Adversarially Robust Estimate and Risk Analysis in Linear Regression

Yue Xing
Purdue University

Ruizhi Zhang
University of Nebraska-Lincoln

Guang Cheng
Purdue University

Abstract

Adversarially robust learning aims to design algorithms that are robust to small adversarial perturbations on input variables. Beyond the existing studies on the predictive performance to adversarial samples, our goal is to understand the statistical properties of adversarially robust estimates and analyze adversarial risk in the setup of linear regression models. By discovering the statistical minimax rate of convergence of adversarially robust estimators, we emphasize incorporating model information, e.g., sparsity, in adversarially robust learning. Further, we reveal an explicit connection between adversarial and standard estimates and propose a straightforward two-stage adversarial learning framework that facilitates utilizing model structure information to improve adversarial robustness. In theory, the consistency of the adversarially robust estimator is proven and its Bahadur representation is also developed for the statistical inference purpose. The proposed estimator converges in a sharp rate under either a low-dimensional or a sparse scenario. Moreover, our theory confirms two phenomena in adversarially robust learning: adversarial robustness hurts generalization, and unlabeled data improves generalization. In the end, we conduct numerical simulations to verify our theory.

1 INTRODUCTION

The development of machine/deep learning methods has led to breakthrough performance in various areas of application. However, some recent research revealed that these powerful but delicate models are vulnerable to random perturbation and adversarial attacks. For example, well-designed malicious adversarial input may induce wrong decision making when filtering junk emails or detecting malicious binary programs Zhang et al. (2017); Papernot et al. (2017). On the other hand, by studying adversarial samples, one can improve the adversarial robustness of algorithms in practice. The existing literature focused on generating adversarial samples, e.g., Papernot et al. (2016, 2017), adversarial training, e.g., Goodfellow et al. (2015); Kurakin et al. (2017); Wang et al. (2019), invariance/interpretability to detect adversarial samples, e.g., Xu et al. (2018); Tao et al. (2018); Ma et al. (2019); Etmann et al. (2019); Carmon et al. (2019) and theoretical studies of adversarially robust learning, e.g., Xu et al. (2009a,b); Xu and Mannor (2012). In particular, some studies Yin et al. (2019); Raghunathan et al. (2019) showed that adversarial training leads to a worse generalization performance, while Schmidt et al. (2018); Zhai et al. (2019); Najafi et al. (2019) argued that the adversarial robustness requires more (labeled/unlabeled) data to enhance generalization performance. Besides, the trade-off between standard performance and adversarial performance is carefully characterized in Zhang et al. (2019); Javanmard et al. (2020).

Adversarially robust estimation in the literature is often formulated as an empirical "min-max" problem: minimizing the empirical risk under the worst-case attack (which maximizes the loss) on the training data. Unfortunately, this formulation does not directly consider the structural information of the model such as sparsity and grouping, e.g., Shaham et al. (2015); Sinha et al. (2018); Wang et al. (2019), which may be utilized to improve adversarial robustness. The structure information is particularly needed in the high-dimensional regime, i.e., data dimension p is much larger than sample size n, where the empirical (adversarial) risk may no longer converge to the population risk Mei et al. (2018).

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The above concern raises two questions: (1) whether the statistical minimax[1] rate of the estimation error of *any* linear adversarial estimator will get changed given certain structure information for the standard model, and (2) whether we can utilize this information to get a better adversarially robust estimator.

Our contributions can be summarized as follows:

- In Section 3, by studying the form of adversarial risk, we figure out the minimax lower bound of estimation error, which reveals the potential to improve the estimation efficiency through utilizing model information.
- In Section 4, we design a two-stage adversarially robust learning framework that nicely connects adversarially robust estimation with standard estimation. The model structure information can be easily embedded into the standard estimator, and is further carried over to the adversarially robust estimate through this two-stage learning procedure. For statistical inference, we develop the Bahadur representation result (He and Shao, 1996) that implies the asymptotic normality of the proposed estimate under certain conditions. Besides, by analyzing the upper bound for the estimation error, we reveal the benefit of incorporating sparsity information into the adversarial estimation procedure, in which the estimator reaches the minimax optimal rate of convergence.
- Besides the above two main contributions, in Section 5, we utilize our theory to verify two arguments in adversarially robust learning: adversarially robust learning hurts generalization, and adversarial robustness can be improved using unlabeled data.

Two related works are appearing very recently. The first one Javanmard et al. (2020) mainly investigated the trade-off between adversarial risk and standard risk under an isotropic condition of the covariate. Rather, we focus on improving adversarial robustness by utilizing prior knowledge on the model and studying statistical properties of the adversarially robust estimate itself, in contrast with the generalization studies by Schmidt et al. (2018); Zhang et al. (2019); Zhai et al. (2019); Najafi et al. (2019). Another recent work Dan et al. (2020) studied the sharp statistical bound in adversarially robust *classification*. In the regression setup, our theorems reveal that an adversarially robust estimate is different from a standard estimate even in the rate of convergence: for noiseless case, standard model estimators can exactly recover the correct model, but the lower bound for adversarially robust model is always nonzero. Our lower bound for sparse model is also new. **Notation.** We use boldface font for vectors, e.g., $\mathbf{x}$, and capital letters for matrices, e.g., $\mathbf{A}$. The ℓ_2 norm of a vector $\mathbf{u}$ is denoted as $\|\mathbf{u}\|_2$ (or $\|\mathbf{u}\|$ for simplicity). The $p\times p$ identity matrix is denoted by $\mathbf{I}_p$.The induced spectral norm of a matrix $\mathbf{A}\in\mathbb{R}^{p\times p}$ is denoted by $\|\mathbf{A}\|$, i.e., $\|\mathbf{A}\| := \sup\{\|\mathbf{A}\mathbf{x}\| : \|\mathbf{x}\| = 1\}$. We denote by $\lambda_i(\mathbf{A}), i\in\{1,2,\cdots,p\}$, its eigenvalues in decreasing order. For a symmetric matrix $\mathbf{A}$, denote $\|\mathbf{x}\|_{\mathbf{A}}^2 = \mathbf{x}^\top\mathbf{A}\mathbf{x}$. For two matrices $\mathbf{A},\mathbf{B}$, we denote $\langle\mathbf{A},\mathbf{B}\rangle_F$ as the Frobenius inner product, which is the sum of component-wise inner product of two matrices. The Frobenius norm of $\mathbf{A}$ is denoted by $\|\mathbf{A}\|_F$.

2 PROPERTIES OF ADVERSARIAL RISK

Consider a linear regression model

$$y = \mathbf{x}^\top\theta_0 + \epsilon, \tag{1}$$

where $\mathbb{E}\mathbf{x} = \mathbf{0}$, $\mathrm{Var}(\mathbf{x}) = \Sigma$, and ϵ is a noise term (independent of $\mathbf{x}$) with $\mathbb{E}(\epsilon) = 0$ and $\mathrm{Var}(\epsilon) = \sigma^2$. Throughout this paper, we assume that $\mathbf{x}\in\mathbb{R}^p$ follows a p-dimensional Gaussian distribution and Σ has a bounded largest eigenvalue (away from ∞) and a bounded smallest eigenvalue (away from 0) as p increases. The noise variance σ^2 and $\|\theta_0\|$ are allowed to diverge in p, and the signal-to-noise ratio $\|\theta_0\|_\Sigma/\sigma$ needs to be large enough, say bounded away from 0.

The (population) adversarial risk is defined as follows

$$\begin{aligned} R_0(\theta,\delta) &:= \mathbb{E}_{\mathbf{x}}\max_{\|\mathbf{x}^*-\mathbf{x}\|_2\le\delta}\left[((\mathbf{x}^*)^\top\theta - \mathbf{x}^\top\theta_0)^2\right] \qquad (2)\\ &= \|\theta-\theta_0\|_\Sigma^2 + 2\delta c_0\|\theta-\theta_0\|_\Sigma\|\theta\| + \delta^2\|\theta\|^2, \end{aligned}$$

where $c_0 := \sqrt{2/\pi}$. The corresponding minimizer of (2) is denoted by $\theta^*(\delta)$, i.e.,

$$\theta^*(\delta) := \arg\min_\theta R_0(\theta,\delta).$$

We may just use θ^* when no confusion arises.

In the proposition below, we study the shape of R_0, and establish an analytical form of $\theta^*(\delta)$, which suggests the construction of adversarially robust estimator (to be specified later). Define

$$\theta(\lambda) := (\Sigma+\lambda\mathbf{I}_p)^{-1}\Sigma\theta_0,$$

and two thresholds of δ:

$$\delta_1 = \frac{c_0\|\theta_0\|}{\|\theta_0\|_{\Sigma^{-1}}} \text{ and } \delta_2 = \frac{\|\theta_0\|_{\Sigma^2}}{c_0\|\theta_0\|_\Sigma}.$$

[1] In this paper, "min-max" refers to the optimization problem considered in adversarially robust learning, while "minimax" refers to the statistical lower bound on the estimation error.

Proposition 1. *The risk $R_0(\theta, \delta)$ is a convex function w.r.t. θ, and has positive definite Hessian for any $\theta \neq \mathbf{0}, \theta \neq \theta_0$. In addition, the global minimizer of $R_0(\theta, \delta)$ can be written as*

$$\theta^*(\delta) := \theta(\lambda^*(\delta)) \tag{3}$$

where $\lambda^*(\delta)$ depends on $(\delta, \Sigma, \theta_0)$. (1) If $\delta \leq \delta_1$, then $\lambda^*(\delta) = 0$ such that $\theta^* = \theta_0$, and there is no stationary point for $R_0(\theta, \delta)$. (2) If $\delta \geq \delta_2$, then $\lambda^*(\delta) = \infty$ such that $\theta^* = \mathbf{0}$, and there is no stationary point for $R_0(\theta, \delta)$. (3) If $\delta_1 < \delta < \delta_2$, then there is a unique stationary point $\theta(\lambda^*(\delta))$ of $R_0(\theta, \delta)$, which is the global optimum. Here $\lambda^*(\delta)$ is the solution of the following equation w.r.t. λ:

$$\lambda\left(1 + \frac{\delta c_0 \|\theta(\lambda)\|}{\|\theta(\lambda) - \theta_0\|_\Sigma}\right) = \delta c_0 \frac{\|\theta(\lambda) - \theta_0\|_\Sigma}{\|\theta(\lambda)\|} + \delta^2. \tag{4}$$

The proof of Proposition 1 is in Appendix B.

For a general Σ, it is hard to obtain an explicit solution for θ^* by solving (4). However, when $\Sigma = \mathbf{I}_p$, one can write down the explicit formula of $\theta^*(\delta)$, which is actually a re-scaled version of θ_0. In this case, $\delta_1 = c_0$, $\delta_2 = 1/c_0$, and $\lambda^*(\delta) = (\delta^2 - \delta c_0)/(1 - \delta c_0)$ when $\delta \in (\delta_1, \delta_2)$. Moreover, the adversarial risk and standard risk of the adversarially robust model become

$$R_0(\theta^*(\delta), \delta) = \begin{cases} \delta^2 \|\theta_0\|^2 & \delta \leq c_0 \\ \frac{\delta^2(1-c_0^2)}{\delta^2 + 1 - 2\delta c_0} \|\theta_0\|^2 & c_0 \leq \delta \leq 1/c_0 \\ \|\theta_0\|^2 & \delta \geq 1/c_0 \end{cases}$$

$$R_0(\theta^*(\delta), 0) = \begin{cases} 0 & \delta \leq c_0 \\ \frac{\delta^2(\delta - c_0)^2}{(\delta^2 + 1 - 2\delta c_0)^2} \|\theta_0\|^2 & c_0 \leq \delta \leq 1/c_0 \\ \|\theta_0\|^2 & \delta \geq 1/c_0 \end{cases}.$$

Similar as $R_0(\theta^*(\delta), \delta)$, the standard risk of the adversarially robust model $R_0(\theta^*(\delta), 0)$ also increases as δ and reaches the same level as $R_0(\theta^*(\delta), \delta)$ when $\delta > 1/c_0$; see Figure 1 below. This result echoes with Javanmard et al. (2020); Raghunathan et al. (2019) that the adversarially robust model leads to a worse performance when testing data is un-corrupted.

Remark 1. *Besides adversarial risk, we define adversarial* **prediction** *risk as*

$$R(\theta, \delta) := \mathbb{E}_{\mathbf{x}, y} \max_{\|\mathbf{x}^* - \mathbf{x}\| \leq \delta} \left[\left((\mathbf{x}^*)^\top \theta - y\right)^2\right].$$

The properties of R are similar as R_0 when $\epsilon \sim N(0, \sigma^2)$, and we focus on R_0 in this paper.

3 MINIMAX LOWER BOUND

In this section, through figuring out the minimax lower bounds of the estimation error, we argue that it is essential to incorporate sparsity information of (θ_0, Σ) in $(\widehat{\theta}_0, \widehat{\Sigma})$ in sparse model. For minimax lower bound in standard learning problems, studies can be found in Dicker et al. (2016); Mourtada (2019) for dense case and Verzelen (2010); Ye and Zhang (2010); Raskutti et al. (2011) for sparse case.

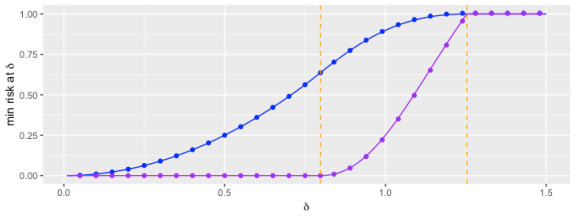

Figure 1: $R_0(\theta^*(\delta), \delta)$ and $R_0(\theta^*(\delta), 0)$ correspond to blue and purple curves, respectively. Here, $\Sigma = \mathbf{I}_p$ and $\|\theta_0\|^2 = 1$. Dashed lines represent the two thresholds $\delta_1 = c_0$ (left) and $\delta_2 = 1/c_0$ (right). Curve: theoretical values. Dots: simulations with $p = 10$ and $n = 10000$.

The following two theorems present the lower bounds of $\mathbb{E}\|\hat{\theta} - \theta^*\|^2$ for dense/sparse models respectively.

Theorem 1. *When $\sigma/\|\theta_0\| < \infty$, $\sigma^2 p/(\|\theta_0\|^2 n) \to 0$, and $(p \log^2 n)/n \to 0$, if $\|\theta_0\| \leq R$, $0 < c_1 \leq \lambda_{\min}(\Sigma) \leq \lambda_{\max}(\Sigma) \leq c_2 < \infty$, $\delta > 0$, then there exists some constant $\delta > 0$ such that*

$$\inf_{\widehat{\theta}} \sup_{\Sigma, \theta_0, \delta} \mathbb{E}\|\widehat{\theta} - \theta^*\|^2 = \Omega\left(\frac{p\sigma^2}{n} \vee \frac{pR^2}{n}\right),$$

The estimator $\widehat{\theta}$ refers to any estimator $\widehat{\theta}(X, Y, \delta)$, and θ^* is a function of $(\theta_0, \Sigma, \delta)$.

For sparse model, the sparsity of θ_0 is directly controlled through the size of active set of θ_0. In terms of the sparsity of Σ, we follow Cai et al. (2010) to consider a family of sparse covariance matrix as follows:

$$\mathcal{F}_\alpha = \Big\{\Sigma : \max_j \sum_i \{|\sigma_{ij}| : |i - j| > k\} \leq M k^{-\alpha} \ \forall k, \\ \lambda_{\max}(\Sigma) \leq M_0, \ \lambda_{\min}(\Sigma) \geq m_0 > 0\Big\}.$$

Theorem 2. *When $\sigma/\|\theta_0\| < \infty$, if $\|\theta_0\| \leq R$ and $\|\theta_0\|_0 \leq s$, $0 < c_1 \leq \lambda_{\min}(\Sigma) \leq \lambda_{\max}(\Sigma) \leq c_2 < \infty$, $\delta > 0$, then for any $0 < s < p$ and $\alpha > 0$, there exists some constant $\delta > 0$ such that*

$$\inf_{\widehat{\theta}} \sup_{\Sigma \in \mathcal{F}_\alpha, \theta_0, \delta} \mathbb{E}\|\widehat{\theta} - \theta^*\|^2 \\ = \Omega\left(s\sigma^2 \frac{1 + \log(p/s)}{n} \vee R^2 n^{-\frac{2\alpha}{2\alpha+1}}\right).$$

The proof of the above two theorems utilizes some tools in Mourtada (2019); Verzelen (2010); Cai et al.

(2010). A difficulty compared with existing literature in standard learning is that the relationship between θ_0 and θ^* is nonlinear, and θ^* further depends on Σ. The details are in Appendix C.

To compare Theorem 1 and 2, the lower bound for sparse model is much smaller than the one for dense model. This indicates a potential improvement for adversarially robust estimators if the algorithm can utilize the sparsity information (if there is). As discussed in Belkin et al. (2019); Xing et al. (2020), for the high-dimensional model, if we do not consider the sparsity information, the resulting model is not consistent in both standard and adversarially robust learning problems.

To compare with standard learning problem, the results in Theorem 1 and 2 are different from those in standard learning. Such a difference implies it is hard to train adversarially robust models. In standard learning, when $\sigma^2 = 0$, the lower bound is exactly zero since some estimators of θ_0 can achieve zero estimation error. However, when $\delta > 0$, even if $\sigma^2 = 0$, the lower bound is not zero.

Remark 2. *Similar to our results, Dan et al. (2020) provided a minimax lower bound of generalization error under the adversarially robust classification setup. However, they only considered the dense case corresponding to our Theorem 1, but not for the sparse case.*

4 TWO-STAGE ADVERSARIAL ROBUST ESTIMATOR

In this section, we demonstrate a two-stage procedure for constructing adversarially robust estimators based on the explicit relation pointed out in the previous section. This relation allows us to incorporate specific model information, such as sparsity, into adversarially robust estimates through standard estimates. The idea of the proposed method is similar to the estimators in Dan et al. (2020); Carmon et al. (2019) and the method is straightforward. We emphasize that such a simple two-stage method is powerful enough to achieve minimax optimal.

4.1 Estimator description

There are two stages in the proposed method. In the first stage, consistent estimators of the true parameter θ_0, denoted as $\widehat{\theta}_0$, and matrix Σ, denoted as $\widehat{\Sigma}$, are obtained from standard statistical procedures. In the second stage, the robust estimator of θ^*, which minimizes the adversarial risk, is constructed as follows:

$$\widehat{\theta}(\delta) := \widehat{\theta}(\widehat{\lambda}^*(\delta)) := (\widehat{\Sigma} + \widehat{\lambda}^*(\delta)\mathbf{I}_p)^{-1}\widehat{\Sigma}\widehat{\theta}_0, \tag{5}$$

where $\widehat{\lambda}^*(\delta)$ is a plug-in estimate of $\lambda^*(\delta)$ depending on $\widehat{\theta}_0$ and $\widehat{\Sigma}$. Alternatively speaking, $\widehat{\theta}(\delta)$ may be obtained by minimizing an empirical version of (2):

$$\begin{aligned}\widehat{R}_0(\theta,\delta) &:= \widehat{R}_0(\theta,\widehat{\theta}_0,\widehat{\Sigma},\delta) \\ &= \|\theta-\widehat{\theta}_0\|_{\widehat{\Sigma}}^2 + 2\delta c_0\|\theta-\widehat{\theta}_0\|_{\widehat{\Sigma}}\|\theta\| + \|\theta\|^2.\end{aligned} \tag{6}$$

According to the proof of Proposition 1, the empirical risk $\widehat{R}_0(\theta,\delta)$ shares similar properties as adversarial risk $R_0(\theta,\delta)$ in Proposition 1. We may simply use $\widehat{\theta}$ instead of $\widehat{\theta}(\delta)$ when no confusion arises.

4.2 Consistency

We first show that for any level of attack δ, the adversarial excess risk converges to zero, i.e., (7), as long as the standard estimates of θ_0 and Σ are consistent with proper rates and p does not grow too fast. Next, combining with the convex properties of R_0, the upper bound in (7) implies the consistency of $\widehat{\theta}$ in estimating θ^*; see Theorem 4. This consistency result will be used in deriving the generalization error in Theorem 5 later.

Theorem 3. *For any consistent estimators $\widehat{\theta}_0$ and $\widehat{\Sigma}$, with probability tending to 1,*

$$\begin{aligned}&\sup_{\delta\geq 0}\left|R_0(\theta^*(\delta),\delta) - R_0(\widehat{\theta}(\delta),\delta)\right| \\ =\ & O\left(\|\widehat{\theta}_0-\theta_0\|\|\theta_0\|\right) + O\left(\|\theta_0\|^2\sqrt{\|\widehat{\Sigma}-\Sigma\|}\right).\end{aligned} \tag{7}$$

To illustrate Theorem 3 in details, we use $\widehat{\theta}_0 = (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{y}$ and $\widehat{\Sigma} = \mathbf{X}^\top\mathbf{X}/n$ to construct $\widehat{\theta}$. Based on Theorem 2 in Hsu et al. (2012) (taking ridge penalty as zero) and Theorem 3, with probability tending to 1, we have

$$\frac{R_0(\widehat{\theta},\delta) - R_0(\theta^*,\delta)}{\|\theta_0\|_\Sigma^2 + \sigma^2} = o(1), \tag{8}$$

which implies the adversarial excess risk of $\widehat{\theta}$ converges to zero as long as $(p\log n)/n \to 0$.

The proof of Theorem 3 is postponed to Appendix C. We also postpone an analog of Theorem 3 for the adversarial prediction risk R to Appendix A (for the statement) and C (for the proof). Note that the upper bound in (7) is not tight, but enough to justify the adversarial risk consistency of $\widehat{\theta}(\delta)$.

We next use an example to illustrate how sparsity information can be utilized in the proposed framework.

Example 1 (Sparse Standard Estimates)**.** *Assume matrix belongs to the family $\mathcal{F}_\alpha$, then using the sparse estimator $\widehat{\Sigma}$ in Cai et al. (2010), we have*

$$\mathbb{E}\|\widehat{\Sigma}-\Sigma\|^2 = O\left(n^{-\frac{2\alpha}{2\alpha+1}} + \frac{\log p}{n}\right).$$

Assume $\widehat{\theta}_0$ is the LASSO estimate obtained under proper penalization. Denote $s < n$ as the number of nonzero coefficients in θ_0. When $\mathbf{x}$ follows Gaussian and the noise ϵ satisfies $\mathbb{E}\exp\{t\epsilon^2\} < \infty$ for some $t > 0$, based on Bickel et al. (2009); Jeng et al. (2018), we have with probability tending to 1,

$$\|\widehat{\theta}_0 - \theta_0\| = O\left(\sigma\sqrt{\frac{s\log p}{n}}\right).$$

Therefore, (8) holds under weaker conditions, say $(\sigma s\log p)/n \to 0$ and $(\log p)/n \to 0$. On the other hand, we point out that $\widehat{\theta}$ (θ^*) does not inherit the sparsity of $\widehat{\theta}_0$ (θ_0) according to (5) and (3).

