PROVABLE MORE DATA HURT IN HIGH DIMENSIONAL LEAST SQUARES ESTIMATOR

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ABSTRACT

This paper investigates the finite-sample prediction risk of the high-dimensional least squares estimator. We derive the central limit theorem for the prediction risk when both the sample size and the number of features tend to infinity. Furthermore, the finite-sample distribution and the confidence interval of the prediction risk are provided. Our theoretical results demonstrate the sample-wise non-monotonicity of the prediction risk and confirm "more data hurt" phenomenon.

1 INTRODUCTION

More data hurt refers to the phenomenon that training on more data can hurt the prediction performance of the learned model, especially for some deep learning tasks. Loog et al. (2019) shows that various standard learners can lead to sample-wise non-monotonicity. Nakkiran et al. (2019) experimentally confirms the sample-wise non-monotonicity of the test accuracy on deep neural networks. This challenges the conventional understanding in large sample properties: if an estimator is consistent, more data makes the estimator more stable and improves its finite-sample performance. Nakkiran (2019) considers adding one single data point to a linear regression task and analyzes its marginal effect to the test risk. Dereziński et al. (2019) gives an exact non-asymptotic risk of the high-dimensional least squares estimator and observes the sample-wise non-monotonicity on MSE. For adversarially robust models, Min et al. (2020) proves that more data may increase the gap between the generalization error of adversarially-trained models and standard models. Chen et al. (2020) shows that more training data causes the generalization error to increase in the strong adversary regime. In this work, we derive the finite-sample distribution of the prediction risk under linear models and prove the *"more data hurt"* phenomenon from an asymptotic point of view.

Intuitively, the *"more data hurt"* stems from the *"double descent"* risk curve: as the model complexity increases, the prediction risk of the learned model first decreases and then increases, and then decreases again. The *double descent* phenomenon can be precisely quantified for certain simple models (Hastie et al. (2019); Mei & Montanari (2019); Ba et al. (2019); Belkin et al. (2019); Bartlett et al. (2020); Xing et al. (2019)). Among these works, Hastie et al. (2019) and Mei & Montanari (2019) use the tools from random matrix theory and explicitly prove the double descent curve of the asymptotic risk of linear regression and random features regression in high dimensional setup. Ba et al. (2019) gives the asymptotic risk of two-layer neural networks when either the first or the second layer is trained using a gradient flow.

The second decline of the prediction risk in the double descent curve is highly related to the *more data hurt* phenomenon. In the over-parameterized regime when the model complexity is fixed while the sample size increases, the degree of over-parameterization decreases and becomes close to the interpolation boundary (for example $p/n = 1$ in Hastie et al. (2019)), in which a high prediction risk is achieved. However, the existing asymptotic results, which focus on the first order limit of the prediction risk, cannot exactly guarantee the *more data hurt* phenomenon. Hence, in this work, we characterize the second-order fluctuations of the prediction risk and make attempts to fill this gap. We employ the linear regression task in Hastie et al. (2019) and Nakkiran (2019), and introduce new tools from the random matrix theory, e.g. the central limit theorem for linear spectral statistics in Bai & Silverstein (2004); Bai et al. (2007), to derive the central limit theorem of the prediction risk.

Consider a linear regression task with n data points and p features, the setup of the *more data hurt* is similar to that in the classical asymptotic analysis in Van der Vaart (2000). According to the

classical asymptotic analysis with p fixed and $n \to \infty$, the least square estimator is unbiased and $\sqrt{n}$-consistent to the ground truth. This implies that the more data will not hurt and even improve the prediction performance when $p < n$ and the sample size is sufficiently large. However, the story is very different in the overparameterized regime. The prediction risk doesn't decrease monotonously with n when $p > n$. More data does hurt in the overparametrized case. In the following, we will justify this phenomenon by developing the CLT results as both n and p tend to infinity. We assume $p/n \to c$, and denote $0 < n_1 < n_2 < +\infty$, $c_1 = p/n_1$ and $c_2 = p/n_2$. Then the direct comparison of the prediction risk between sample sizes n_1 and n_2 can be decomposed into three parts: (i) the gap between the finite-sample risk under $n = n_1$ and the asymptotic risk with $c = c_1$; (ii) the gap between the finite-sample risk under $n = n_2$ and the asymptotic risk with $c = c_2$; (iii) the comparison between two asymptotic risks under $c = c_1$ and $c = c_2$. Theorem 1 and 2 of Hastie et al. (2019) give answers to the task (iii). For (i) and (ii), we develop the convergence rate and the limiting distribution of the prediction risk as $n, p \to +\infty$, $p/n \to c$ in this paper. Thus the finite-sample distribution of the prediction risk can be approximated by its limiting distribution. Furthermore, the confidence interval of the finite-sample risk can be obtained as well.

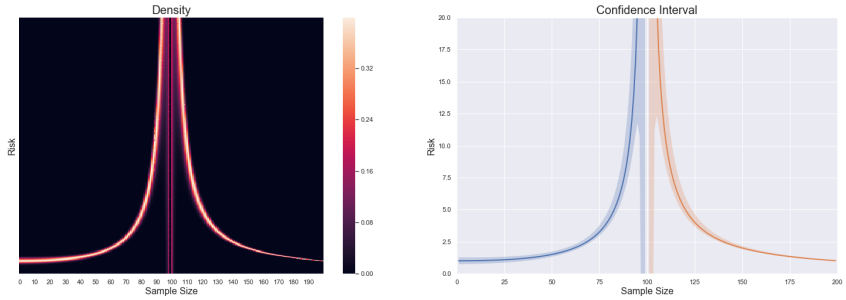

Figure 1: Sample-wise double descent. We take $p = 100$ and $1 \leq n \leq 200$. **Left**: The conditional density of the prediction risk when sample size varies from 1 to 200. According to the conditional distribution of the prediction risk, we can observe the sample-wise double descent phenomenon. **Right**: The 95%-confidence band (point-wise) of the prediction risk. In the overparameterized regime $1 \leq n < 100$, there exists some pairs (n_1, n_2), $1 \leq n_1 < n_2 < 100$ such that the upper boundary of the confidence interval at n_1 is smaller than the lower boundary of the confidence interval at n_2. This confirms the more data hurt phenomenon.

We summarize our findings as follows:

- The finite-sample distribution of the prediction risk is derived and the sample-wise double descent is characterized in Theorem 4.2 and Theorem 4.5 (see Figure 1). Under certain assumptions, the more data hurt phenomenon can be confirmed by comparing the confidence intervals built via the central limit theorems.
- Two different types of prediction risk in the linear regression model are considered in Section 4, one conditional risk given both the training data and regression coefficient, the other conditional risk given the training data only. The regression coefficient is set to be either random or nonrandom to cover more cases. Different convergence rates and limiting distributions of both prediction risk are derived under various scenarios.
- Our results incorporate non-Gaussian observations. For Gaussian data, the limiting mean and variance in the central limit theorems have simpler forms, see Section 4.2 and 4.3 for more details.

The main goal of this paper is to study the asymptotic behaviour of two different types of prediction risk in the linear regression model. The rest of this paper is organized as follows. Section 3 introduces the model settings and two different prediction risk. Section 4 presents the main results on CLTs for the two types of risk. Section 5 conducts simulation experiments to verify the main results. All the technical proofs and lemmas are relegated to the appendix in the supplementary file.

2 RELATED WORK

Double Descent The *double descent* curve describes how generalization ability changes as model capacity increases. It subsumes the classical bias-variance trade-off, a U-shape curve, and further show that the test error exhibits a second drop when the model capacity exceeds the interpolation threshold (Belkin et al. (2018); Geiger et al. (2019); Spigler et al. (2019); Advani & Saxe (2017)). The *double descent* phenomenon has been quantified for certain models, including two-layer neural networks via non-asymptotic bounds or asymptotic risk (Belkin et al. (2019); Muthukumar et al. (2020); Hastie et al. (2019); Mei & Montanari (2019); Ba et al. (2019)). As our results are based on the linear regression model, we mainly focus on the literature of linear models. Muthukumar et al. (2020) and Bartlett et al. (2020) derive the generalization bounds for overparametrized linear models and show the benefits of the interpolation. Hastie et al. (2019) gives the first order limit of the generalization error for linear regressions as $n, p \to +\infty$. Dereziński et al. (2019) provides an exact non-asymptotic expression for *double descent* of the high-dimensional least square estimator. Montanari et al. (2019), Deng et al. (2019) and Kini & Thrampoulidis (2020) investigate the shape asymptotics of binary classification tasks with the max-margin solution and the maximum likelihood solution. Emami et al. (2020) and Gerbelot et al. (2020a) consider the *double descent* in generalized linear models. Furthermore, the *double descent* phenomenon is also observed on linear tasks with various problems and assumptions, e.g. LeJeune et al. (2020); Gerbelot et al. (2020b); Javanmard et al. (2020); Dar & Baraniuk (2020); Xu & Hsu (2019); Dar et al. (2020). Xing et al. (2019) sharply quantifies the benefit of interpolation in the nearest neighbours algorithm. Mei & Montanari (2019) derives the limit risk on the random features model and shows that minimum generalization error is achieved by highly overparametrized interpolators. Ba et al. (2019) gives the limit risk of the regression problem under two-layer neural networks. However, the existing asymptotic results focus on the first order limit of prediction risk and do not indicate the convergence rate. In this work, we are the first to develop results on second-order fluctuations of the prediction risk in linear regressions and provide its corresponding confidence intervals. The more data hurt phenomenon is further justified from the asymptotic point of view.

Random Matrix Theory The primary tool for analyzing the second-order fluctuations of prediction risk comes from random matrix theory. In particular, Bai & Silverstein (2004) refines the central limit theorem for linear spectral statistics of the large dimensional sample covariance matrix with general population and the population is not necessary to be Gaussian. Such central limit theorems are also developed for other random matrix ensembles, see Sinai & Soshnikov (1998); Bai & Yao (2005); Zheng (2012). Other than the central limit theorem for linear spectral statistics, Bai et al. (2007) and Pan & Zhou (2008) study the asymptotic fluctuation of eigenvectors of sample covariance matrices. Bai & Yao (2008) considers quadratic forms like the type $\mathbf{x}_0^{\mathrm{T}}\mathbf{A}\mathbf{x}_0$. All these technical tools and results are adopted and fully utilized in this paper, especially those based on Stieltjes transform are closely related to the prediction risk studied in this paper.

3 PRELIMINARIES

3.1 PROBLEM, DATA AND ESTIMATOR

Suppose that the training data $\{(\mathbf{x}_i, \mathrm{y}_i) \in \mathbb{R}^p \times \mathbb{R}, i = 1, 2, \ldots, n\}$ is generated from the model (ground truth or teacher model):

$$\mathrm{y}_i = \boldsymbol{\beta}^{\mathrm{T}}\mathbf{x}_i + \epsilon_i, \quad \text{and} \quad (\mathbf{x}_i, \epsilon_i) \sim (P_{\mathbf{x}}, P_{\epsilon}), \quad i = 1, 2, \ldots, n, \tag{1}$$

where the randomness across $i = 1, \ldots, n$ is independent. Here, $P_{\mathbf{x}}$ is a distribution on $\mathbb{R}^p$ such that $\mathbb{E}(\mathbf{x}_i) = \mathbf{0}$, $\mathrm{Cov}(\mathbf{x}_i) = \boldsymbol{\Sigma}$, and P_{ϵ} is a distribution on $\mathbb{R}$ such that $\mathbb{E}(\epsilon_i) = 0$, $\mathrm{Var}(\epsilon_i) = \sigma^2$. To proceed further, we denote

$$\mathbf{X}_{n\times p} = (\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n)^{\mathrm{T}}, \quad \mathbf{y} = (\mathrm{y}_1, \mathrm{y}_2, \ldots, \mathrm{y}_n)^{\mathrm{T}}.$$

The minimum ℓ_2 norm (min-norm) least squares estimator, of $\mathbf{y}$ on $\mathbf{X}$, is defined by

$$\hat{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta}} \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|^2 = (\mathbf{X}^{\mathrm{T}}\mathbf{X})^{+}\mathbf{X}^{\mathrm{T}}\mathbf{y}, \tag{2}$$

where $(\mathbf{X}^{\mathrm{T}}\mathbf{X})^{+}$ denotes the Moore-Penrose pseudoinverse of $\mathbf{X}^{\mathrm{T}}\mathbf{X}$.

