

## Auxiliary Learning and its Statistical Understanding

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### Supplementary Material

## Appendix A: Verification Details

### Appendix A.1: Verification for the form of $\mathbb{W}$

For the sake of simplicity, we write  $\mathbb{W}_1 = \{w \in \mathbb{R}^{K+1} : Bw = \beta^{(0)}\}$  and  $\mathbb{W}_2 = \{e_1 + \Theta u : u \in \mathbb{R}^{K-d+1}\}$ . Then it suffices to show that  $\mathbb{W}_1 = \mathbb{W}_2$ . On one side, for any  $w \in \mathbb{W}_2$ , we can find  $u$  such that  $w = e_1 + \Theta u$ . We then have  $Bw = B(e_1 + \Theta u) = \beta^{(0)} + B\Theta u$ . In fact, we should have  $B\Theta u = \mathbf{0}_p$ ; otherwise we have  $u^\top \Theta^\top B^\top B \Theta u > 0$ , which is a contradiction since  $\Theta^\top B^\top B \Theta = \mathbf{O}_{K-d+1}$ . Then  $Bw = \beta^{(0)}$  and thus  $w \in \mathbb{W}_1$ , indicating  $\mathbb{W}_2 \subset \mathbb{W}_1$ . On the other side, for any  $w \in \mathbb{W}_1$ , we should have  $B(w - e_1) = \mathbf{0}$ . Recall that  $\text{rank}(B) = d$ ,  $\text{rank}(\Theta) = K + d - 1$ , and  $B\Theta = \mathbf{O}_{p \times (K+d-1)}$ . Therefore,  $\Theta$  is a basis of the null space for  $B$ . It follows that there exists  $u \in \mathbb{R}^{K+d-1}$  such that  $w - e_1 = \Theta u$ . Therefore,  $w \in \mathbb{W}_2$  and  $\mathbb{W}_1 \subset \mathbb{W}_2$ . Consequently, we have  $\mathbb{W}_1 = \mathbb{W}_2$ .

### Appendix A.2: Derivation of $w^*$

We start with solving  $w^* = \arg \min_{w \in \mathbb{W}} \mathcal{P}(w) = \arg \min_{w \in \mathbb{W}} w^\top \Sigma_\epsilon w$ . Recall that for any  $w \in \mathbb{W}$ , there exists some  $u \in \mathbb{R}^{K+1-d}$  such that  $w = e_1 + \Theta u$ . Therefore, minimizing  $w^\top \Sigma_\epsilon w$  under the constraint  $w \in \mathbb{W}$  is equivalent to minimizing  $(e_1 + \Theta u)^\top \Sigma_\epsilon (e_1 + \Theta u)$  with

respect to  $u \in \mathbb{R}^{K+1-d}$ . Define  $\mathcal{Q}(u) = (e_1 + \Theta u)^\top \Sigma_\varepsilon (e_1 + \Theta u)$ , which is convex with respect to  $u$ . The first-order derivative of  $\mathcal{Q}(u)$  is given by  $\dot{\mathcal{Q}}(u) = \partial \mathcal{Q}(u) / \partial u = \Theta^\top \Sigma_\varepsilon e_1 + \Theta^\top \Sigma_\varepsilon \Theta u$ . Setting this derivative to zero, we find  $u^* = -(\Theta^\top \Sigma_\varepsilon \Theta)^{-1} \Theta^\top \Sigma_\varepsilon e_1$ . Finally, substituting  $u^*$  into the expression for  $w$ , we obtain the optimal weight  $w^* = e_1 - \Theta(\Theta^\top \Sigma_\varepsilon \Theta)^{-1} \Theta^\top \Sigma_\varepsilon e_1$ .

## Appendix B: The Proof of Theorem 1

Write  $H = \Sigma_\varepsilon^{1/2} \Theta (\Theta^\top \Sigma_\varepsilon \Theta)^{-1} \Theta \Sigma_\varepsilon^{1/2}$  and  $\hat{H} = \hat{\Sigma}_\varepsilon^{1/2} \hat{\Theta} (\hat{\Theta} \hat{\Sigma}_\varepsilon \hat{\Theta})^{-1} \hat{\Theta} \hat{\Sigma}_\varepsilon^{1/2}$ . We then have  $w^* = e_1 - \Sigma_\varepsilon^{-1/2} H \Sigma_\varepsilon^{1/2} e_1$  and  $\hat{w}^* = e_1 - \hat{\Sigma}_\varepsilon^{-1/2} \hat{H} \hat{\Sigma}_\varepsilon^{1/2} e_1$ . Then

$$\begin{aligned} \|\hat{\beta}_{\hat{w}^*} - \hat{\beta}_{w^*}\|_2 &= \|\hat{B}(\hat{w}^* - w^*)\|_{\text{op}} \leq \|\hat{B}\|_{\text{op}} \|\hat{w}^* - w^*\|_{\text{op}} \\ &\leq \|\hat{B}\|_{\text{op}} \|\hat{\Sigma}_\varepsilon^{-1/2} \hat{H} \hat{\Sigma}_\varepsilon^{1/2} - \Sigma_\varepsilon^{-1/2} H \Sigma_\varepsilon^{1/2}\|_{\text{op}} \\ &\leq \|\hat{B}\|_{\text{op}} \left\{ \|\hat{\Sigma}_\varepsilon^{-1/2} - \Sigma_\varepsilon^{-1/2}\|_{\text{op}} \|\hat{\Sigma}_\varepsilon^{1/2}\|_{\text{op}} + \tau_{\min}^{-1/2} \|\hat{H} - H\|_{\text{op}} \|\hat{\Sigma}_\varepsilon^{1/2}\|_{\text{op}} \right. \\ &\quad \left. + \tau_{\min}^{-1/2} \|\hat{\Sigma}_\varepsilon^{1/2} - \Sigma_\varepsilon^{1/2}\|_{\text{op}} \right\}. \end{aligned}$$

