

# GAUSSIAN AND BOOTSTRAP APPROXIMATIONS FOR HIGH-DIMENSIONAL U-STATISTICS AND THEIR APPLICATIONS\*

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This paper studies the Gaussian and bootstrap approximations for the probabilities of a non-degenerate U-statistic belonging to the hyperrectangles in  $\mathbb{R}^d$  when the dimension  $d$  is large. A two-step Gaussian approximation procedure that does not impose structural assumptions on the data distribution is proposed. Subject to mild moment conditions on the kernel, we establish the explicit rate of convergence uniformly in the class of all hyperrectangles in  $\mathbb{R}^d$  that decays polynomially in sample size for a high-dimensional scaling limit, where the dimension can be much larger than the sample size. We also provide computable approximation methods for the quantiles of the maxima of centered U-statistics. Specifically, we provide a unified perspective for the empirical bootstrap, the randomly reweighted bootstrap, and the Gaussian multiplier bootstrap with the jackknife estimator of covariance matrix as randomly reweighted quadratic forms and we establish their validity. We show that all three methods are inferentially first-order equivalent for high-dimensional U-statistics in the sense that they achieve the same uniform rate of convergence over all  $d$ -dimensional hyperrectangles. In particular, they are asymptotically valid when the dimension  $d$  can be as large as  $O(e^{n^c})$  for some constant  $c \in (0, 1/7)$ .

The bootstrap methods are applied to statistical applications for high-dimensional non-Gaussian data including: (i) principled and data-dependent tuning parameter selection for regularized estimation of the covariance matrix and its related functionals; (ii) simultaneous inference for the covariance and rank correlation matrices. In particular, for the thresholded covariance matrix estimator with the bootstrap selected tuning parameter, we show that [for a class of subgaussian data, error bounds of the bootstrapped thresholded covariance matrix estimator can be much tighter than those of the minimax estimator with a universal threshold](#). In addition, we also show that the Gaussian-like convergence rates can be achieved for heavy-tailed data, which are less conservative than those obtained by the Bonferroni technique that ignores the dependency in the underlying data distribution.

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\*First version: January 30, 2016. This version: February 20, 2017.

<sup>†</sup>Research partially supported by NSF grant DMS-1404891 and UIUC Research Board Award RB15004.

**1. Introduction.** Let  $X_1^n = \{X_1, \dots, X_n\}$  be a sample of independent and identically distributed (iid) random vectors in  $\mathbb{R}^p$  with the distribution  $F$ . Let  $h : \mathbb{R}^p \times \mathbb{R}^p \rightarrow \mathbb{R}^d$  be a fixed and measurable function such that  $h(x_1, x_2) = h(x_2, x_1)$  for all  $x_1, x_2 \in \mathbb{R}^p$  and  $\mathbb{E}|h_k(X_1, X_2)| < \infty$  for all  $k = 1, \dots, d$ . Consider the U-statistic of order two

$$(1) \quad U_n = \frac{1}{n(n-1)} \sum_{1 \leq i \neq j \leq n} h(X_i, X_j).$$

In this paper, we consider the uniform approximation of the probabilities of  $U_n$  over a class of the Borel subsets in  $\mathbb{R}^d$ . More specifically, let  $T_n = \sqrt{n}(U_n - \theta)/2$ , where  $\theta = \mathbb{E}[h(X_1, X_2)]$  is the parameter of interest, and  $\mathcal{A}^{re}$  be the class of all hyperrectangles  $A$  in  $\mathbb{R}^d$  of the form

$$(2) \quad A = \{x \in \mathbb{R}^d : a_j \leq x_j \leq b_j \text{ for all } j = 1, \dots, d\},$$

where  $-\infty \leq a_j \leq b_j \leq \infty$  for  $j = 1, \dots, d$ . Our main goal are to construct a random vector  $T_n^{\natural}$  in  $\mathbb{R}^d$  and to derive non-asymptotic bounds for

$$(3) \quad \rho^{re}(T_n, T_n^{\natural}) = \sup_{A \in \mathcal{A}^{re}} |\mathbb{P}(T_n \in A) - \mathbb{P}(T_n^{\natural} \in A)|.$$