3.2 BIAS, VARIANCE AND RISK

Similar to Hastie et al. (2019), we define two different types of out-of-sample prediction risk. The first one is given by

$$R_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) = \mathbb{E}\big[(\mathbf{x}_0^{\mathrm{T}}\hat{\boldsymbol{\beta}} - \mathbf{x}_0^{\mathrm{T}}\boldsymbol{\beta})^2 \big| \mathbf{X}\big] = \mathbb{E}\big[\|\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}\|_{\boldsymbol{\Sigma}}^2 \big| \mathbf{X}\big],$$

where $\mathbf{x}_0 \sim P_{\mathbf{x}}$ is a test point and is independent of the training data, and $\|\boldsymbol{\beta}\|_{\boldsymbol{\Sigma}}^2$ stands for $\boldsymbol{\beta}^{\mathrm{T}}\boldsymbol{\Sigma}\boldsymbol{\beta}$. Here $\boldsymbol{\beta}$ is assumed to be a random vector independent of $\mathbf{x}_0$. In this definition, the expectation $\mathbb{E}$ stands for the conditional expectation for $\mathbf{x}_0$, $\hat{\boldsymbol{\beta}}$ and $\boldsymbol{\beta}$ when $\mathbf{X}$ is given. According to the bias-variance decomposition, we have $R_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) := B_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) + V_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta})$, where

$$B_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) = \mathbb{E}\Big\{\|\mathbb{E}(\hat{\boldsymbol{\beta}}|\mathbf{X}) - \boldsymbol{\beta}\|_{\boldsymbol{\Sigma}}^2 \big| \mathbf{X}\Big\} \quad \text{and} \quad V_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) = \mathrm{Tr}\{\mathrm{Cov}(\hat{\boldsymbol{\beta}}|\mathbf{X})\boldsymbol{\Sigma}\}. \tag{3}$$

Plugging the model (1) into the min-norm estimator (2), the bias and variance terms can be rewritten as

$$B_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) = \mathbb{E}\big\{\boldsymbol{\beta}^{\mathrm{T}}\Pi\boldsymbol{\Sigma}\Pi\boldsymbol{\beta} \big| \mathbf{X}\big\} \quad \text{and} \quad V_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) = \frac{\sigma^2}{n}\,\mathrm{Tr}(\hat{\boldsymbol{\Sigma}}^{+}\boldsymbol{\Sigma}),$$

where $\hat{\boldsymbol{\Sigma}} = \mathbf{X}^{\mathrm{T}}\mathbf{X}/n$ is the (uncentered) sample covariance matrix of $\mathbf{X}$, and $\boldsymbol{\Pi} = \boldsymbol{I}_p - \hat{\boldsymbol{\Sigma}}^{+}\hat{\boldsymbol{\Sigma}}$ is the projection onto the null space of $\mathbf{X}$.

The second type of out-of-sample prediction risk is defined as

$$R_{\mathbf{X},\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) = \mathbb{E}\big[(\mathbf{x}_0^{\mathrm{T}}\hat{\boldsymbol{\beta}} - \mathbf{x}_0^{\mathrm{T}}\boldsymbol{\beta})^2 \big| \mathbf{X}, \boldsymbol{\beta}\big] = \mathbb{E}\big[\|\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}\|_{\boldsymbol{\Sigma}}^2 \big| \mathbf{X}, \boldsymbol{\beta}\big],$$

where

$$B_{\mathbf{X},\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) = \boldsymbol{\beta}^{\mathrm{T}}\Pi\boldsymbol{\Sigma}\Pi\boldsymbol{\beta} \quad \text{and} \quad V_{\mathbf{X},\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) = V_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) = \frac{\sigma^2}{n}\,\mathrm{Tr}(\hat{\boldsymbol{\Sigma}}^{+}\boldsymbol{\Sigma}).$$

In this definition, the parameter $\boldsymbol{\beta}$ is assumed to be given. The expectation $\mathbb{E}$ is the conditional expectation for $\mathbf{x}_0$ and $\hat{\boldsymbol{\beta}}$ when $\mathbf{X}$ and $\boldsymbol{\beta}$ are given. This is consistent with the common-used testing procedure, in which a trained model is evaluated by the average loss on unseen testing data. Our main goal is to study the asymptotic behavior of the two types of out-of-sample prediction risk $R_{\mathbf{X}}$ and $R_{\mathbf{X},\boldsymbol{\beta}}$ as $n, p \to +\infty$ and $p/n \to c \in (0, +\infty)$.

4 MAIN RESULTS

Before stating our main results, we briefly highlight the challenges we faced in proving the *more data hurt* phenomenon. First, the finite-sample behaviour of prediction risk is required. Hastie et al. (2019) gives the first-order limit of both $R_{\mathbf{X},\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta})$ and $R_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta})$ as $n, p \to +\infty$ and $p/n \to c \in (0, +\infty)$. However, to prove the *more data hurt* phenomenon, we should fix p and investigate the finite-sample risk with different sample sizes n. This implies that only knowing the first-order limit is not enough, the convergence rate is also needed. To solve this problem, we have derived the central limit theorems for $R_{\mathbf{X},\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta})$ and $R_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta})$ respectively, which characterize the second-order fluctuations of the risk. Then we can figure out the finite-sample behavior of the risk by computing the gap between the risk and its limit. The confidence intervals of the risk can be further obtained. Second, the parameter $\boldsymbol{\beta}$ also contributes randomness to the finite-sample risk, which further influences the convergence rate. To analyze the contribution of $\boldsymbol{\beta}$, we need to make use of the technical tools and asymptotic results for eigenvectors and quadratic forms developed in Bai et al. (2007) and Bai & Yao (2008). Another interesting finding is that, in the overparameterized regime such that $p > n$, the two types of out-of-sample prediction risk $R_{\mathbf{X},\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta})$ and $R_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta})$ enjoy different convergence rates.

4.1 ASSUMPTIONS AND MORE NOTATIONS

Throughout this paper, we consider the limiting distributions and the convergence rates of the out-of-sample prediction risk when $n, p \to \infty$ such that $p/n = c_n \to c \in (0, \infty)$. If $c > 1$, the sample

size n is smaller than the number of parameters p, we call this case *"overparametrized"*. Otherwise when $c < 1$, we call it *"underparameterized"*.

As follows are some notations used in this paper. The $p \times p$ identity matrix is denoted by $\boldsymbol{I}_p$. For a symmetric matrix $\boldsymbol{A} \in \mathbb{R}^{p\times p}$, we define its empirical spectral distribution as

$$F^{\boldsymbol{A}}(x) = \frac{1}{p}\sum_{i=1}^{p} \mathbb{1}\{\lambda_i(\boldsymbol{A}) \le x\}$$

where $\mathbb{1}\{\cdot\}$ is the indicator function, and $\lambda_i(\boldsymbol{A})$, $i = 1, 2, \dots p$ are the eigenvalues of $\boldsymbol{A}$. What's more, the notation $\xrightarrow{d}$ stands for the convergence in distribution. Throughout this paper, $Z_{\alpha/2}$ is the $\alpha/2$ upper quantile of the standard normal distribution, $\lambda_{\max}(\boldsymbol{A})$ and $\lambda_{\min}(\boldsymbol{A})$ denote the largest and smallest eigenvalues of $\boldsymbol{A}$ respectively.

In the following, we will derive confidence intervals for both risks under various combinations of model assumptions for c, $\mathbf{X}$ and $\boldsymbol{\beta}$. Here we list all the assumptions needed in different scenarios:

(A) $\mathbf{x}_j \sim P_{\mathbf{x}}$ is of the form $\mathbf{x}_j = \boldsymbol{\Sigma}^{1/2}\mathbf{z}_j$, where $\mathbf{z}_j$ is a p-length random vector with i.i.d. entries that have zero mean, unit variance, and a finite 4-th order moment $\mathbb{E}(\mathbf{z}_{ij}^4) = \nu_4$, $i = 1, \cdots, p$, $j = 1, \cdots, n$.

(B1) $\boldsymbol{\Sigma}$ is a deterministic positive definite matrix, such that $\lambda(\boldsymbol{\Sigma}) \ge c_0 > 0$, for all n, p and a constant c_0. As $p \to \infty$, we assume that the empirical spectral distribution $F^{\boldsymbol{\Sigma}}$ converges weakly to a measure H.

(B2) $\boldsymbol{\Sigma}$ is an identity matrix, $\boldsymbol{\Sigma} = \boldsymbol{I}_p$.

(C1) $\boldsymbol{\beta}$ is a nonrandom constant vector, and $\|\boldsymbol{\beta}\|_2^2 = \boldsymbol{\beta}^{\mathrm{T}}\boldsymbol{\beta} = r^2$.

(C2) $\boldsymbol{\beta} \sim P_{\boldsymbol{\beta}}$ is independent of $\mathbf{X}$ and follows multivariate Gaussian distribution $N_p(0, \frac{r^2}{p}\boldsymbol{I}_p)$.

4.2 Underparametrized asymptotics

In this section, we focus on the risk of the min-norm estimator (2) in the underparametrized regime. According to Theorem 1 of Hastie et al. (2019), both $B_{\mathbf{X},\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta})$ and $B_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta})$ converge to $\sigma^2 c/(1-c)$ almost surely. The following theorems show that both $B_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta})$ and $B_{\mathbf{X},\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta})$ converge to $\sigma^2 c/(1-c)$ at the rate of $1/p$. Furthermore, the limiting distributions are derived by making use of the CLT for linear spectral statistics of large-dimensional sample covariance matrices.

Theorem 4.1. *Suppose that the training data is generated from the model* (1)*, and the assumptions* (A) *and* (B1) *hold. Then the first type of out-of-sample prediction risk* $R_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta})$ *of the min-norm estimator* (2) *satisfies that, as* $n, p \to \infty$ *such that* $p/n = c_n \to c < 1$*,*

$$p\Big(R_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) - \frac{c_n\sigma^2}{1-c_n}\Big) \xrightarrow{d} N(\mu_c, \sigma_c^2), \tag{4}$$

where

$$\mu_c = \frac{c^2\sigma^2}{(c-1)^2} + \frac{\sigma^2 c^2(\nu_4 - 3)}{1-c} \quad \textit{and} \quad \sigma_c^2 = \frac{2c^3\sigma^4}{(c-1)^4} + \frac{c^3\sigma^4(\nu_4-3)}{(1-c)^2}.$$

Conclusively,

$$P(L_{\alpha,c} \le R_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) \le U_{\alpha,c}) \to 1 - \alpha, \tag{5}$$

where $1-\alpha$ *is the confidence level and*

$$L_{\alpha,c} = \frac{c_n\sigma^2}{1-c_n} + \frac{1}{p}(\mu_c - Z_{\alpha/2}\sigma_c), \quad U_{\alpha,c} = \frac{c_n\sigma^2}{1-c_n} + \frac{1}{p}(\mu_c + Z_{\alpha/2}\sigma_c).$$

Under the assumptions of Theorem 4.1, we know that $\boldsymbol{\Pi} = \boldsymbol{I}_p - \hat{\boldsymbol{\Sigma}}^{+}\hat{\boldsymbol{\Sigma}} = \mathbf{0}$ and

$$B_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) = B_{\mathbf{X},\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) = 0, \quad V_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) = V_{\mathbf{X},\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) = \frac{\sigma^2}{n}\operatorname{Tr}(\hat{\boldsymbol{\Sigma}}^{+}\boldsymbol{\Sigma}).$$

Thus $R_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta})$ equals to $R_{\mathbf{X},\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta})$ and the two risk share the same asymptotic limit.