4.3 Bahadur representation and convergence rate

We next study statistical properties of the adversarially robust estimator $\widehat{\theta}$ by establishing its Bahadur representation He and Shao (1996) that implies asymptotic normality in some cases.

Theorem 4. *Assume both $\|\widehat{\theta}_0-\theta_0\|/\|\theta_0\|$ and $\|\widehat{\Sigma}-\Sigma\|$ converge to zero in probability.*

(1) If $\delta \in (\delta_1, \delta_2)$, then $\widehat{\theta} - \theta^*$ is a linear combination of $\widehat{\theta}_0 - \theta_0$ and $\widehat{\Sigma} - \Sigma$ in the main term:

$$\begin{aligned}&\widehat{\theta} - \theta^*\\ =\ &\mathbf{M}_1(\theta^*, \theta_0, \Sigma)(\widehat{\theta}_0 - \theta_0)\\ &+(\theta^* - \theta_0)^\top(\widehat{\Sigma} - \Sigma)(\theta^* - \theta_0)\mathbf{M}_2(\theta^*, \theta_0, \Sigma)\\ &+\mathbf{M}_3(\theta^*, \theta_0, \Sigma)(\widehat{\Sigma} - \Sigma)(\theta^* - \theta_0) + o_p(\|\widehat{\theta} - \theta^*\|),\end{aligned}$$

where $\mathbf{M}_1$, $\mathbf{M}_2$, and $\mathbf{M}_3$ are functions of $(\delta, \theta_0, \Sigma, \theta^*)$, and detailed formulas are postponed to Appendix A.

(2) If $\delta < \delta_1$, then $\widehat{\theta} - \theta^* = \widehat{\theta}_0 - \theta_0 + o_p(\|\widehat{\Sigma} - \Sigma\|) + o_p(\|\widehat{\theta}_0 - \theta_0\|)$.

(3) If $\delta > \delta_2$, we have $\widehat{\theta} - \theta^* = o_p(\|\widehat{\Sigma} - \Sigma\|) + o_p(\|\widehat{\theta}_0 - \theta_0\|)$.

The proof for Theorem 4 is postponed to Appendix C. We next illustrate how the Bahadur representation can be used to infer the asymptotic normality of $\widehat{\theta}$.

Example 2 (Least Square Estimate)**.** *Consider the least square estimate (OLS)*

$$\widehat{\theta}_0 = (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{y}, \qquad \widehat{\Sigma} = \frac{1}{n}\mathbf{X}^\top\mathbf{X}.$$

It is trivial to see that $\widehat{\theta} = \mathbf{0}$ in probability when $\delta > \delta_2$ based on Theorems 1 and 4. When $\delta \in [0, \delta_1)$, the asymptotic normality of $\sqrt{n/p}(\widehat{\theta} - \theta^*)$ trivially follows the fact that $\widehat{\theta} = \widehat{\theta}_0$ in probability and $\theta^* = \theta_0$. When $\delta \in (\delta_1, \delta_2)$,

$$\widehat{\theta} - \theta^* = \mathbf{m}_1 + \mathbf{m}_2 + \mathbf{m}_3 + o_p(\|\widehat{\theta} - \theta^*\|),$$

where

$$\begin{aligned}\mathbf{m}_1 &= \mathbf{M}_1\left[\frac{\Sigma^{-1}}{n}\sum_{i=1}^n x_i\epsilon_i\right],\\ \mathbf{m}_2 &= \mathbf{M}_2\left[\frac{1}{n}\sum_{i=1}^n(\theta^* - \theta_0)^\top(x_ix_i^\top - \Sigma)(\theta^* - \theta_0)\right],\\ \mathbf{m}_3 &= \mathbf{M}_3\left[\frac{1}{n}\sum_{i=1}^n(x_ix_i^\top - \Sigma)(\theta^* - \theta_0)\right].\end{aligned}$$

If p is fixed and $\delta \in (\delta_1, \delta_2)$, then $\sqrt{n}(\widehat{\theta} - \theta^*)$ asymptotically converges to a zero-mean Gaussian. For inference purpose, we need to estimate $Var(\widehat{\theta})$. Since $x_i\epsilon_i$ and $(x_ix_i^\top - \Sigma)$ in $\mathbf{m}_1, \mathbf{m}_2, \mathbf{m}_3$ are both i.i.d. random variables, and x_i follows Gaussian distribution, one can figure out the variance of $\widehat{\theta}$. As a result, replacing $(\theta^*, \theta_0, \Sigma, \delta)$ with $(\widehat{\theta}, \widehat{\theta}_0, \widehat{\Sigma}, \delta)$, one can obtain an estimate of $Var(\widehat{\theta})$. As a side remark, if p diverges in n, we have $\|\widehat{\theta} - \theta^*\|/\sqrt{\|\theta_0\|_\Sigma^2 + \sigma^2} = O_p(\sqrt{p/n})$.

Furthermore, when using dense/sparse estimators of (θ_0, Σ), our proposed two-stage estimator achieves minimax rate optimal in dense/sparse models respectively. The upper bound of $\mathbb{E}\|\widehat{\theta} - \theta^*\|^2$ can be developed from Theorem 4:

Corollary 1. *Denote $v^2 = \|\theta_0\|_\Sigma^2 + \sigma^2$. When $(p\log n)/n \to 0$, $\widehat{\theta}_0$ is the OLS estimate, and $\widehat{\Sigma}$ is the sample matrix, we have*

$$\mathbb{E}\|\widehat{\theta} - \theta^*\|^2 = \Theta\left(\frac{v^2p}{n}\right).$$

Combining upper bound result in the above corollary and lower bound in Theorem 1 together, one can see that using OLS estimate as $\widehat{\theta}_0$ and sample covariance matrix as $\widehat{\Sigma}$ in the two-stage method reaches minimax optimal in dense models. Besides, as stated in the following result, using the sparse estimators in Example 1, our proposed two-stage estimator reaches the minimax rate as in Theorem 2:

Corollary 2. *For sparse models, when $(\log p)/n \to 0$, $\sigma^2(s\log p)/(n\|\theta_0\|^2) \to 0$, $\widehat{\theta}_0$ is the LASSO estimate and $\widehat{\Sigma}$ is the sparse covariance estimator in Cai et al. (2010), it satisfies that*

$$\mathbb{E}\|\widehat{\theta} - \theta^*\|^2 = O\left(\frac{s\sigma^2\log p}{n} + v^2n^{-\frac{2\alpha}{2\alpha+1}}\right).$$

If $\log_s(p) > 1 + c_s$ for some constant $c_s > 0$, the above results are minimax-optimal.

5 PROPERTIES OF THE METHOD

This section provides additional properties of the proposed method beyond the consistency and convergence rate. In particular, we use theorems associated

with our method to verify two arguments in the existing literature: (1) generalization of adversarially robust learning is worse than standard learning; (2) one can improve the generalization of adversarially robust learning through utilizing extra unlabeled data.

5.1 Adversarial learning hurts generalization

We study the generalization of our proposed estimator. From the minimax lower bound theorems in Section 3, it is easy to see that the excess risk when $\delta > 0$ may converge in a slower rate than the one when $\epsilon = 0$. Besides this, we work on the multiplicative constants of excess risk and generalization error and reveal that those constants are larger when $\epsilon > 0$ as well.

Based on Theorem 4, the generalization error (9) and the estimation error of minimal adversarial risk (10) can be decomposed as follows:

$$\begin{aligned} & R_0(\widehat{\theta},\delta) - \widehat{R}_0(\widehat{\theta},\delta) \qquad (9)\\ = \;& e_{1,\Sigma}(\widehat{\Sigma},\delta) + e_{1,\theta_0}(\widehat{\theta}_0,\delta) + o_p(R_0(\widehat{\theta},\delta) - \widehat{R}_0(\widehat{\theta},\delta)),\\ & R_0(\theta^*,\delta) - \widehat{R}_0(\widehat{\theta},\delta) \qquad (10)\\ = \;& e_{2,\Sigma}(\widehat{\Sigma},\delta) + e_{2,\theta_0}(\widehat{\theta}_0,\delta) + o_p(R_0(\theta^*,\delta) - \widehat{R}_0(\widehat{\theta},\delta)). \end{aligned}$$

The term e_{j,θ_0} ($e_{j,\Sigma}$) represents the error component that is *only* caused by the estimation error of $\widehat{\theta}_0$ ($\widehat{\Sigma}$). We next characterizes the forms of $e_{j,\Sigma}$ and e_{j,θ_0} with precise multiplicative constants.

Theorem 5. *Under the same conditions as in Proposition 1, if $\|\widehat{\Sigma}-\Sigma\| \to 0$ and $\|\widehat{\theta}_0-\theta_0\|/\|\theta_0\| \to 0$, then when $\delta < \delta_1$,*

$$\begin{aligned} e_{1,\Sigma}(\widehat{\Sigma},\delta) &= o_p(\|\widehat{\Sigma}-\Sigma\|\|\theta_0\|^2),\\ e_{1,\theta_0}(\widehat{\theta}_0,\delta) &= \|\widehat{\theta}_0-\theta_0\|_\Sigma^2 + 2c_0\delta\|\theta_0\|\|\widehat{\theta}_0-\theta_0\|_\Sigma\\ &\quad + o_p(\|\widehat{\theta}_0-\theta_0\|\|\theta_0\|),\\ e_{2,\Sigma}(\widehat{\Sigma},\delta) &= o_p(\|\widehat{\Sigma}-\Sigma\|\|\theta_0\|^2),\\ e_{2,\theta_0}(\widehat{\theta}_0,\delta) &= -2\delta^2\theta_0^\top(\widehat{\theta}_0-\theta_0) + o_p(\|\widehat{\theta}_0-\theta_0\|\|\theta_0\|). \end{aligned}$$

If $\delta > \delta_1$, we have

$$\begin{aligned} e_{1,\Sigma}(\widehat{\Sigma},\delta) &= -c_\Sigma(\delta)\frac{(\theta^*-\theta_0)^\top(\widehat{\Sigma}-\Sigma)(\theta^*-\theta_0)}{\|\theta^*-\theta_0\|_\Sigma^2}\\ &\quad + o_p(\|\widehat{\Sigma}-\Sigma\|\|\theta_0\|^2),\\ e_{1,\theta_0}(\widehat{\theta}_0,\delta) &= 2c_{\theta_0}(\delta)\frac{(\widehat{\theta}_0-\theta_0)^\top\Sigma(\theta^*-\theta_0)}{\|\theta^*-\theta_0\|_\Sigma}\\ &\quad + o_p(\|\widehat{\theta}_0-\theta_0\|\|\theta_0\|),\\ e_{2,\Sigma}(\widehat{\Sigma},\delta) &= e_{1,\Sigma}(\widehat{\Sigma},\delta) + o_p(\|\widehat{\Sigma}-\Sigma\|\|\theta_0\|^2),\\ e_{2,\theta_0}(\widehat{\theta}_0,\delta) &= e_{1,\theta_0}(\widehat{\theta}_0,\delta) + + o_p(\|\widehat{\theta}_0-\theta_0\|\|\theta_0\|). \end{aligned}$$

where the multiplicative constants $c_\Sigma(\delta) := \|\theta^*-\theta_0\|_\Sigma^2 + \delta c_0\|\theta^*\|\|\theta^*-\theta_0\|_\Sigma$ and $c_{\theta_0}(\delta) := \|\theta^*-\theta_0\|_\Sigma + \delta c_0\|\theta^*\|$ are monotone increasing functions in δ. Recall that θ^* is a function of δ.

The proof of Theorem 5 is postponed to Appendix C.

To better understand Theorem 5, we plot the changes of $|e_{1,\theta_0}|$, $|e_{1,\Sigma}|$, and $|e_{2,\theta_0}|$ w.r.t. δ by assuming $\Sigma = \mathbf{I}_p$ in Figure 2. In the left plot, $|e_{1,\theta_0}|$ firstly increases in δ linearly until $\delta = \delta_1$, then jumps to the second regime and grows until it converges to $2|(\widehat{\theta}_0-\theta_0)^\top\Sigma\theta_0|$ after $\delta > \delta_2$. In the middle plot, $|e_{1,\Sigma}|$ is almost zero when $\delta < \delta_1$, then increases when $\delta \in (\delta_1,\delta_2)$ and finally converges when $\delta > \delta_2$. And, $|e_{2,\Sigma}|$ shares a similar pattern. The pattern of $|e_{2,\theta_0}|$ is similar as $|e_{1,\theta_0}|$ except that it smoothly transits into the second regime, as shown in the right plot. The empirical and theoretical curves match very well in Figure 2.

5.2 Reducing estimation error through additional unlabeled data

Unlabeled data is commonly used in semi-supervised learning, e.g. locally-weighted nearest neighbors algorithm (Cannings et al., 2020). Besides, in the context of adversarially robust learning, some studies also observed the benefits of using extra unlabeled data (Raghunathan et al., 2019).

We study the effect of extra unlabeled data on the minimax lower bounds and the upper bounds of our proposed method under different scenarios. With the existence of extra unlabeled data, the minimax lower bounds become smaller. Besides, these data also help reduce the upper bounds by improving the accuracy of $\widehat{\Sigma}$:

Theorem 6. *Under the conditions in Theorem 1, if there are extra n_1 samples of unlabeled data, the lower bound becomes $\Omega((p\sigma^2/n) \vee (pR^2/(n+n_1)))$.*

Under the conditions in Theorem 2, if there are extra n_1 samples of unlabeled data, the lower bound becomes

$$\Omega\left(s\sigma^2\frac{\log(p/s)}{n} \vee R^2(n+n_1)^{-\frac{2\alpha}{2\alpha+1}}\right).$$

In terms of the upper bounds, since the estimation of $\widehat{\Sigma}$ is only related to $\mathbf{x}$, one can directly utilize these extra unlabeled data into the two-stage framework. The following result is extended from Theorem 4:

Corollary 3. *Under the conditions in Corollary 1, if there are extra n_1 samples of unlabeled data, the upper bound becomes $O((p\sigma^2/n) \vee (pR^2/(n+n_1)))$.*

Under the conditions in Corollary 2, if there are extra n_1 samples of unlabeled data, the bound becomes

$$O\left(s\sigma^2\frac{\log(p/s)}{n} \vee R^2(n+n_1)^{-\frac{2\alpha}{2\alpha+1}}\right).$$

To summarize, as both lower bounds and upper bounds are reduced, it is essential to utilize extra un-

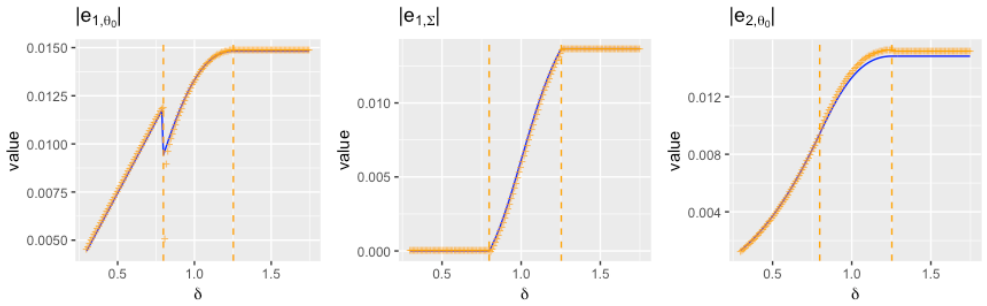

Figure 2: The value of $|e_{1,\theta_0}|$, $|e_{1,\Sigma}|$, and $|e_{2,\theta_0}|$ as functions of δ. Assume $\|\theta_0\| = 1$, $\Sigma = \mathbf{I}_p$. Blue curve is obtained from Theorem 5 given $(\widehat{\theta}_0, \widehat{\Sigma})$. Orange points are obtained from simulation. $n = 1000$, $\sigma^2 = 1$. The two vertical dashed lines in each figure represent δ_1 and δ_2.

labeled data for adversarially robust learning. A numerical illustration is also given in the next section of the experiments.

6 NUMERICAL EXPERIMENTS

In numerical experiments, we consider Example 2, and adopt LASSO/sparse estimators in the first stage to improve adversarial robustness.

We consider the following specifications of (θ_0, Σ): θ_0 is randomly generated from $\partial B(0,1)$, the sphere of a $\mathcal{L}_2$ ball; the diagonal elements in Σ are $\Sigma_{ii} = 2r + |\tau_i|$, where τ_i's follow i.i.d. standard Gaussian, and the other elements in Σ are r. Under this design of Σ, coordinates of $\mathbf{x}$ are correlated with each other, and the smallest and largest eigenvalues are within a reasonable range as p increases. Each experiment was repeated 500 times with $\sigma^2 = 1$. Define $\widehat{\Sigma} = \mathbf{X}^\top \mathbf{X}/n$ for non-sparse Σ.

Empirical coverage when p is fixed. As mentioned in Example 2, $\sqrt{n}(\widehat{\theta} - \theta^*)$ asymptotically converges to a zero-mean Gaussian when $\delta < \delta_2$. We use empirical coverage to verify this statement. In this experiment, $\theta_0 = (1,2)^\top$ and $\Sigma_{ii} = i$ for $i = 1, 2$ with $\Sigma_{12} = 0.5$. For each δ, we repeat the experiment of estimating θ^* for 1000 times using 1000 samples, and calculate the 95% empirical coverage for θ_1^* and θ_2^*. In Figure 3, when $\delta < 1.9$, the magnitude of θ_i^*'s are away from zero, and the empirical coverage for both θ_i^*'s are close to 0.95. When $\delta > 1.9$, θ_i^*'s are almost zero, and the corresponding empirical coverages are a little bit away from 0.95.

Sparse coefficients. In this experiment, we verify that LASSO helps to obtain a better adversarially robust estimate. We take $p = 50$, $n = 300$, and assume Σ is known. Cross-validation is applied to choose the penalty that minimizes the (standard) prediction risk. This is implemented by library `glmnet` in R.

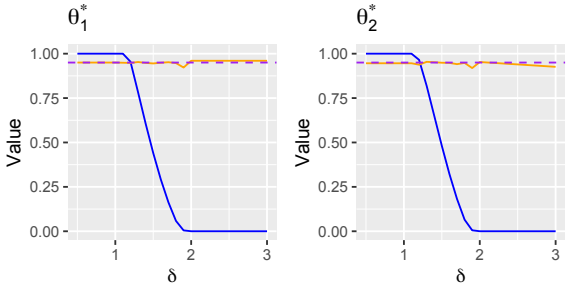

Figure 3: Value of θ_i^* and the 95% Empirical Coverage. Blue line: θ_i^*/θ_{0i}. Orange line: 95% Empirical Coverage. Purple dased line: 0.95. The 95% coverage for both θ_1^* and θ_2^* are close to 0.95 when $\delta < 1.9$.

We consider both lower-dimensional dense (Table 1) case with $(p, n) = (50, 300)$ and high-dimensional sparse scenario with $(p, n) = (300, 200)$. For high-dimensional sparse model, to make it clear on the difference between $\widehat{\theta}_{OLS}$ and $\widehat{\theta}_{LASSO}$, we present the results given Σ is known/unknown. In the dense coefficient model, although we can select a λ such that the LASSO estimator leads to a smaller standard risk than the OLS estimator, its corresponding adversarial risk gets worse with an increasing δ. For the sparse model, for all choices of δ, LASSO has a smaller adversarial risk than OLS. The results for unknown Σ are similar to the case when Σ is known, in the sense that LASSO is also better than OLS.

In addition, $R_0(\widehat{\theta}_{LASSO}, \delta)$ is always smaller when Σ is known than when Σ is unknown. This also verifies that unlabeled data helps improve the adversarial robustness (the comparison is not applicable to $R_0(\widehat{\theta}_{OLS}, \delta)$ since $\widehat{\theta}_{OLS}$ is not consistent).

Sparse matrix. We use sparse matrix estimator to verify that it helps enhancing adversarial robustness. To generate sparse matrix, we consider Σ such that $\Sigma_{ii} = 1$, and $\Sigma_{ij} = r|i-j|^{-\alpha-1}$ when $j \neq i$, where $r = 0.6$ and $\alpha = 0.2$. This choice of (r, α) ensures that all eigenvalues of Σ are positive. We take $p = 300$, $n =$

Table 1: Comparison between OLS and LASSO for dense θ_0 with known Σ. $p = 50$, $n = 300$, $r = 0.1$, $\sigma^2 = 1$. Σ is known. Standard deviation is provided for $R_0(\theta^*, \delta) - R_0(\widehat{\theta}_{OLS}, \delta)$ and $R_0(\theta^*, \delta) - R_0(\widehat{\theta}_{LASSO}, \delta)$.

δ	$R_0(\theta^*, \delta)$	$R_0(\widehat{\theta}_{OLS}, \delta)$	$R_0(\widehat{\theta}_{LASSO}, \delta)$	$R_0(\theta_0, \delta)$	$R_0(0, \delta)$
0.5	0.2489	0.8545(0.1413)	**0.633**(0.0795)	0.25	0.9997
0.8	0.5847	**0.8436**(0.0867)	0.8516(0.0858)	0.64	0.9997
0.9	0.6862	**0.8715**(0.65)	0.8888(0.0762)	0.81	0.9997

Table 2: Comparison between OLS and LASSO for sparse θ_0 . The first 10 elements of θ_0 are $1/\sqrt{10}$. $p = 300$, $n = 200$, $r = 0.1$, $\sigma^2 = 1$.

Σ	δ	$R_0(\theta^*, \delta)$	$R_0(\widehat{\theta}_{OLS}, \delta)$	$R_0(\widehat{\theta}_{LASSO}, \delta)$	$R_0(\theta_0, \delta)$	$R_0(0, \delta)$
known	0.5	0.25	6.1134(1.0171)	**0.7486**(0.1200)	0.25	1.8943
	1	0.7847	2.7114(0.4124)	**0.9941**(0.0752)	1	1.8943
	2	1.3088	1.4912(0.0431)	**1.3684**(0.0453)	4	1.8943
	3	1.6088	1.7522(0.0641)	**1.6435**(0.1033)	9	1.8943
unknown	0.5	0.25	2.3533(0.2551)	**0.8212**(0.0984)	0.25	1.8943
	1	0.7847	1.5830(0.1368)	**1.1414**(0.0732)	1	1.8943
	2	1.3088	1.5023(0.0341)	**1.4716**(0.0358)	4	1.8943
	3	1.6088	1.7040(0.0250)	**1.6930**(0.0494)	9	1.8943

Table 3: Comparison between $\widehat{\Sigma}$ and $\widehat{\Sigma}_{sparse}$. $p = 300$, $n = 200$, $\sigma^2 = 1$. θ_0 is known. $\widehat{\Sigma}_{sparse}$ performs slightly better when Σ is sparse.