When  $p$  (and therefore  $d$ ) is fixed, the classical central limit theorems (CLT) for approximating  $T_n$  by a Gaussian random vector  $T_n^{\natural} \sim N(0, \Gamma)$ , where  $\Gamma = \text{Cov}(g(X_1))$  and  $g(X_1) = \mathbb{E}[h(X_1, X_2)|X_1] - \theta$ , have been extensively studied in literature [34, 3, 37, 32, 25, 35, 33, 59, 3, 67, 31, 36, 37, 59]. Recently, due to the explosive data enrichment, regularized estimation and dimension reduction of high-dimensional data (i.e.  $d$  is large or even much larger than  $n$ ) have attracted a lot of research attentions such as covariance matrix estimation [9, 10, 29, 19], graphical models [27, 66, 11], discriminant analysis [47], factor models [30, 43], among many others. Those problems all involve the consistent estimation of an expectation  $\mathbb{E}[h(X_1, X_2)]$  of U-statistics of order two. Below are three examples.

**EXAMPLE 1.1.** The sample mean vector  $\bar{X}_n = n^{-1} \sum_{i=1}^n X_i$  is an unbiased estimator of  $\mathbb{E}X_1$  and  $\bar{X}_n$  can be written as a U-statistic of form (1) with the linear kernel  $h(x_1, x_2) = (x_1 + x_2)/2$  for  $x_1, x_2 \in \mathbb{R}^p$  and  $d = p$ .

**EXAMPLE 1.2.** Let  $d = p \times p$ . The sample covariance matrix  $\hat{S}_n = (n-1)^{-1} \sum_{i=1}^n (X_i - \bar{X}_n)(X_i - \bar{X}_n)^\top$  is an unbiased estimator of the covariance matrix  $\Sigma = \text{Cov}(X_1)$ . Here,  $\hat{S}_n$  is a matrix-valued U-statistic of form (1) with the quadratic kernel  $h(x_1, x_2) = (x_1 - x_2)(x_1 - x_2)^\top/2$  for  $x_1, x_2 \in \mathbb{R}^p$ .

EXAMPLE 1.3. The covariance matrix quantifies the linear dependency in a random vector. The rank correlation is another measure for the nonlinear dependency in a random vector. Two generic vectors  $y = (y_1, y_2)$  and  $z = (z_1, z_2)$  in  $\mathbb{R}^2$  are said to be *concordant* if  $(y_1 - z_1)(y_2 - z_2) > 0$ . For  $m, k = 1, \dots, p$ , define

$$\tau_{mk} = \frac{1}{n(n-1)} \sum_{1 \leq i \neq j \leq n} \mathbf{1}\{(X_{im} - X_{jm})(X_{ik} - X_{jk}) > 0\}.$$

Then, Kendall's tau rank correlation coefficient matrix  $T = \{\tau_{mk}\}_{m,k=1}^p$  is a matrix-valued U-statistic with a bounded kernel. It is clear that  $\tau_{mk}$  quantifies the monotonic dependency between  $(X_{1m}, X_{1k})$  and  $(X_{2m}, X_{2k})$  and it is an unbiased estimator of  $\mathbb{P}((X_{1m} - X_{2m})(X_{1k} - X_{2k}) > 0)$ , i.e. the probability that  $(X_{1m}, X_{1k})$  and  $(X_{2m}, X_{2k})$  are concordant.

In this paper, we are interested in the following central questions: *how does the dimension impact the asymptotic behavior of U-statistics and how can we make practical statistical inference when  $d \rightarrow \infty$ ?* Bounds on (3) with the explicit dependence on  $d$  are particularly useful in large-scale statistical inference problems. In particular, motivation of this paper comes from the estimation and inference problems for large covariance matrix and its related functionals [50, 66, 57, 53, 65, 12, 10, 19, 20]. To establish rate of convergence for the regularized estimators or to approximate the limiting null distribution of  $\ell^\infty$ -tests in high-dimensions, a key issue is to characterize the distribution of the supremum norm  $|U_n - \mathbb{E}U_n|_\infty$  that relates to the probabilities of  $\mathbb{P}(T_n \in A)$  for  $A$  belonging to the family of max-hyperrectangles in  $\mathbb{R}^d$  of the form  $A = \{x \in \mathbb{R}^d : x_j \leq a \text{ for all } j = 1, \dots, d\}$  and  $-\infty \leq a \leq \infty$ .