Theorem 4.2. *Under the assumptions of Theorem 4.1, the second type of out-of-sample prediction risk $R_{\mathbf{X},\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})$ of the min-norm estimator* (2) *satisfies that, as $n,p\to\infty$ such that $p/n=c_n\to c<1$,*

$$p\big(R_{\mathbf{X},\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})-\frac{c_n\sigma^2}{1-c_n}\big)\xrightarrow{d}N(\mu_c,\sigma_c^2),$$

and

$$P(L_{\alpha,c}\le R_{\mathbf{X},\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})\le U_{\alpha,c})\to 1-\alpha,$$

where μ_c, σ_c^2, $L_{\alpha,c}$ and $U_{\alpha,c}$ are the same as those in Theorem 4.1.

4.3 Overparametrized asymptotics

In this section, we consider the min-norm estimator (2) in the overparametrized case. The bias term , either $B_{\mathbf{X}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})$ or $B_{\mathbf{X},\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})$, is generally nonzero when $c>1$. According to Lemma 2 of Hastie et al. (2019), both $B_{\mathbf{X}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})$ and $B_{\mathbf{X},\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})$ converge to $r^2(1-1/c)$ as $n,p\to+\infty$ and $p/n\to c>1$. This implies that the bias term can influence the asymptotic behavior of the prediction risk, including the convergence rate. Hence to derive the CLT of the out-of-sample prediction risk, we need to consider both the bias and variance terms in (3).

In the following, we investigate the asymptotic properties of the two prediction risk $R_{\mathbf{X}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})$ and $R_{\mathbf{X},\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})$ under various combinations of the assumptions (A1), (B2) for $\mathbf{X}$ and scenarios (C1), (C2) for $\boldsymbol{\beta}$. We start with the case when $\boldsymbol{\beta}$ is a constant vector.

Theorem 4.3. *Suppose that the training data is generated from the model (1), and the assumptions* (A)*,* (B2) *and* (C1) *hold. Then the first type of out-of-sample prediction risk, $R_{\mathbf{X}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})$, of the min-norm estimator* (2) *satisfies that, as $n,p\to\infty$ such that $p/n=c_n\to c>1$,*

$$\sqrt{p}\Big\{R_{\mathbf{X}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})-(1-\frac{1}{c_n})r^2-\frac{\sigma^2}{c_n-1}\Big\}\xrightarrow{d}N(\mu_{c,1},\sigma_{c,1}^2),\tag{6}$$

where $\mu_{c,1}=0$ and $\sigma_{c,1}^2=\frac{2(c-1)}{c^2}r^4$. A more practical version is to replace $\mu_{c,1}$ and $\sigma_{c,1}^2$ with

$$\begin{aligned}\tilde{\mu}_{c,1} &= \frac{1}{\sqrt{p}}\Big\{\frac{c\sigma^2}{(1-c)^2}+\frac{\sigma^2(\nu_4-3)}{c-1}\Big\},\\ \tilde{\sigma}_{c,1}^2 &= \frac{2(c-1)}{c^2}r^4+\frac{1}{p}\Big\{\frac{2c^3\sigma^4}{(1-c)^4}+\frac{c\sigma^4(\nu_4-3)}{(c-1)^2}\Big\}.\end{aligned}$$

Conclusively,

$$P(L_{\alpha,c}\le R_{\mathbf{X}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})\le U_{\alpha,c})\to 1-\alpha,\tag{7}$$

where $1-\alpha$ is the confidence level and

$$\begin{aligned}L_{\alpha,c} &= (1-\frac{1}{c_n})r^2+\frac{\sigma^2}{c_n-1}+\frac{1}{\sqrt{p}}(\tilde{\mu}_{c,1}-Z_{\alpha/2}\tilde{\sigma}_{c,1}),\\ U_{\alpha,c} &= (1-\frac{1}{c_n})r^2+\frac{\sigma^2}{c_n-1}+\frac{1}{\sqrt{p}}(\tilde{\mu}_{c,1}+Z_{\alpha/2}\tilde{\sigma}_{c,1}).\end{aligned}$$

Remark 4.1. *Under assumption (C1), $B_{\mathbf{X}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})=B_{\mathbf{X},\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})$ and $R_{\mathbf{X}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})=R_{\mathbf{X},\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})$. Thus Theorem 4.3 still holds if we replace $R_{\mathbf{X}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})$ with $R_{\mathbf{X},\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})$.*

Next we consider the case when $\boldsymbol{\beta}$ is a random vector that follows Assumption (C2), we have

Theorem 4.4. *Suppose that the training data is generated from the model* (1)*, and the assumptions* (A)*,* (B2) *and* (C2) *hold. Then, as $n,p\to\infty$ such that $p/n=c_n\to c>1$, the first type of out-of-sample prediction risk, $R_{\mathbf{X}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})$, of the min-norm estimator* (2) *satisfies,*

$$p\Big\{R_{\mathbf{X}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})-(1-\frac{1}{c_n})r^2-\frac{\sigma^2}{c_n-1}\Big\}\xrightarrow{d}N(\mu_{c,2},\sigma_{c,2}^2),$$

where

$$\mu_{c,2}=\frac{c\sigma^2}{(1-c)^2}+\frac{\sigma^2(\nu_4-3)}{c-1}\quad\textit{and}\quad\sigma_{c,2}^2=\frac{2c^3\sigma^4}{(1-c)^4}+\frac{c\sigma^4(\nu_4-3)}{(c-1)^2}.$$

Hence we have

$$P(L_{\alpha,c} \leq R_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) \leq U_{\alpha,c}) \to 1 - \alpha,$$

where

$$\begin{aligned} L_{\alpha,c} &= \frac{\sigma^2}{c_n - 1} + (1 - \frac{1}{c_n})r^2 + \frac{1}{p}(\mu_{c,2} - Z_{\alpha/2}\sigma_{c,2}), \\ U_{\alpha,c} &= \frac{\sigma^2}{c_n - 1} + (1 - \frac{1}{c_n})r^2 + \frac{1}{p}(\mu_{c,2} + Z_{\alpha/2}\sigma_{c,2}). \end{aligned}$$

As for $R_{\mathbf{X},\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta})$, we have the following theorem.

Theorem 4.5. *Suppose that the training data is generated from the model* (1)*, and the assumptions* (A)*,* (B2) *and* (C2) *hold. Then, as $n, p \to \infty$ such that $p/n = c_n \to c > 1$, the second type of out-of-sample prediction risk, $R_{\mathbf{X},\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta})$, of the min-norm estimator* (2) *satisfies,*

$$\sqrt{p}\Big\{R_{\mathbf{X},\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) - (1 - \frac{1}{c_n})r^2 - \frac{\sigma^2}{c_n - 1}\Big\} \xrightarrow{d} N(\mu_{c,3}, \sigma_{c,3}^2), \tag{8}$$

where $\mu_{c,3} = 0$ and $\sigma_{c,3}^2 = 2(1 - \frac{1}{c})r^4$. A more practical version is to replace $\mu_{c,3}$ and $\sigma_{c,3}^2$ with

$$\begin{aligned} \tilde{\mu}_{c,3} &= \frac{1}{\sqrt{p}}\left\{\frac{c\sigma^2}{(1-c)^2} + \frac{\sigma^2(\nu_4 - 3)}{c - 1}\right\}, \\ \tilde{\sigma}_{c,3}^2 &= 2(1 - \frac{1}{c})r^4 + \frac{1}{p}\left\{\frac{2c^3\sigma^4}{(1-c)^4} + \frac{c\sigma^4(\nu_4 - 3)}{(c-1)^2}\right\}, \end{aligned}$$

and the corresponding $(1 - \alpha)$-confidence interval is given by

$$P(L_{\alpha,c} \leq R_{\mathbf{X},\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) \leq U_{\alpha,c}) \to 1 - \alpha, \tag{9}$$

with

$$\begin{aligned} L_{\alpha,c} &= \frac{\sigma^2}{c_n - 1} + (1 - \frac{1}{c_n})r^2 + \frac{1}{\sqrt{p}}(\tilde{\mu}_{c,3} - Z_{\alpha/2}\tilde{\sigma}_{c,3}), \\ U_{\alpha,c} &= \frac{\sigma^2}{c_n - 1} + (1 - \frac{1}{c_n})r^2 + \frac{1}{\sqrt{p}}(\tilde{\mu}_{c,3} + Z_{\alpha/2}\tilde{\sigma}_{c,3}). \end{aligned}$$

Remark 4.2. *If we compare the results in Theorem 4.3 and 4.5, we will find out that $R_{\mathbf{X}}$ with constant β and $R_{\mathbf{X},\boldsymbol{\beta}}$ with random β share the same first-order limit and second-order error rate $O(p^{-1/2})$. This is quite intuitive because both risk treat β as a constant. Their differences are reflected in their limiting variances. Nevertheless, it's very interesting to observe from Theorem 4.4 that, $R_{\mathbf{X}}$ with random β under the overparametrized case has a smaller second-order error rate $O(p^{-1})$. It enjoys the same rate as the underparametrized case in Theorem 4.1. A possible explanation would be that averaging over random β can partially offset the curse of dimensionality so that $R_{\mathbf{X}}$ achieves the same error rate for all p, n combinations.*

Remark 4.3. *It's worth mentioning that the only assumption regarding data distribution is Assumption (A), where only finite fourth order moment is required. Non-Gaussianity allows our theoretical results more widely applied.*

5 Experiments

In this section, we carry out simulation experiments to examine the central limit theorems and the corresponding confidence intervals in Theorem 4.2 and Theorem 4.5. We generate data points from the linear model (1) and directly compute the prediction risk via the bias-variance decomposition in (3). The generative distribution $P_{\mathbf{x}}$ is taken to be the standard normal distribution. The noise distribution P_ϵ is taken to be $N(0, 1)$. In the following, we present the gap between the finite-sample distribution of the prediction risk and the corresponding limiting distribution to check the central limit theorems and use the cover rate to measure the effectiveness of the confidence intervals. More simulation results are relegated to the Appendix due to space limitations.

Example 1. This example examines the results in Theorem 4.2. We define a statistic

$$T_n = \frac{p}{\sigma_c}\Big(R_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) - \sigma^2 \frac{c_n}{1 - c_n}\Big) - \frac{\mu_c}{\sigma_c}.$$

According to Theorem 4.2, T_n weakly converges to the standard normal distribution as $n, p \to \infty$. In this example, $c = 2/3$ and $p = 100, 200, 400$. The finite-sample distribution of T_n is presented by the histogram of T_n in Figure 2 with 1000 repetitions, where the solid blue curve stands for standard normal density function. It can be seen that the finite-sample distribution of T_n is very consistent with the standard normal distribution, especially when n, p become larger. When $\alpha = 0.05$, the empirical cover rates of the 95%-confidence interval are 93.1%, 93.9% and 95.2% for $p = 100$, 200 and 400 respectively. All these experiments verify the correctness of our theoretical results.

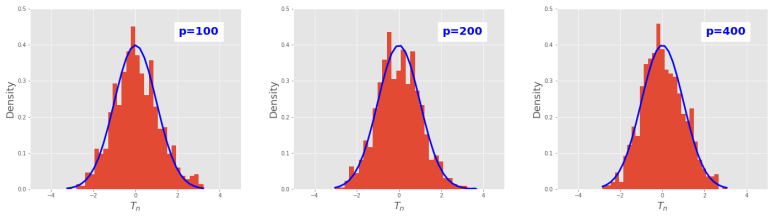

Figure 2: The histogram of T_n. The solid line is the density of the standard normal distribution.

Example 2. This example verifies the results in Theorem 4.5. Here we define two statistics:

$$\begin{aligned} T_{n,0} &= \frac{\sqrt{p}}{\sigma_{c,3}}\Big\{R_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) - (1 - \frac{1}{c_n})r^2 - \frac{\sigma^2}{c_n - 1}\Big\} - \frac{\mu_{c,3}}{\sigma_{c,3}}, \\ T_{n,1} &= \frac{\sqrt{p}}{\tilde{\sigma}_{c,3}}\Big\{R_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) - (1 - \frac{1}{c_n})r^2 - \frac{\sigma^2}{c_n - 1}\Big\} - \frac{\tilde{\mu}_{c,3}}{\tilde{\sigma}_{c,3}}. \end{aligned}$$

According to Theorem 4.5, both $T_{n,0}$ and $T_{n,1}$ weakly converge to the standard normal distribution as $n, p \to +\infty$. We take $c = 3/2$ and $p = 150, 300, 450$. Similarly the finite-sample distributions of $T_{n,0}$ and $T_{n,1}$ are presented by the histogram of $T_{n,0}$ and $T_{n,1}$ with 1000 repetitions. The comparison between these two statistics is shown in Figure 3. It can also be seen that the finite sample distributions of $T_{n,0}$ and $T_{n,1}$ both match the standard normal distribution quite well. The empirical cover rates of the 95%-confidence interval (9) are 93.8%, 94.7% and 94.4% for $p = 150$, 300 and 600 respectively, which further shows the validity of our theoretical results.