Consequently, it suffices to prove the following inequalities, i.e., (B.1)—(B.4). Their detailed proofs are presented in Appendix C.

$$P \left( \|\hat{B} - B\|_{\text{op}} > C_1 \sqrt{\frac{p+K}{N}} \right) \leq C_2 \exp\{- (p+K)\}, \quad (\text{B.1})$$

$$P \left\{ \|\hat{\Sigma}_\varepsilon^{1/2} - \Sigma_\varepsilon^{1/2}\|_{\text{op}} > C_3 \left( \sqrt{\frac{K}{N}} + \frac{p}{N} \right) \right\} \leq 2 \exp(-K), \quad (\text{B.2})$$

$$P \left\{ \|\hat{\Sigma}_\varepsilon^{-1/2} - \Sigma_\varepsilon^{-1/2}\|_{\text{op}} > C_4 \left( \sqrt{\frac{K}{N}} + \frac{p}{N} \right) \right\} \leq 2 \exp(-K), \quad (\text{B.3})$$

$$P \left\{ \|\hat{H} - H\|_{\text{op}} > C_5 \left( \sqrt{\frac{K+d}{N}} + \frac{p}{N} \right) \right\} \leq C_6 \exp(-K). \quad (\text{B.4})$$

The detailed proof of (B.1) is given in Lemma 1. The results of (B.2) and (B.3) are given in Lemma 2. The inequality (B.4) is proved in Lemma 3.

Based on (B.1)—(B.4), we have  $\|\hat{B}\|_{\text{op}} \leq \|\hat{B} - B\|_{\text{op}} + \|B\|_{\text{op}} \leq 2\|B\|_{\text{op}}$  as long as  $N > N_0$  for some sufficiently large constant  $N_0$ . Similarly, we have  $\|\hat{\Sigma}_\varepsilon^{1/2}\|_{\text{op}} \leq 2\|\Sigma_\varepsilon^{1/2}\|_{\text{op}}$  as  $N > N_0$  for the same  $N_0$ . It follows that  $\|\hat{\beta}_{\hat{w}^*} - \hat{\beta}_{w^*}\|_2 \leq 4\tau_{\max}^{3/2} \|\hat{\Sigma}_\varepsilon^{-1/2} - \Sigma_\varepsilon^{-1/2}\|_{\text{op}} + \tau_{\min}^{-1/2} \tau_{\max}^{3/2} \|\hat{H} - H\|_{\text{op}} +$

$\tau_{\min}^{-1/2} \tau_{\max} \|\widehat{\Sigma}_\varepsilon^{1/2} - \Sigma_\varepsilon^{1/2}\|_{\text{op}}$ . Then by (B.2)—(B.4), we have

$$P \left\{ \left\| \widehat{\beta}_{\widehat{w}^*} - \widehat{\beta}_{w^*} \right\|_{\text{op}} > C_7 \left( \sqrt{\frac{K+d}{N}} + \frac{p}{N} \right) \right\} \leq C_8 \exp(-K),$$

for some constants  $C_7$  and  $C_8$  as long as  $N > N_0$  for the same constant  $N_0$ . This concludes the entire proof.

## Appendix C: Some Useful Lemmas for Theorem 1

**Lemma 1.** (Convergence Rate of  $\widehat{B}$ ) Assume the same conditions as Theorem 1. Then  $\|\widehat{B} - B\|_{\text{op}} \leq C_1 \sqrt{(p+K)/N}$  holds with probability at least  $1 - C_2 \exp\{-(p+K)\}$  as long as  $N > N_0$  for some sufficiently large constant  $N_0$ . Here  $C_1$  and  $C_2$  are constants independent of  $p$ ,  $K$ , and  $N$ .

*Proof.* Note that  $\widehat{B} - B = (\mathbb{X}^\top \mathbb{X})^{-1} \mathbb{X}^\top \mathcal{E}$ , where  $\mathbb{X} = (X_1, \dots, X_N)^\top \in \mathbb{R}^{N \times p}$ ,  $\mathcal{E} = (\varepsilon^{(0)}, \dots, \varepsilon^{(K)}) \in \mathbb{R}^{N \times (K+1)}$ , and  $\varepsilon^{(k)} = (\varepsilon_1^{(k)}, \dots, \varepsilon_N^{(k)})^\top \in \mathbb{R}^N$ . Then we have

$$\begin{aligned} \|\widehat{B} - B\|_{\text{op}} &\leq \|\widehat{\Sigma}_{xx}^{-1}\|_{\text{op}} \|N^{-1} \mathbb{X}^\top \mathcal{E}\|_{\text{op}} \\ &\leq \left\{ \lambda_{\min}(\Sigma_{xx}) - \lambda_{\max}(\Sigma_{xx} - \widehat{\Sigma}_{xx}) \right\}^{-1} \|N^{-1} \mathbb{X}^\top \mathcal{E}\|_{\text{op}}, \end{aligned}$$

where the last inequality is due to the fact that  $\lambda_{\min}(A) \geq \lambda_{\min}(B) - \lambda_{\max}(B - A)$  for two arbitrary but symmetric matrices  $A$  and  $B$ . Then it suffices to prove the following two inequalities

$$P\left(\|\widehat{\Sigma}_{xx} - \Sigma_{xx}\|_{\text{op}} > \tau_{\min}/2\right) \leq C_1 \exp(-C_2 N), \quad (\text{C.1})$$

$$P\left(\|N^{-1} \mathbb{X}^\top \mathcal{E}\|_{\text{op}} > t\right) \leq C_3 \exp\left\{2(p+K) - C_4 N \min\left(\frac{t^2}{4C_{\text{sub}}^4}, \frac{t}{2C_{\text{sub}}^2}\right)\right\}. \quad (\text{C.2})$$