Our first main contribution is to provide a Gaussian approximation scheme for the high-dimensional *non-degenerate* U-statistics. Different from the CLT type results for the sums of independent random vectors [21, 23], which are directly approximated by the Gaussian counterparts with the matching first and second moments, approximation of the U-statistics is more subtle because of its dependency and nonlinearity structures. Here, we propose a *two-step* Gaussian approximation method in Section 2. In the first step, we approximate the U-statistics by the leading component of a linear form in the Hoeffding decomposition (a.k.a. the Hájek projection); in the second step, the linear term is further approximated by the Gaussian random vectors. To approximate the distribution of U-statistics by a linear form, a maximal moment inequality is developed to control the nonlinear and *canonical*, i.e. *completely degenerate*, form of the reminder term. Then the linear projection is handled by the recent development of Gaussian approximation in

high-dimensions [21, 23, 69, 68]. Explicit rate of convergence of the Gaussian approximation for high-dimensional U-statistics uniformly in the class of all hyperrectangles in  $\mathbb{R}^d$  is established for unbounded kernels subject to sub-exponential and uniform polynomial moment conditions. Specifically, under either moment conditions, we show that the validity of the Gaussian approximation holds for a high-dimensional scaling limit, where  $d$  can be larger or even much larger than  $n$ . In our results, symmetry of U-statistics is an key ingredient in the Hoeffding decomposition. Therefore our result can be viewed as nonlinear generalizations of the Gaussian approximation for the high-dimensional sample mean vector of iid  $X_1, \dots, X_n$ .

The second contribution of this paper is to provide *computable* methods for approximating the probabilities  $\mathbb{P}(T_n \in A)$  uniformly for  $A \in \mathcal{A}^{re}$ . This allows us to compute the quantiles of the maxima  $|U_n - \mathbb{E}U_n|_\infty$ . Since the covariance matrix  $\Gamma$  of the Hájek projection of the centered U-statistics depends on the underlying data distribution  $F$  which is unknown in many real applications, a practically feasible alternative is to use data-dependent approaches such as the bootstrap to approximate  $\mathbb{P}(T_n \in A)$ , where the insight is to implicitly construct a consistent estimator of  $\Gamma$  under the supremum norm. In Section 3, we provide a unified perspective for the empirical bootstrap, the randomly reweighted bootstrap, and the Gaussian multiplier bootstrap with the jackknife estimator of covariance matrix as randomly reweighted quadratic forms and we establish their validity. Specifically, we show that all three methods are inferentially first-order equivalent for high-dimensional U-statistics in the sense that they achieve the same uniform rate of convergence over  $\mathcal{A}^{re}$ . In particular, they are asymptotically valid when the dimension  $d$  can be as large as  $O(e^{n^c})$  for some constant  $c \in (0, 1/7)$ . One important feature of the Gaussian and bootstrap approximations is that no structural assumption on the distribution  $F$  is made and the strong dependency in  $F$  is allowed, which in fact helps the Gaussian and bootstrap approximations.

In Section 4, we apply the proposed bootstrap method to a number of important high-dimensional problems, including the data-dependent tuning parameter selection in the thresholded covariance matrix estimator and the simultaneous inference of the covariance and Kendall's tau rank correlation matrices. Two additional applications for the estimation problems of the sparse precision matrix and the sparse linear functionals of the precision matrix are given in the Supplemental Materials (SM). In those problems, we show that the Gaussian like convergence rates can be achieved for non-Gaussian data with heavy-tails, which are less conservative than those obtained by the Bonferroni technique that ignores the dependency in the

underlying data distribution. For the sparse covariance matrix estimation problem, we also show that the thresholded estimator with the tuning parameter selected by the bootstrap procedure adapts the dependency and moment in the underlying data distribution and therefore the bounds can be much tighter than those of the minimax estimator with a universal threshold that ignores the dependency in  $F$  [10, 19, 13].

To establish the Gaussian approximation result and the validity of the bootstrap methods, a key step is to bound the expected supremum norm of the second-order canonical term in the Hoeffding decomposition of the U-statistics and establish its non-asymptotic maximal moment inequalities. An alternative simple data splitting approach by reducing the U-statistics to sums of iid random vectors can give the exact rate for bounding the moments in the non-degenerate case [61, 49, 41, 28]. Nonetheless, the reduction to the iid summands in terms of data splitting does not exploit the complete degeneracy structure of the canonical term and it does not lead to the convergence result in the Gaussian approximation for the non-degenerate U-statistics; see Section 5.1 for details. In addition, unlike the Hoeffding decomposition approach, the data splitting approximation is not asymptotically tight in distribution and therefore it is less useful in making inference of the high-dimensional U-statistics.