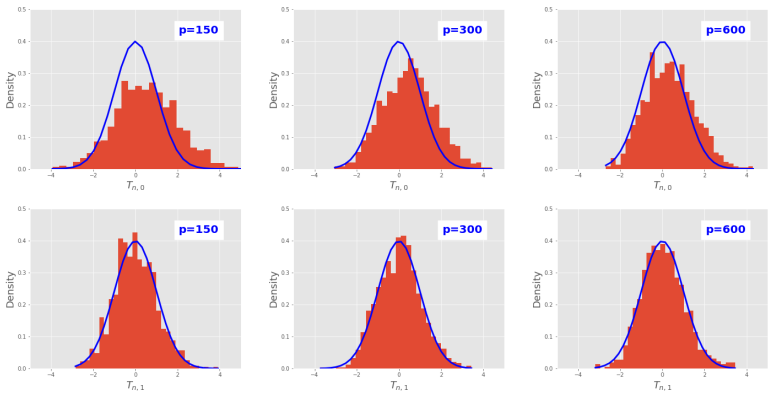

Figure 3: The histogram of $T_{n,0}$ and $T_{n,1}$. The solid line is the density of the standard normal distribution.

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A PROOF OF THEOREM 4.1 AND THEOREM 4.2

Let $\mathbf{X} = \mathbf{Z}\boldsymbol{\Sigma}^{1/2}$. According to the Bai-Yin theorem (Bai & Yin (2008)), the smallest eigenvalue of $\mathbf{Z}^{\mathrm{T}}\mathbf{Z}/n$ is almost surely larger than $(1-\sqrt{c})^2/2$ for sufficiently large n. Thus

$$\lambda_{min}(\frac{1}{n}\mathbf{X}^{\mathrm{T}}\mathbf{X}) \geq c_0\lambda_{\min}(\frac{1}{n}\mathbf{Z}^{\mathrm{T}}\mathbf{Z}) \geq \frac{c_0}{2}(1-\sqrt{c})^2,$$

which implies that the matrix $\mathbf{X}^{\mathrm{T}}\mathbf{X}/n$ is almost surely invertible for large n. By Section 3.2, $\boldsymbol{\Pi} = \mathbf{0}$, $B_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) = B_{\mathbf{X},\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) = 0$ and $V_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) = V_{\mathbf{X},\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta})$. Thus the CLT of $R_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta})$ is same to that of $R_{\mathbf{X},\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta})$. For simplicity, we focus on $R_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta})$ in the following. Notice that

$$\begin{aligned} V_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) &= \frac{\sigma^2}{n}\operatorname{Tr}(\hat{\boldsymbol{\Sigma}}^{-1}\boldsymbol{\Sigma}) \\ &= \frac{\sigma^2}{n}\operatorname{Tr}\Big(\boldsymbol{\Sigma}^{-1/2}\big(\frac{\mathbf{Z}^{\mathrm{T}}\mathbf{Z}}{n}\big)^{-1}\boldsymbol{\Sigma}^{-1/2}\boldsymbol{\Sigma}\Big) \\ &= \frac{\sigma^2}{n}\sum_{i=1}^{p}\frac{1}{s_i} = \frac{\sigma^2 p}{n}\int\frac{1}{s}dF_{\mathbf{Z}}(s) \end{aligned}$$

where $F_{\mathbf{Z}}$ is the spectral measure of $\mathbf{Z}^{\mathrm{T}}\mathbf{Z}/n$. According to Theorem 1 of Hastie et al. (2019), as $n, p \to \infty$ such that $p/n = c_n \to c \in (0, \infty)$, $F_{\mathbf{Z}}(x)$ weakly converges to the standard Marcenko-Pastur law $F_c(x)$ and

$$V_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) \to \sigma^2 c\int\frac{1}{s}dF_c(s) = \sigma^2\frac{c}{1-c}.$$

Here the standard Marcenko-Pastur law $F_c(x)$ has a density function

$$p_c(x) = \begin{cases} \frac{1}{2\pi cx}\sqrt{(b-x)(x-a)}, & \text{if } a \leq x \leq b, \\ 0, & \text{o.w.}, \end{cases}$$

where $a = (1-\sqrt{c})^2$, $b = (1+\sqrt{c})^2$ and $p_c(x)$ has a point mass $1-\frac{1}{c}$ at the origin if $c > 1$. Hence

$$\begin{aligned} R_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) - \sigma^2\frac{c_n}{1-c_n} &= \frac{\sigma^2 p}{n}\int\frac{1}{s}dF_Z(s) - \sigma^2 c_n\int\frac{1}{s}dF_{c_n}(s) \\ &= \sigma^2 c_n\int\frac{1}{s}\big(dF_Z(s) - dF_{c_n}(s)\big). \end{aligned}$$

According to Theorem 1.1 of Bai & Silverstein (2004),

$$p\Big(R_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) - \sigma^2\frac{c_n}{1-c_n}\Big) \xrightarrow{d} N(\mu_c, \sigma_c^2), \tag{10}$$

where

$$\begin{aligned} \mu_c &= -\frac{\sigma^2 c}{2\pi i}\oint_\gamma\frac{1}{z}\frac{c\underline{m}(z)^3(1+\underline{m}(z))^{-3}}{\{1-c\underline{m}(z)^2(1+\underline{m}(z))^{-2}\}^2}dz \\ &\quad -\frac{\sigma^2 c(\nu_4-3)}{2\pi i}\oint_\gamma\frac{1}{z}\frac{c\underline{m}(z)^3(1+\underline{m}(z))^{-3}}{1-c\underline{m}(z)^2(1+\underline{m}(z))^{-2}}dz, \end{aligned} \tag{11}$$

$$\begin{aligned} \sigma_c^2 &= -\frac{\sigma^4 c^2}{2\pi^2}\oint_{\mathcal{C}_1}\oint_{\mathcal{C}_2}\frac{1}{z_1 z_2}\frac{1}{(\underline{m}(z_1)-\underline{m}(z_2))^2}\frac{d}{dz_1}\underline{m}(z_1)\frac{d}{dz_2}\underline{m}(z_2)dz_1dz_2 \\ &\quad -\frac{\sigma^4 c^3(\nu_4-3)}{4\pi^2}\oint_{\mathcal{C}_1}\oint_{\mathcal{C}_2}\frac{1}{z_1 z_2}\frac{1}{(1+\underline{m}(z_1))^2(1+\underline{m}(z_2))^2}d\underline{m}(z_1)d\underline{m}(z_2). \end{aligned} \tag{12}$$

Here the contours in (11) and (12) are closed and taken in the positive direction in the complex plane, enclosing the support of $F_{\mathbf{Z}}$, i.e. $[(1-\sqrt{c})^2, (1+\sqrt{c})^2]$. The Stieltjes transform $\underline{m}(z)$ satisfies the equation

$$z = -\frac{1}{\underline{m}} + \frac{c}{1+\underline{m}}.$$

To further simplify the integrations in μ_c and σ_c, let $z = 1 + \sqrt{c}(r\xi + \frac{1}{r\xi}) + c$ and perform change of variables, then we have

$$\underline{m}(z) = -\frac{1}{1+\sqrt{c}r\xi}, \quad dz = \sqrt{c}(r - \frac{1}{r\xi^2})d\xi, \quad d\underline{m} = \frac{\sqrt{c}r}{(1+\sqrt{c}r\xi)^2}d\xi$$

and when ξ moves along the unit circle $|\xi| = 1$ on the complex plane, z will orbit around the center point $1 + c$ along an ellipse which enclosing the support of $F_{\mathbf{Z}}$. Thus

$$\begin{aligned}
\mu_c &= -\frac{\sigma^2 c}{2\pi i}\oint_\gamma \frac{1}{z}\frac{c\underline{m}(z)^3(1+\underline{m}(z))^{-3}}{(1-c\underline{m}(z)^2(1+\underline{m}(z))^{-2})^2}dz \\
&\quad -\frac{\sigma^2 c(\nu_4-3)}{2\pi i}\oint_\gamma \frac{1}{z}\frac{c\underline{m}(z)^3(1+\underline{m}(z))^{-3}}{1-c\underline{m}(z)^2(1+\underline{m}(z))^{-2}}dz \\
&= \frac{\sigma^2 c}{2\pi i}\oint_{|\xi|=1}\frac{1}{r(\sqrt{c}+r\xi)(1+\sqrt{c}r\xi)(\xi-\frac{1}{r})(\xi+\frac{1}{r})}d\xi \\
&\quad +\frac{\sigma^2 c(\nu_4-3)}{2\pi i}\oint_{|\xi|=1}\frac{1}{r\xi^2(\sqrt{c}+r\xi)(1+\sqrt{c}r\xi)}d\xi \\
&= \frac{\sigma^2 c^2}{(c-1)^2} + \frac{\sigma^2 c^2(\nu_4-3)}{1-c}.
\end{aligned}$$

As for σ_c^2, note that

$$\begin{aligned}
&\frac{1}{2\pi i}\oint_{\gamma_1}\frac{1}{z_1(\underline{m}_1-\underline{m}_2)^2}d\underline{m}_1 \\
=\ & \frac{1}{2\pi i}\oint_{|\xi_1|=1}\frac{1}{1+\sqrt{c}(r_1\xi_1+\frac{1}{r_1\xi_1})+c}\cdot\frac{\sqrt{c}\,r_1}{(\underline{m}_2+\frac{1}{1+\sqrt{c}r_1\xi_1})^2(1+\sqrt{c}r_1\xi_1)^2}d\xi_1 \\
=\ & \frac{1}{2\pi i}\oint_{|\xi_1|=1}\frac{\sqrt{c}\,r_1\xi_1}{(\xi_1+\frac{\sqrt{c}}{r_1})(r_1\xi_1\sqrt{c}+1)\left\{(r_1\xi_1\sqrt{c}+1)\underline{m}_2+1\right\}^2}d\xi_1 \\
=\ & \frac{c}{(c-1)\left\{(c-1)\underline{m}_2-1\right\}^2},
\end{aligned}$$

therefore

$$\begin{aligned}
&-\frac{\sigma^4 c^2}{2\pi^2}\oiint\frac{1}{z_1z_2(\underline{m}_1-\underline{m}_2)^2}d\underline{m}_1 d\underline{m}_2 \\
=\ & \frac{2\sigma^4 c^2}{2\pi i}\oint_{|\xi_2|=1}\frac{c}{z_2(c-1)\left\{(c-1)\underline{m}_2-1\right\}^2}d\underline{m_2} \\
=\ & \frac{2\sigma^4 c^2}{2\pi i}\oint_{|\xi_2|=1}\frac{\sqrt{c}\,r_2^2\xi_2}{(c-1)(1+\sqrt{c}\,r_2\xi_2)(\sqrt{c}+r_2\xi_2)^3}d\xi_2 = \frac{2c^3\sigma^4}{(c-1)^4}.
\end{aligned}$$

Meanwhile,

$$\begin{aligned}
&\frac{1}{2\pi i}\oint_{\gamma_1}\frac{1}{z_1}\frac{1}{(1+\underline{m}(z_1))^2}d\underline{m}(z_1) \\
=\ & \frac{1}{2\pi i}\oint_{|\xi|=1}\frac{1}{\sqrt{c}\xi(1+\sqrt{c}r\xi)(\sqrt{c}+r\xi)}d\xi = \frac{1}{c-1},
\end{aligned}$$

hence

$$-\frac{\sigma^4 c^3(\nu_4-3)}{4\pi^2}\oint_{\mathcal{C}_1}\oint_{\mathcal{C}_2}\frac{1}{z_1z_2}\frac{1}{(1+\underline{m}(z_1))^2(1+\underline{m}(z_2))^2}d\underline{m}(z_1)d\underline{m}(z_2) = \frac{\sigma^4 c^3(\nu_4-3)}{(1-c)^2},$$

and

$$\sigma_c^2 = \frac{2c^3\sigma^4}{(c-1)^4} + \frac{\sigma^4 c^3(\nu_4-3)}{(1-c)^2}.$$