$\delta = 2$	$R_0(\theta^*, \delta)$	$R_0(\theta^*_{\widehat{\Sigma}}, \delta)$	$R_0(\theta^*_{\widehat{\Sigma}_{sparse}}, \delta)$	$R_0(\theta_0, \delta)$
Dense	1.8865	**2.0576**(0.1841)	4.8769(0.1044)	4.0000
Sparse	2.9807	3.0652(0.0279)	**3.0293**(0.0279)	4.0000

200 so that the difference between $\widehat{\Sigma}$ and $\widehat{\Sigma}_{sparse}$ is obvious. The attack level δ is set to be 2 in this comparison. For simplicity, we assume θ_0 is known in the comparison of matrix estimators. The sparse covariance estimator $\widehat{\Sigma}_{sparse}$ was obtained based on the method in Cai et al. (2010). In Table 3, the adversarial excess risk is reduced from 0.0845 ($R_0(\theta^*_{\widehat{\Sigma}}, \delta) - R_0(\theta^*, \delta)$) to 0.0486 ($R_0(\theta^*_{\widehat{\Sigma}_{sparse}}, \delta) - R_0(\theta^*, \delta)$), which shows the effectiveness of $\widehat{\Sigma}_{sparse}$. In addition to the sparse matrix, we also consider dense covariance matrix generated in the same way as previous experiments by taking $r = 0.6$. When the true matrix is dense, using a sparse estimate is not appropriate; thus, the corresponding adversarial risk is much higher.

7 CONCLUSIONS AND FUTURE DIRECTIONS

In this paper, we figure out the minimax lower bound of estimation error of adversarially robust model in linear regression setup, which indicates the importance of incorporating model information in adversarially robust learning. In addition, we propose a two-stage adversarially robust learning method based on an explicit relation between adversarially robust estimator and standard estimator. The proposed two-stage estimator can encode model information (e.g., sparsity) into standard estimators, through which the robustness of adversarially robust estimator could be improved and reach minimax optimal convergence rate. Our investigation in the generalization error also verifies that adversarial robustness hurts generalization.

One future direction is to relax the distributional assumption on $(\mathbf{x}, y)$, say $\mathbf{x}$ follows non-Gaussian distribution. Although there is a wide range of data that may follow Gaussian assumption, e.g., abalone data and other biological data, many other data may not follow Gaussian, e.g., image data. The constant c_0 in our framework currently depends on the Gaussian assumption, and there is potential to relax it. Another direction is concerned with sparse adversarially robust learning, say sparse $\widehat{\theta}$, which could be useful in both compressing and robustifying deep neural networks Guo et al. (2018). The first step is to understand how the sparsity of θ_0 (together with other model assumptions) implies the sparsity of θ^*, which in turn determines the sparsity of $\widehat{\theta}$. An example can be found in Allen-Zhu and Li (2020) for linear sparse coding model. However, more careful studies would be needed in the future.

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A More theoretical results

This section provides some supplementary theorems.

A.1 Results regarding to prediction risk (an analog of Theorem 3)

For consistent estimates $(\widehat{\theta}_0, \widehat{\Sigma}, \widehat{\sigma}^2)$, with probability tending to 1, we have

$$\begin{aligned}\sup_{\delta\geq 0}\left|R(\theta^*(\delta),\delta)-R(\widetilde{\theta}(\delta),\delta)\right| &= O\left(\|\widehat{\theta}_0-\theta_0\|\|\theta_0\|\right)+O\left(\|\theta_0\|^2\sqrt{\|\widehat{\Sigma}-\Sigma\|}\right)\\ &\quad +O\left(\widehat{\sigma}^2-\sigma^2\right)+O\left(\|\theta_0\|(\widehat{\sigma}-\sigma)\right).\end{aligned}$$

A.2 Definitions in Theorem 4

$$\begin{aligned}\mathbf{M}_1(\theta^*,\theta_0,\Sigma) &= \mathbf{H}(\theta^*,\theta_0,\Sigma)^{-1}\mathbf{M}(\theta^*,\theta_0,\Sigma),\\ \mathbf{M}_2(\theta^*,\theta_0,\Sigma) &= -\delta c_0\mathbf{H}(\theta^*,\theta_0,\Sigma)^{-1}\left(\frac{\Sigma(\theta^*-\theta_0)}{2\|\theta^*-\theta_0\|_\Sigma\|\theta^*\|}-\frac{\|\theta^*\|\theta^*}{2\|\theta^*-\theta_0\|_\Sigma^3}\right),\end{aligned}$$

$$\begin{aligned}\mathbf{M}_3(\theta^*,\theta_0,\Sigma) &= -(1+\delta c_0 A(\theta^*,\theta_0,\Sigma)),\\ \mathbf{M}(\theta^*,\theta_0,\Sigma) &= \Sigma+\delta c_0 A(\theta^*,\theta_0,\Sigma)\Sigma+\frac{\delta c_0 A(\theta^*,\theta_0,\Sigma)}{\|\theta^*-\theta_0\|_\Sigma^2}\Sigma(\theta^*-\theta_0)(\theta^*-\theta_0)^\top\Sigma\\ &\quad +\delta\frac{c_0}{A(\theta^*,\theta_0,\Sigma)\|\theta^*\|_2^2}\theta^*(\theta^*)^\top,\end{aligned}$$

where $A(\theta^*,\theta_0,\Sigma)=\|\theta^*\|/\|\theta^*-\theta_0\|_\Sigma$. The matrix $\mathbf{H}(\theta^*,\theta_0,\Sigma)$ is the Hessian matrix of R_0.

B Proofs in Section 2

There are two parts of Proposition 1: the statement about Hessian, and the optimal solution θ^*. We prove them separately.

B.1 Positive definite Hessian

Proof of Proposition 1 for Positive Definite Hessian. Expand the adversarial risk at $\mathbf{x}$ as

$$\begin{aligned}\max_{\|x^*-x\|\leq\delta}\left[((x^*)^\top\theta-\mathbf{x}^\top\theta_0)^2\right] &= \max_{\|x^*-x\|\leq\delta}\left[(\mathbf{x}^*-\mathbf{x})^\top\theta+\mathbf{x}^\top(\theta-\theta_0)\right]^2\\ &= \left(\delta\|\theta\|+|\mathbf{x}^\top(\theta-\theta_0)|\right)^2.\end{aligned}$$

Since $\mathbf{x}$ follows Gaussian, for any fixed $\theta-\theta_0$, $\mathbf{x}^\top(\theta-\theta_0)$ follows Gaussian as well. Let $Z=\mathbf{x}^\top(\theta-\theta_0)$. Note that $\mathbf{x}\sim N(\mathbf{0},\Sigma)$, we have $Z\sim N(0,\|\theta-\theta_0\|_\Sigma^2)$ and

$$\begin{aligned}R_0(\theta,\delta) &= \mathbb{E}_Z(|Z|+\delta\|\theta\|)^2\\ &= \|\theta-\theta_0\|_\Sigma^2+2\delta c_0\|\theta\|\|\theta-\theta_0\|_\Sigma+\delta^2\|\theta\|_2^2.\end{aligned}$$

Taking the gradient of $R_0(\theta,\delta)$ with respect to θ yields

$$\begin{aligned}\nabla_\theta R_0(\theta,\delta) &= 2\left[\Sigma(\theta-\theta_0)+\delta c_0\frac{\|\theta-\theta_0\|_\Sigma}{\|\theta\|}\theta+\delta c_0\frac{\|\theta\|}{\|\theta-\theta_0\|_\Sigma}\Sigma(\theta-\theta_0)+\delta^2\theta\right]\\ &= 2\left[\left(\mathbf{I}_p+\delta c_0\frac{\|\theta\|}{\|\theta-\theta_0\|_\Sigma}\right)\Sigma(\theta-\theta_0)+\left(\delta c_0\frac{\|\theta-\theta_0\|_\Sigma}{\|\theta\|}+\delta^2\right)\theta\right].\end{aligned}$$

Denote $A=\|\theta\|/\|\theta-\theta_0\|_\Sigma$, then $\frac{\partial^2 R_0}{2\partial\theta^2}$ becomes

$$\mathbf{H}:=\frac{\partial^2 R_0}{2\partial\theta^2}=\Sigma+\delta c_0 A\Sigma+\left(\frac{\delta c_0}{A}+\delta^2\right)\mathbf{I}_p+\delta c_0\Sigma(\theta-\theta_0)\left(\frac{\partial A}{\partial\theta}\right)^\top+\delta c_0\theta\left(\frac{\partial 1/A}{\partial\theta}\right)^\top. \tag{11}$$

To show that R_0 is convex, it sufficies to show that H is positive definite.

In $\mathbf{H}$, the two partial derivatives are

$$\frac{\partial A}{\partial \theta} = \frac{\partial}{\partial \theta}\frac{\|\theta\|}{\|\theta-\theta_0\|_\Sigma} = \frac{\theta}{\|\theta\|\|\theta-\theta_0\|_\Sigma} - \frac{\|\theta\|\Sigma(\theta-\theta_0)}{\|\theta-\theta_0\|_\Sigma^3},$$

and

$$\frac{\partial 1/A}{\partial \theta} = \frac{\Sigma(\theta-\theta_0)}{\|\theta\|\|\theta-\theta_0\|_\Sigma} - \frac{\|\theta-\theta_0\|_\Sigma\theta}{\|\theta\|^3}.$$

Thus

$$\begin{aligned}
\Sigma(\theta-\theta_0)\left(\frac{\partial A}{\partial \theta}\right)^\top &= \frac{1}{\|\theta\|\|\theta-\theta_0\|_\Sigma}\Sigma(\theta-\theta_0)\theta^\top - \frac{\|\theta\|}{\|\theta-\theta_0\|_\Sigma^3}\Sigma(\theta-\theta_0)(\theta-\theta_0)^\top\Sigma, \\
&= \frac{1}{\|\theta\|\|\theta-\theta_0\|_\Sigma}\Sigma(\theta-\theta_0)\theta^\top - \frac{A}{\|\theta-\theta_0\|_\Sigma^2}\Sigma(\theta-\theta_0)(\theta-\theta_0)^\top\Sigma, \\
\theta\left(\frac{\partial 1/A}{\partial \theta}\right)^\top &= \frac{1}{\|\theta\|\|\theta-\theta_0\|_\Sigma}\theta(\theta-\theta_0)^\top\Sigma - \frac{\|\theta-\theta_0\|_\Sigma}{\|\theta\|^3}\theta\theta^\top, \\
&= \frac{1}{\|\theta\|\|\theta-\theta_0\|_\Sigma}\theta(\theta-\theta_0)^\top\Sigma - \frac{1}{A\|\theta\|^2}\theta\theta^\top.
\end{aligned}$$

Then $\mathbf{H}$ can be represented as

$$\begin{aligned}
& \Sigma + \delta c_0 A\Sigma + \left(\frac{\delta c_0}{A} + \delta^2\right)\mathbf{I}_p + \delta c_0\Sigma(\theta-\theta_0)\left(\frac{\partial A}{\partial \theta}\right)^\top + \delta c_0\theta\left(\frac{\partial 1/A}{\partial \theta}\right)^\top \\
= & \left(\Sigma - \frac{1}{\|\theta-\theta_0\|_\Sigma^2}\Sigma(\theta-\theta_0)(\theta-\theta_0)^\top\Sigma\right)Ac_0\delta \\
& + \left(\mathbf{I}_p - \frac{1}{\|\theta\|^2}\theta\theta^\top\right)\frac{c_0\delta}{A} \\
& + \left(\Sigma + \delta^2\mathbf{I}_p + \frac{\delta c_0}{\|\theta\|\|\theta-\theta_0\|_\Sigma}\theta(\theta-\theta_0)^\top\Sigma + \frac{\delta c_0}{\|\theta\|\|\theta-\theta_0\|_\Sigma}\Sigma(\theta-\theta_0)\theta^\top\right) \\
:= & \mathbf{M}_1 Ac_0\delta + \mathbf{M}_2\frac{c_0\delta}{A} + \mathbf{M}_3.
\end{aligned}$$

Since Σ is positive definite, for any vector $\mathbf{a} \neq \mathbf{0}$, and $\theta \neq \theta_0, \theta \neq \mathbf{0}$, by Cauchy inequality,

$$\begin{aligned}
\mathbf{a}^\top\mathbf{M}_1\mathbf{a} &= \mathbf{a}^\top\Sigma\mathbf{a} - \frac{\left(\mathbf{a}^\top\Sigma(\theta-\theta_0)\right)^2}{\|\theta-\theta_0\|_\Sigma^2} \geq 0, \\
\mathbf{a}^\top\mathbf{M}_2\mathbf{a} &= \mathbf{a}^\top\mathbf{a} - \frac{(\mathbf{a}^\top\theta)^2}{\|\theta\|^2} \geq 0,
\end{aligned}$$

which imply $\mathbf{M}_1$ and $\mathbf{M}_2$ are positive semi-definite.

For $\mathbf{M}_3$, we have

$$\begin{aligned}
\mathbf{M}_3 = & \left[\delta\mathbf{I}_p + \frac{c_0}{\|\theta\|\|\theta-\theta_0\|_\Sigma}\Sigma(\theta-\theta_0)\theta^\top\right]\left[\delta\mathbf{I}_p + \frac{c_0}{\|\theta\|\|\theta-\theta_0\|_\Sigma}\Sigma(\theta-\theta_0)\theta^\top\right]^\top \\
& + \Sigma - \frac{c_0^2}{\|\theta-\theta_0\|_\Sigma^2}\Sigma(\theta-\theta_0)(\theta-\theta_0)^\top\Sigma.
\end{aligned}$$

Since $c_0 = \sqrt{2/\pi} < 1$, for any vector $\mathbf{a} \neq \mathbf{0}$, and $\theta \neq \theta_0, \theta \neq \mathbf{0}$,

$$\mathbf{a}^\top\left(\Sigma - \frac{c_0^2}{\|\theta-\theta_0\|_\Sigma^2}\Sigma(\theta-\theta_0)(\theta-\theta_0)^\top\Sigma\right)\mathbf{a} > \mathbf{a}^\top\mathbf{M}_1\mathbf{a} \geq 0.$$

□

B.2 Optimal solution

Proof of Proposition 1 for θ^*. We first consider the case where Σ is a diagonal matrix. Recall that the gradient of $R_0(\theta,\delta)$ is

$$\begin{aligned}\nabla_\theta R_0(\theta,\delta) &= 2\left[\Sigma(\theta-\theta_0)+\delta c_0\frac{\|\theta-\theta_0\|_\Sigma}{\|\theta\|}\theta+\delta c_0\frac{\|\theta\|}{\|\theta-\theta_0\|_\Sigma}\Sigma(\theta-\theta_0)+\delta^2\theta\right]\\ &= 2\left[\left(\mathbf{I}_p+\delta c_0\frac{\|\theta\|}{\|\theta-\theta_0\|_\Sigma}\right)\Sigma(\theta-\theta_0)+\left(\delta c_0\frac{\|\theta-\theta_0\|_\Sigma}{\|\theta\|}+\delta^2\right)\theta\right].\end{aligned}$$

Note the gradient $\nabla_\theta R_0(\theta,\delta)$ is well-defined in $\mathbb{R}^p/\{\mathbf{0},\theta_0\}$ and $R_0(\theta,\delta)\to+\infty$ as $\|\theta\|\to+\infty$. Thus, the global minimizer θ^* of $R_0(\theta,\delta)$ should only be $\mathbf{0},\theta_0$ or the stationary point of $R_0(\theta,\delta)$. Note if $\nabla_\theta R_0(\theta,\delta)=\mathbf{0}$, we have $\eta\Sigma(\theta-\theta_0)=-\theta$ for some $\eta>0$, or equivalently,

$$\theta_\eta=(\eta\Sigma+\mathbf{I}_p)^{-1}\eta\Sigma\theta_0=\left[\mathbf{I}_p-(\eta\Sigma+\mathbf{I}_p)^{-1}\right]\theta_0.$$

Since when $\eta\to0$, $\theta_\eta\to\mathbf{0}$ and when $\eta\to+\infty$, $\theta_\eta\to\theta_0$, the global minimizer of $R_0(\theta,\delta)$ should has the form as $\left[I-(\eta\Sigma+\mathbf{I}_p)^{-1}\right]\theta_0$ for some $\eta\in[0,\infty]$. Define

$$\begin{aligned}r(\eta) &= R_0(\theta_\eta,\delta), &(12)\\ \theta_\eta &= (\mathbf{I}_p-(\eta\Sigma+\mathbf{I}_p)^{-1})\theta_0, &(13)\\ H(\eta) &= \frac{\sqrt{\theta_0^\top(\frac{\Sigma}{\eta\Sigma+\mathbf{I}_p})^2\theta_0}}{\sqrt{\theta_0^\top\frac{\Sigma}{(\eta\Sigma+\mathbf{I}_p)^2}\theta_0}}, &(14)\\ g(\eta) &= 1-\frac{\delta c_0}{H(\eta)}+\eta(\delta c_0H(\eta)-\delta^2). &(15)\end{aligned}$$

We have

$$\begin{aligned}r'(\eta)=\frac{\partial}{\partial\eta}R_0(\theta_\eta,\delta) &= (\nabla_\theta R_0(\theta_\eta))^\top\frac{\partial}{\partial\eta}\theta_\eta\\ &= -2g(\eta)(\theta-\theta_0)^\top\Sigma(\eta\Sigma+\mathbf{I}_p)^{-1}\Sigma(\theta-\theta_0). &(16)\end{aligned}$$

By Lemma 1 below, if $\delta\le\delta_1$, $g(\eta)>0$. Thus, $r(\eta)$ is decreasing and the global minimizer of $R_0(\theta,\delta)$ is $\theta_{\eta=+\infty}=\theta_0$. If $\delta\ge\delta_2$, $g(\eta)<0$. Thus, $r(\eta)$ is increasing and the global minimizer of $R_0(\theta,\delta)$ is $\theta_{\eta=0}=\mathbf{0}$. If $\delta_1<\delta<\delta_2$, there exists a unique positive number η^* (as denoted as $\eta^*(\delta)$) such that $g(\eta^*)=0$. Moreover, note

$$g(\eta)=\left(1+\delta c_0\frac{\|\theta_\eta\|}{\|\theta_\eta-\theta_0\|_\Sigma}\right)-\eta\left(\delta c_0\frac{\|\theta_\eta-\theta_0\|_\Sigma}{\|\theta_\eta\|}+\delta^2\right),$$

thus, η^* is the unique solution to (4). Finally, $g(\eta)>0$ when $\eta\in[0,\eta^*)$, and $g(\eta)<0$ when $\eta\in(\eta^*,\infty)$. Thus, by (16), $r(\eta)$ is decreasing when $\eta\in[0,\eta^*)$, is increasing when $\eta\in(\eta^*,\infty)$. Thus, $R_0(\theta,\delta)$ gets the global minimum when $\theta=\theta_{\eta=\eta^*}$.

For the general positive definite matrix Σ, we consider the orthogonal decomposition of Σ and let $\Sigma=\mathbf{U}^\top\mathbf{D}\mathbf{U}$ where $\mathbf{D}$ is a $p\times p$ diagonal matrix and $\mathbf{U}$ is an orthogonal matrix. Let $\theta=\mathbf{U}\theta,\theta_0=\mathbf{U}\theta_0$. Then the adversarial prediction risk $R_0(\theta,\delta)$ in (2) becomes

$$R_0(\theta,\delta)=R_0(U^\top\theta,\delta)=\|\theta-\theta_0\|_{\mathbf{D}}^2+2\delta c_0\|\theta\|\|\theta-\theta_0\|_{\mathbf{D}}+\delta^2\|\theta\|_2^2. \tag{17}$$

Note $\mathbf{D}$ is a diagonal matrix. Applying the results from Proposition 1 yields $\theta^*=(\mathbf{I}_p-(\eta^*\mathbf{D}+\mathbf{I}_p)^{-1})\theta_0$. Therefore, since $\theta=\mathbf{U}\theta,\theta_0=\mathbf{U}\theta_0$, $\theta^*=(\mathbf{I}_p-(\eta^*\Sigma+\mathbf{I}_p)^{-1})\theta_0$, which completes the proof. □

Lemma 1. *Suppose Σ is a p by p diagonal matrix. Define functions $H(\eta)$ and $g(\eta)$ as in (14) and (15), then*

1. *If $\delta\ge\delta_2$, $g(\eta)<0$ for all $\eta>0$.*
2. *If $\delta\le\delta_1$, $g(\eta)>0$ for all $\eta\ge0$.*

3. *If $\delta_1 < \delta < \delta_2$, there exists a unique positive number η^* such that $g(\eta) = 0$. Moreover, $g(\eta) > 0$ when $\eta \in [0, \eta^*)$, and $g(\eta) < 0$ when $\eta \in (\eta^*, \infty)$.*

Here $\delta_1 = \frac{c_0\|\theta_0\|}{\|\theta_0\|_{\Sigma^{-1}}}$ and $\delta_2 = \frac{\|\theta_0\|_{\Sigma^2}}{c_0\|\theta_0\|_\Sigma}$.

Proof of Lemma 1. By Lemma 2 below, we have for any $\eta \geq 0$, $\delta_1/c_0 \leq H(\eta) \leq \delta_2 c_0$. Therefore, $g(\eta) > 0$ if $\delta \leq \delta_1$ and $g(\eta) < 0$ if $\delta \geq \delta_2$.

