$ -axis is plotted on a log scale.