Let

$$T_n = \frac{p}{\sigma_c}\Big(R_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) - \sigma^2 \frac{c_n}{1-c_n} - \frac{\mu_c}{p}\Big).$$

According to (10), we have

$$P(L_{\alpha,c} \leq R_{\mathbf{X},\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) \leq U_{\alpha,c}) = P(-Z_{\alpha/2} \leq T_n \leq Z_{\alpha/2}) \to 1-\alpha,$$

where

$$\begin{aligned} L_{\alpha,c} &= \sigma^2 \frac{c_n}{1-c_n} + \frac{1}{p}(\mu_c - Z_{\alpha/2}\sigma_c), \\ U_{\alpha,c} &= \sigma^2 \frac{c_n}{1-c_n} + \frac{1}{p}(\mu_c + Z_{\alpha/2}\sigma_c). \end{aligned}$$

□

B PROOF OF THEOREM 4.3

Notice that

$$\begin{aligned} B_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) &= \boldsymbol{\beta}^{\mathrm{T}}(\boldsymbol{I}_p - \hat{\boldsymbol{\Sigma}}^{+}\hat{\boldsymbol{\Sigma}})\boldsymbol{\beta} \\ &= \lim_{z\to 0^+} \boldsymbol{\beta}^{\mathrm{T}}\big(\boldsymbol{I}_p - (\hat{\boldsymbol{\Sigma}} + z\boldsymbol{I}_p)^{-1}\hat{\boldsymbol{\Sigma}}\big)\boldsymbol{\beta} \\ &= \lim_{z\to 0^+} z\boldsymbol{\beta}^{\mathrm{T}}(\hat{\boldsymbol{\Sigma}} + z\boldsymbol{I}_p)^{-1}\boldsymbol{\beta}. \end{aligned}$$

Since $\boldsymbol{\beta}$ is a constant vector, we can make use of the results in Theorem 3 in Bai et al. (2007) and Theorem 1.3 in Pan & Zhou (2008) regarding eigenvectors. Their works investigate the sample covariance matrix $\mathbf{A}_p = \boldsymbol{T}_p^{1/2}\mathbf{X}_p^{\mathrm{T}}\mathbf{X}_p\boldsymbol{T}_p^{1/2}/n$, where $\boldsymbol{T}_p$ is an $p \times p$ nonnegative definite Hermitian matrix with a square root $\boldsymbol{T}_p^{1/2}$ and $\mathbf{X}_p$ is an $n \times p$ matrix with i.i.d. entries $(\mathrm{x}_{ij})_{n\times p}$. Let $\boldsymbol{U}_p\boldsymbol{\Lambda}_p\boldsymbol{U}_p^{\mathrm{T}}$ denote the spectral decomposition of $\mathbf{A}_p$ where $\boldsymbol{\Lambda}_p = \mathrm{diag}(\lambda_1, \cdots, \lambda_p)$ and $\boldsymbol{U}_p$ is a unitary matrix consisting of the orthonormal eigenvectors of $\mathbf{A}_p$. Assume that $\boldsymbol{x}_p$ is an arbitrary nonrandom unit vector and $\boldsymbol{y} = (y_1, y_2, \cdots, y_p)^{\mathrm{T}} = \boldsymbol{U}_p^{\mathrm{T}}\boldsymbol{x}_p$, two empirical distribution functions based on eigenvectors and eigenvalues are defined as

$$F_1^{\mathbf{A}_p}(x) = \sum_{i=1}^{p} |y_i|^2 \mathbb{1}(\lambda_i \leq x), \quad F^{\mathbf{A}_p}(x) = \frac{1}{p}\sum_{i=1}^{p} \mathbb{1}(\lambda_i \leq x).$$

Then for a bounded continuous function $g(x)$, we have

$$\sum_{j=1}^{p} |\mathrm{y}_j|^2 g(\lambda_j) - \frac{1}{p}\sum_{j=1}^{p} g(\lambda_j) = \int g(x) dF_1^{\boldsymbol{A}_p}(x) - \int g(x) dF^{\boldsymbol{A}_p}(x).$$

The results in Bai et al. (2007) and Pan & Zhou (2008) show that

Lemma B.1. (Theorem 3 Bai et al. (2007) and Theorem 1.3 Pan & Zhou (2008)) *Suppose that*

(1) x_{ij}*'s are i.i.d. satisfying* $\mathbb{E}(\mathrm{x}_{ij}) = 0$, $\mathbb{E}(|\mathrm{x}_{ij}|^2) = 1$ *and* $\mathbb{E}(|\mathrm{x}_{ij}|^4) < \infty$*;*

(2) $\boldsymbol{x}_p \in \mathbb{C}^p$, $\|\boldsymbol{x}_p\| = 1$, $\lim_{n,p\to\infty} p/n = c \in (0, \infty)$*;*

(3) $\boldsymbol{T}_p$ *is nonrandom Hermitian non-negative definite with with its spectral norm bounded in* p*, with* $H_p = F^{\boldsymbol{T}_p} \xrightarrow{d} H$ *a proper distribution function and* $\boldsymbol{x}_p^{\mathrm{T}}(\boldsymbol{T}_p - z\boldsymbol{I}_p)^{-1}\boldsymbol{x}_p \to m_{F^H}(z)$*, where* $m_{F^H}(z)$ *denotes the Stieltjes transform of* $H(t)$*;*

(4) $g_1, \cdots, g_k$ *are analytic functions on an open region of the complex plain which contains the real interval*

$$\Big[\liminf_p \lambda_{min}(\boldsymbol{T}_p)\mathbb{1}_{(0,1)}(c)(1-\sqrt{c})^2,\ \limsup_p \lambda_{max}(\boldsymbol{T}_p)\mathbb{1}_{(0,1)}(c)(1+\sqrt{c})^2\Big];$$

(5) as $n, p \to \infty$,

$$\sup_z \sqrt{n}\Big\|\boldsymbol{x}_p^{\mathrm{T}}\big(\underline{m}_{F^{c_n,H_p}}(z)\boldsymbol{T}_p - \boldsymbol{I}_p\big)^{-1}\boldsymbol{x}_p - \int \frac{1}{1+t\underline{m}_{F^{c_n,H_p}}(z)}dH_n(t)\Big\| \to 0.$$

Define $G_p(x) = \sqrt{n}(F_1^{\boldsymbol{A}_p}(x) - F^{\boldsymbol{A}_p}(x))$, then the random vectors

$$\Big(\int g_1(x)dG_p(x), \cdots, \int g_k(x)dG_p(x)\Big)$$

forms a tight sequence and converges weakly to a Gaussian vector $\mathrm{x}_{g_1}, \cdots, \mathrm{x}_{g_k}$ with mean zero and covariance function

$$\mathrm{Cov}(\mathrm{x}_{g_1}, \mathrm{x}_{g_2}) = -\frac{1}{2\pi^2}\int_{\mathbb{C}_1}\int_{\mathbb{C}_2} g_1(z_1)g_2(z_2)\frac{(z_2\underline{m}_2 - z_1\underline{m}_1)^2}{c^2 z_1 z_2 (z_2 - z_1)(\underline{m}_2 - \underline{m}_1)}dz_1 dz_2.$$

The contours $\mathbb{C}_1$, $\mathbb{C}_2$ are disjoint, both contained in the analytic region for the functions $(g_1, \cdots, g_k)$ and enclose the support of F^{c_n,H_p} for all large p.

(6) If $H(x)$ satisfies

$$\int \frac{dH(t)}{(1+t\underline{m}(z_1))(1+t\underline{m}(z_2))} = \int \frac{dH(t)}{1+t\underline{m}(z_1)}\int \frac{dH(t)}{1+t\underline{m}(z_2)},$$

then the covariance function can be further simplified to

$$\mathrm{Cov}(\mathrm{x}_{g_1}, \mathrm{x}_{g_2}) = \frac{2}{c}\Big(\int g_1(x)g_2(x)dF^{c,H}(x) - \int g_1(x)dF^{c,H}(x)\int g_2(x)dF^{c,H}(x)\Big).$$

Recall that $B_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) = \lim_{z\to 0^+} z\boldsymbol{\beta}^{\mathrm{T}}(\hat{\boldsymbol{\Sigma}} + z\boldsymbol{I}_p)^{-1}\boldsymbol{\beta}$. Let $g(x) = 1/(x+z)$ and $\boldsymbol{x}_p = \boldsymbol{\beta}/r$. Then we have

$$\int g(x)dG_n(x) = \sqrt{n}\Big(\frac{1}{r^2}\boldsymbol{\beta}^{\mathrm{T}}(\hat{\boldsymbol{\Sigma}} + z\boldsymbol{I}_p)^{-1}\boldsymbol{\beta} - \int g(x)dF_{c_n}(x)\Big),$$

where $F_{c_n}(x)$ is the standard Marcenko-Pastur law. It is not difficult to check that under Assumptions (A1), (B1) and (C1), all the conditions *(1)-(6)* in Lemma B.1 are satisfied.

To proceed further, denote $a = (1-\sqrt{c})^2$, $b = (1+\sqrt{c})^2$. If c is replaced by c_n, a and b are denoted by a_n and b_n respectively. By some algebraic calculations, we have

$$\begin{aligned}\int g(x)dF_{c_n}(x) &= (1-\frac{1}{c_n})\cdot\frac{1}{z} + \int_{a_n}^{b_n}\frac{1}{x+z}\cdot\frac{1}{2\pi c_n x}\sqrt{(b_n-x)(x-a_n)}dx \\ &= (1-\frac{1}{c_n})\cdot\frac{1}{z} - \frac{-1+c_n+z-\sqrt{c_n^2+2c_n(z-1)+(1+z)^2}}{2c_n z},\end{aligned}$$

and

$$\begin{aligned}\mathrm{Var}(\mathrm{x}_g) &= \frac{2}{c}\Big(\int\{g(x)\}^2 dF_c(x) - \big\{\int g(x)dF_c(x)\big\}^2\Big) \\ &= \frac{2}{c}\Big((1-\frac{1}{c})\cdot\frac{1}{z^2} + \int_a^b \frac{1}{(x+z)^2}\cdot\frac{1}{2\pi c x}\sqrt{(b-x)(x-a)}dx\Big) \\ &\quad -\frac{2}{c}\Big((1-\frac{1}{c})\cdot\frac{1}{z} + \int_a^b \frac{1}{x+z}\cdot\frac{1}{2\pi c x}\sqrt{(b-x)(x-a)}dx\Big)^2.\end{aligned}$$

Therefore,

$$\lim_{z\to 0^+} z\int g(x)dF_{c_n}(x) = 1 - \frac{1}{c_n} \quad \text{and} \quad \lim_{z\to 0^+} z^2\mathrm{Var}(\mathrm{x}_g) = \frac{2(c-1)}{c^3}.$$

Furthermore, as $n, p \to \infty$, $p/n = c_n \to c > 1$,

$$\sqrt{n}\Big(B_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) - (1-\frac{1}{c_n})r^2\Big) \xrightarrow{d} N\Big(0, \frac{2(c-1)}{c^3}r^4\Big).$$

This can be rewritten as

$$\sqrt{p}\Big(B_{\mathbf{X}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})-(1-\frac{1}{c_n})r^2\Big)\xrightarrow{d}N\Big(0,\frac{2(c-1)}{c^2}r^4\Big).$$