Moreover, note $H(\eta = 0) = \delta_2 c_0, H(\eta = \infty) = \delta_1/c_0$. When $\delta_1 < \delta < \delta_2$, $g(\eta = 0) = 1 - \delta/\delta_2 > 0$ and $g(\eta = \infty) = -\infty$. There must exist a positive solution to $g(\eta) = 0$. Next, we will show the solution is unique. Assume η^* is the smallest η such that $g(\eta) = 0$. Then we claim $g(\eta)$ is decreasing as $\eta \geq \eta^*$. In fact, if $g(\eta^*) = 0$, we have $1 - \frac{\delta c_0}{H(\eta^*)} \leq 0$ and $\delta c_0 H(\eta^*) - \delta^2 < 0$. By Lemma 3, $H(\eta)$ is a decreasing function when $\eta \geq 0$. Thus, $g(\eta)$ is decreasing as $\eta \geq \eta^*$ and $g(\eta) < g(\eta^*) = 0$ for $\eta > \eta^*$. Therefore, there is one unique η^* such that $g(\eta^*) = 0$. Moreover, $g(\eta) > 0$ when $\eta \in [0, \eta^*)$, and $g(\eta) < 0$ when $\eta \in (\eta^*, \infty)$. □

Lemma 2. *If $\Sigma = diag(d_1, d_2, \cdots, d_p)$ is a diagonal matrix, where all $d_i > 0$, then for any $\eta \geq 0$,*

$$\left(\theta_0^\top \left(\frac{1}{\Sigma}\right)\theta_0\right)\left(\theta_0^\top \left(\frac{\Sigma}{\eta\Sigma + \mathbf{I}_p}\right)^2 \theta_0\right) \geq \left(\theta_0^\top \frac{\Sigma}{(\eta\Sigma + \mathbf{I}_p)^2}\theta_0\right)(\theta_0^\top\theta_0) \tag{18}$$

$$(\theta_0^\top\Sigma^2\theta_0)\left(\theta_0^\top \frac{\Sigma}{(\eta\Sigma + \mathbf{I}_p)^2}\theta_0\right) \geq (\theta_0^\top\Sigma\theta_0)\left(\theta_0^\top \left(\frac{\Sigma}{\eta\Sigma + \mathbf{I}_p}\right)^2 \theta_0\right) \tag{19}$$

Proof of Lemma 2. To prove Lemma 2, we expand all terms in

$$\begin{aligned}
&\left(\theta_0^\top \left(\frac{1}{\Sigma}\right)\theta_0\right)\left(\theta_0^\top \left(\frac{\Sigma}{\eta\Sigma + \mathbf{I}_p}\right)^2 \theta_0\right) = \left(\sum_{i=1}^p \frac{1}{d_i}(\theta_0^i)^2\right)\left(\sum_{i=1}^p (\frac{d_i}{\eta d_i + 1})^2(\theta_0^i)^2\right) \\
= &-\sum_{i=1}^p \frac{d_i}{(\eta d_i + 1)^2}(\theta_0^i)^4 + \sum_{1\leq i\leq j\leq p}\sum \left[\frac{1}{d_i}(\theta_0^i)^2(\frac{d_j}{\eta d_j + 1})^2(\theta_0^j)^2 + \frac{1}{d_j}(\theta_0^j)^2(\frac{d_i}{\eta d_i + 1})^2(\theta_0^i)^2\right] \\
= &-\sum_{i=1}^p \frac{d_i}{(\eta d_i + 1)^2}(\theta_0^i)^4 + \sum_{1\leq i\leq j\leq p}\sum \left[\left(\frac{1}{d_i}(\frac{d_j}{\eta d_j + 1})^2 + \frac{1}{d_j}(\frac{d_i}{\eta d_i + 1})^2\right)(\theta_0^i\theta_0^j)^2\right]
\end{aligned}$$

$$\begin{aligned}
&\left(\theta_0^\top \frac{\Sigma}{(\eta\Sigma + \mathbf{I}_p)^2}\theta_0\right)(\theta_0^\top\theta_0) = \left(\sum_{i=1}^p \frac{d_i}{(\eta d_i + 1)^2}(\theta_0^i)^2\right)\left(\sum_{i=1}^p (\theta_0^i)^2\right) \\
= &-\sum_{i=1}^p \frac{d_i}{(\eta d_i + 1)^2}(\theta_0^i)^4 + \sum_{1\leq i\leq j\leq p}\sum \left[\frac{d_i}{(\eta d_i + 1)^2}(\theta_0^i)^2(\theta_0^j)^2 + \frac{d_j}{(\eta d_j + 1)^2}(\theta_0^j)^2(\theta_0^i)^2\right] \\
= &-\sum_{i=1}^p \frac{d_i}{(\eta d_i + 1)^2}(\theta_0^i)^4 + \sum_{1\leq i\leq j\leq p}\sum \left[\left(\frac{d_i}{(\eta d_i + 1)^2} + \frac{d_j}{(\eta d_j + 1)^2}\right)(\theta_0^i\theta_0^j)^2\right]
\end{aligned}$$

By rearrangement inequality, for any i and j, we have

$$\left(\frac{1}{d_i}(\frac{d_j}{\eta d_j + 1})^2 + \frac{1}{d_j}(\frac{d_i}{\eta d_i + 1})^2\right) \geq \left(\frac{d_i}{(\eta d_i + 1)^2} + \frac{d_j}{(\eta d_j + 1)^2}\right),$$

which yields the inequality in (18). Similarly we can show (19). □

Lemma 3. *If $\Sigma = diag(d_1, d_2, \cdots, d_p)$ is a diagonal matrix, where all $d_i > 0$, then for any $\eta_1 > \eta_2$,*

$$\left(\theta_0^\top (\frac{\Sigma}{\eta_1\Sigma + \mathbf{I}_p})^2\theta_0\right)\left(\theta_0^\top (\frac{\Sigma}{(\eta_2\Sigma + \mathbf{I}_p)^2})\theta_0\right) < \left(\theta_0^\top (\frac{\Sigma}{\eta_2\Sigma + \mathbf{I}_p})^2\theta_0\right)\left(\theta_0^\top (\frac{\Sigma}{(\eta_1\Sigma + \mathbf{I}_p)^2}.)\theta_0\right).$$

Proof of Lemma 3. Using the same techniques as in the proof of Lemma 2, it suffices to show that for any $d_i \neq d_j$,

$$\begin{aligned} & \left(\frac{d_i}{\eta_1 d_i+1}\right)^2 \frac{d_j}{(\eta_2 d_j+1)^2}+\left(\frac{d_j}{\eta_1 d_j+1}\right)^2 \frac{d_i}{(\eta_2 d_i+1)^2} \\ < & \left(\frac{d_i}{\eta_2 d_i+1}\right)^2 \frac{d_j}{(\eta_1 d_j+1)^2}+\left(\frac{d_j}{\eta_2 d_j+1}\right)^2 \frac{d_i}{(\eta_1 d_i+1)^2}, \end{aligned}$$

which is equivalent to

$$\frac{d_i-d_j}{(\eta_1 d_i+1)^2(\eta_2 d_j+1)^2}<\frac{d_i-d_j}{(\eta_1 d_j+1)^2(\eta_2 d_i+1)^2}. \tag{20}$$

The last inequality (20) always hold no matter $d_i > d_j$ or $d_i < d_j$ by the rearrangement inequality, which completes the proof. □

C Proofs in Section 3 and 4

C.1 Theorem 1

Lemma 4. *Assume $R > c_1\sigma$ for some constant c_1. Also Assume $\lambda_{\max}(\Sigma)$ and $\lambda_{\min}(\Sigma)$ are bounded and bounded away from zero. When $(p\log^2 n)/n \to 0$,*

$$\inf_{\widehat{\theta}} \sup_{\delta,\sigma<\|\theta_0\|\leq\sqrt{R^2+\sigma^2},\Sigma} \mathbb{E}\|\widehat{\theta}-\theta^*(\delta)\|^2=\Omega\left(\frac{\sigma^2 p}{n}\right). \tag{21}$$

Proof of Lemma 4. We first consider a relaxation where $\|\theta_0\|$ is unbounded, then add back the condition on $\|\theta_0\|$ into the bound to show that these conditions does not change the rate of the lower bound.

Assume θ_0 follows $N(0,\sigma^2/(\alpha n)\mathbf{I}_p)$ and $\alpha = o(1)$. Denote $\widehat{\Sigma}_n = \mathbf{X}^\top\mathbf{X}/n$, and $\widehat{\theta}_{n,\alpha} = (\widehat{\Sigma}_n+\alpha\mathbf{I}_p)^{-1}\mathbf{X}^\top\mathbf{y}/n$. Given $(\mathbf{X},\mathbf{y})$, it follows that $\theta_0|(\mathbf{X},\mathbf{y}) \sim N(\widehat{\theta}_{n,\alpha},(\sigma^2/n)(\widehat{\Sigma}_n+\alpha\mathbf{I}_p)^{-1})$, and

$$\begin{aligned} \inf_{\widehat{\theta}} \sup_{\delta,\theta_0,\Sigma} \mathbb{E}\|\widehat{\theta}-\theta^*(\delta)\|^2 &\geq \inf_{\widehat{\theta}} \sup_{\delta,\theta_0,\Sigma=\mathbf{I}_p} \mathbb{E}\|\widehat{\theta}-\theta^*(\delta)\|^2 \\ &\geq \inf_{\widehat{\theta}} \sup_{\delta} \mathbb{E}\left[\mathbb{E}_{\theta_0|\mathbf{X},\mathbf{y},\Sigma=\mathbf{I}_p}\|\widehat{\theta}-\theta^*(\delta)\|^2\right]. \end{aligned}$$

Observe that

$$\begin{aligned} & \inf_{\widehat{\theta}} \sup_{\delta} \mathbb{E}\left[\mathbb{E}_{\theta_0|\mathbf{X},\mathbf{y},\Sigma=\mathbf{I}_p}\|\widehat{\theta}-\theta^*(\delta)\|^2\right] \\ = & \inf_{\widehat{\theta}} \sup_{\delta} \mathbb{E}\left(\|\widehat{\theta}-\mathbb{E}_{\theta_0|\mathbf{X},\mathbf{y},\Sigma=\mathbf{I}_p}[\theta^*(\delta)]\|^2+\mathbb{E}_{\theta_0|\mathbf{X},\mathbf{y},\Sigma=\mathbf{I}_p}\|\mathbb{E}_{\theta_0|\mathbf{X},\mathbf{y},\Sigma=\mathbf{I}_p}[\theta^*(\delta)]-\theta^*(\delta)\|^2\right) \\ \geq & \sup_{\delta} \mathbb{E}\left[\mathbb{E}_{\theta_0|\mathbf{X},\mathbf{y},\Sigma=\mathbf{I}_p}\|\mathbb{E}_{\theta_0|\mathbf{X},\mathbf{y},\Sigma=\mathbf{I}_p}[\theta^*(\delta)]-\theta^*(\delta)\|^2\right]. \end{aligned}$$

When $\Sigma = \mathbf{I}_p$, by Proposition 1, we know that $\theta^*(\delta) = (1-\kappa(\delta))\theta_0$ for some function κ that only depends on δ. In addition, based on equation (A.5) in Lemma A.6 of Ing and Lai (2011), we have $\|\widehat{\Sigma}_n-\mathbf{I}_p\| = o(1)$ and $tr(\widehat{\Sigma}^{-1}) = \Theta(p)$ with probability tending to 1. Thus for $\alpha = o(1)$,

$$\begin{aligned} \mathbb{E}_{\theta_0|\mathbf{X},\mathbf{y},\Sigma=\mathbf{I}_p}\|\theta^*(\delta)-\mathbb{E}_{\theta_0|\mathbf{X},\mathbf{y},\Sigma=\mathbf{I}_p}[\theta^*(\delta)]\|^2 &= (1-\kappa(\delta))^2\mathbb{E}_{\theta_0|\mathbf{X},\mathbf{y},\Sigma=\mathbf{I}_p}\|\theta_0-\widehat{\theta}_{n,\alpha}\|^2 \\ &= (1-\kappa(\delta))^2\frac{\sigma^2}{n}tr\left((\widehat{\Sigma}_n+\alpha\mathbf{I}_p)^{-1}\right) \\ &= (1-\kappa(\delta))^2\frac{\sigma^2}{n}tr\left(\widehat{\Sigma}_n^{-1}-\alpha(\widehat{\Sigma}_n+\alpha\mathbf{I}_p)^{-1}\widehat{\Sigma}_n^{-1}\right) \\ &= \left(1+O\left(\frac{1}{\lambda_{\max}(\widehat{\Sigma}_n)/\alpha+1}\right)\right)(1-\kappa(\delta))^2\frac{\sigma^2}{n}tr\left(\widehat{\Sigma}_n^{-1}\right) \\ &= (1+o(1))(1-\kappa(\delta))^2\frac{\sigma^2}{n}tr\left(\widehat{\Sigma}_n^{-1}\right). \end{aligned}$$

The above derivation is for unbounded θ_0. Now we show that adding back the constraint $\|\theta_0\| \le R$ does not change the order of this bound.

Take $\alpha = (pR^2)/(n)$, and denote $\Pi(c) = \{(\mathbf{X},\mathbf{y}) \mid \|\widehat{\theta}_{n,\alpha}\| \in (\sigma(1+c), \sqrt{R^2+\sigma^2}(1-c)],\ \|\widehat{\Sigma}_n - \mathbf{I}_p\| = o(1)\}$. Recall that $R \ge c_1\sigma$ for some constant $c_1 > 0$, thus there exists some small constant $c > 0$, such that $P((\mathbf{X},\mathbf{y}) \in \Pi(c)) > c_2$ for some constant $c_2 > 0$.

For any $(\mathbf{X},\mathbf{y}) \in \Pi(c)$, from the conditional distribution $\theta_0|\mathbf{X},\mathbf{y}$ and the assumption that $(p\log^2 n)/n \to 0$, one can show that

$$\begin{aligned} & \mathbb{E}_{\theta_0|\mathbf{X},\mathbf{y},\Sigma=\mathbf{I}_p} \left\| \mathbb{E}_{\theta_0|\mathbf{X},\mathbf{y},\Sigma=\mathbf{I}_p} \left[\theta^*(\delta) 1_{\{\|\theta_0\| \in (\sigma,\sqrt{R^2+\sigma^2}]\}}\right] - \left[\theta^*(\delta) 1_{\{\|\theta_0\| \in (\sigma,\sqrt{R^2+\sigma^2}]\}}\right] \right\|^2 \\ = \ & (1+o(1)) \mathbb{E}_{\theta_0|\mathbf{X},\mathbf{y},\Sigma=\mathbf{I}_p} \|\theta^*(\delta) - \mathbb{E}_{\theta_0|\mathbf{X},\mathbf{y},\Sigma=\mathbf{I}_p}[\theta^*(\delta)]\|^2. \end{aligned}$$

Consequently,

$$\begin{aligned} & \inf_{\widehat{\theta}} \sup_{\delta, \sigma < \|\theta_0\| \le \sqrt{R^2+\sigma^2}, \Sigma} \mathbb{E}\|\widehat{\theta} - \theta^*(\delta)\|^2 \\ = \ & \inf_{\widehat{\theta}} \sup_{\delta,\theta_0,\Sigma} \mathbb{E}\left[\|\widehat{\theta} - \theta^*(\delta)\|^2 1_{\{\|\theta_0\| \in (\sigma,\sqrt{R^2+\sigma^2}]\}}\right] \\ \ge \ & \inf_{\widehat{\theta}} \sup_{\delta} \mathbb{E}\left[1_{\{(\mathbf{X},\mathbf{y}) \in \Pi(c)\}} \left(\mathbb{E}_{\theta_0|\mathbf{X},\mathbf{y},\Sigma=\mathbf{I}_p} \|\widehat{\theta} - \theta^*(\delta)\|^2 1_{\{\|\theta_0\| \in (\sigma,\sqrt{R^2+\sigma^2}]\}}\right)\right] \\ \ge \ & (1+o(1)) \sup_{\delta} \mathbb{E}\left[1_{\{(\mathbf{X},\mathbf{y}) \in \Pi(c)\}} \left(\mathbb{E}_{\theta_0|\mathbf{X},\mathbf{y},\Sigma=\mathbf{I}_p} \|\theta^* - \mathbb{E}_{\theta_0|\mathbf{X},\mathbf{y},\Sigma=\mathbf{I}_p}[\theta^*]\|^2\right)\right] \\ = \ & \Omega\left(\frac{\sigma^2 p}{n}\right). \end{aligned}$$

□

Lemma 5. *Assume $(p\log^2 n)/n \to 0$, then for any θ_0, when $\lambda_{\min}(\Sigma)$ and $\lambda_{\max}(\Sigma)$ are both bounded and bounded away from zero, for any nonzero θ_0,*

$$\inf_{\widehat{\theta}} \sup_{\delta,\Sigma} \mathbb{E}\|\widehat{\theta} - \theta^*(\delta)\|^2 = \Omega\left(\frac{p\|\theta_0\|^2}{n}\right). \tag{22}$$

Proof of Lemma 5. We impose a prior distribution on Σ. Assume Σ follows $IW(\nu,\Lambda)$ with $\Lambda = (\nu-p-1)\mathbf{I}_p$ and $\nu = n+p+1$. In this case, we have $\mathbb{E}\Sigma = \frac{\Lambda}{\nu-p-1} = \mathbf{I}_p$, and

$$\Sigma|\mathbf{X} \sim IW(n+\nu, \Lambda + n\widehat{\Sigma}_n).$$

Similar as Lemma 4, we first relax the condition on the eigenvalues on Σ to obtain a bound, then add back the conditions back to the bound.

Based on the distribution of $\Sigma|\mathbf{X}$, we have

$$\begin{aligned} \inf_{\widehat{\theta}} \sup_{\delta} \mathbb{E}\left[\mathbb{E}_{\Sigma|\mathbf{X}}\|\widehat{\theta} - \theta^*(\delta)\|^2\right] &= \inf_{\widehat{\theta}} \sup_{\delta} \mathbb{E}\left(\|\widehat{\theta} - \mathbb{E}_{\Sigma|\mathbf{X}}\theta^*(\delta)\|^2 + \mathbb{E}_{\Sigma|\mathbf{X}}\|\mathbb{E}_{\Sigma|\mathbf{X}}(\theta^*) - \theta^*\|^2\right) \\ &\ge \sup_{\delta} \mathbb{E}\left[\mathbb{E}_{\Sigma|\mathbf{X}}\|\mathbb{E}_{\Sigma|\mathbf{X}}(\theta^*) - \theta^*\|^2\right]. \end{aligned} \tag{23}$$

Denote $\lambda = \lambda^*((n\widehat{\Sigma}_n + \Lambda)/(n+\nu-p-1), \theta_0, \delta)$. For any $\delta > 0$,

$$\begin{aligned} & \mathbb{E}_{\Sigma|\mathbf{X}}\|\mathbb{E}_{\Sigma|\mathbf{X}}(\theta^*) - \theta^*\|^2 \\ \ge \ & \frac{1}{2}\mathbb{E}_{\Sigma|\mathbf{X}}\|(\mathbb{E}_{\Sigma|\mathbf{X}}(\Sigma+\lambda\mathbf{I}_p)^{-1}\Sigma\theta_0) - (\Sigma+\lambda\mathbf{I}_p)^{-1}\Sigma\theta_0)\|^2 \\ & -\mathbb{E}_{\Sigma|\mathbf{X}}\left\|\mathbb{E}_{\Sigma|\mathbf{X}}(\theta^*) - \mathbb{E}_{\Sigma|\mathbf{X}}(\Sigma+\lambda\mathbf{I}_p)^{-1}\Sigma\theta_0 - \theta^* + (\Sigma+\lambda\mathbf{I}_p)^{-1}\Sigma\theta_0\right\|^2 \\ = \ & \frac{1}{2}\mathbb{E}_{\Sigma|\mathbf{X}}\|(\mathbb{E}_{\Sigma|\mathbf{X}}(\Sigma+\lambda\mathbf{I}_p)^{-1}\Sigma\theta_0) - (\Sigma+\lambda\mathbf{I}_p)^{-1}\Sigma\theta_0)\|^2 \\ & -\mathbb{E}_{\Sigma|\mathbf{X}}\left\|\mathbb{E}_{\Sigma|\mathbf{X}}(\lambda^*(\Sigma)-\lambda)(\Sigma+\lambda^*(\Sigma)\mathbf{I}_p)^{-1}(\Sigma+\lambda\mathbf{I}_p)^{-1}\Sigma\theta_0 - (\lambda^*(\Sigma)-\lambda)(\Sigma+\lambda^*(\Sigma)\mathbf{I}_p)^{-1}(\Sigma+\lambda\mathbf{I}_p)^{-1}\Sigma\theta_0\right\|^2 \\ = \ & \frac{1}{2}\mathbb{E}_{\Sigma|\mathbf{X}}\|(\mathbb{E}_{\Sigma|\mathbf{X}}(\Sigma+\lambda\mathbf{I}_p)^{-1}\Sigma\theta_0) - (\Sigma+\lambda\mathbf{I}_p)^{-1}\Sigma\theta_0)\|^2 - O\left(\mathbb{E}\|\Sigma - \mathbb{E}_{\Sigma|\mathbf{X}}\Sigma\|^4\|\theta_0\|^2\right). \end{aligned} \tag{24}$$

When $(p\log^2 n)/n \to 0$, $\mathbb{E}\|\Sigma - \mathbb{E}_{\Sigma|\mathbf{X}}\Sigma\|^4 = O(((p\log n)/n)^2) = o(p/n)$ based on equation (A.5) in Lemma A.6 of Ing and Lai (2011). As will be shown later, the dominant term is in $\Theta(p\|\theta_0\|^2/n)$, therefore $\mathbb{E}\|\Sigma - \mathbb{E}_{\Sigma|\mathbf{X}}\Sigma\|^4\|\theta_0\|^2$ is only a remainder term. Furthermore,

$$\begin{aligned} & \mathbb{E}_{\Sigma|\mathbf{X}}\|(\mathbb{E}_{\Sigma|\mathbf{X}}(\Sigma+\lambda\mathbf{I}_p)^{-1}\Sigma\theta_0) - (\Sigma+\lambda\mathbf{I}_p)^{-1}\Sigma\theta_0)\|^2 \\ = \;& \lambda^2\mathbb{E}_{\Sigma|\mathbf{X}}\|(\mathbb{E}_{\Sigma|\mathbf{X}}(\Sigma+\lambda\mathbf{I}_p)^{-1}\theta_0) - (\Sigma+\lambda\mathbf{I}_p)^{-1}\theta_0\|^2 \\ := \;& \lambda^2\psi(\lambda). \end{aligned}$$

Based on Lemma 6 below, when $\lambda \geq 0$,

$$\begin{aligned} & \psi(0) = \theta_0^\top \mathbf{V}_n \theta_0, \\ & \frac{\partial\psi(\lambda)}{\partial\lambda} \leq 0, \\ & \frac{\partial\psi(\lambda)}{\partial\lambda}\bigg|_{\lambda=0} = -\Theta(\theta_0^\top\mathbf{V}_n\theta_0), \\ & \frac{\partial^2\psi(\lambda)}{\partial\lambda^2} \geq 0, \end{aligned}$$

where

$$\mathbf{V}_{n,i,j} \;=\; \sum_{k=1}^{p} Cov_{\Sigma|X}(\Sigma^{-1}_{i,k}, \Sigma^{-1}_{k,j}).$$

From the formula in Nydick (2012),

$$Cov_{\Sigma|X}(\Sigma^{-1}_{i,k}, \Sigma^{-1}_{k,j}) \;=\; (n+\nu)\left((\Lambda+n\widehat{\Sigma}_n)^{-1}_{i,k}(\Lambda+n\widehat{\Sigma}_n)^{-1}_{k,j} + (\Lambda+n\widehat{\Sigma}_n)^{-1}_{i,j}(\Lambda+n\widehat{\Sigma}_n)^{-1}_{k,k}\right).$$

Consequently, there exists some constant $\epsilon > 0$ such that, when δ is chosen such that the corresponding λ satisfies $0 < \lambda < \epsilon$, then

$$\mathbb{E}_{\Sigma|\mathbf{X}}\|\mathbb{E}_{\theta_0,\Sigma|\mathbf{X},\mathbf{y}}(\theta^*) - \mathbb{E}_{\theta_0|\mathbf{X},\mathbf{y}}[\theta^*|\Sigma]\|^2 = \Omega\left(\frac{tr(\widehat{\Sigma}_n^{-1})\lambda_{\min}(\widehat{\Sigma}_n^{-1})\|\theta_0\|^2}{n}\right).$$

Note that the above bound does not have restriction on Σ.