The detailed proofs are given in the following STEP 1 and STEP 2. With the help of (C.1) and (C.2), we then have

$$\begin{aligned} P\left(\|\widehat{B} - B\|_{\text{op}} > \delta\right) &\leq P\left(\|\widehat{\Sigma}_{xx} - \Sigma_{xx}\|_{\text{op}} > \tau_{\min}/2\right) + P\left(2\tau_{\min}^{-1} \|N^{-1} \mathbb{X}^\top \mathcal{E}\| > \delta\right) \\ &\leq 2C_3 \exp\left\{2(p+K) - C_4 N \min(C_5^2 \delta^2, C_5 \delta)\right\}, \end{aligned} \quad (\text{C.3})$$

where  $C_5 = \tau_{\min}/(4C_{\text{sub}}^2)$  is a constant. Recall that by Condition (C4),  $p/N \rightarrow 0$  holds as

$N \rightarrow \infty$ . Therefore, we should have  $p/N \leq \sqrt{p/N}$  as long as  $N > N_0$  for the same constant  $N_0$ . Subsequentl, we take

$$\delta = \frac{1}{\mathcal{C}_5} \max \left( \sqrt{\frac{3(p+K)}{\mathcal{C}_4 N}}, \frac{3(p+K)}{\mathcal{C}_4 N} \right) = \frac{1}{\mathcal{C}_5} \sqrt{\frac{3(p+K)}{\mathcal{C}_4 N}}.$$

Then (C.3) suggests that  $\|\widehat{B} - B\|_{\text{op}} \leq C_1 \sqrt{(p+K)/N}$  holds with probability at least  $1 - C_2 \exp\{- (p+K)\}$ , where  $C_1 = 3/(\sqrt{\mathcal{C}_4} \mathcal{C}_5)$  and  $C_2 = 2\mathcal{C}_3$  are constants. This leads to the conclusion of Lemma 1. We next verify the inequalities (C.1) and (C.2) in the following two steps.

STEP 1: PROOF OF (C.1). By condition (C1), we know  $X_i$  is an independently and identically distributed sub-Gaussian random variable. Therefore, we can apply Theorem 6.5 of Wainwright (2019) and obtain

$$P \left\{ C_{\text{sub}}^{-2} \left\| \widehat{\Sigma}_{xx} - \Sigma_{xx} \right\|_{\text{op}} \geq C_1 \left( \sqrt{\frac{p}{N}} + \frac{p}{N} \right) + \epsilon \right\} \leq C_2 \exp \left\{ - C_3 N \min(\epsilon, \epsilon^2) \right\}, \quad (\text{C.4})$$

where  $C_1, C_2$  and  $C_3$  are some fixed constants. Next define  $\epsilon = \tau_{\min}/(4C_{\text{sub}})$ . Then by Condition (C2) that  $p/N \rightarrow 0$  as  $N \rightarrow \infty$ , we should have  $C_1 C_{\text{sub}}^2 (\sqrt{p/N} + p/N) + C_{\text{sub}}^2 \epsilon \leq \tau_{\min}/2$  as long as  $N > N_0$  for some sufficiently large constant  $N_0$ . Therefore, by the inequality (C.4) we know that as long as  $N > N_\delta$ , we have

$$P \left( \|\Sigma_{xx} - \widehat{\Sigma}_{xx}\|_{\text{op}} \geq \tau_{\min}/2 \right) \leq C_2 \exp(-C_4 N), \quad (\text{C.5})$$

where  $C_4 = C_3 \min \left\{ \tau_{\min}/(4C_{\text{sub}}), \tau_{\min}^2/(16C_{\text{sub}}^4) \right\}$  is a constant independent of  $N$ .

STEP 2: PROOF OF (C.2). We consider an  $\varepsilon$ -net to bound the term  $\|N^{-1} \mathbb{X}^\top \mathcal{E}\|_{\text{op}}^2$ . Let  $\varepsilon = 1/3$  and we can find two  $\varepsilon$ -nets  $\mathcal{U}$  and  $\mathcal{V}$  of the unit spheres  $\mathcal{S}^{p-1}$  and  $\mathcal{S}^K$  with

cardinalities  $|\mathcal{U}| \leq 7^p \leq e^{2p}$  and  $|\mathcal{V}| \leq 7^{K+1} \leq e^{2(K+1)}$ , respectively (Vershynin, 2018, Corollary 4.2.13). Then we have  $\|N^{-1}\mathbb{X}^\top \mathcal{E}\|_{\text{op}} \leq 2 \max_{u \in \mathcal{U}, v \in \mathcal{V}} |N^{-1}(\mathcal{E}v)^\top(\mathbb{X}u)|$  (Vershynin, 2018, Lemma 4.4.1). Note that  $N^{-1}(\mathcal{E}v)^\top(\mathbb{X}u) = N^{-1} \sum_{i=1}^N \tilde{X}_i \tilde{\varepsilon}_i$ , where  $\tilde{X}_i = X_i^\top u \in \mathbb{R}$  and  $\tilde{\varepsilon}_i = \varepsilon_i^\top v \in \mathbb{R}$ . Here  $\tilde{X}_i$  and  $\tilde{\varepsilon}_i$  are independent sub-Gaussian variables with  $\|\tilde{X}_i\|_{\psi_2} \leq C_{\text{sub}}$  and  $\|\tilde{\varepsilon}_i\|_{\psi_2} \leq C_{\text{sub}}$  by Condition (C1). We further note that  $\tilde{X}_i \tilde{\varepsilon}_i$  are sub-exponential variables with  $E(\tilde{X}_i \tilde{\varepsilon}_i) = \mathbf{0}$  and  $\|\tilde{X}_i \tilde{\varepsilon}_i\|_{\psi_1} \leq \|\tilde{X}_i\|_{\psi_2} \|\tilde{\varepsilon}_i\|_{\psi_2} \leq C_{\text{sub}}^2$  (Vershynin, 2018, Lemma 2.7.7). Then for some fixed positive constant  $C_5$  and  $C_6$ , we have