Next we deal with the variance term $V_{\mathbf{X}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})$. According to the Assumption *(B1)*, the variance term is

$$V_{\mathbf{X}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})=\frac{\sigma^2}{n}\operatorname{Tr}\{\hat{\boldsymbol{\Sigma}}^+\}=\frac{\sigma^2}{n}\sum_{i=1}^n\frac{1}{s_i},$$

where s_i, $i=1,\ldots,n$ are the nonzero eigenvalues of $\mathbf{X}^{\mathrm{T}}\mathbf{X}/n$. Let $\{t_i,\ i=1,\ldots n\}$ denote the non-zero eigenvalues of $\mathbf{X}\mathbf{X}^{\mathrm{T}}/p$, then we have

$$V_{\mathbf{X}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})=\frac{\sigma^2}{p}\sum_{i=1}^n\frac{1}{t_i}=\frac{\sigma^2 n}{p}\int\frac{1}{t}dF_{\mathbf{X}\mathbf{X}^{\mathrm{T}}/p}(t)\to\frac{\sigma^2}{c-1}.$$

By interchanging the role of p and n, from the result in Theorem 4.1, as $n,p\to\infty$, $p/n=c_n\to c>1$, we have,

$$\sum_{i=1}^n\frac{1}{t_i}-\frac{n}{1-c_n'}\xrightarrow{d}N\Big(\frac{c'}{(c'-1)^2}+\frac{c'(\nu_4-3)}{1-c'},\ \frac{2c'}{(c'-1)^4}+\frac{c'(\nu_4-3)}{(1-c')^2}\Big).$$

where $c_n'=n/p=1/c_n$, $c'=1/c$. This result can be rewritten as

$$\sum_{i=1}^n\frac{1}{t_i}-\frac{p}{c_n-1}\xrightarrow{d}N\Big(\frac{c}{(1-c)^2}+\frac{(\nu_4-3)}{c-1},\ \frac{2c^3}{(1-c)^4}+\frac{c(\nu_4-3)}{(c-1)^2}\Big).$$

Hence the CLT of $V_{\mathbf{X}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})$ is given by

$$p\Big(V_{\mathbf{X}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})-\frac{\sigma^2}{c_n-1}\Big)\xrightarrow{d}N\Big(\frac{c\sigma^2}{(1-c)^2}+\frac{\sigma^2(\nu_4-3)}{c-1},\ \frac{2c^3\sigma^4}{(1-c)^4}+\frac{c\sigma^4(\nu_4-3)}{(c-1)^2}\Big).$$

Notice that $\operatorname{Cov}\Big(B_{\mathbf{X}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta}),\ V_{\mathbf{X}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})\Big)=0$. According to the consistency rate and the limiting distribution of $B_{\mathbf{X}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})$ and $V_{\mathbf{X}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})$, we know that the bias $B_{\mathbf{X}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})$ is the leading term of $R_{\mathbf{X}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})$. This implies that

$$\sqrt{p}\Big\{R_{\mathbf{X}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})-(1-\frac{1}{c_n})\|\boldsymbol{\beta}\|_2^2-\frac{\sigma^2}{c_n-1}\Big\}\xrightarrow{d}N\big(0,\sigma_{c,1}^2\big),$$

where $\sigma_{c,1}^2=2(c-1)r^4/c^2$. A practical version of this CLT is given by

$$\sqrt{p}\Big\{R_{\mathbf{X}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})-(1-\frac{1}{c_n})\|\boldsymbol{\beta}\|_2^2-\frac{\sigma^2}{c_n-1}\Big\}\xrightarrow{d}N\big(\tilde{\mu}_{c,1},\tilde{\sigma}_{c,1}^2\big),$$

where

$$\begin{aligned}\tilde{\mu}_{c,1}&=\frac{1}{\sqrt{p}}\Big\{\frac{c\sigma^2}{(1-c)^2}+\frac{\sigma^2(\nu_4-3)}{c-1}\Big\},\\ \tilde{\sigma}_{c,1}^2&=\frac{2(c-1)}{c^2}r^4+\frac{1}{p}\Big\{\frac{2c^3\sigma^4}{(1-c)^4}+\frac{c\sigma^4(\nu_4-3)}{(c-1)^2}\Big\}.\end{aligned}$$

C Proof of theorem 4.4

First we consider the bias term $B_{\mathbf{X}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})$. By Assumption (A1), (B1), and (C2),

$$\begin{aligned}B_{\mathbf{X}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})&=\mathbb{E}[\boldsymbol{\beta}^{\mathrm{T}}\Pi\boldsymbol{\Sigma}\Pi\boldsymbol{\beta}|\mathbf{X}]=\mathbb{E}[\boldsymbol{\beta}^{\mathrm{T}}\Pi\boldsymbol{\beta}|\mathbf{X}]\\&=\operatorname{Tr}\Big\{(\boldsymbol{I}_p-\hat{\boldsymbol{\Sigma}}^+\hat{\boldsymbol{\Sigma}})\mathbb{E}(\boldsymbol{\beta}\boldsymbol{\beta}^{\mathrm{T}}|\mathbf{X})\Big\}\\&=\frac{r^2}{p}\operatorname{Tr}\{\boldsymbol{I}_p-\hat{\boldsymbol{\Sigma}}^+\hat{\boldsymbol{\Sigma}}\}=r^2(1-n/p).\end{aligned}$$

Alternatively, we can rewrite the bias as

$$\begin{aligned} B_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) &= \lim_{z\to 0^+} \mathbb{E}[\boldsymbol{\beta}^{\mathrm{T}}(\boldsymbol{I}_p - (\hat{\boldsymbol{\Sigma}} + z\boldsymbol{I}_p)^{-1}\hat{\boldsymbol{\Sigma}})\boldsymbol{\beta}|\mathbf{X}] \\ &= \lim_{z\to 0^+} \mathbb{E}[z\boldsymbol{\beta}^{\mathrm{T}}(\hat{\boldsymbol{\Sigma}} + z\boldsymbol{I}_p)^{-1}\boldsymbol{\beta}|\mathbf{X}] \\ &= \lim_{z\to 0^+} z\frac{r^2}{p}\operatorname{Tr}(\hat{\boldsymbol{\Sigma}} + z\boldsymbol{I}_p)^{-1}. \end{aligned}$$

Define that $f_n(z) = z\frac{r^2}{p}\operatorname{Tr}(\hat{\boldsymbol{\Sigma}} + z\boldsymbol{I}_p)^{-1}$. Notice that $|f_n(z)|$ and $|f_n'(z)|$ are bounded above. By the Arzela-Ascoli theorem, we deduce that $f_n(z)$ converges uniformly to its limit. Under Assumption *(C2)*, by the Moore-Osgood theorem, almost surely,

$$\begin{aligned} \lim_{n,p\to\infty} B_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) &= \lim_{z\to 0^+}\lim_{n,p\to\infty} z\frac{r^2}{p}\operatorname{Tr}(\hat{\boldsymbol{\Sigma}} + z\boldsymbol{I}_p)^{-1} \\ &= \lim_{z\to 0^+}\lim_{n,p\to\infty} z\frac{r^2}{p}\operatorname{Tr}\left(\frac{1}{n}\mathbf{X}\mathbf{X}^{\mathrm{T}} + z\boldsymbol{I}_n\right)^{-1}, \end{aligned}$$

In fact,

$$\lim_{n,p\to\infty} B_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) = r^2 \lim_{z\to 0^+}\lim_{n,p\to\infty} z m_n(-z),$$

where $m_n(z)$ is the Stieltjes transform of empirical spectral distribution of $\hat{\boldsymbol{\Sigma}} = \mathbf{X}^{\mathrm{T}}\mathbf{X}/n$. According to Theorem 2.1 in Zheng et al. (2015) and Lemma 1.1 in Bai & Silverstein (2004), the truncated version of $p(m_n(z) - m(z))$ converges weakly to a two-dimensional Gaussian process $M(\cdot)$ satisfying

$$\mathbb{E}[M(z)] = \frac{c\underline{m}^3(1+\underline{m})}{\{(1+\underline{m})^2 - c\underline{m}^2\}^2} + \frac{c(\nu_4 - 3)\underline{m}^3}{(1+\underline{m})\{(1+\underline{m})^2 - c\underline{m}^2\}},$$

and

$$\begin{aligned} \operatorname{Cov}\big(M(z_1), M(z_2)\big) &= 2\Big\{\frac{\underline{m}'(z_1)\underline{m}'(z_2)}{(\underline{m}(z_1) - \underline{m}(z_2))^2} - \frac{1}{(z_1 - z_2)^2}\Big\} \\ &\quad + \frac{c(\nu_4 - 3)\underline{m}'(z_1)\underline{m}'(z_2)}{(1+\underline{m}(z_1))^2(1+\underline{m}(z_2))^2}, \end{aligned}$$

where $\underline{m} = \underline{m}(z)$ represents the Stieltjes transform of limiting spectral distribution of companion matrix $\mathbf{X}\mathbf{X}^{\mathrm{T}}/n$ satisfying the equation

$$z = -\frac{1}{\underline{m}} + \frac{c}{1+\underline{m}}, \quad \underline{m}(z) = -\frac{1-c}{z} + cm(z).$$

When $p > n$, we can actually solve $\underline{m}(z)$ equation and obtain that

$$\begin{aligned} \underline{m}(z) &= \frac{-1 + c - z + \sqrt{-4z + (1-c+z)^2}}{2z}, \\ m(z) &= \frac{1 - c - z + \sqrt{-4z + (1-c+z)^2}}{2cz}. \end{aligned}$$

Therefore, by some algebraic calculations, we have

$$\begin{aligned} \lim_{n,p\to\infty} B_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) &= \lim_{n,p\to\infty} r^2 \lim_{z\to 0^+} z m_n(-z) = r^2 \lim_{z\to 0^+}\left\{zm(-z) + z(1 - \frac{1}{c})\frac{1}{z}\right\} \\ &= \lim_{n,p\to\infty} r^2 \lim_{z\to 0^+} z\frac{n}{p}\underline{m}_n(z) = r^2\frac{1}{c}\lim_{z\to 0^+} z\underline{m}(-z) \\ &= r^2(1 - \frac{1}{c}). \end{aligned}$$

Moreover,

$$\begin{aligned} \operatorname{Var}\big(M(z)\big) &= \lim_{z_1\to z_2 = z} \operatorname{Cov}\big(M(z_1), M(z_2)\big) \\ &= \frac{2\underline{m}'(z)\underline{m}'''(z) - 3(\underline{m}''(z))^2}{6(\underline{m}'(z))^2} + \frac{c(\nu_4 - 3)(\underline{m}'(z))^2}{(1+\underline{m}(z))^4}. \end{aligned}$$

By substituting of the explicit form of $\underline{m}(z)$, we can easily derive that

$$\lim_{z\to 0^+} z\mathbb{E}[M(-z)] = 0, \quad \lim_{z\to 0^+} z^2 \mathrm{Var}(M(-z)) = 0,$$

which means that the second order limit of $B_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta})$ is still $r^2(1-1/c)$. All in all, $B_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta})$ is identical with a constant $r^2(1-1/c)$ in distribution.

On the other hand, by Assumption (B1),

$$V_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) = \frac{\sigma^2}{n}\,\mathrm{Tr}\{\hat{\boldsymbol{\Sigma}}^+\} = \frac{\sigma^2}{n}\sum_{i=1}^{n}\frac{1}{s_i},$$

where s_i, $i = 1, \ldots, n$ are the nonzero eigenvalues of $\mathbf{X}^{\mathrm{T}}\mathbf{X}/n$. Similar to the proof of Theorem 4.3, the CLT of $V_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta})$ is given by

$$p\Big(V_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) - \frac{\sigma^2}{c_n - 1}\Big) \xrightarrow{d} N\Big(\frac{c\sigma^2}{(1-c)^2} + \frac{\sigma^2(\nu_4 - 3)}{c-1},\ \frac{2c^3\sigma^4}{(1-c)^4} + \frac{c\sigma^4(\nu_4-3)}{(c-1)^2}\Big).$$

Combining the results of $B_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta})$ and $V_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta})$, we have

$$p\Big\{R_{\mathbf{X}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) - r^2(1 - \frac{1}{c_n}) - \frac{\sigma^2}{c_n - 1}\Big\} \xrightarrow{d} N(\mu_{c,2}, \sigma_{c,2}^2),$$

where

$$\mu_{c,2} = \frac{c\sigma^2}{(1-c)^2} + \frac{\sigma^2(\nu_4-3)}{c-1}, \quad \sigma_{c,2}^2 = \frac{2c^3\sigma^4}{(1-c)^4} + \frac{c\sigma^4(\nu_4-3)}{(c-1)^2}.$$

D PROOF OF THEOREM 4.5

Note that under Assumption *(B1)* and *(C2)*, $B_{\mathbf{X},\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) = \boldsymbol{\beta}^{\mathrm{T}}\Pi\boldsymbol{\beta} = \boldsymbol{\beta}^{\mathrm{T}}(\boldsymbol{I}_p - \hat{\boldsymbol{\Sigma}}^+\hat{\boldsymbol{\Sigma}})\boldsymbol{\beta}$. If we directly consider $\boldsymbol{\beta}^{\mathrm{T}}(\boldsymbol{I}_p - \hat{\boldsymbol{\Sigma}}^+\hat{\boldsymbol{\Sigma}})\boldsymbol{\beta}$, we can make use of the asymptotic results for quadratic forms Theorem 7.2 in Bai & Yao (2008) stated as follows.