Now we add back the condition where $\lambda_{\min}(\Sigma)$ and $\lambda_{\max}(\Sigma)$ are both bounded and bounded away from zero. When $(p\log^2 n)/n \to 0$ and $c_1 \leq \lambda_{\min}(\widehat{\Sigma}_n) \leq \lambda_{\max}(\widehat{\Sigma}_n) \leq c_2$, since $\Sigma \to \mathbb{E}_{\Sigma|\mathbf{X}}\Sigma$, there exists some constant $c > 0$ such that

$$\begin{aligned} & \mathbb{E}_{\Sigma|\mathbf{X}}\|(\mathbb{E}_{\Sigma|\mathbf{X}}\Sigma^{-1}\theta_0 1_{\{\lambda_{\max}(\Sigma),\lambda_{\min}(\Sigma)\in(c_1-c,c_2+c)\}}) - \Sigma^{-1}\theta_0 1_{\{\lambda_{\max}(\Sigma),\lambda_{\min}(\Sigma)\in(c_1-c,c_2+c)\}}\|^2 \\ = \;& (1+o(1))\mathbb{E}_{\Sigma|\mathbf{X}}\|(\mathbb{E}_{\Sigma|\mathbf{X}}\Sigma^{-1}\theta_0) - \Sigma^{-1}\theta_0\|^2. \end{aligned}$$

Furthermore, since with probability tending to 1, $\|\widehat{\Sigma}_n - \mathbf{I}_p\| = o(1)$, we also have with probability tending to 1, $\lambda^*((n\widehat{\Sigma}_n+\Lambda)/(n+\nu-p-1), \theta_0, \delta) = (1+o(1))\lambda^*(\mathbf{I}_p, \theta_0, \delta)$. Therefore, denote δ_1^* and δ_2^* be the δ's such that $\lambda^*(\mathbf{I}_p, \theta_0, \delta) = 0^+$ and $\lambda^*(\mathbf{I}_p, \theta_0, \delta) = \epsilon$ respectively, then when $\delta \in (\delta_1^* + \varepsilon, \delta_2^* - \varepsilon)$ for some small $\varepsilon > 0$, with probability tending to 1,

$$\lambda^*((n\widehat{\Sigma}_n+\Lambda)/(n+\nu-p-1), \theta_0, \delta) \in (0, \epsilon).$$

Recall that the prior distribution of Σ is $IW(\nu, \Lambda)$, so there exists some $(C_1, C_2, c) > 0$ such that with probability

tending to 1, $\lambda_{\min}(\widehat{\Sigma}_n) > C_1 + c, \lambda_{\max}(\widehat{\Sigma}_n) < C_2 - c$. Therefore, taking $0 < C_1 + c < 1 < C_2 - c < \infty$,

$$
\begin{aligned}
& \inf_{\widehat{\theta}} \sup_{\delta, \lambda_{\min}(\Sigma) > C_1, \lambda_{\max}(\Sigma) < C_2} \mathbb{E}\|\widehat{\theta} - \theta^*(\delta)\|^2 && (25)\\
= \; & \inf_{\widehat{\theta}} \sup_{\delta, \Sigma} \mathbb{E}\|\widehat{\theta} - \theta^*(\delta)\|^2 1_{\{\lambda_{\min}(\Sigma) > C_1, \lambda_{\max}(\Sigma) < C_2\}} && (26)\\
\geq \; & (1 + o(1)) \sup_{\delta} \mathbb{E}\left[1_{\{\lambda_{\min}(\widehat{\Sigma}_n) > C_1 + c, \lambda_{\max}(\widehat{\Sigma}_n) < C_2 - c\}} \mathbb{E}_{\Sigma|\mathbf{X}} \|\mathbb{E}_{\theta_0, \Sigma|\mathbf{X}, \mathbf{y}}(\theta^*) - \mathbb{E}_{\theta_0|\mathbf{X}, \mathbf{y}}[\theta^*|\Sigma]\|^2\right] && (27)\\
\geq \; & (1 + o(1)) \sup_{\delta \in (\delta_1^* + \varepsilon, \delta_2^* - \varepsilon)} \mathbb{E}\Bigg[1_{\{\lambda^*((n\widehat{\Sigma}_n + \Lambda)/(n + \nu - p - 1), \theta_0, \delta) \in (0, \epsilon)\}} 1_{\{\lambda_{\min}(\widehat{\Sigma}_n) > C_1 + c, \lambda_{\max}(\widehat{\Sigma}_n) < C_2 - c\}} \\
& \qquad \times \mathbb{E}_{\Sigma|\mathbf{X}} \|\mathbb{E}_{\theta_0, \Sigma|\mathbf{X}, \mathbf{y}}(\theta^*) - \mathbb{E}_{\theta_0|\mathbf{X}, \mathbf{y}}[\theta^*|\Sigma]\|^2\Bigg] && (28)\\
= \; & \Omega\left(\frac{p\|\theta_0\|^2}{n}\right).
\end{aligned}
$$

From (25) to (26), we use the fact that the exact choice of Σ in (25) will automatically leads to $1_{\{\lambda_{\min}(\Sigma) > C_1, \lambda_{\max}(\Sigma) < C_2\}} = 1$, thus moving the eigenvalue conditions from sup to indicator function does not change the result.

From (26) to (27), we change from "choosing the exact Σ" to "Σ satisfies a prior distribution", so the equality becomes inequality. Further, since under our choice of prior distribution of Σ, $\Sigma|\widehat{\Sigma}_n \to \widehat{\Sigma}_n$, we replace $1_{\{\lambda_{\min}(\Sigma) > C_1, \lambda_{\max}(\Sigma) < C_2\}}$ to $1_{\{\lambda_{\min}(\widehat{\Sigma}_n) > C_1 + c, \lambda_{\max}(\widehat{\Sigma}_n) < C_2 - c\}}$. The estimator $\widehat{\theta}$ is eliminated due to (23).

From (27) to (28), we restrict the choice of δ into a certain range. □

Lemma 6. *When $(p \log n)/n \to 0$, and all eigenvalues of $\widehat{\Sigma}_n$ are finite and bounded away from zero,*

$$
\begin{aligned}
& \psi(0) = \theta_0^\top \mathbf{V}_n \theta_0, \\
& \frac{\partial \psi(\lambda)}{\partial \lambda} \leq 0, \quad \left.\frac{\partial \psi(\lambda)}{\partial \lambda}\right|_{\lambda = 0} = -\Theta(\theta_0^\top \mathbf{V}_n \theta_0), \\
& \frac{\partial^2 \psi(\lambda)}{\partial \lambda^2} \geq 0,
\end{aligned}
$$

Proof of Lemma 6. Recall that the definition of ψ is

$$
\psi(\lambda) = \mathbb{E}_{\Sigma|\mathbf{X}} \|(\mathbb{E}_{\Sigma|\mathbf{X}}(\Sigma + \lambda \mathbf{I}_p)^{-1}\theta_0) - (\Sigma + \lambda \mathbf{I}_p)^{-1}\theta_0\|^2,
$$

thus when $\lambda = 0$, we have

$$
\psi(0) = \mathbb{E}_{\Sigma|\mathbf{X}} \left\| \left[\Sigma^{-1} - \mathbb{E}_{\Sigma|\mathbf{X}}(\Sigma^{-1})\right] \theta_0 \right\|^2 = \theta_0^\top \mathbf{V}_n \theta_0.
$$

On the other hand,

$$
\begin{aligned}
\frac{\partial \psi(\lambda)}{\partial \lambda} &= \frac{\partial}{\partial \lambda} \mathbb{E}_{\Sigma|\mathbf{X}} \|(\mathbb{E}_{\Sigma|\mathbf{X}}(\Sigma + \lambda \mathbf{I}_p)^{-1}\theta_0) - (\Sigma + \lambda \mathbf{I}_p)^{-1}\theta_0\|^2 \\
&= \mathbb{E}_{\Sigma|\mathbf{X}} \frac{\partial}{\partial \lambda} \left\|(\mathbb{E}_{\Sigma|\mathbf{X}}(\Sigma + \lambda \mathbf{I}_p)^{-1}\theta_0) - (\Sigma + \lambda \mathbf{I}_p)^{-1}\theta_0\right\|^2 \\
&= 2\mathbb{E}_{\Sigma|\mathbf{X}} \left[(\mathbb{E}_{\Sigma|\mathbf{X}}(\Sigma + \lambda \mathbf{I}_p)^{-1}\theta_0) - (\Sigma + \lambda \mathbf{I}_p)^{-1}\theta_0\right]^\top \frac{\partial}{\partial \lambda} \left[(\mathbb{E}_{\Sigma|\mathbf{X}}(\Sigma + \lambda \mathbf{I}_p)^{-1}\theta_0) - (\Sigma + \lambda \mathbf{I}_p)^{-1}\theta_0\right] \\
&= -2\mathbb{E}_{\Sigma|\mathbf{X}} \left[(\mathbb{E}_{\Sigma|\mathbf{X}}(\Sigma + \lambda \mathbf{I}_p)^{-1}\theta_0) - (\Sigma + \lambda \mathbf{I}_p)^{-1}\theta_0\right]^\top \left[(\mathbb{E}_{\Sigma|\mathbf{X}}(\Sigma + \lambda \mathbf{I}_p)^{-2}\theta_0) - (\Sigma + \lambda \mathbf{I}_p)^{-2}\theta_0\right] \\
&= 2(\mathbb{E}_{\Sigma|\mathbf{X}}(\Sigma + \lambda \mathbf{I}_p)^{-1}\theta_0)^\top (\mathbb{E}_{\Sigma|\mathbf{X}}(\Sigma + \lambda \mathbf{I}_p)^{-2}\theta_0) - 2\mathbb{E}_{\Sigma|\mathbf{X}} \theta_0^\top (\Sigma + \lambda \mathbf{I}_p)^{-3}\theta_0 \\
&\leq 0,
\end{aligned}
$$

$$\begin{aligned}\frac{\partial^2\psi(\lambda)}{\partial\lambda^2} &= \frac{\partial^2}{\partial\lambda^2}\mathbb{E}_{\Sigma|\mathbf{X}}\|(\mathbb{E}_{\Sigma|\mathbf{X}}(\Sigma+\lambda\mathbf{I}_p)^{-1}\theta_0)-(\Sigma+\lambda\mathbf{I}_p)^{-1}\theta_0\|^2\\ &= 2\mathbb{E}_{\Sigma|\mathbf{X}}\left[(\mathbb{E}_{\Sigma|\mathbf{X}}(\Sigma+\lambda\mathbf{I}_p)^{-2}\theta_0)-(\Sigma+\lambda\mathbf{I}_p)^{-2}\theta_0\right]^\top\left[(\mathbb{E}_{\Sigma|\mathbf{X}}(\Sigma+\lambda\mathbf{I}_p)^{-2}\theta_0)-(\Sigma+\lambda\mathbf{I}_p)^{-2}\theta_0\right]\\ &\quad +4\mathbb{E}_{\Sigma|\mathbf{X}}\left[(\mathbb{E}_{\Sigma|\mathbf{X}}(\Sigma+\lambda\mathbf{I}_p)^{-1}\theta_0)-(\Sigma+\lambda\mathbf{I}_p)^{-1}\theta_0\right]^\top\left[(\mathbb{E}_{\Sigma|\mathbf{X}}(\Sigma+\lambda\mathbf{I}_p)^{-3}\theta_0)-(\Sigma+\lambda\mathbf{I}_p)^{-3}\theta_0\right]\\ &\geq 0.\end{aligned}$$

When $(p\log n)/n\to 0$, and all eigenvalues of $\widehat{\Sigma}_n$ are finite and bounded away from zero,

$$\begin{aligned}&\theta_0^\top\left(\mathbb{E}_{\Sigma|\mathbf{X}}\Sigma^{-1}\mathbb{E}_{\Sigma|\mathbf{X}}\Sigma^{-2}-\mathbb{E}_{\Sigma|\mathbf{X}}\Sigma^{-3}\right)\theta_0\\ =\;&\theta_0^\top\left(-\mathbb{E}_{\Sigma|\mathbf{X}}(\Sigma^{-1}-\mathbb{E}_{\Sigma|\mathbf{X}}\Sigma^{-1})^3-2\mathbb{E}_{\Sigma|\mathbf{X}}\Sigma^{-1}\mathbb{E}_{\Sigma|\mathbf{X}}(\Sigma^{-1}-\mathbb{E}_{\Sigma|\mathbf{X}}\Sigma^{-1})^2\right)\theta_0\\ =\;&-\Theta(1)\theta_0^\top\mathbf{V}_n\theta_0.\end{aligned}$$

□

Proof of Theorem 1. In Lemma 4 and 5, we obtain two lower bounds for $\mathbb{E}\|\widehat{\theta}-\theta^*\|^2$, therefore the final lower bound just takes the larger one of these two bounds.

□

C.2 Theorem 2

Proof of Theorem 2. Similar as Theorem 1, we have the following decomposition:

$$\begin{aligned}&\inf_{\widehat{\theta}}\sup_{\delta,\|\theta_0\|\leq R,\|\theta_0\|_0\leq s,\Sigma}\mathbb{E}\|\widehat{\theta}-\theta^*\|^2\\ \geq\;&\left(\inf_{\widehat{\theta}}\sup_{\delta=0,\|\theta_0\|\leq R,\|\theta_0\|_0\leq s,\Sigma=\mathbf{I}_p}\mathbb{E}\|\widehat{\theta}-\theta^*\|^2\right)\vee\left(\inf_{\widehat{\theta}}\sup_{\delta,\theta_0=(1,0,0,\ldots)^\top,\Sigma}\mathbb{E}\|\widehat{\theta}-\theta^*\|^2\right).\end{aligned}\tag{29}$$

For the first part of bound in (29), it is directly followed from Proposition 4.3 of Verzelen (2010): for some constant $L>0$,

$$\inf_{\widehat{\theta}}\sup_{\delta=0,\|\theta_0\|\leq R,\|\theta_0\|_0\leq s,\Sigma=\mathbf{I}_p}\mathbb{E}\|\widehat{\theta}-\theta^*\|^2\geq(sLR^2)\wedge\frac{sL\sigma^2(1+\log(p/s))}{n}.$$

Since we assume $\|\theta_0\|/\sigma$ to be bounded away from zero, the above result becomes

$$\inf_{\widehat{\theta}}\sup_{\delta=0,\|\theta_0\|\leq R,\|\theta_0\|_0\leq s,\Sigma=\mathbf{I}_p}\mathbb{E}\|\widehat{\theta}-\theta^*\|^2=\Omega\left(\frac{s\sigma^2(1+\log(p/s))}{n}\right).$$

The above bound also holds for $\delta>0$ since when $\Sigma=\mathbf{I}_p$, $\theta^*=(1-\kappa(\delta))\theta_0$.

For the second part of bound in (29), we use Assouad's method and modify the proof in Cai et al. (2010). Consider $\Sigma_1=\mathbf{I}_p$ and $\Sigma_2=\mathbf{I}_p+\mathbf{D}$, where $\mathbf{D}_{1,j}=\mathbf{D}_{j,1}=n^{-(\alpha+1)/(2\alpha+1)}$ for $j=1,\ldots,n^{1/(2\alpha+1)}$. Denote $k=n^{1/(2\alpha+1)}$ and $a=n^{-(\alpha+1)/(2\alpha+1)}$, then $\mathbf{D}$ is just a matrix where the first k elements in the first row and first column are a.

Denote P_Σ as the density of $N(0,\Sigma)$. Based on Assouad's Lemma, for any δ and θ_0, for some constant $C>0$ (which is independent with (δ,θ_0)),

$$\inf_{\widehat{\theta}}\sup_{\Sigma}\|\widehat{\theta}-\theta^*(\Sigma,\delta)\|^2\geq C\|\theta^*(\Sigma_1,\delta)-\theta^*(\Sigma_2,\delta)\|^2\|P_{\Sigma_1}\wedge P_{\Sigma_2}\|,$$

where $\|P_{\Sigma_1}\wedge P_{\Sigma_2}\|=\int P_{\Sigma_1}(x)\wedge P_{\Sigma_2}(x)dx$. The notation $\theta^*(\Sigma,\delta)$ is to emphasize the choice of Σ.

From Lemma 6 of Cai et al. (2010), we have

$$\|P_{\Sigma_1}\wedge P_{\Sigma_2}\|\geq c.$$

As a result, our remaining task becomes to quantify $\|\theta^*(\Sigma_1,\delta)-\theta^*(\Sigma_2,\delta)\|^2$. Consider $\theta_0=(1,0,0,...,0)^\top$, for a given δ such that $\lambda_1:=\lambda^*(\theta_0,\Sigma_1,\delta)>0$, we have

$$\lambda_1-\delta c_0\lambda_1\frac{\|(\Sigma_1+\lambda_1\mathbf{I}_p)^{-1}\theta_0\|_{\Sigma_1}}{\|(\Sigma_1+\lambda_1\mathbf{I}_p)^{-1}\Sigma_1\theta_0\|}+\delta c_0\frac{\|(\Sigma_1+\lambda_1\mathbf{I}_p)^{-1}\Sigma_1\theta_0\|}{\|(\Sigma_1+\lambda_1\mathbf{I}_p)^{-1}\theta_0\|_{\Sigma_1}}-\delta^2=0. \tag{30}$$

Similarly, denote $\lambda_2:=\lambda^*(\theta_0,\Sigma_2,\delta)$, then

$$\lambda_2-\delta c_0\lambda_2\frac{\|(\Sigma_2+\lambda_2\mathbf{I}_p)^{-1}\theta_0\|_{\Sigma_2}}{\|(\Sigma_2+\lambda_2\mathbf{I}_p)^{-1}\Sigma_2\theta_0\|}+\delta c_0\frac{\|(\Sigma_2+\lambda_2\mathbf{I}_p)^{-1}\Sigma_2\theta_0\|}{\|(\Sigma_2+\lambda_2\mathbf{I}_p)^{-1}\theta_0\|_{\Sigma_2}}-\delta^2=0. \tag{31}$$

It is easy to observe that $\lambda_1-\lambda_2=O(\|\Sigma_1-\Sigma_2\|)$. However, since our aim is to figure out the lower bound of $\|\widehat{\theta}-\theta^*\|$, we want the lower bound of $|\lambda_1-\lambda_2|$. To characterize $\lambda_1-\lambda_2$ in details, observe that

$$\begin{aligned}
&\|(\Sigma_2+\lambda_2\mathbf{I}_p)^{-1}\theta_0\|_{\Sigma_2}-\|(\Sigma_1+\lambda_2\mathbf{I}_p)^{-1}\theta_0\|_{\Sigma_1}\\
=\;&\frac{1}{2\|(\Sigma_1+\lambda_2\mathbf{I}_p)^{-1}\theta_0\|_{\Sigma_1}}\left[\theta_0^\top(\Sigma_2+\lambda_2\mathbf{I}_p)^{-1}\Sigma_2(\Sigma_2+\lambda_2\mathbf{I}_p)^{-1}\theta_0-\theta_0^\top(\Sigma_1+\lambda_2\mathbf{I}_p)^{-1}\Sigma_1(\Sigma_1+\lambda_2\mathbf{I}_p)^{-1}\theta_0\right]+o\\
=\;&\frac{1}{2\|(\Sigma_1+\lambda_2\mathbf{I}_p)^{-1}\theta_0\|_{\Sigma_1}}\theta_0^\top\left[(\Sigma_2+\lambda_2\mathbf{I}_p)^{-1}-(\Sigma_1+\lambda_2\mathbf{I}_p)^{-1}-\lambda_2(\Sigma_2+\lambda_2\mathbf{I}_p)^{-2}+\lambda_2(\Sigma_1+\lambda_2\mathbf{I}_p)^{-2}\right]\theta_0+o\\
=\;&\frac{\theta_0^\top\left[-(\Sigma_2+\lambda_2\mathbf{I}_p)^{-1}\mathbf{D}(\Sigma_1+\lambda_2\mathbf{I}_p)^{-1}+\lambda_2(\Sigma_2+\lambda_2\mathbf{I}_p)^{-1}\mathbf{D}(\Sigma_1+\lambda_2\mathbf{I}_p)^{-1}\left((\Sigma_2+\lambda_2\mathbf{I}_p)^{-1}+(\Sigma_1+\lambda_2\mathbf{I}_p)^{-1}\right)\right]\theta_0}{2\|(\Sigma_1+\lambda_2\mathbf{I}_p)^{-1}\theta_0\|_{\Sigma_1}}+o\\
=\;&\frac{\theta_0^\top\left[-(\Sigma_1+\lambda_2\mathbf{I}_p)^{-1}\mathbf{D}(\Sigma_1+\lambda_2\mathbf{I}_p)^{-1}+2\lambda_2(\Sigma_1+\lambda_2\mathbf{I}_p)^{-1}\mathbf{D}(\Sigma_1+\lambda_2\mathbf{I}_p)^{-2}\right]\theta_0}{2\|(\Sigma_1+\lambda_2\mathbf{I}_p)^{-1}\theta_0\|_{\Sigma_1}}+o\\
=\;&\frac{1}{2\|(\Sigma_1+\lambda_2\mathbf{I}_p)^{-1}\theta_0\|_{\Sigma_1}}\frac{\lambda_2-1}{(1+\lambda_2)^3}(2k-1)a+o\\
=\;&\frac{\lambda_2-1}{2(1+\lambda_2)^2}(2k-1)a+o,
\end{aligned}$$

and

$$\begin{aligned}
&\|(\Sigma_2+\lambda_2\mathbf{I}_p)^{-1}\Sigma_2\theta_0\|-\|(\Sigma_1+\lambda_2\mathbf{I}_p)^{-1}\Sigma_1\theta_0\|\\
=\;&\frac{1}{2\|(\Sigma_1+\lambda_2\mathbf{I}_p)^{-1}\Sigma_1\theta_0\|}\theta_0^\top\left[-2\lambda_2\left((\Sigma_2+\lambda_2\mathbf{I}_p)^{-1}-(\Sigma_1+\lambda_2\mathbf{I}_p)^{-1}\right)+\lambda_2^2\left((\Sigma_2+\lambda_2\mathbf{I}_p)^{-2}-(\Sigma_1+\lambda_2\mathbf{I}_p)^{-2}\right)\right]\theta_0+o\\
=\;&\frac{1}{2\|(\Sigma_1+\lambda_2\mathbf{I}_p)^{-1}\Sigma_1\theta_0\|}\theta_0^\top\left[2\lambda_2(\Sigma_1+\lambda_2\mathbf{I}_p)^{-1}\mathbf{D}(\Sigma_1+\lambda_2\mathbf{I}_p)^{-1}-2\lambda_2^2(\Sigma_1+\lambda_2\mathbf{I}_p)^{-1}\mathbf{D}(\Sigma_1+\lambda_2\mathbf{I}_p)^{-2}\right]\theta_0+o\\
=\;&\frac{1}{2\|(\Sigma_1+\lambda_2\mathbf{I}_p)^{-1}\Sigma_1\theta_0\|}\frac{2\lambda_2}{(1+\lambda_2)^3}(2k-1)a+o\\
=\;&\frac{\lambda_2}{(1+\lambda_2)^2}(2k-1)a+o.
\end{aligned}$$