$$\begin{aligned} P\left(\|N^{-1}\mathbb{X}^\top \mathcal{E}\|_{\text{op}} > t\right) &\leq |\mathcal{U}| |\mathcal{V}| P\left(\left|\frac{1}{N} \sum_{i=1}^N \tilde{X}_i \tilde{\varepsilon}_i\right| > \frac{t}{2}\right) \\ &\leq C_5 \exp\left\{2(p+K) - C_6 N \min\left(\frac{t^2}{4C_{\text{sub}}^4}, \frac{t}{2C_{\text{sub}}^2}\right)\right\}. \end{aligned} \quad (\text{C.6})$$

□

**Lemma 2.** (Convergence Rate of  $\widehat{\Sigma}_\varepsilon^{1/2}$  and  $\widehat{\Sigma}_\varepsilon^{-1/2}$ ) Assume the same conditions as Theorem 1. We then have  $\|\widehat{\Sigma}_\varepsilon^{1/2} - \Sigma_\varepsilon^{1/2}\|_{\text{op}} \leq C_1(\sqrt{K/N} + p/N)$  and  $\|\widehat{\Sigma}_\varepsilon^{-1/2} - \Sigma_\varepsilon^{-1/2}\|_{\text{op}} \leq C_2(\sqrt{K/N} + p/N)$  hold with a probability at least  $1 - 2\exp(-K)$  as long as  $N > N_0$  for some sufficiently large constant  $N_0$ . Here  $C_1$  and  $C_2$  are constants independent of  $K$ ,  $N$ , and  $N_0$ .

*Proof.* We first argue the conclusion that  $\|\widehat{\Sigma}_\varepsilon - \Sigma_\varepsilon\|_{\text{op}} \leq C(\sqrt{K/N} + p/N)$  holds with a probability at least  $1 - 2\exp(-K)$  as long as  $N > N_0$ . We prove this conclusion in Lemma 4. Then by Lemma 4, we should have  $\widehat{\Sigma}_\varepsilon$  to be consistent as  $N \rightarrow \infty$ . Define  $\Delta = \widehat{\Sigma}_\varepsilon^{1/2} - \Sigma_\varepsilon^{1/2}$ , we should have  $\|\Delta\|_{\text{op}} \rightarrow_p 0$  as  $N \rightarrow \infty$ . We next study the probabilistic upper bound for  $\|\Delta\|_{\text{op}}$ . Note that  $\widehat{\Sigma}_\varepsilon = (\Sigma_\varepsilon^{1/2} + \Delta)(\Sigma_\varepsilon^{1/2} + \Delta) = \Sigma_\varepsilon + \Sigma_\varepsilon^{1/2}\Delta + \Delta\Sigma_\varepsilon^{1/2} + \Delta^2$ . It follows that  $\|\widehat{\Sigma}_\varepsilon^{-1/2} - \Sigma_\varepsilon^{-1/2}\|_{\text{op}} \leq C_0\|\widehat{\Sigma}_\varepsilon - \Sigma_\varepsilon\|_{\text{op}}$  for some constant  $C_0$ . Then by Lemma 4, we should have  $\|\Delta\|_{\text{op}} = \|\widehat{\Sigma}_\varepsilon^{1/2} - \Sigma_\varepsilon^{1/2}\|_{\text{op}} \leq C_1(\sqrt{K/N} + p/N)$  holds for some constant  $C_0$  with a probability

at least  $1 - 2 \exp(-K)$  as long as  $N > N_0$ . Further note that  $\widehat{\Sigma}_\varepsilon^{-1/2} - \Sigma_\varepsilon^{-1/2} = (\widehat{\Sigma}_\varepsilon^{1/2} - \Sigma_\varepsilon^{1/2})\widehat{\Sigma}_\varepsilon^{-1} - \Sigma_\varepsilon^{-1/2}(\widehat{\Sigma}_\varepsilon - \Sigma_\varepsilon)\widehat{\Sigma}_\varepsilon^{-1}$ . This suggests that  $\|\widehat{\Sigma}_\varepsilon^{-1/2} - \Sigma_\varepsilon^{-1/2}\|_{\text{op}} \leq C_2(\sqrt{K/N} + p/N)$  holds with a probability at least  $1 - 2 \exp(-K)$  as long as  $N > N_0$  for some sufficiently large constant  $N_0$  and a constant  $C_2$ .  $\square$

**Lemma 3.** (*Convergence rate of  $\widehat{H}$* ) Assume the same conditions as Theorem 1. Then  $\|\widehat{H} - H\|_{\text{op}} \leq C_1 \left\{ \sqrt{(K+d)/N} + (p/N) \right\}$  holds with a probability at least  $1 - C_2 \exp(-K)$  as long as  $N > N_0$  for some sufficiently large constant  $N_0$ .