Lemma D.1. (Theorem 7.2 in Bai & Yao (2008)) *Let $\{\boldsymbol{A}_n = [a_{ij}(n)]\}$ be a sequence of $n \times n$ real symmetric matrices, $\{\mathbf{x}_i\}_{i\in\mathbb{N}}$ be a sequence of i.i.d. K dimensional real random vectors, with $\mathbb{E}(\mathbf{x}_i) = 0$, $\mathbb{E}(\mathbf{x}_i\mathbf{x}_i^{\mathrm{T}}) = (\gamma_{ij})_{K\times K}$ and $\mathbb{E}[\|\mathbf{x}_i\|^4] < \infty$. Denote*

$$\mathbf{x}_i = (\mathrm{x}_{\ell i})_{K\times 1}, \quad \mathbf{X}(\ell) = (\mathrm{x}_{\ell 1}, \cdots, \mathrm{x}_{\ell n})^{\mathrm{T}}, \quad \ell = 1, \cdots, K,\ i = 1, \cdots, n,$$

assume the following limits exist

$$\omega = \lim_{n\to\infty}\frac{1}{n}\sum_{i=1}^{n} a_{ii}^2(n), \quad \theta = \lim_{n\to\infty}\frac{1}{n}\,\mathrm{Tr}\,\boldsymbol{A}_n^2.$$

Then the K-dimensional random vectors

$$\mathbf{z}_n = (\mathrm{z}_{n,\ell})_{K\times 1}, \quad \mathrm{z}_{n,\ell} = \frac{1}{\sqrt{n}}\big(\mathbf{X}(\ell)^{\mathrm{T}}\boldsymbol{A}_n\mathbf{X}(\ell) - \gamma_{\ell\ell}\,\mathrm{Tr}\{\boldsymbol{A}_n\}\big), \quad 1 \le \ell \le K,$$

converge weakly to a zero-mean Gaussian vector with covariance matrix $\boldsymbol{D} = \boldsymbol{D}_1 + \boldsymbol{D}_2$ where

$$[\boldsymbol{D}_1]_{\ell\ell'} = \omega\left\{\mathbb{E}(x_{\ell 1}^2 x_{\ell' 1}^2) - \gamma_{\ell\ell}\gamma_{\ell'\ell'}\right\},\ [\boldsymbol{D}_2]_{\ell\ell'} = (\theta - \omega)(\gamma_{\ell\ell'}\gamma_{\ell'\ell} + \gamma_{\ell\ell'}^2),\ 1 \le \ell, \ell' \le K.$$

According to the results in Lemma D.1, let $\boldsymbol{A}_n = \Pi = \boldsymbol{I}_p - \hat{\boldsymbol{\Sigma}}^+\hat{\boldsymbol{\Sigma}}$, then we have, as $p \to \infty$,

$$\sqrt{p}\Big\{\boldsymbol{\beta}^{\mathrm{T}}\Pi\boldsymbol{\beta} - \frac{r^2}{p}\,\mathrm{Tr}(\Pi)\Big\} \xrightarrow{d} N(0, d^2 = d_1^2 + d_2^2),$$

where

$$\omega = \lim_{p\to\infty}\frac{1}{p}\sum_{i=1}^{p}\Pi_{ii}^2, \quad \theta = \lim_{p\to\infty}\frac{1}{p}\,\mathrm{Tr}(\Pi^2) = 1 - \frac{1}{c},$$

and

$$\begin{aligned} d_1^2 &= \omega\left\{\mathbb{E}(x_{\ell 1}^2 x_{\ell 1}^2) - \gamma_{\ell\ell}^2\right\} = \omega\big(\frac{p^2}{r^4}\,\mathbb{E}(\beta_i^4) - 1\big)r^4, \\ d_2^2 &= (\theta-\omega)(\gamma_{\ell\ell}^2 + \gamma_{\ell\ell}^2) = 2(\theta-\omega)r^4. \end{aligned}$$

Since in the proof of Theorem 4.4, we have already shown that

$$\frac{r^2}{p}\,\mathrm{Tr}(\Pi) = r^2(1-\frac{n}{p}).$$

In particular, if $\boldsymbol{\beta}$ follows multivariate Gaussian distribution, i.e. $\boldsymbol{\beta} \sim N_p(0, \frac{r^2}{p}\boldsymbol{I}_p)$, then as $p \to \infty$,

$$\sqrt{p}\Big\{B_{\mathbf{X},\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta}) - r^2(1-\frac{n}{p})\Big\} \xrightarrow{d} N\Big(0, 2(1-\frac{1}{c})r^4\Big).$$

Moreover, $V_{\mathbf{X},\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta}) = V_{\mathbf{X}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})$, we have already proved in Theorem 4.4 that

$$p(V_{\mathbf{X},\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta}) - \frac{\sigma^2}{c_n-1}) \xrightarrow{d} N\Big(\frac{c\sigma^2}{(1-c)^2} + \frac{\sigma^2(\nu_4-3)}{c-1},\ \frac{2c^3\sigma^4}{(1-c)^4} + \frac{c\sigma^4(\nu_4-3)}{(c-1)^2}\Big).$$

Note that $\mathrm{Cov}(B_{\mathbf{X},\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta}),\ V_{\mathbf{X},\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})) = 0$. According to the consistency rate of $B_{\mathbf{X},\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})$ and $V_{\mathbf{X},\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})$, we know that the bias $B_{\mathbf{X}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})$ is the leading term of $R_{\mathbf{X},\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta})$. This implies that

$$\sqrt{p}\Big\{R_{\mathbf{X},\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta}) - r^2(1-\frac{1}{c_n}) - \frac{\sigma^2}{c_n-1}\Big\} \xrightarrow{d} N(0,\sigma_{c,3}^2),$$

where $\sigma_{c,3}^2 = 2r^4(1-1/c)$. A practical version of this CLT is given by

$$\sqrt{p}\Big\{R_{\mathbf{X},\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta}) - r^2(1-\frac{1}{c_n}) - \frac{\sigma^2}{c_n-1}\Big\} \xrightarrow{d} N(\tilde{\mu}_{c,3},\tilde{\sigma}_{c,3}^2),$$

where

$$\begin{aligned} \tilde{\mu}_{c,3} &= \frac{1}{\sqrt{p}}\Big\{\frac{c\sigma^2}{(1-c)^2} + \frac{\sigma^2(\nu_4-3)}{c-1}\Big\}, \\ \tilde{\sigma}_{c,3}^2 &= 2(1-\frac{1}{c})r^4 + \frac{1}{p}\Big\{\frac{2c^3\sigma^4}{(1-c)^4} + \frac{c\sigma^4(\nu_4-3)}{(c-1)^2}\Big\}. \end{aligned}$$

E MORE EXPERIMENTS

E.1 MORE RESULTS OF EXAMPLE 1

This example checks Theorem 4.2. We define a statistic

$$T_n = \frac{p}{\sigma_c}\Big(R_{\mathbf{X}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta}) - \sigma^2\frac{c_n}{1-c_n}\Big) - \frac{\mu_c}{\sigma_c}.$$

According to Theorem 4.2, T_n weakly converges to the standard normal distribution as $n, p \to \infty$. In this example, $c = 1/2$ and $p = 50, 100, 200$. To make sure the assumption (A) holds, the generative distribution $P_{\mathbf{x}}$ is taken to be the standard normal distribution, the centered gamma with shape 4.0 and scale 0.5, and the normalized Student-t distribution with 6.0 degree of freedom. The finite-sample distribution of T_n is estimated by the histogram of T_n under 1000 repetitions. The results are presented in Figure 4. One can find that the finite-sample distribution of T_n tends to the standard normal distribution as $n, p \to +\infty$. When $\alpha = 0.05$, the empirical cover rates of the 95%-confidence interval are reported in Figure 5.

E.2 MORE RESULTS OF EXAMPLE 2

The Example 2 checks Theorem 4.5. Here we consider the standardized statistics:

$$\begin{aligned} T_{n,0} &= \frac{\sqrt{p}}{\sigma_{c,3}}\Big\{R_{\mathbf{X}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta}) - (1-\frac{1}{c_n})r^2 - \frac{\sigma^2}{c_n-1}\Big\} - \frac{\mu_{c,3}}{\sigma_{c,3}}, \\ T_{n,1} &= \frac{\sqrt{p}}{\tilde{\sigma}_{c,3}}\Big\{R_{\mathbf{X}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta}) - (1-\frac{1}{c_n})r^2 - \frac{\sigma^2}{c_n-1}\Big\} - \frac{\tilde{\mu}_{c,3}}{\tilde{\sigma}_{c,3}}. \end{aligned}$$

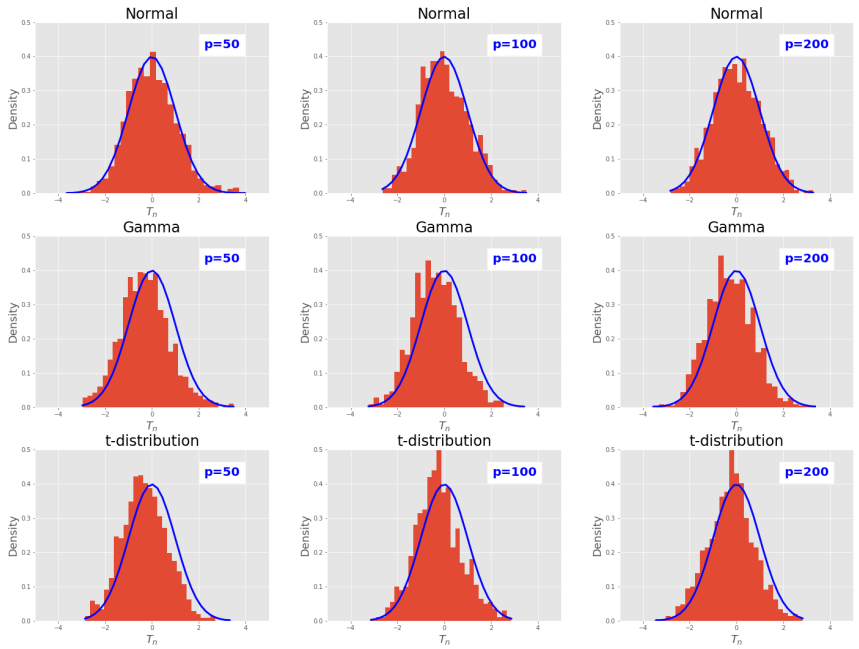

Figure 4: The histogram of T_n. The solid line is the density of the standard normal distribution.

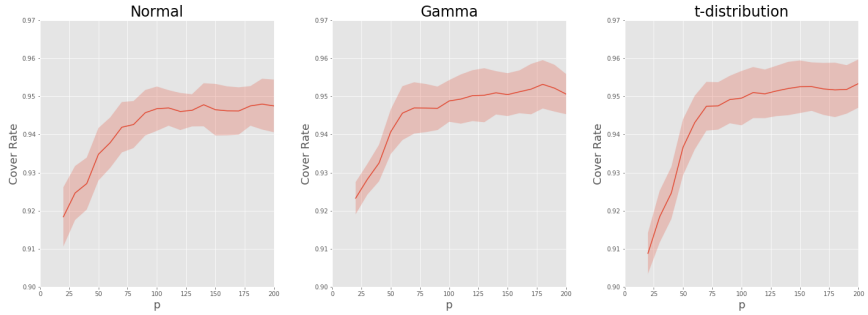

Figure 5: The cover rate of the confidence interval (5) as p creases. The confidence level is 95%.