Therefore, denote $\Delta_1=A(\theta_0,\Sigma_2,\delta,\lambda_2)-A(\theta_0,\Sigma_1,\delta,\lambda_2)$, with

$$A(\theta_0,\Sigma,\delta,\lambda)=\frac{\|(\Sigma+\lambda\mathbf{I}_p)^{-1}\Sigma\theta_0\|}{\|(\Sigma+\lambda\mathbf{I}_p)^{-1}\theta_0\|_\Sigma},$$

then

$$\begin{aligned}
A(\theta_0,\Sigma_2,\delta,\lambda_2)=\;&\left(\|(\Sigma_1+\lambda\mathbf{I}_p)^{-1}\Sigma_1\theta_0\|+\frac{\lambda_2}{(1+\lambda_2)^2}(2k-a)+o\right)\\
&\times\left(\frac{1}{\|(\Sigma_1+\lambda\mathbf{I}_p)^{-1}\theta_0\|_{\Sigma_1}}-\frac{1}{\|(\Sigma_1+\lambda\mathbf{I}_p)^{-1}\theta_0\|_{\Sigma_1}^2}\frac{\lambda_2-1}{2(1+\lambda_2)^2}(2k-a)+o\right)\\
=\;&-\frac{\|(\Sigma_1+\lambda\mathbf{I}_p)^{-1}\Sigma_1\theta_0\|}{\|(\Sigma_1+\lambda\mathbf{I}_p)^{-1}\theta_0\|_{\Sigma_1}^2}\frac{\lambda_2-1}{2(1+\lambda_2)^2}(2k-1)a+\frac{1}{\|(\Sigma_1+\lambda\mathbf{I}_p)^{-1}\theta_0\|_{\Sigma_1}}\frac{\lambda_2}{(1+\lambda_2)^2}(2k-1)a+o\\
&+A(\theta_0,\Sigma_1,\delta,\lambda_2)\\
=\;&-\frac{\lambda_2-1}{2(1+\lambda_2)}(2k-1)a+\frac{\lambda_2}{1+\lambda_2}(2k-1)a+A(\theta_0,\Sigma_1,\delta,\lambda_2)+o\\
=\;&\frac{1}{2}(2k-1)a+A(\theta_0,\Sigma_1,\delta,\lambda_2)+o.
\end{aligned}$$

Hence $\Delta_1 = (2k-1)a + o$.

Denote $\varepsilon = \lambda_2 - \lambda_1$. Note that $A(\theta_0, \Sigma_1, \delta, \lambda) = 1$ for any $\lambda \geq 0$ since $\Sigma_1 = \mathbf{I}_p$. Therefore, (30) minus (31) leads to

$$\begin{aligned}
0 &= -\varepsilon - \delta c_0 \lambda_1 \frac{1}{A(\theta_0, \Sigma_1, \delta, \lambda_1)} + \delta c_0 \lambda_2 \frac{1}{A(\theta_0, \Sigma_2, \delta, \lambda_2)} - \delta c_0 \Delta_1 + A(\theta_0, \Sigma_1, \delta, \lambda_1) - A(\theta_0, \Sigma_1, \delta, \lambda_2) \\
&= -\varepsilon - \delta c_0 \lambda_1 \frac{1}{A(\theta_0, \Sigma_1, \delta, \lambda_1)} + \delta c_0 (\lambda_1 + \varepsilon) \left[\frac{1}{A(\theta_0, \Sigma_1, \delta, \lambda_2)} - \frac{\Delta_1}{A^2(\theta_0, \Sigma_1, \delta, \lambda_2)} \right] - \delta c_0 \Delta_1 + o \\
&= -\varepsilon + \delta c_0 \lambda_1 \left(\frac{1}{A(\theta_0, \Sigma_1, \delta, \lambda_2)} - \frac{1}{A(\theta_0, \Sigma_1, \delta, \lambda_1)} \right) + \varepsilon \frac{\delta c_0}{A(\theta_0, \Sigma_1, \delta, \lambda_2)} - \frac{\lambda_1 \delta c_0 \Delta_1}{A^2(\theta_0, \Sigma_1, \delta, \lambda_2)} - \delta c_0 \Delta_1 + o \\
&= -\varepsilon + \varepsilon \frac{\delta c_0}{A(\theta_0, \Sigma_1, \delta, \lambda_2)} - \frac{\lambda_1 \delta c_0 \Delta_1}{A^2(\theta_0, \Sigma_1, \delta, \lambda_2)} - \delta c_0 \Delta_1 + o \\
&= -\varepsilon + \varepsilon \delta c_0 - \lambda_1 \delta c_0 \Delta_1 - \delta c_0 \Delta_1 + o.
\end{aligned}$$

Consequently,

$$\varepsilon = \delta c_0 \frac{\lambda_1 + 1}{\delta c_0 - 1} \Delta_1 + o,$$

and hence

$$\begin{aligned}
& (\Sigma_1 + \lambda_1 \mathbf{I}_p)^{-1} \Sigma_1 \theta_0 - (\Sigma_2 + \lambda_2 \mathbf{I}_p)^{-1} \Sigma_2 \theta_0 \\
= \; & (\Sigma_1 + \lambda_1 \mathbf{I}_p)^{-1} \Sigma_1 \theta_0 - (\Sigma_2 + \lambda_2 \mathbf{I}_p)^{-1} \Sigma_1 \theta_0 + (\Sigma_2 + \lambda_2 \mathbf{I}_p)^{-1} \Sigma_1 \theta_0 - (\Sigma_2 + \lambda_2 \mathbf{I}_p)^{-1} \Sigma_2 \theta_0 \\
= \; & (\Sigma_1 + \lambda_1 \mathbf{I}_p)^{-1} (\mathbf{D} + \varepsilon \mathbf{I}_p)(\Sigma_2 + \lambda_1 \mathbf{I}_p)^{-1} \Sigma_1 \theta_0 - (\Sigma_2 + \lambda_2 \mathbf{I}_p)^{-1} \mathbf{D} \theta_0 \\
= \; & (\Sigma_1 + \lambda_1 \mathbf{I}_p)^{-1} (\mathbf{D} + \varepsilon \mathbf{I}_p)(\Sigma_1 + \lambda_1 \mathbf{I}_p)^{-1} \Sigma_1 \theta_0 - (\Sigma_1 + \lambda_1 \mathbf{I}_p)^{-1} \mathbf{D} \theta_0 + o \\
= \; & \frac{1}{(1+\lambda_1)^2} (\mathbf{D} + \varepsilon \mathbf{I}_p) \theta_0 - \frac{1}{1+\lambda_1} \mathbf{D} \theta_0 + o.
\end{aligned}$$

Since

$$\varepsilon \theta_0 + \mathbf{D} \theta_0 = \begin{bmatrix} \varepsilon + a \\ a \\ \cdots \\ a \\ 0 \\ \cdots \end{bmatrix},$$

and recall that $k = n^{1/(2\alpha+1)}$ and $a = n^{-(\alpha+1)/(2\alpha+1)}$, when δ is chosen such that $\varepsilon = \Theta(ka)$, we have

$$\left\| (\Sigma_1 + \lambda_1 \mathbf{I}_p)^{-1} \Sigma_1 \theta_0 - (\Sigma_2 + \lambda_2 \mathbf{I}_p)^{-1} \Sigma_2 \theta_0 \right\|^2 = \Omega(k^2 a^2) = \Omega\left(n^{-\frac{2\alpha}{2\alpha+1}} \right).$$

As a result, we conclude that

$$\inf_{\widehat{\theta}} \sup_{\delta, \|\theta_0\| \leq R, \|\theta_0\|_0 \leq s, \Sigma} \|\widehat{\theta} - \theta^*\|^2 = \Omega\left(R^2 n^{-\frac{2\alpha}{2\alpha+1}} \right). \tag{32}$$

□

C.3 Proof of Theorem 3

Proof of Theorem 3. There exacts a constant $\delta' > \delta_1$ such that as $\delta \geq \delta'$, $\widehat{\theta} = \theta^* = 0$. Thus, we have $R_0(\widehat{\theta}, \delta) - R_0(\theta^*, \delta) = 0$ when $\delta \geq \delta'$. Next, we will show for any $\delta \leq \delta'$, (7) always hold.

To simplify notations, denote $\widehat{\theta}(\lambda) = \widehat{\theta}_0 - (\widehat{\Sigma}/\lambda + \mathbf{I}_p)^{-1} \widehat{\theta}_0$ and $\theta(\lambda) = \theta_0 - (\Sigma/\lambda + \mathbf{I}_p)^{-1} \theta_0$, $\widehat{R}(\theta, \delta) = R_n(\theta, \widehat{\theta}_0, \widehat{\Sigma}, \delta)$ as in (6). Then

$$R_0(\widehat{\theta}(\lambda), \delta) - \widehat{R}_0(\widehat{\theta}(\lambda), \delta) = \|\widehat{\theta}(\lambda) - \theta_0\|_\Sigma^2 + 2\delta c_0 \|\widehat{\theta}(\lambda)\| \|\widehat{\theta}(\lambda) - \theta_0\|_\Sigma - \|\widehat{\theta}(\lambda) - \widehat{\theta}_0\|_{\widehat{\Sigma}}^2 - 2\delta c_0 \|\widehat{\theta}(\lambda)\| \|\widehat{\theta}(\lambda) - \widehat{\theta}_0\|_{\widehat{\Sigma}}.$$

From the formula of $\widehat{\theta}(\lambda)$, we have $\sup_\lambda \|2\widehat{\theta}(\lambda) - \theta_0 - \widehat{\theta}_0\|$ and $\|\widehat{\theta}(\lambda) - \widehat{\theta}_0\|$ are always in $O(\|\theta_0\|)$, therefore

$$\begin{aligned}\left|\|\widehat{\theta}(\lambda) - \theta_0\|_\Sigma^2 - \|\widehat{\theta}(\lambda) - \widehat{\theta}_0\|_{\widehat{\Sigma}}^2\right| &= (\widehat{\theta}_0 - \theta_0)^\top \Sigma(2\widehat{\theta}(\lambda) - \theta_0 - \widehat{\theta}_0) - \|\widehat{\theta}(\lambda) - \widehat{\theta}_0\|_{\widehat{\Sigma}-\Sigma}^2 \\ &= O(\|\widehat{\theta}_0 - \theta_0\|\|\theta(\lambda) - \theta_0\|) + O(\|\theta(\lambda) - \theta_0\|^2\|\widehat{\Sigma} - \Sigma\|).\end{aligned}$$

Based on similar arguments,

$$\begin{aligned}\left|\|\widehat{\theta}(\lambda) - \theta_0\|_\Sigma - \|\widehat{\theta}(\lambda) - \widehat{\theta}_0\|_{\widehat{\Sigma}}\right| &= \left|\|\widehat{\theta}(\lambda) - \theta_0\|_\Sigma - \|\widehat{\theta}(\lambda) - \widehat{\theta}_0\|_\Sigma + \|\widehat{\theta}(\lambda) - \widehat{\theta}_0\|_\Sigma - \|\widehat{\theta}(\lambda) - \widehat{\theta}_0\|_{\widehat{\Sigma}}\right| \\ &= O(\|\widehat{\theta}_0 - \theta_0\|) + O\left(\|\theta(\lambda) - \theta_0\|\sqrt{\|\widehat{\Sigma} - \Sigma\|}\right).\end{aligned}$$

Thus,

$$\left|\|\widehat{\theta}(\lambda)\|\|\widehat{\theta}(\lambda) - \theta_0\|_\Sigma - \|\widehat{\theta}(\lambda)\|\|\widehat{\theta}(\lambda) - \widehat{\theta}_0\|_{\widehat{\Sigma}}\right| = O(\|\theta(\lambda)\|\|\widehat{\theta}_0 - \theta_0\|) + O\left(\|\theta(\lambda)\|\|\theta(\lambda) - \theta_0\|\sqrt{\|\widehat{\Sigma} - \Sigma\|}\right).$$

Therefore, uniformly for all λ:

$$\begin{aligned}&R_0(\widehat{\theta}(\lambda), \delta) - \widehat{R}_0(\widehat{\theta}(\lambda), \delta) \qquad (33)\\ =\ &O(\|\widehat{\theta}_0 - \theta_0\|\|\theta(\lambda) - \theta_0\|) + O(\|\theta(\lambda) - \theta_0\|^2\|\widehat{\Sigma} - \Sigma\|) + O(\delta\|\theta(\lambda)\|\|\widehat{\theta}_0 - \theta_0\|) + O\left(\delta\|\theta(\lambda)\|\|\theta(\lambda) - \theta_0\|\sqrt{\|\widehat{\Sigma} - \Sigma\|}\right) \qquad (34)\end{aligned}$$

When $\delta \to \infty$, $\delta\|\theta(\lambda)\|/\|\theta_0\|$ converges to some constant. For any $\delta > 0$, $\delta\|\theta^*\|/\|\theta_0\|$ is finite. As a result,

$$R_0(\widehat{\theta}(\lambda), \delta) - \widehat{R}_0(\widehat{\theta}(\lambda), \delta) = O\left(\|\widehat{\theta}_0 - \theta_0\|\|\theta_0\|\right) + O\left(\|\theta_0\|\sqrt{\|\widehat{\Sigma} - \Sigma\|}\right). \qquad (35)$$

By similar derivations, we can get uniformly for all λ:

$$R_0(\theta(\lambda), \delta) - \widehat{R}_0(\theta(\lambda), \delta) = O\left(\|\widehat{\theta}_0 - \theta_0\|\|\theta_0\|\right) + O\left(\|\theta_0\|\sqrt{\|\widehat{\Sigma} - \Sigma\|}\right). \qquad (36)$$

From the definition of R and $\widehat{R}$, we have

$$R_0(\widehat{\theta}, \delta) - R_0(\theta^*, \delta) = R_0(\widehat{\theta}, \delta) - \widehat{R}_0(\widehat{\theta}, \delta) + \widehat{R}_0(\widehat{\theta}, \delta) - \widehat{R}_0(\theta^*, \delta) + \widehat{R}_0(\theta^*, \delta) - R_0(\theta^*, \delta).$$

Since $\widehat{\lambda}$ is the minimizer of $\widehat{R}(\widehat{\theta}(\lambda), \delta)$, it becomes

$$\widehat{R}(\widehat{\theta}, \delta) - \widehat{R}(\theta^*, \delta) < 0.$$

By the universal bounds in (35), (36), we obtain

$$R_0(\widehat{\theta}, \delta) - R_0(\theta^*, \delta) = O\left(\|\widehat{\theta}_0 - \theta_0\|\|\theta_0\|\right) + O\left(\|\theta_0\|\sqrt{\|\widehat{\Sigma} - \Sigma\|}\right).$$

□

C.4 Theorem 4

Proof of Theorem 4. In the proof, we first assume $\|\theta_0\|$ and σ^2 are finite, then extend to unbounded $\|\theta_0\|$ and σ^2 in the end. For simplification, we define

$$R_0(\theta_1, \theta_2, \Sigma) = \|\theta_1 - \theta_2\|_\Sigma^2 + 2\delta c_0\|\theta_1\|\|\theta_1 - \theta_2\|_\Sigma + \delta^2\|\theta_1\|_2^2.$$

We will prove the theorem based on different scenarios of δ. Denote θ^*, $\widetilde{\theta}$, and $\widehat{\theta}$ as the minimizers of $R_0(\cdot, \theta_0, \Sigma)$, $R_0(\cdot, \widehat{\theta}_0, \Sigma)$, and $R_0(\cdot, \widehat{\theta}_0, \widehat{\Sigma})$. Then we consider the partial derivative of $R_0(\theta_1, \theta_2, \Sigma)$,

$$\frac{\partial R_0(\theta_1, \theta_2, \Sigma)}{\partial \theta_1} = 2\left[(1 + \delta c A(\theta_1, \theta_2, \Sigma))\,\Sigma(\theta_1 - \theta_2) + \left(\delta c \frac{1}{A(\theta_1, \theta_2, \Sigma)} + \delta^2\right)\theta_1\right],$$

where $A(\theta_1, \theta_2, \Sigma) = \|\theta_1\|/\|\theta_1 - \theta_2\|_\Sigma$.

Case 1: When $\delta_1 < \delta < \delta_2$, based on Proposition 1, the minimizer θ^* is neither θ_0 nor 0. Thus, for large n (such that the probability of $\widehat{\theta}$ being 0 or $\widehat{\theta}_0$ can be ignored), from the first order optimality condition of θ^*, $\widetilde{\theta}$, and $\widehat{\theta}$, we first have

$$\begin{aligned}
\mathbf{0} &= \frac{\partial R_0}{2\partial\theta_1}(\widehat{\theta},\widehat{\theta}_0,\widehat{\Sigma}) - \frac{\partial R_0}{2\partial\theta_1}(\theta^*,\theta_0,\Sigma) \\
&= \left[\left(1+\delta c A(\widehat{\theta},\widehat{\theta}_0,\widehat{\Sigma})\right)\widehat{\Sigma}(\widehat{\theta}-\widehat{\theta}_0) + \left(\delta c\frac{1}{A(\widehat{\theta},\widehat{\theta}_0,\widehat{\Sigma})}+\delta^2\right)\widehat{\theta}\right] - \\
&\quad \left[\left(1+\delta c A(\theta^*,\theta_0,\Sigma)\right)\Sigma(\theta^*-\theta_0) + \left(\delta c\frac{1}{A(\theta^*,\theta_0,\Sigma)}+\delta^2\right)\theta^*\right] \\
&= \left[\left(1+\delta c A(\widehat{\theta},\widehat{\theta}_0,\widehat{\Sigma})\right)\Sigma(\widehat{\theta}-\widehat{\theta}_0) + \left(\delta c\frac{1}{A(\widehat{\theta},\widehat{\theta}_0,\widehat{\Sigma})}+\delta^2\right)\widehat{\theta}\right] - \\
&\quad \left[\left(1+\delta c A(\theta^*,\theta_0,\Sigma)\right)\Sigma(\theta^*-\theta_0) + \left(\delta c\frac{1}{A(\theta^*,\theta_0,\Sigma)}+\delta^2\right)\theta^*\right] \\
&\quad + \left(1+\delta c A(\widehat{\theta},\widehat{\theta}_0,\widehat{\Sigma})\right)(\widehat{\Sigma}-\Sigma)(\widehat{\theta}-\widehat{\theta}_0). \qquad (37)
\end{aligned}$$

Consider the Taylor expansions of $A(\widehat{\theta},\widehat{\theta}_0,\widehat{\Sigma})$, $\frac{1}{A(\widehat{\theta},\widehat{\theta}_0,\widehat{\Sigma})}$ at $(\theta^*,\theta_0,\Sigma)$. For both A and $1/A$, we observe that

$$\begin{aligned}
A(\widehat{\theta},\widehat{\theta}_0,\widehat{\Sigma}) &= A(\theta^*,\theta_0,\Sigma) + \left(\frac{\partial A}{\partial\theta_1}(\theta^*,\theta_0,\Sigma)\right)^\top(\widehat{\theta}-\theta^*) + \left(\frac{\partial A}{\partial\theta_2}(\theta^*,\theta_0,\Sigma)\right)^\top(\widehat{\theta}_0-\theta_0) \\
&\quad + \frac{(\theta^*-\theta_0)^\top(\widehat{\Sigma}-\Sigma)(\theta^*-\theta_0)}{2\|\theta^*-\theta_0\|_\Sigma\|\theta^*\|} + O\left(\frac{\|\widehat{\theta}-\theta^*\|^2}{\|\theta_0\|^2}\right) \\
\frac{1}{A(\widehat{\theta},\widehat{\theta}_0,\widehat{\Sigma})} &= \frac{1}{A(\theta^*,\theta_0,\Sigma)} + \left(\frac{\partial 1/A}{\partial\theta_1}(\theta^*,\theta_0,\Sigma)\right)^\top(\widehat{\theta}-\theta^*) + \left(\frac{\partial 1/A}{\partial\theta_2}(\theta^*,\theta_0,\Sigma)\right)^\top(\widehat{\theta}_0-\theta_0) \\
&\quad - \|\theta^*\|\frac{(\theta^*-\theta_0)^\top(\widehat{\Sigma}-\Sigma)(\theta^*-\theta_0)}{2\|\theta^*-\theta_0\|_\Sigma^3} + O\left(\frac{\|\widehat{\theta}-\theta^*\|^2}{\|\theta_0\|^2}\right)
\end{aligned}$$

Moreover,

$$\begin{aligned}
&\left(1+\delta c A(\widehat{\theta},\widehat{\theta}_0,\widehat{\Sigma})\right)(\widehat{\Sigma}-\Sigma)(\widehat{\theta}-\widehat{\theta}_0) \\
=\ &\left(1+\delta c A(\theta^*,\theta_0,\Sigma)\right)(\widehat{\Sigma}-\Sigma)(\theta^*-\theta_0) + O(\|\widehat{\theta}-\theta^*\|^2/\|\theta_0\|) + O(\|\widehat{\theta}_0-\theta_0\|^2/\|\theta_0\|) + O(\|\widehat{\Sigma}-\Sigma\|^2\|\theta_0\|)
\end{aligned}$$