*Proof.* We consider the symmetric matrices  $M = \Sigma_\varepsilon^{-1/2} B^\top B \Sigma_\varepsilon^{-1/2}$  and  $\widehat{M} = \widehat{\Sigma}_\varepsilon^{-1/2} (\widehat{B}^\top \widehat{B} - \sum_{k=d+1}^{K+1} \widehat{\lambda}_k \widehat{\nu}_k \widehat{\nu}_k^\top) \widehat{\Sigma}_\varepsilon^{-1/2}$ , where  $\widehat{\lambda}_k$  is the  $k$ -th largest eigenvalue of  $\widehat{B}^\top \widehat{B}$  and  $\widehat{\nu}_k$  is the associated eigenvector. Then we have  $M \Sigma_\varepsilon^{1/2} \Theta = \mathbf{O}$  and  $\widehat{M} \widehat{\Sigma}_\varepsilon^{1/2} \widehat{\Theta} = \mathbf{O}$ , where  $\mathbf{O}$  is a zero matrix. We conduct the eigenvalue decomposition on  $M$  and  $\widehat{M}$  as  $M = \sum_{k=1}^{K+1} \lambda_k^* \nu_k^* \nu_k^{*\top}$  and  $\widehat{M} = \sum_{k=1}^{K+1} \widehat{\lambda}_k^* \widehat{\nu}_k^* \widehat{\nu}_k^{*\top}$ , where  $\lambda_k^*$  and  $\widehat{\lambda}_k^*$  are the  $k$ -th largest eigenvalues and  $\nu_k^*$  and  $\widehat{\nu}_k^*$  are the associated eigenvectors of  $M$  and  $\widehat{M}$ , respectively. Let  $\Theta^* = (\nu_{d+1}^*, \dots, \nu_{K+1}^*) \in \mathbb{R}^{(K+1) \times (K-d+1)}$  and  $\widehat{\Theta}^* = (\widehat{\nu}_{d+1}^*, \dots, \widehat{\nu}_{K+1}^*) \in \mathbb{R}^{(K+1) \times (K-d+1)}$ . Then we have  $\Theta^*$  and  $\widehat{\Theta}^*$  as matrices with orthogonal columns, satisfying  $M \Theta^* = \mathbf{O}$  and  $\widehat{M} \widehat{\Theta}^* = \mathbf{O}$ . Under the condition that  $\widehat{\lambda}_d^* > 0$ , we should have  $\mathcal{S}(\Sigma_\varepsilon^{1/2} \Theta) = \mathcal{S}(\Theta^*)$  and  $\mathcal{S}(\widehat{\Sigma}_\varepsilon^{1/2} \widehat{\Theta}) = \mathcal{S}(\widehat{\Theta}^*)$  with projection matrices  $H$  and  $\widehat{H}$ , respectively. Therefore, we have  $\|H - \widehat{H}\|_{\text{op}} = \|\widehat{\Theta}^* \widehat{\Theta}^{*\top} - \Theta^* \Theta^{*\top}\|_{\text{op}} = \|\sin \theta(\widehat{\Theta}^*, \Theta^*)\|_{\text{op}}$ ; see Lemma 2.5 of Chen et al. (2021). Here  $\sin \theta(\widehat{\Theta}^*, \Theta^*) = \text{diag}(\sin \theta_k^* : 0 \leq k \leq K) \in \mathbb{R}^{(K+1) \times (K+1)}$ , where  $\theta_k^* = \arccos(\sigma_k^*)$  and  $\sigma_k^*$  is the  $k$ -th largest singular value of  $\widehat{\Theta}^{*\top} \Theta^*$ . Note that  $\lambda_d^* \geq \tau_{\min}^{-1}$  and  $\widehat{\lambda}_k^* = 0$  for any  $d < k \leq K+1$ . Under the condition that  $\widehat{\lambda}_k^* > 0$  for  $1 \leq k \leq d$ , we can apply the Davis-Kahan Theorem (Chen et al., 2021, Theorem 2.7) as

$$\|\widehat{H} - H\|_{\text{op}} = \left\| \sin \theta(\widehat{\Theta}^*, \Theta^*) \right\|_{\text{op}} \leq \left( \frac{\tau_{\max}}{\tau_{\min}} \right) \left\| \widehat{M} - M \right\|_{\text{op}}. \quad (\text{C.7})$$



We write  $\widehat{M} = \widehat{\Sigma}_\varepsilon^{-1/2}(\widehat{B}^\top \widehat{B} - \sum_{k=d+1}^{K+1} \widehat{\lambda}_k \widehat{\nu}_k \widehat{\nu}_k^\top) \widehat{\Sigma}_\varepsilon^{-1/2} = \widehat{\Sigma}_\varepsilon^{-1/2} \widehat{B}^\top \widehat{B} \widehat{\Sigma}_\varepsilon^{-1/2} - \widehat{\Sigma}_\varepsilon^{-1/2} \widehat{\Theta} \widehat{\Lambda} \widehat{\Theta}^\top \widehat{\Sigma}_\varepsilon^{-1/2}$ , where  $\widehat{\Lambda} = \text{diag}(\widehat{\lambda}_k : d < k \leq K+1) \in \mathbb{R}^{(K+1) \times (K+1)}$ . Then  $\|\widehat{M} - M\|_{\text{op}}$  can be further bounded by  $M_1 + M_2$ , where  $M_1 = \|\widehat{\Sigma}_\varepsilon^{-1/2} \widehat{B}^\top \widehat{B} \widehat{\Sigma}_\varepsilon^{-1/2} - \Sigma_\varepsilon^{-1/2} B^\top B \Sigma_\varepsilon^{-1/2}\|_{\text{op}}$  and  $M_2 = \|\widehat{\Sigma}_\varepsilon^{-1/2} \widehat{\Theta} \widehat{\Lambda} \widehat{\Theta}^\top \widehat{\Sigma}_\varepsilon^{-1/2}\|_{\text{op}}$ .