According to the central limit theorem (8) and its practical version, both $T_{n,0}$ and $T_{n,1}$ weakly converge to the standard normal distribution as $n, p \to +\infty$. We take $c = 2$ and $p = 100, 200, 400$. The finite-sample distributions of $T_{n,0}$ and $T_{n,1}$ are estimated by the histogram of $T_{n,0}$ and $T_{n,1}$ under 1000 repetitions. The results are presented in Figure 6 and Figure 7. When $\alpha = 0.05$, the empirical cover rates of the 95%-confidence interval (9) are reported in Figure 8.

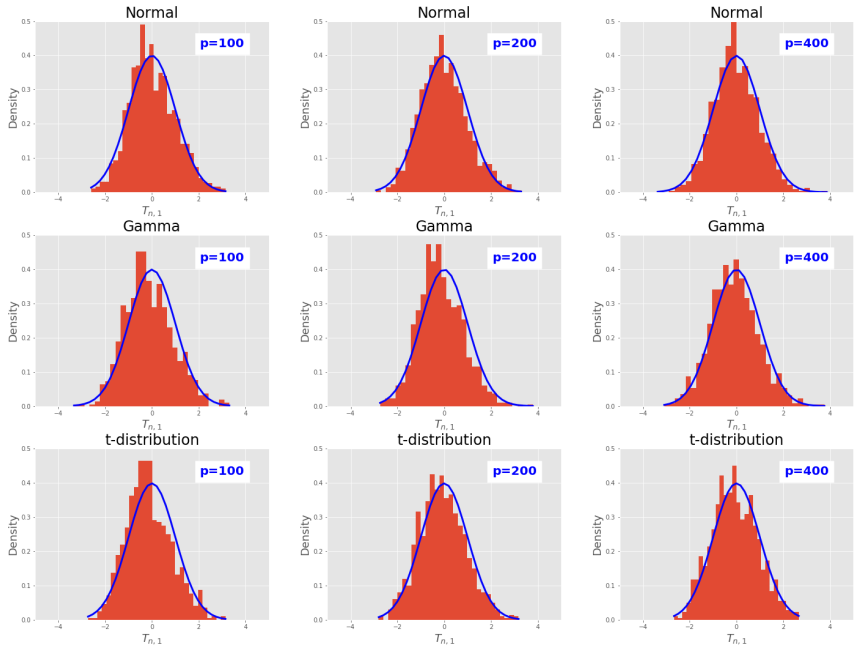

Figure 6: The histogram of $T_{n,1}$. The solid line is the density of the standard normal distribution.

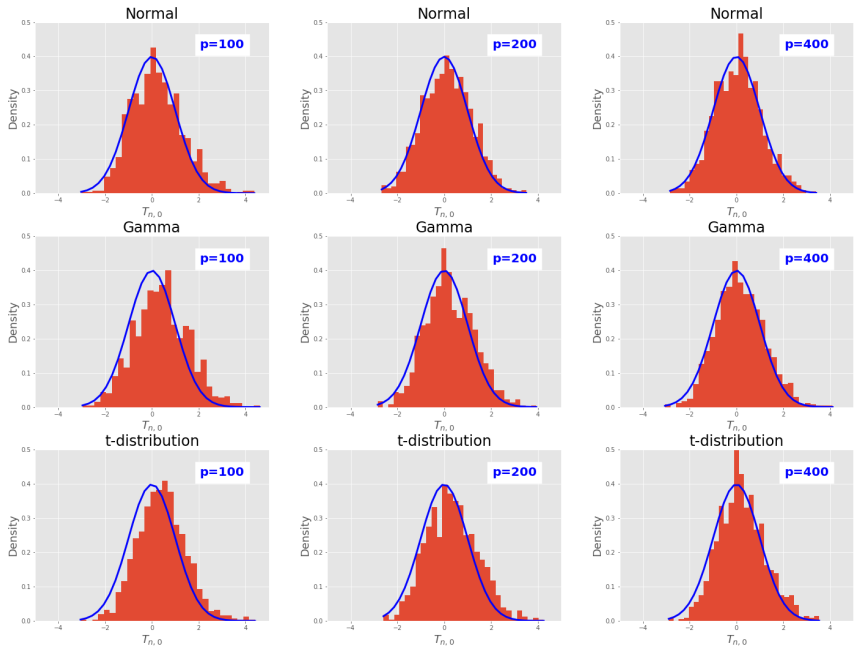

Figure 7: The histogram of $T_{n,0}$. The solid line is the density of the standard normal distribution.

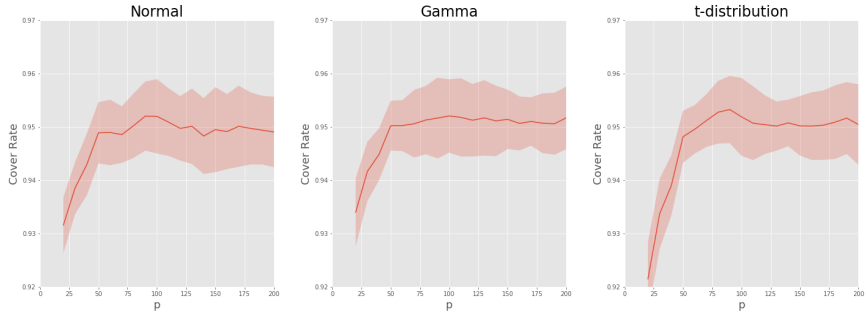

Figure 8: The cover rate of the confidence interval (9) as p creases. The confidence level is 95%.

E.3 EXAMPLE 3

This example checks Theorem 4.3. To proceed further, we denote two statistics:

$$T_{n,2} = \frac{\sqrt{p}}{\sigma_{c,1}}\Big\{R_{\mathbf{X}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta}) - (1-\frac{1}{c_n})r^2 - \frac{\sigma^2}{c_n-1}\Big\} - \frac{\mu_{c,1}}{\sigma_{c,1}},$$
$$T_{n,3} = \frac{\sqrt{p}}{\tilde{\sigma}_{c,1}}\Big\{R_{\mathbf{X}}(\hat{\boldsymbol{\beta}},\boldsymbol{\beta}) - (1-\frac{1}{c_n})r^2 - \frac{\sigma^2}{c_n-1}\Big\} - \frac{\tilde{\mu}_{c,1}}{\tilde{\sigma}_{c,1}}.$$

According to the central limit theorem (6) and its practical version, both $T_{n,2}$ and $T_{n,3}$ weakly converge to the standard normal distribution as $n, p \to +\infty$. We take $c = 2$ and $p = 100, 200, 400$. The finite-sample distributions of $T_{n,2}$ and $T_{n,3}$ are estimated by the histogram of $T_{n,2}$ and $T_{n,3}$ under 1000 repetitions. The results are presented at Figure 9 and Figure 10. One can see that the finite-sample distributions of $T_{n,2}$ and $T_{n,3}$ are close to the standard normal distribution, and the finite-sample performance of $T_{n,3}$ is better than that of $T_{n,2}$. When $\alpha = 0.05$, the empirical cover rates of the 95%-confidence interval (7) are reported in Figure 11.

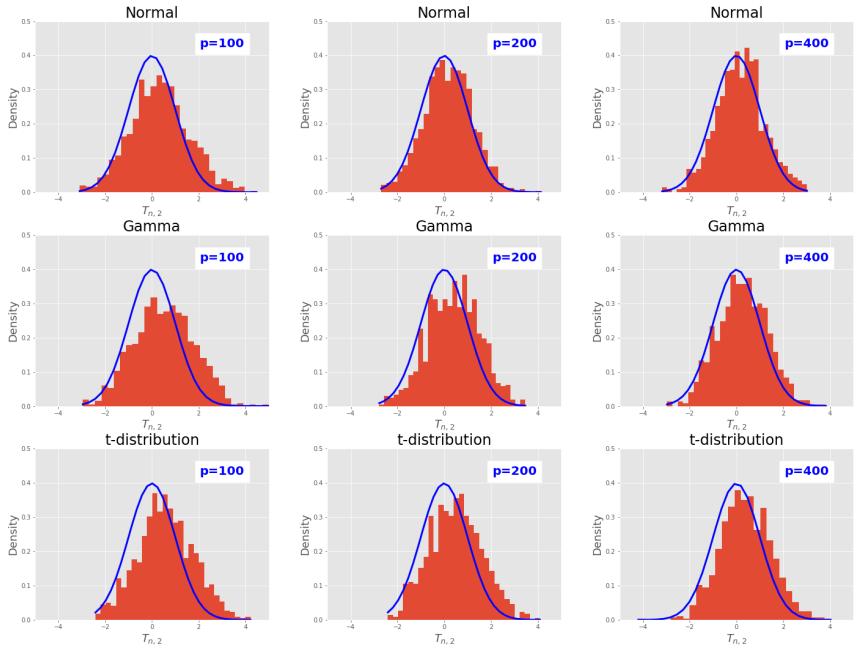

Figure 9: The histogram of $T_{n,2}$. The solid line is the density of the standard normal distribution.

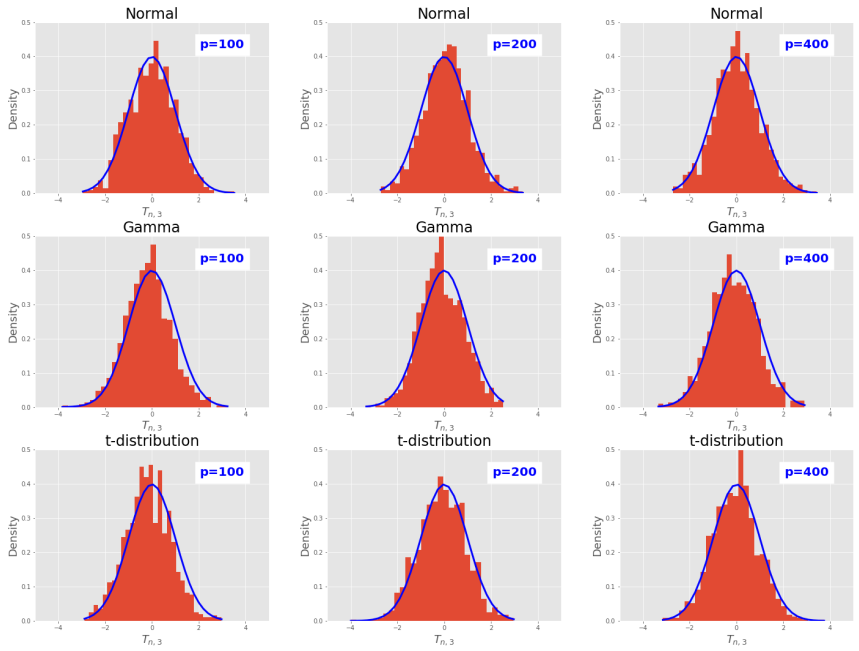

Figure 10: The histogram of $T_{n,3}$. The solid line is the density of the standard normal distribution.

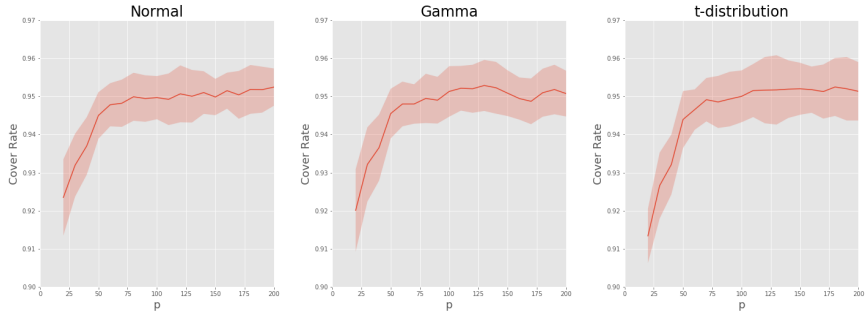

Figure 11: The cover rate of the confidence interval (7) as p creases. The confidence level is 95%.