Combined with (37) yields

$$\begin{aligned}
&\Sigma(\widehat{\theta}-\theta^*+\theta_0-\widehat{\theta}_0) + \delta c A(\theta^*,\theta_0,\Sigma)\Sigma(\widehat{\theta}-\theta^*+\theta_0-\widehat{\theta}_0) + \left(\frac{\delta c}{A(\theta^*,\theta_0,\Sigma)}+\delta^2\right)(\widehat{\theta}-\theta^*) \\
&+\delta c\Sigma(\theta^*-\theta_0)\left(\frac{\partial A}{\partial\theta_1}(\theta^*,\theta_0,\Sigma)\right)^\top(\widehat{\theta}-\theta^*) + \delta c\theta^*\left(\frac{\partial 1/A}{\partial\theta_1}(\theta^*,\theta_0,\Sigma)\right)^\top(\widehat{\theta}-\theta^*) + \\
&\delta c\Sigma(\theta^*-\theta_0)\left(\frac{\partial A}{\partial\theta_2}(\theta^*,\theta_0,\Sigma)\right)^\top(\widehat{\theta}_0-\theta_0) + \delta c\theta^*\left(\frac{\partial 1/A}{\partial\theta_2}(\theta^*,\theta_0,\Sigma)\right)^\top(\widehat{\theta}_0-\theta_0) \\
&+\delta c\frac{(\theta^*-\theta_0)^\top(\widehat{\Sigma}-\Sigma)(\theta^*-\theta_0)}{\|\theta^*-\theta_0\|_\Sigma\|\theta^*\|}\Sigma(\theta^*-\theta_0) - \delta c\|\theta^*\|\frac{(\theta^*-\theta_0)^\top(\widehat{\Sigma}-\Sigma)(\theta^*-\theta_0)}{\|\theta^*-\theta_0\|_\Sigma^3}\theta^* \\
&+\left(1+\delta c A(\theta^*,\theta_0,\Sigma)\right)(\widehat{\Sigma}-\Sigma)(\theta^*-\theta_0) \\
&+O\left(\frac{\|\widehat{\theta}-\theta^*\|^2}{\|\theta_0\|}\right) = 0.
\end{aligned}$$

Thus the difference between $\widehat{\theta}$ and θ^* is dominated by $\widehat{\theta}_0 - \theta_0$, and $\widehat{\Sigma} - \Sigma$:

$$\begin{aligned}\widehat{\theta} - \theta^* &= [\mathbf{H}(\theta^*, \theta_0, \Sigma)]^{-1} \left[\mathbf{M}(\theta^*, \theta_0, \Sigma)(\widehat{\theta}_0 - \theta_0) - \delta c \frac{(\theta^* - \theta_0)^\top (\widehat{\Sigma} - \Sigma)(\theta^* - \theta_0)}{2\|\theta^* - \theta_0\|_\Sigma \|\theta^*\|} \Sigma(\theta^* - \theta_0) \right. \\ &\quad \left. + \delta c \|\theta^*\| \frac{(\theta^* - \theta_0)^\top (\widehat{\Sigma} - \Sigma)(\theta^* - \theta_0)}{2\|\theta^* - \theta_0\|_\Sigma^3} \theta^* - (1 + \delta c A(\theta^*, \theta_0, \Sigma)) (\widehat{\Sigma} - \Sigma)(\theta^* - \theta_0) \right] \\ &\quad + O\left(\frac{\|\widehat{\theta} - \theta^*\|^2}{\|\theta_0\|} \right), \end{aligned} \tag{38}$$

where

$$\begin{aligned}\mathbf{H}(\theta^*, \theta_0, \Sigma) &= \Sigma + \delta c A(\theta^*, \theta_0, \Sigma)\Sigma + \left(\frac{\delta c}{A(\theta^*, \theta_0, \Sigma)} + \delta^2 \right) \mathbf{I}_p + \delta c \Sigma(\theta^* - \theta_0) \left(\frac{\partial A}{\partial \theta_1}(\theta^*, \theta_0, \Sigma) \right)^\top \\ &\quad + \delta c \theta^* \left(\frac{\partial 1/A}{\partial \theta_1}(\theta^*, \theta_0, \Sigma) \right)^\top \end{aligned}$$

is the Hessian matrix of the population risk defined in (11) at point $\theta = \theta^*$, which is positive-definite by Proposition 1.

$$\begin{aligned}\mathbf{M}(\theta^*, \theta_0, \Sigma) &= \Sigma + \delta c A(\theta^*, \theta_0, \Sigma)\Sigma - \delta c \Sigma(\theta^* - \theta_0) \left(\frac{\partial A}{\partial \theta_2}(\theta^*, \theta_0, \Sigma) \right)^\top - \delta c \theta^* \left(\frac{\partial 1/A}{\partial \theta_2}(\theta^*, \theta_0, \Sigma) \right)^\top \\ &= \Sigma + \delta c A(\theta^*, \theta_0, \Sigma)\Sigma + \frac{\delta c A(\theta^*, \theta_0, \Sigma)}{\|\theta^* - \theta_0\|_\Sigma^2} \Sigma(\theta^* - \theta_0)(\theta^* - \theta_0)^\top \Sigma \\ &\quad + \delta \frac{c}{A(\theta^*, \theta_0, \Sigma)\|\theta^*\|_2^2} \theta^* (\theta^*)^\top, \end{aligned}$$

which is also positive definite.

Case 2: δ is either smaller than δ_1 or larger than δ_2. Recall that $\delta_1 = \frac{c_0 \|\theta_0\|}{\sqrt{\theta_0^\top (\Sigma^{-1}) \theta_0}}$ and $\delta_2 = \frac{\sqrt{\theta_0^\top \Sigma^2 \theta_0}}{c_0 \sqrt{\theta_0^\top \Sigma \theta_0}}$.

$$\begin{aligned}\widehat{\delta}_1 - \delta_1 &= \frac{\partial \delta_1}{\partial \theta_0}(\widehat{\theta}_0 - \theta_0) + \left\langle \frac{\partial \delta_1}{\partial \Sigma}, \widehat{\Sigma} - \Sigma \right\rangle_F + O\left(\frac{\|\widehat{\theta}_0 - \theta_0\|^2}{\|\theta_0\|^2} \right) + O(\|\widehat{\Sigma} - \Sigma\|^2), \\ \widehat{\delta}_2 - \delta_2 &= \frac{\partial \delta_2}{\partial \theta_0}(\widehat{\theta}_0 - \theta_0) + \left\langle \frac{\partial \delta_2}{\partial \Sigma}, \widehat{\Sigma} - \Sigma \right\rangle_F + O\left(\frac{\|\widehat{\theta}_0 - \theta_0\|^2}{\|\theta_0\|^2} \right) + O(\|\widehat{\Sigma} - \Sigma\|^2). \end{aligned}$$

Therefore, if $\widehat{\theta}_0 - \theta_0$ and $\widehat{\Sigma} - \Sigma$ are consistent, with probability tending to one, δ will smaller than $\widehat{\delta}_1$ or greater than $\widehat{\delta}_2$. Thus, $\widehat{\theta}$ will be either $\widehat{\theta}_0$ or 0 depending on δ.

□

C.5 Theorem 5

Proof of Theorem 5. The decomposition of generalizations can be directly obtained from Taylor expansion. When $\delta < \delta_1$, since $\widehat{\delta}_1 - \delta_1 \to 0$, we have

$$\begin{aligned}R_0(\widehat{\theta}, \delta) - \widehat{R}_0(\widehat{\theta}, \delta) &= \mathbf{1}\{\widehat{\delta}_1 \geq \delta\} \left[\|\widehat{\theta}_0 - \theta_0\|_\Sigma^2 - \|\widehat{\theta}_0 - \widehat{\theta}_0\|_{\widehat{\Sigma}}^2 + 2\delta c_0 \|\widehat{\theta}_0\| \left(\sqrt{\|\widehat{\theta}_0 - \theta_0\|_\Sigma^2} - \sqrt{\|\widehat{\theta}_0 - \widehat{\theta}_0\|_{\widehat{\Sigma}}^2} \right) \right] \\ &\quad + \mathbf{1}\{\widehat{\delta}_1 < \delta\} \left[\|\widehat{\theta} - \theta_0\|_\Sigma^2 - \|\widehat{\theta} - \widehat{\theta}_0\|_{\widehat{\Sigma}}^2 + 2\delta c_0 \|\widehat{\theta}\| \left(\sqrt{\|\widehat{\theta} - \theta_0\|_\Sigma^2} - \sqrt{\|\widehat{\theta} - \widehat{\theta}_0\|_{\widehat{\Sigma}}^2} \right) \right] \\ &= \|\widehat{\theta}_0 - \theta_0\|_\Sigma^2 + 2\delta c_0 \|\theta_0\| \|\widehat{\theta}_0 - \theta_0\|_\Sigma + o_p(R_0(\widehat{\theta}, \delta) - \widehat{R}_0(\widehat{\theta}, \delta)). \end{aligned}$$

When $\delta > \delta_1$,

$$\begin{aligned}
& R_0(\widehat{\theta},\delta) - \widehat{R}_0(\widehat{\theta},\delta) \\
= \; & \mathbf{1}\{\widehat{\delta}_1 < \delta\}\left[\|\widehat{\theta}-\theta_0\|_\Sigma^2 - \|\widehat{\theta}-\widehat{\theta}_0\|_{\widehat{\Sigma}}^2 + 2\delta c_0\|\widehat{\theta}\|\left(\sqrt{\|\widehat{\theta}-\theta_0\|_\Sigma^2} - \sqrt{\|\widehat{\theta}-\widehat{\theta}_0\|_{\widehat{\Sigma}}^2}\right)\right] \\
& +\mathbf{1}\{\widehat{\delta}_1 \geq \delta\}\left[\|\widehat{\theta}_0-\theta_0\|_\Sigma^2 - \|\widehat{\theta}_0-\widehat{\theta}_0\|_{\widehat{\Sigma}}^2 + 2\delta c_0\|\widehat{\theta}_0\|\left(\sqrt{\|\widehat{\theta}_0-\theta_0\|_\Sigma^2} - \sqrt{\|\widehat{\theta}_0-\widehat{\theta}_0\|_{\widehat{\Sigma}}^2}\right)\right] \\
= \; & \|\widehat{\theta}-\theta_0\|_\Sigma^2 - \|\widehat{\theta}-\theta_0\|_{\widehat{\Sigma}}^2 + \|\widehat{\theta}-\theta_0\|_{\widehat{\Sigma}}^2 - \|\widehat{\theta}-\widehat{\theta}_0\|_{\widehat{\Sigma}}^2 \\
& +2\delta c_0\|\theta^*\|\left(\sqrt{\|\widehat{\theta}-\theta_0\|_\Sigma^2} - \sqrt{\|\widehat{\theta}-\widehat{\theta}_0\|_\Sigma^2}\right) + 2\delta c_0\|\theta^*\|\left(\sqrt{\|\widehat{\theta}-\widehat{\theta}_0\|_\Sigma^2} - \sqrt{\|\widehat{\theta}-\widehat{\theta}_0\|_{\widehat{\Sigma}}^2}\right) \\
& +o_p(R(\widehat{\theta},\delta) - \widehat{R}(\widehat{\theta},\delta)) \\
= \; & (\theta^*-\theta_0)^\top(\Sigma-\widehat{\Sigma})(\theta^*-\theta_0) + 2(\widehat{\theta}_0-\theta_0)^\top\Sigma(\theta^*-\theta_0) + 2\delta c_0\|\theta^*\|\frac{(\widehat{\theta}_0-\theta_0)^\top\Sigma(\theta^*-\theta_0)}{\sqrt{\|\theta^*-\theta_0\|_\Sigma^2+\sigma^2}} \\
& +o_p(R(\widehat{\theta},\delta) - \widehat{R}(\widehat{\theta},\delta)).
\end{aligned}$$

Next we present the statement "$\|\theta^*-\theta_0\|_\Sigma + c_0\delta\|\theta^*\|$ is an increasing function in δ for any Σ and θ_0". From (4) in Proposition 1, the first-order optimality condition to minimize population adversarial loss is

$$\lambda\left(1+\delta c_0\frac{\|\theta(\lambda)\|_2}{\|\theta(\lambda)-\theta_0\|_\Sigma}\right) = \left(\delta c_0\frac{\|\theta(\lambda)-\theta_0\|_\Sigma}{\|\theta(\lambda)\|_2} + \delta^2\right),$$

which is a quadratic function of δ (take $A = \|\theta(\lambda)\|/\|\theta(\lambda)-\theta_0\|_\Sigma$):

$$\delta^2 + \delta\left(\frac{c_0}{A} - \lambda c_0 A\right) - \lambda = 0.$$

Therefore, δ can be written as a function of λ:

$$\delta = \frac{1}{2}\left[\lambda c_0 A - \frac{c_0}{A} + \sqrt{\left(\lambda c_0 A - \frac{c_0}{A}\right)^2 + 4\lambda}\right],$$

thus

$$\begin{aligned}
c_0\delta\|\theta(\lambda)\| &= c_0\delta A\|\theta(\lambda)-\theta_0\|_\Sigma \\
&= \frac{c_0\|\theta(\lambda)-\theta_0\|_\Sigma}{2}\left[\lambda c_0 A^2 - c_0 + \sqrt{(\lambda c_0 A^2 - c_0)^2 + 4\lambda A^2}\right].
\end{aligned}$$

Therefore,

$$\begin{aligned}
& \frac{\partial}{\partial\lambda}\left(\|\theta(\lambda)-\theta_0\|_\Sigma + c_0\delta\|\theta(\lambda)\|\right) \\
= \; & \frac{\partial}{\partial\lambda}\|\theta(\lambda)-\theta_0\|_\Sigma\left\{1+\frac{c_0}{2}\left[\lambda c_0 A^2 - c_0 + \sqrt{(\lambda c_0 A^2 - c_0)^2 + 4\lambda A^2}\right]\right\} \\
= \; & \left\{1+\frac{c_0}{2}\left[\lambda c_0 A^2 - c_0 + \sqrt{(\lambda c_0 A^2 - c_0)^2 + 4\lambda A^2}\right]\right\}\left(\frac{\partial}{\partial\lambda}\|\theta(\lambda)-\theta_0\|_\Sigma\right) \\
& +\|\theta(\lambda)-\theta_0\|_\Sigma\frac{\partial}{\partial\lambda}\left\{1+\frac{c_0}{2}\left[\lambda c_0 A^2 - c_0 + \sqrt{(\lambda c_0 A^2 - c_0)^2 + 4\lambda A^2}\right]\right\}.
\end{aligned}$$

The derivatives becomes

$$\frac{\partial}{\partial\lambda}\|\theta(\lambda)-\theta_0\|_\Sigma = \frac{1}{2\|\theta(\lambda)-\theta_0\|_\Sigma}\frac{\partial\|\theta(\lambda)-\theta_0\|_\Sigma^2}{\partial\lambda} \tag{39}$$

and

$$\begin{aligned}
&\frac{\partial}{\partial\lambda}\left\{1+\frac{c_0}{2}\left[\lambda c_0A^2-c_0+\sqrt{(\lambda c_0A^2-c_0)^2+4\lambda A^2}\right]\right\}\\
=\;&\frac{c_0}{2}\left[c_0A^2+\frac{2c_0A^2(\lambda c_0A^2-c_0)+4A^2}{2\sqrt{(\lambda c_0A^2-c_0)^2+4\lambda A^2}}\right]+\frac{c_0}{2}\left[\lambda c_0+\frac{2\lambda c_0(\lambda c_0A^2-c_0)+4\lambda}{2\sqrt{(\lambda c_0A^2-c_0)^2+4\lambda A^2}}\right]\frac{\partial A^2}{\partial\lambda}\\
=\;&\frac{c_0}{2}\left[c_0A^2+\frac{c_0A^2(\lambda c_0A^2-c_0)+2A^2}{\sqrt{(\lambda c_0A^2-c_0)^2+4\lambda A^2}}\right]+\frac{c_0}{2}\left[\lambda c_0+\frac{\lambda c_0(\lambda c_0A^2-c_0)+2\lambda}{\sqrt{(\lambda c_0A^2-c_0)^2+4\lambda A^2}}\right]\frac{\partial A^2}{\partial\lambda},
\end{aligned}$$

where

$$\frac{\partial A^2}{\partial\lambda}=\frac{1}{\|\theta(\lambda)-\theta_0\|_\Sigma^2}\frac{\partial\|\theta(\lambda)\|^2}{\partial\lambda}-\frac{\|\theta(\lambda)\|^2}{\|\theta(\lambda)-\theta_0\|_\Sigma^4}\frac{\partial\|\theta(\lambda)-\theta_0\|_\Sigma^2}{\partial\lambda}. \tag{40}$$

For any $\lambda\geq 0$, one can check that

$$\frac{c_0}{2}\left[c_0A^2+\frac{2c_0A^2(\lambda c_0A^2-c_0)+4A^2}{2\sqrt{(\lambda c_0A^2-c_0)^2+4\lambda A^2}}\right]\geq 0,$$

and

$$\|\theta(\lambda)-\theta_0\|_\Sigma\frac{c_0}{2}\left[c_0A^2+\frac{2c_0A^2(\lambda c_0A^2-c_0)+4A^2}{2\sqrt{(\lambda c_0A^2-c_0)^2+4\lambda A^2}}\right]=\frac{\|\theta(\lambda)-\theta_0\|_\Sigma^2}{\|\theta(\lambda)-\theta_0\|}\frac{c_0}{2}\left[c_0A^2+\frac{c_0A^2(\lambda c_0A^2-c_0)+2A^2}{2\sqrt{(\lambda c_0A^2-c_0)^2+4\lambda A^2}}\right]. \tag{41}$$

The coefficient w.r.t $\partial\|\theta(\lambda)-\theta_0\|_\Sigma^2/\partial\lambda$ is

$$\begin{aligned}
&\frac{1}{2\|\theta(\lambda)-\theta_0\|_\Sigma}\left\{1+\frac{c_0}{2}\left[\lambda c_0A^2-c_0+\sqrt{(\lambda c_0A^2-c_0)^2+4\lambda A^2}\right]\right\}\\
&-\frac{A^2}{\|\theta(\lambda)-\theta_0\|_\Sigma}\frac{c_0}{2}\left[\lambda c_0+\frac{\lambda c_0(\lambda c_0A^2-c_0)+2\lambda}{\sqrt{(\lambda c_0A^2-c_0)^2+4\lambda A^2}}\right]\\
=\;&\frac{1}{2\|\theta(\lambda)-\theta_0\|_\Sigma}\left\{1+\frac{c_0}{2}\left[\lambda c_0A^2-c_0+\sqrt{(\lambda c_0A^2-c_0)^2+4\lambda A^2}\right]-c_0A^2\left[\lambda c_0+\frac{\lambda c_0(\lambda c_0A^2-c_0)+2\lambda}{\sqrt{(\lambda c_0A^2-c_0)^2+4\lambda A^2}}\right]\right\}.
\end{aligned}$$

The coefficient w.r.t $\partial\|\theta(\lambda)\|^2/\partial\lambda$ is

$$\frac{1}{\|\theta(\lambda)-\theta_0\|_\Sigma}\frac{c_0}{2}\left[\lambda c_0+\frac{\lambda c_0(\lambda c_0A^2-c_0)+2\lambda}{\sqrt{(\lambda c_0A^2-c_0)^2+4\lambda A^2}}\right].$$

Decompose Σ as $PDP^\top$ and take $\beta_0=P^\top\theta_0$, then

$$\frac{\partial\|\theta(\lambda)-\theta_0\|_\Sigma^2}{\partial\lambda}=\frac{\partial}{\partial\lambda}\beta_0^\top\left(\frac{\lambda^2D}{(D+\lambda\mathbf{I}_p)^2}\right)\beta_0=2\lambda\beta_0^\top\left(\frac{D^2}{(D+\lambda\mathbf{I}_p)^3}\right)\beta_0,$$

and

$$\frac{\partial\|\theta(\lambda)\|^2}{\partial\lambda}=\frac{\partial}{\partial\lambda}\beta_0^\top\left(\frac{D^2}{(D+\lambda\mathbf{I}_p)^2}\right)\beta_0=2\beta_0^\top\left(\frac{D^2}{(D+\lambda\mathbf{I}_p)^3}\right)\beta_0,$$

$$\|\theta(\lambda)-\theta_0\|_\Sigma^2=\beta_0^\top\left(\frac{\lambda^2D^2+\lambda^3\mathbf{I}_p}{(D+\lambda\mathbf{I}_p)^3}\right)\beta_0.$$