For the term  $M_1$ , simple algebra suggests that  $M_1 \leq M_{11} + M_{12}$ , where

$$M_{11} = \left\| \widehat{\Sigma}_\varepsilon^{-1/2} \right\|_{\text{op}}^2 \left\| \widehat{B}^\top \widehat{B} - B^\top B \right\|_{\text{op}},$$

$$M_{12} = \tau_{\max} \left( \left\| \widehat{\Sigma}_\varepsilon^{-1/2} \right\|_{\text{op}} + \left\| \Sigma_\varepsilon^{-1/2} \right\|_{\text{op}} \right) \left\| \widehat{\Sigma}_\varepsilon^{-1/2} - \Sigma_\varepsilon^{-1/2} \right\|_{\text{op}}.$$

Furthermore, note that  $M_2 \leq \|\widehat{\Sigma}_\varepsilon^{-1/2}\|_{\text{op}}^2 |\widehat{\lambda}_{d+1}|$ , which is due to the fact that  $\|\widehat{V}\|_{\text{op}} = \widehat{\lambda}_{d+1}$ . Recall that  $\widehat{\lambda}_d \geq 0$  and  $\lambda_{d+1} = 0$ . Then by Weyl's inequality, we should have  $\widehat{\lambda}_{d+1} = |\widehat{\lambda}_{d+1} - \lambda_{d+1}| \leq \|\widehat{B}^\top \widehat{B} - B^\top B\|_{\text{op}}$  (Chen et al., 2021, Lemma 2.2). Consequently, we have  $M_2 \leq \|\widehat{\Sigma}_\varepsilon^{-1/2}\|_{\text{op}}^2 \|\widehat{B}^\top \widehat{B} - B^\top B\|_{\text{op}}$ . Thus we have  $\|\widehat{M} - M\|_{\text{op}} \leq 2M_{11} + M_{12}$ . Next by Lemma 2, we should have

$$M_{11} \leq M'_{11} = 4 \|\widehat{\Sigma}_\varepsilon^{-1/2}\|_{\text{op}}^2 \|\widehat{B}^\top \widehat{B} - B^\top B\|_{\text{op}},$$

$$M_{12} \leq M'_{12} = 3 \|\Sigma_\varepsilon^{-1/2}\|_{\text{op}} \|\widehat{\Sigma}_\varepsilon^{-1/2} - \Sigma_\varepsilon^{-1/2}\|_{\text{op}},$$

as long as  $N > N_0$  for some sufficiently large constant  $N_0$ . Then by Lemma 2 and Lemma

5, we obtain the probabilistic upper bound for  $\|\widehat{H} - H\|_{\text{op}}$  as

$$\begin{aligned} P \left\{ \|\widehat{H} - H\|_{\text{op}} > \frac{4C_1\tau_{\max}}{\tau_{\min}^2} \left( \sqrt{\frac{K+d}{N}} + \frac{p}{N} \right) + \frac{3C_2\tau_{\max}}{\tau_{\min}^{3/2}} \left( \sqrt{\frac{K}{N}} + \frac{p}{N} \right) \right\} \\ \leq P \left\{ \|\widehat{B}^\top \widehat{B} - B^\top B\|_{\text{op}} > C_1 \left( \sqrt{\frac{K+d}{N}} + \frac{p}{N} \right) \right\} \\ + P \left\{ \|\widehat{\Sigma}_\varepsilon^{-1/2} - \Sigma_\varepsilon^{-1/2}\|_{\text{op}} > C_2 \left( \sqrt{\frac{K}{N}} + \frac{p}{N} \right) \right\} \leq C_3 \exp(-K). \end{aligned}$$

Consequently, we should have  $P \left[ \|\widehat{H} - H\|_{\text{op}} > C_4 \{ \sqrt{(K+d)/N} + (p/N) \} \right] \leq C_3 \exp(-K)$

holds as long as  $N > N_0$  for the same constant  $N_0$  as mentioned before.  $\square$

**Lemma 4.** (*Convergence Rate of  $\widehat{\Sigma}_\varepsilon$ .*) Assume the same conditions as Theorem 1. We then have  $\|\widehat{\Sigma}_\varepsilon - \Sigma_\varepsilon\|_{\text{op}} \leq C(\sqrt{K/N} + p/N)$  holds with a probability at least  $1 - 2 \exp(-K)$  as long as  $N > N_0$  for some sufficiently large constant  $N_0$ . Here  $C$  is a constant independent of  $K$ ,  $N$ , and  $N_0$ .

*Proof.* Recall that  $\widehat{\Sigma}_\varepsilon = N^{-1}(\mathbb{Y} - \mathbb{X}\widehat{B})^\top(\mathbb{Y} - \mathbb{X}\widehat{B}) = N^{-1}\mathcal{E}^\top(I_N - H_{\mathbb{X}})\mathcal{E} \in \mathbb{R}^{(K+1) \times (K+1)}$ , where  $\mathbb{Y} = (Y_i^{(0)}, \dots, Y_i^{(K)}) \in \mathbb{R}^{N \times (K+1)}$ , and  $H_{\mathbb{X}} = \mathbb{X}(\mathbb{X}^\top \mathbb{X})^{-1}\mathbb{X}$ . It follows that  $E(\widehat{\Sigma}_\varepsilon) = \{(N-p)/N\}\Sigma_\varepsilon$ . Therefore, we should have  $\|\widehat{\Sigma}_\varepsilon - \Sigma_\varepsilon\|_{\text{op}} \leq \|\widehat{\Sigma}_\varepsilon - E(\widehat{\Sigma}_\varepsilon)\|_{\text{op}} + \tau_{\max}p/N$ . Then it suffices to prove the following inequality as

$$P \left\{ \|\widehat{\Sigma}_\varepsilon - E(\widehat{\Sigma}_\varepsilon)\|_{\text{op}} > \delta \right\} \leq 2 \exp \left\{ 4K - C_1 N \min \left( \frac{\delta^2}{4C_{\text{sub}}^4}, \frac{\delta}{2C_{\text{sub}}} \right) \right\}. \quad (\text{C.8})$$