*Relation to the existing literature.* For univariate U-statistics, the empirical bootstrap was studied in [7, 2] and the randomly reweighted bootstrap of the form (15) was proposed in [40, 38], where a different class of random weights  $w_i$  was considered satisfying  $w_i = \xi_i / (n^{-1} \sum_{i=1}^n \xi_i)$  such that  $\xi_i$  are iid non-negative random variables and  $\mathbb{E}\xi_i^2 < \infty$ . Weights of such form contain the Bayesian bootstrap as a special case [58, 46]. The randomly reweighted bootstrap with iid mean-zero weights was considered for the non-degenerate case in [64] and for the degenerate case in [26]. More general exchangeably weighted bootstraps can be found in [48, 39, 56]. However, none of those results in literature can be used to establish the bootstrap validity for high-dimensional U-statistics when  $d \gg n$ . The Gaussian and bootstrap approximations for the maxima of sums of high-dimensional independent random vectors were considered in [23, 21]. For an iid sample, this corresponds to a U-statistic with the kernel  $h(x_1, x_2) = (x_1 + x_2)/2$  for  $x_1, x_2 \in \mathbb{R}^d$ . Thus, our results are nonlinear generalizations of those in [23, 21] when  $X_1, \dots, X_n$  are iid.

The current paper supersedes and improves the preliminary work [18] (available as an arXiv preprint) by the author. In [18], a Gaussian multiplier bootstrap was proposed by estimating the individual Hájek projection terms using the idea of decoupling on an independent dataset. The boot-

strap validity therein is established under the Kolmogorov distance, which is a subset of  $\mathcal{A}^{re}$  corresponding to max-hyperrectangles in  $\mathbb{R}^d$ . In addition, the rate of convergence in [18] is sub-optimal while the rate derived in this paper is nearly optimal; see Remark 3 for detailed comparisons.

*Notations and definitions.* For a vector  $x$ , we use  $|x|_1 = \sum_j |x_j|$ ,  $|x| := |x|_2 = (\sum_j x_j^2)^{1/2}$ , and  $|x|_\infty = \max_j |x_j|$  to denote its entry-wise  $\ell^1$ ,  $\ell^2$ , and  $\ell^\infty$  norms, respectively. For a matrix  $M$ , we use  $|M|_F = (\sum_{i,j} M_{ij}^2)^{1/2}$  and  $\|M\|_2 = \max_{|a|=1} |Ma|$  to denote its Frobenius and spectral norms, respectively. We shall use  $C, C_1, C_2, \dots$  to denote positive constants that do not depend on  $n$  and  $d$  and whose values may change from place to place. Denote  $a \vee b = \max(a, b)$ ,  $a \wedge b = \min(a, b)$ ,  $a \asymp b$  if  $C_1 a \leq b \leq C_2 b$  for some constants  $C_1, C_2 > 0$ . For a random variable  $X$ , we write  $\|X\|_q = (\mathbb{E}|X|^q)^{1/q}$  for  $q > 0$ . For  $r = 1, \dots, n$ , we shall write  $x_1^r = (x_1, \dots, x_r)$  and  $\mathbb{E}h = \mathbb{E}h(X_1^r)$  for the random variables  $X_1, \dots, X_r$  taking values in a measurable space  $(S, \mathcal{S})$  and a measurable function  $h : S^r \rightarrow \mathbb{R}^d$ . For two vectors  $x, y \in \mathbb{R}^d$ , we use  $x \leq y$  (or  $x > y$ ) to mean that  $x_j \leq y_j$  (or  $x_j > y_j$ ) for all  $j = 1, \dots, d$ . We use  $\mathcal{L}(X)$  to denote the law or distribution of the random variable  $X$ . For  $\alpha > 0$ , let  $\psi_\alpha(x) = \exp(x^\alpha) - 1$  be a function defined on  $[0, \infty)$  and  $L_{\psi_\alpha}$  be the collection of all real-valued random variables  $\xi$  such that  $\mathbb{E}[\psi_\alpha(|\xi|/C)] < \infty$  for some  $C > 0$ . For  $\xi \in L_{\psi_\alpha}$ , we define  $\|\xi\|_{\psi_\alpha} = \inf\{C > 0 : \mathbb{E}[\psi_\alpha(|\xi|/C)] \leq 1\}$ . Then, for  $\alpha \in [1, \infty)$ ,  $\|\cdot\|_{\psi_\alpha}$  is an Orlicz norm and  $(L_{\psi_\alpha}, \|\cdot\|_{\psi_\alpha})$  is a Banach space [44]. For  $\alpha \in (0, 1)$ ,  $\|\cdot\|_{\psi_\alpha}$  is a quasi-norm, i.e. there exists a constant  $C(\alpha) > 0$  such that  $\|\xi_1 + \xi_2\|_{\psi_\alpha} \leq C(\alpha)(\|\xi_1\|_{\psi_\alpha} + \|\xi_2\|_{\psi_\alpha})$  holds for all  $\xi_1, \xi_2 \in L_{\psi_\alpha}$  [1]. We denote the Kolmogorov distance between two real-valued random variables  $X$  and  $Y$  as  $\rho(X, Y) = \sup_{t \in \mathbb{R}} |\mathbb{P}(X \leq t) - \mathbb{P}(Y \leq t)|$ . Throughout the paper, we assume that  $n \geq 4$  and  $d \geq 3$ .