Combining all the above results, we have

$$
\begin{aligned}
&\frac{\partial}{\partial\lambda}\left(\|\theta(\lambda)-\theta_0\|_\Sigma+c_0\delta\|\theta(\lambda)\|\right)\\
=\;&\frac{\beta_0^\top\left(\frac{\lambda D^2}{(D+\lambda\mathbf{I}_p)^3}\right)\beta_0}{\|\theta(\lambda)-\theta_0\|_\Sigma}\left\{1+\frac{c_0}{2}\left[\lambda c_0A^2-c_0+\sqrt{\left(\lambda c_0A^2-c_0\right)^2+4\lambda A^2}\right]\right.\\
&\qquad\left.-c_0A^2\left[\lambda c_0+\frac{\lambda c_0(\lambda c_0A^2-c_0)+2\lambda}{\sqrt{\left(\lambda c_0A^2-c_0\right)^2+4\lambda A^2}}\right]-c_0\left[c_0+\frac{c_0(\lambda c_0A^2-c_0)+2}{\sqrt{\left(\lambda c_0A^2-c_0\right)^2+4\lambda A^2}}\right]\right\}\\
&+\frac{\beta_0^\top\left(\frac{\lambda^2D^2+\lambda^3D}{(D+\lambda\mathbf{I}_p)^3}\right)\beta_0}{\|\theta(\lambda)-\theta_0\|_\Sigma}\frac{c_0}{2}\left[c_0A^2+\frac{c_0A^2(\lambda c_0A^2-c_0)+2A^2}{\sqrt{\left(\lambda c_0A^2-c_0\right)^2+4\lambda A^2}}\right]\\
=\;&\frac{\beta_0^\top\left(\frac{\lambda D^2}{(D+\lambda\mathbf{I}_p)^3}\right)\beta_0}{\|\theta(\lambda)-\theta_0\|_\Sigma}\left\{1+\frac{c_0}{2}\left[\lambda c_0A^2-c_0+\sqrt{\left(\lambda c_0A^2-c_0\right)^2+4\lambda A^2}\right]\right.\\
&\qquad\left.-\frac{c_0}{2}A^2\left[\lambda c_0+\frac{\lambda c_0(\lambda c_0A^2-c_0)+2\lambda}{\sqrt{\left(\lambda c_0A^2-c_0\right)^2+4\lambda A^2}}\right]-c_0\left[c_0+\frac{c_0(\lambda c_0A^2-c_0)+2}{\sqrt{\left(\lambda c_0A^2-c_0\right)^2+4\lambda A^2}}\right]\right\}\\
&+\frac{\beta_0^\top\left(\frac{\lambda^3D}{(D+\lambda\mathbf{I}_p)^3}\right)\beta_0}{\|\theta(\lambda)-\theta_0\|_\Sigma}\frac{c_0}{2}\left[c_0A^2+\frac{c_0A^2(\lambda c_0A^2-c_0)+2A^2}{\sqrt{\left(\lambda c_0A^2-c_0\right)^2+4\lambda A^2}}\right]\\
=\;&\frac{\beta_0^\top\left(\frac{\lambda D^2}{(D+\lambda\mathbf{I}_p)^3}\right)\beta_0}{\|\theta(\lambda)-\theta_0\|_\Sigma}\left\{1-\frac{3c_0^2}{2}+\frac{c_0}{2}\sqrt{\left(\lambda c_0A^2-c_0\right)^2+4\lambda A^2}-\left(\frac{c_0}{2}A^2\lambda+c_0\right)\left[\frac{c_0(\lambda c_0A^2-c_0)+2}{\sqrt{\left(\lambda c_0A^2-c_0\right)^2+4\lambda A^2}}\right]\right\}\\
&+\frac{\beta_0^\top\left(\frac{\lambda^3D}{(D+\lambda\mathbf{I}_p)^3}\right)\beta_0}{\|\theta(\lambda)-\theta_0\|_\Sigma}\frac{c_0}{2}\left[c_0A^2+\frac{c_0A^2(\lambda c_0A^2-c_0)+2A^2}{\sqrt{\left(\lambda c_0A^2-c_0\right)^2+4\lambda A^2}}\right]\\
\geq\;&\frac{\beta_0^\top\left(\frac{\lambda D^2}{(D+\lambda\mathbf{I}_p)^3}\right)\beta_0}{\|\theta(\lambda)-\theta_0\|_\Sigma}\left\{1-\frac{3c_0^2}{2}+\frac{c_0}{2}\sqrt{\left(\lambda c_0A^2-c_0\right)^2+4\lambda A^2}-\left(\frac{c_0}{2}A^2\lambda+c_0\right)\left[\frac{c_0(\lambda c_0A^2-c_0)+2}{\sqrt{\left(\lambda c_0A^2-c_0\right)^2+4\lambda A^2}}\right]\right\}\\
&+\frac{\beta_0^\top\left(\frac{\lambda D^2}{(D+\lambda\mathbf{I}_p)^3}\right)\beta_0}{\|\theta(\lambda)-\theta_0\|_\Sigma}\frac{c_0}{2}\left[c_0+\frac{c_0(\lambda c_0A^2-c_0)+2}{\sqrt{\left(\lambda c_0A^2-c_0\right)^2+4\lambda A^2}}\right]\\
=\;&\frac{\beta_0^\top\left(\frac{\lambda D^2}{(D+\lambda\mathbf{I}_p)^3}\right)\beta_0}{\|\theta(\lambda)-\theta_0\|_\Sigma}\left\{1-c_0^2+\frac{c_0}{2}\sqrt{\left(\lambda c_0A^2-c_0\right)^2+4\lambda A^2}-\left(\frac{c_0}{2}A^2\lambda+\frac{c_0}{2}\right)\left[\frac{c_0(\lambda c_0A^2-c_0)+2}{\sqrt{\left(\lambda c_0A^2-c_0\right)^2+4\lambda A^2}}\right]\right\}.
\end{aligned}
$$

Further,

$$
\begin{aligned}
& \sqrt{\left(\lambda c_0 A^2 - c_0\right)^2 + 4\lambda A^2}\left\{1 - c_0^2 + \frac{c_0}{2}\sqrt{\left(\lambda c_0 A^2 - c_0\right)^2 + 4\lambda A^2} - \left(\frac{c_0}{2}A^2\lambda + \frac{c_0}{2}\right)\left[\frac{c_0(\lambda c_0 A^2 - c_0) + 2}{\sqrt{\left(\lambda c_0 A^2 - c_0\right)^2 + 4\lambda A^2}}\right]\right\} \\
\geq\ & \left(1 - c_0^2\right)\sqrt{\left(\lambda c_0 A^2 - c_0\right)^2 + 4\lambda A^2} + \frac{c_0}{2}\left(\left(\lambda c_0 A^2 - c_0\right)^2 + 4\lambda A^2\right) - \frac{c_0 A^2 \lambda}{2}\left(c_0(\lambda c_0 A^2 - c_0) + 2\right) \\
& - \frac{c_0}{2}\left(c_0(\lambda c_0 A^2 - c_0) + 2\right) \\
=\ & \left(1 - c_0^2\right)\sqrt{\left(\lambda c_0 A^2 - c_0\right)^2 + 4\lambda A^2} + \frac{\lambda^2 c_0^3 A^4}{2} - c_0^3\lambda A^2 + \frac{c_0^3}{2} + 2c_0\lambda A^2 - \frac{c_0^3\lambda^2 A^4}{2} + \frac{c_0^3\lambda A^2}{2} - c_0 A^2\lambda \\
& - \frac{c_0^3\lambda A^2}{2} + \frac{c_0^3}{2} - c_0 \\
=\ & \left(1 - c_0^2\right)\sqrt{\left(\lambda c_0 A^2 - c_0\right)^2 + 4\lambda A^2} + \frac{c_0^3}{2} - \frac{c_0^3}{2}\lambda A^2 + c_0\lambda A^2 - \frac{c_0^3\lambda A^2}{2} + \frac{c_0^3}{2} - c_0 \\
=\ & \left(1 - \frac{3c_0^2}{2}\right)\sqrt{\left(\lambda c_0 A^2 - c_0\right)^2 + 4\lambda A^2} + c_0^3 - c_0^3\lambda A^2 + c_0\lambda A^2 - c_0 \\
\geq\ & \left(1 - c_0^2\right)\sqrt{\left(\lambda c_0 A^2 - c_0\right)^2 + 4\lambda A^2} + c_0^3 - c_0.
\end{aligned}
$$

Recall that $c_0 = \sqrt{2/\pi}$, so when $\lambda A^2 > 0$,

$$
\begin{aligned}
\sqrt{\left(\lambda c_0 A^2 - c_0\right)^2 + 4\lambda A^2}^2 - c_0^2 &= \lambda^2 c_0^2 A^4 + c_0^2 - 2\lambda c_0^2 A^2 + 4\lambda A^2 - c_0^2 \\
&= \lambda^2 c_0^2 A^4 - 2\lambda c_0^2 A^2 + 4\lambda A^2 \\
&= A^2\lambda(\lambda c_0^2 - 2c_0^2 + 4) > 0.
\end{aligned}
$$

Therefore, uniformly for all δ, Σ, and θ_0,

$$
\frac{\partial}{\partial\lambda}\left(\|\theta(\lambda) - \theta_0\|_\Sigma + c_0\delta\|\theta(\lambda)\|\right) \geq 0.
$$

□

D Additional numerical experiments

Effectiveness of the two-stage estimator. Here we present the performance of the proposed two-stage estimator. We also provide some other methods for references.

In this experiment, we set $p = 10$ and $n = 1000$ and take $r = 0.1$. From Theorem 4, the adversarial risk of our proposed estimator is close to $R_0(\theta^*, \delta)$. We compare the performance of several estimators:

1. *emp*: take $\widehat{\theta}_0 = (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{y}$ and $\widehat{\Sigma} = \frac{1}{n}\sum_{i=1}^n \mathbf{x}_i\mathbf{x}_i^\top$. Denote as $\widehat{\theta}_{emp}$.
2. *mag*: $\widehat{\theta}_{mag}$ is obtained through taking $\widehat{\Sigma}$ as $\alpha\mathbf{I}_p$, where $\alpha = \|\widehat{\Sigma}\|$.
3. *adv_train(y)*: minimize $\min_\theta \frac{1}{n}\sum_{i=1}^n \max_{\|\mathbf{x}-\mathbf{x}_i\|\leq\delta}[\mathbf{x}^\top\theta - y_i]^2$. Denote as $\widehat{\theta}_y$.
4. *true*: θ^*, for reference.
5. *theta0*: θ_0, for reference.
6. *zero*: $\theta = \mathbf{0}$, for reference.

The results are shown in Figure 4. In the left panel, one can see that $R_0(\widehat{\theta}_{emp}, \delta)$ is close to $R_0(\theta^*, \delta)$. In addition, comparing $\widehat{\theta}_{emp}$ and $\widehat{\theta}_{mag}$, it is important to consider the effect of Σ, and one may not assume $\Sigma \propto \mathbf{I}_p$ and use $\widehat{\theta}_{mag}$. On the other hand, for $\widehat{\theta}_y$, when $\sigma^2 \to 0$, it is expected to converge to θ^* since the adversarial

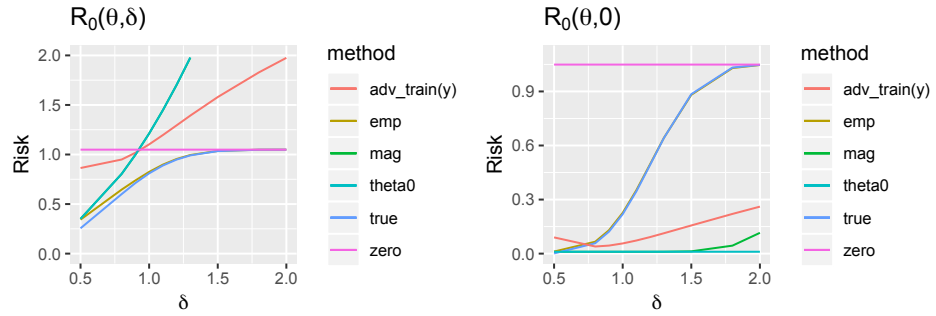

Figure 4: Comparison among Estimators under low dimensional case. Left panel: $R_0(\theta^*, \delta)$ minimizes adversarial risk, and $R_0(\widehat{\theta}_{emp}, \delta)$ is close to $R_0(\theta^*, \delta)$. Right panel: both $R_0(\theta^*, 0)$ and $R_0(\widehat{\theta}, 0)$ increases in δ until $R_0(\mathbf{0}, 0)$.

risk and adversarial prediction are the same when $\delta = 0$. However, when σ^2 gets increasing, its performance in reducing adversarial risk is not as good as $\widehat{\theta}_{emp}$. In terms of $R_0(\theta, 0)$ on the right penal, for both θ^* and $\widehat{\theta}_{emp}$, their standard risk increases in δ until reaches $R_0(\mathbf{0}, 0)$.

We present some more results for other choices of (r, σ^2) from Figure 5 to Figure 11 in Appendix D. Detailed values of $R_0(\theta^*, \delta)$, $R_0(\widehat{\theta}_{emp}, \delta)$, and $Std(R_0(\widehat{\theta}_{emp}, \delta) - R_0(\theta^*, \delta))$ are summarized in Table 4, and similarly the details for $Std(R_0(\widehat{\theta}_{emp}, 0) - R_0(\theta^*, 0))$ in Table 5 in Appendix D.

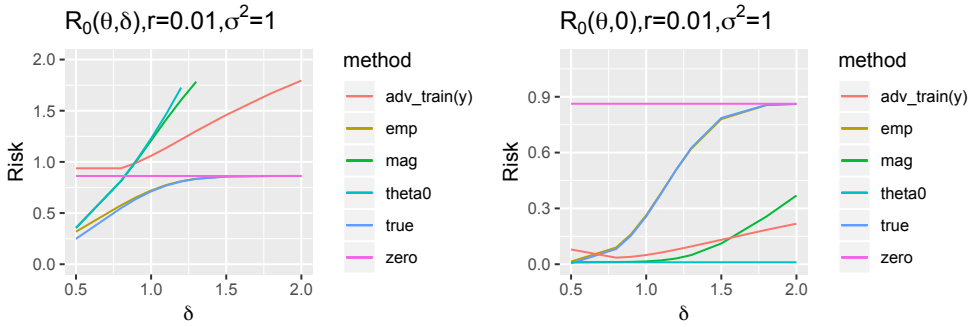

Figure 5: Performance of Two-Stage Estimator

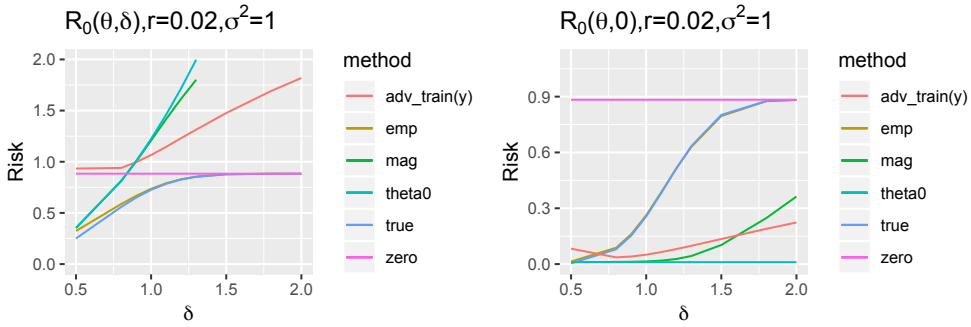

Figure 6: Performance of Two-Stage Estimator

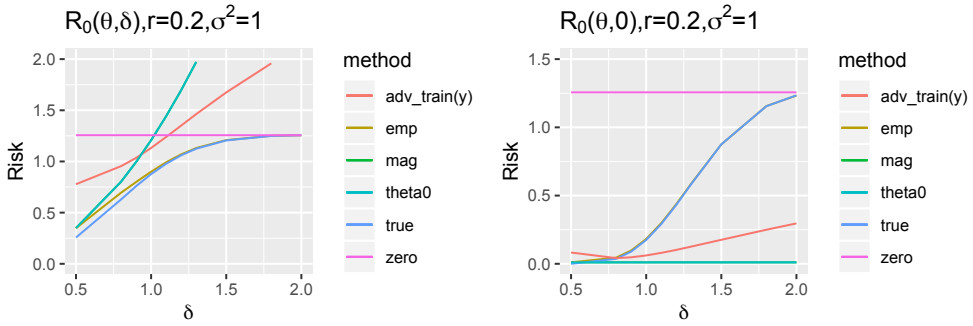

Figure 7: Performance of Two-Stage Estimator

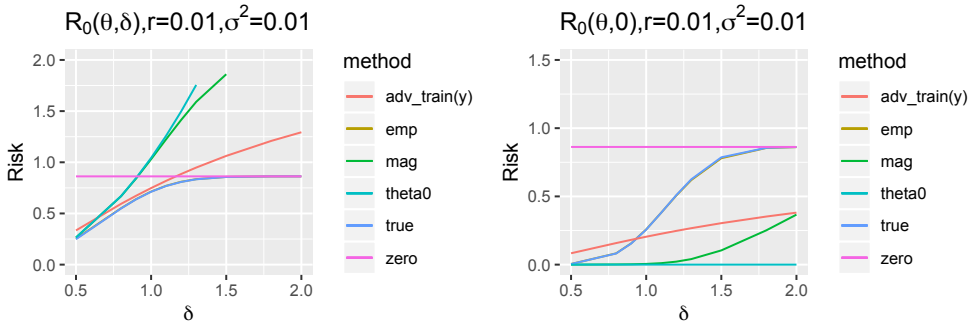

Figure 8: Performance of Two-Stage Estimator

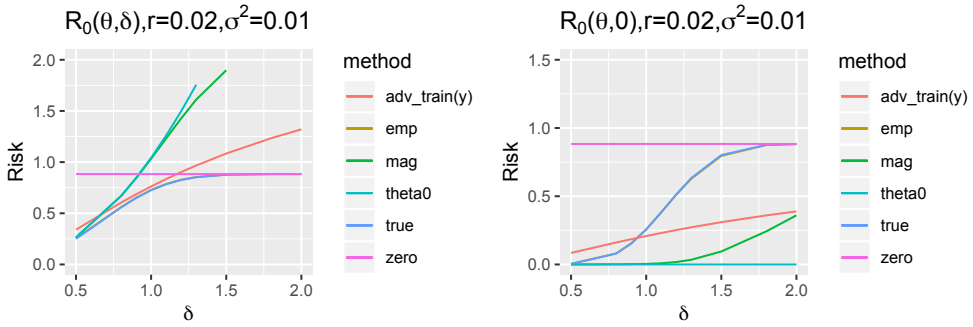

Figure 9: Performance of Two-Stage Estimator

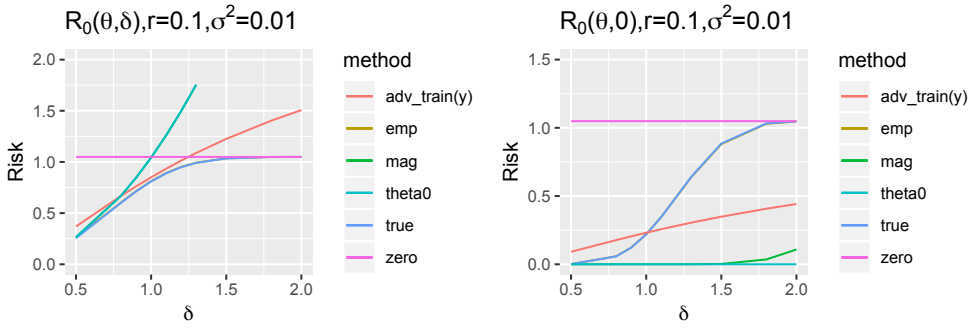

Figure 10: Performance of Two-Stage Estimator

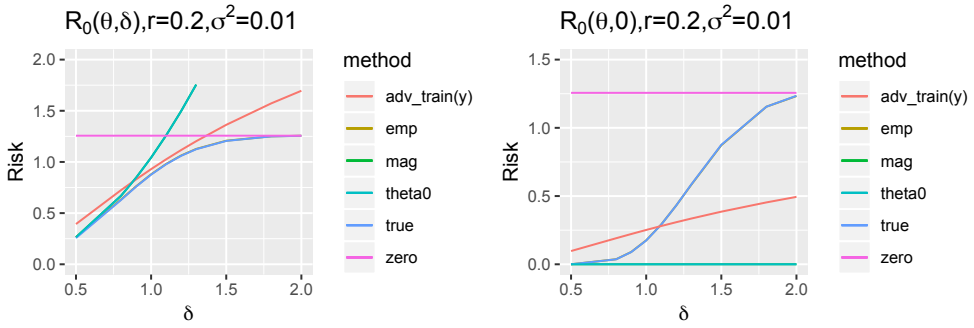

Figure 11: Performance of Two-Stage Estimator

Table 4: Details of $R_0(\theta, \delta)$. "sd" represents $Std(R_0(\widehat{\theta}_{emp}, \delta) - R_0(\theta^*, \delta))$.

r	δ	0.5	0.8	0.9	1	1.1	1.2	1.3	1.5	1.8	2
0.01	true	0.2485	0.5488	0.6381	0.7120	0.7685	0.8082	0.8338	0.8565	0.8622	0.8624
	emp	0.3182	0.5761	0.6539	0.7210	0.7740	0.8117	0.8361	0.8573	0.8622	0.8625
	sd	0.0398	0.0364	0.0242	0.0117	0.0061	0.0044	0.0035	0.0023	0.0005	0.0003
0.02	true	0.2505	0.5575	0.6494	0.7258	0.7845	0.8259	0.8528	0.8769	0.8829	0.8832
	emp	0.3233	0.5864	0.6662	0.7353	0.7902	0.8296	0.8551	0.8777	0.8830	0.8832
	sd	0.0396	0.0378	0.0257	0.0126	0.0064	0.0045	0.0036	0.0024	0.0005	0.0003
0.1	true	0.2558	0.6010	0.7125	0.8097	0.8889	0.9489	0.9911	1.0345	1.0484	1.0491
	emp	0.3430	0.6462	0.7387	0.8247	0.8979	0.9547	0.9950	1.0360	1.0486	1.0491
	sd	0.0367	0.0495	0.0365	0.0216	0.0103	0.0060	0.0047	0.0032	0.0010	0.0004
0.2	true	0.2567	0.6288	0.7585	0.8765	0.9777	1.0603	1.1245	1.2055	1.2497	1.2557
	emp	0.3485	0.6944	0.7991	0.8999	0.9917	1.0694	1.1309	1.2087	1.2505	1.2559
	sd	0.0327	0.0593	0.0487	0.0338	0.0192	0.0096	0.0064	0.0046	0.0023	0.0011

Table 5: Details of $R_0(\theta, 0)$. The minimal $R_0(\theta, 0)$ is 0 through taking $\theta = \theta_0$.

r	δ	0.5	0.8	0.9	1	1.1	1.2	1.3	1.5	1.8	2
0.01	true	0.0045	0.0817	0.1546	0.2568	0.3805	0.5085	0.6251	0.7863	0.8561	0.8618
	emp	0.0143	0.0897	0.1622	0.2633	0.3845	0.5082	0.6208	0.7799	0.8553	0.8613
	sd	0.0060	0.0217	0.0313	0.0416	0.0499	0.0538	0.0562	0.0498	0.0132	0.0088
0.02	true	0.0040	0.0798	0.1528	0.2559	0.3817	0.5132	0.6334	0.8019	0.8765	0.8825
	emp	0.0139	0.0878	0.1605	0.2625	0.3862	0.5135	0.6293	0.7956	0.8755	0.8819
	sd	0.0059	0.0216	0.0315	0.0419	0.0508	0.0548	0.0576	0.0512	0.0140	0.0091
0.1	true	0.0011	0.0579	0.1218	0.2188	0.3460	0.4929	0.6412	0.8849	1.0326	1.0476
	emp	0.0114	0.0661	0.1298	0.2263	0.3526	0.4968	0.6422	0.8811	1.0297	1.0468
	sd	0.0050	0.0185	0.0292	0.0415	0.0536	0.0618	0.0671	0.0666	0.0291	0.0117
0.2	true	0.0000	0.0364	0.0893	0.1745	0.2909	0.4312	0.5846	0.8754	1.1550	1.2345
	emp	0.0104	0.0452	0.0973	0.1819	0.2977	0.4369	0.5878	0.8753	1.1560	1.2332
	sd	0.0043	0.0149	0.0248	0.0370	0.0497	0.0618	0.0702	0.0797	0.0613	0.0394