Recall that by Condition (C1),  $p/N \rightarrow 0$  as  $N \rightarrow \infty$ . Assume  $p/N \leq \sqrt{p/N}$  holds for any  $N > N_0$  with a sufficiently large constant  $N_0$ . Next, in order to apply (C.8), we set

$$\delta = 2C_{\text{sub}} \max \left( \sqrt{\frac{5K}{C_1 N}}, \frac{5K}{C_1 N} \right) = 2C_{\text{sub}} \sqrt{\frac{5K}{C_1 N}}.$$

It follows that  $P(\|\widehat{\Sigma}_\varepsilon - \Sigma_\varepsilon\|_{\text{op}} \geq C_2\sqrt{K/N}) \leq \exp(-K)$ , where  $C_2 = 2\sqrt{5}C_{\text{sub}}/\sqrt{C_1}$  is a constant. Consequently, taking  $C_3 = \max(C_2, \tau_{\min})$ , we can prove that  $\|\widehat{\Sigma}_\varepsilon - \Sigma_\varepsilon\|_{\text{op}} \leq C_3(\sqrt{K/N} + p/N)$  holds with probability at least  $1 - 2\exp(-K)$ . We then verify (C.8) as follows.

**PROOF OF (C.8).** We consider an  $\varepsilon$ -net  $\mathcal{U}$  on the unit sphere with  $\varepsilon = 1/3$ . It follows that  $|\mathcal{U}| \leq e^{2(K+1)}$ . We then have  $\|\widehat{\Sigma}_\varepsilon - E(\widehat{\Sigma}_\varepsilon)\|_{\text{op}} \leq 2 \max_{u,v \in \mathcal{U}} |u^\top \{\widehat{\Sigma}_\varepsilon - E(\widehat{\Sigma}_\varepsilon)\}v|$ . Note that  $\|u^\top \widehat{\Sigma}_\varepsilon v\|_{\psi_1} \leq \|N^{-1}u^\top \mathcal{E}^\top \mathcal{E}v\|_{\psi_1} \leq C_{\text{sub}}^2$ , which suggests that  $u^\top \widehat{\Sigma}_\varepsilon v$  is a sub-exponential variable. Then the Hanson-Wright inequality can be applied to obtain the upper bound as

$$\begin{aligned} P\left\{\|\widehat{\Sigma}_\varepsilon - E(\widehat{\Sigma}_\varepsilon)\|_{\text{op}} > \delta\right\} &\leq \sum_{u,v \in \mathcal{U}} P\left[|u^\top \{\widehat{\Sigma}_\varepsilon - E(\widehat{\Sigma}_\varepsilon)\}v| > \frac{\delta}{2}\right] \\ &\leq 2 \exp\left\{4K - C_1 N \min\left(\frac{\delta^2}{4C_{\text{sub}}^4}, \frac{\delta}{2C_{\text{sub}}}\right)\right\}. \end{aligned}$$

This concludes the entire proof. □

**Lemma 5.** (*Convergence Rate of  $\widehat{B}^\top \widehat{B}$* ) Assume the same conditions as Theorem 1. We then have  $\|\widehat{B}^\top \widehat{B} - B^\top B\|_{\text{op}} \leq C_1 \left\{ \sqrt{(K+d)/N} + p/N \right\}$  holds with a probability at least  $1 - C_2 \exp(-K)$  as long as  $N > N_0$  for some sufficiently large constant  $N_0$ .

*Proof.* Note that  $\|\widehat{B}^\top \widehat{B} - B^\top B\|_{\text{op}} \leq 2\|B^\top(\widehat{B} - B)\|_{\text{op}} + \|\widehat{B} - B\|_{\text{op}}^2$ , where the probabilistic upper bound for  $\|\widehat{B} - B\|_{\text{op}}^2$  can be obtained from Lemma 1. Therefore, it suffices to prove the following inequality

$$P\left\{\|B^\top(\widehat{B} - B)\|_{\text{op}} > \delta\right\} \leq C_1 \exp\left\{(K+d) - C_2 N \min(C_3^2 \delta^2, C_3 \delta)\right\} \quad (\text{C.9})$$

for some constants  $C_1, C_2$ , and  $C_3$  as long as  $N > N_0$  for a sufficiently large constant  $N_0$ .

To apply (C.9), we take

$$\delta = \frac{1}{C_3} \max \left( \sqrt{\frac{2(K+d)}{C_2 N}}, \frac{2(K+d)}{C_2 N} \right) = \frac{1}{C_3} \sqrt{\frac{2(K+d)}{C_2 N}},$$

where the last equation is due to Condition (C4) that  $(p/N) \leq \sqrt{p/N}$  as long as  $N > N_0$ .

It follows that

$$P \left( \|B^\top(\widehat{B} - B)\|_{\text{op}} > C_4 \sqrt{\frac{K+d}{N}} \right) \leq C_5 \exp(-K)$$

as long as  $N > N_0$ . Then by the conclusion of Lemma 1, we should have

$$\begin{aligned} & P \left( \|\widehat{B}^\top \widehat{B} - B^\top B\|_{\text{op}} > 2C_4 \sqrt{\frac{K+d}{N}} + \frac{C_6^2(p+K)}{N} \right) \\ & \leq P \left( \|B^\top(\widehat{B} - B)\|_{\text{op}} > C_4 \sqrt{\frac{K+d}{N}} \right) + P \left( \|\widehat{B} - B\|_{\text{op}} > C_6 \sqrt{\frac{p+K}{N}} \right) \\ & \leq C_5 \exp(-K) + C_7 \exp(-p). \end{aligned}$$

Consequently, we should have  $\|\widehat{B}^\top \widehat{B} - B^\top B\|_{\text{op}} \leq C_8 \left\{ \sqrt{(K+d)/N} + p/N \right\}$  holds with probability at least  $1 - C_9 \exp(-K)$ . This leads to the desired conclusion. Then it only suffices to prove (C.9).

**PROOF OF (C.9).** Note that  $\|B^\top(\widehat{B} - B)\|_{\text{op}} = \|N^{-1}B^\top \widehat{\Sigma}_\varepsilon^{-1} \mathbb{X}^\top \mathcal{E}\|_{\text{op}} \leq \|N^{-1}B^\top(\widehat{\Sigma}_\varepsilon^{-1} - \Sigma_\varepsilon^{-1})\mathbb{X}^\top \mathcal{E}\|_{\text{op}} + \|N^{-1}B^\top \Sigma_\varepsilon^{-1} \mathbb{X}^\top \mathcal{E}\|_{\text{op}}$ . We first study the term  $\|N^{-1}B^\top \Sigma_\varepsilon^{-1} \mathbb{X}^\top \mathcal{E}\|_{\text{op}}$ . Recall that  $\nu_k \in \mathbb{R}^{K+1}$  is the eigenvector corresponding to the  $k$ -th largest eigenvalue of  $B^\top B$ . We then consider two  $\varepsilon$ -nets  $\mathcal{U}$  and  $\mathcal{V}$  of the set  $\{\|x\| = 1 : x \in \mathcal{S}(\nu_k : 1 \leq k \leq d)\}$  and the unit sphere  $\mathcal{S}^K$  with  $\varepsilon = 1/3$ . It follows that  $|\mathcal{U}| \leq e^{2d}$  and  $|\mathcal{V}| \leq e^{2(K+1)}$ . Note that  $\|N^{-1}B^\top \Sigma_\varepsilon^{-1} \mathbb{X}^\top \mathcal{E}\|_{\text{op}} \leq 2 \sup_{u \in \mathcal{U}, v \in \mathcal{V}} |N^{-1}u^\top B^\top \Sigma_\varepsilon^{-1} \mathbb{X}^\top \mathcal{E}v|$ . Further write  $t = \Sigma_\varepsilon^{-1}Bu / \|\Sigma_\varepsilon^{-1}Bu\|$  with  $\|t\| = 1$ . Then  $\|N^{-1}B^\top \Sigma_\varepsilon^{-1} \mathbb{X}^\top \mathcal{E}\|_{\text{op}}$  can be further bounded by

$2\tau_{\max}\tau_{\min}^{-1} \sup_{u \in \mathcal{U}, v \in \mathcal{V}} N^{-1}t^\top \mathbb{X}^\top \mathcal{E}v$ . Subsequently, by Hanson-Wright's inequality, we have

$$\begin{aligned} P\left(\|N^{-1}B^\top \Sigma_\varepsilon^{-1} \mathbb{X}^\top \mathcal{E}\|_{\text{op}} > \delta\right) &\leq |\mathcal{U}||\mathcal{V}|P\left(N^{-1}t^\top \mathbb{X}^\top \mathcal{E}v > \frac{\tau_{\min}\delta}{2\tau_{\max}}\right) \\ &\leq \mathcal{C}_1 \exp\left\{2(K+d) - \mathcal{C}_2 N \min\left(\frac{\tau_{\min}^2 \delta^2}{4\tau_{\max}^2 C_{\text{sub}}^2}, \frac{\tau_{\min}\delta}{2\tau_{\max} C_{\text{sub}}}\right)\right\}, \end{aligned}$$

where  $\mathcal{C}_1 = 2e^2$ . By Lemma 4 that  $\|\widehat{\Sigma}_\varepsilon - \Sigma_\varepsilon\|_{\text{op}} \rightarrow_p 0$  as  $N \rightarrow \infty$ , it follows that  $\|N^{-1}B^\top(\widehat{\Sigma}_\varepsilon^{-1} - \Sigma_\varepsilon^{-1})\mathbb{X}^\top \mathcal{E}\|_{\text{op}} \leq \|N^{-1}B^\top \Sigma_\varepsilon^{-1} \mathbb{X}^\top \mathcal{E}\|_{\text{op}}$  holds almost surely as  $N \rightarrow \infty$ . Therefore, as long as  $N > N_0$  for some constant  $N_0$ , we should have

$$\begin{aligned} &P\left\{\|B^\top(\widehat{B} - B)\|_{\text{op}} > \delta\right\} \\ &\leq \mathcal{C}_3 \exp\left\{2(K+d) - \mathcal{C}_2 N \min\left(\frac{\tau_{\min}^2 \delta^2}{4\tau_{\max}^2 C_{\text{sub}}^2}, \frac{\tau_{\min}\delta}{2\tau_{\max} C_{\text{sub}}}\right)\right\} \end{aligned}$$

for some constants  $\mathcal{C}_2$  and  $\mathcal{C}_3$ . □

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