**2. Gaussian approximation.** In this section, we study the approximation for  $\mathbb{P}(T_n \in A)$  where  $T_n = \sqrt{n}(U_n - \theta)/2$  and  $A \in \mathcal{A}^{re}$ . We shall derive a Gaussian approximation result (GAR) for non-degenerate U-statistics, which is the stepping stone to study various bootstrap procedures in Section 3. Let  $X'$  and  $X$  be two independent random vectors with the distribution  $F$  that are also independent of  $X_1^n$ . In Section 2 and 3, since we consider centered U-statistics  $T_n$ , we assume without loss of generality that  $\theta = 0$ . Define  $g(X) = \mathbb{E}[h(X, X')|X]$  and  $f(X, X') = h(X, X') - g(X) - g(X')$ .

**DEFINITION 2.1.** The kernel  $h : \mathbb{R}^p \times \mathbb{R}^p \rightarrow \mathbb{R}^d$  is said to be: (i) non-degenerate if  $\text{Var}(g_m(X)) > 0$  for all  $m = 1, \dots, d$ ; (ii) degenerate of order one, i.e. completely degenerate or  $F$ -canonical, if  $\mathbb{P}(g(X) = 0) = 1$  or equiva-

lently  $\mathbb{E}[h(x_1, X')] = \mathbb{E}[h(X, x_2)] = \mathbb{E}[h(X, X')] = 0$  for all  $x_1, x_2 \in \mathbb{R}^p$ . The corresponding U-statistic in (1) is non-degenerate if  $h$  is non-degenerate.

Throughout this paper, we only consider the non-degenerate U-statistics and we assume that

- (M.1) There exists a constant  $\underline{b} > 0$  such that  $\mathbb{E}[g_m^2(X)] \geq \underline{b}$  for all  $m = 1, \dots, d$ .

The Hoeffding decomposition of  $T_n$  is given by  $T_n = L_n + R_n$ , where

$$L_n = \frac{1}{\sqrt{n}} \sum_{i=1}^n g(X_i) \quad \text{and} \quad R_n = \frac{1}{2\sqrt{n}(n-1)} \sum_{1 \leq i \neq j \leq n} f(X_i, X_j).$$

Since  $f$  is  $F$ -canonical, we expect that  $L_n$  is the leading term (a.k.a. the Hájek projection) of  $T_n$ . Therefore, we can reasonably expect that  $T_n$  is an approximately linear statistic such that  $\mathcal{L}(T_n) \approx \mathcal{L}(L_n)$ , where the latter can be further approximated by its Gaussian analogue [21, 23]. This motivates the following two-step Gaussian approximation procedure. Let  $\Gamma = \text{Cov}(g(X)) = \mathbb{E}(g(X)g(X)^\top)$  be the  $d \times d$  covariance matrix of  $g(X)$  and  $Y \sim N(0, \Gamma)$  be a  $d$ -dimensional Gaussian random vector. The main result of this section is to establish non-asymptotic error bounds for  $\rho^{re}(T_n, Y)$  under different moment conditions on  $h$ . Let  $q > 0$  and  $B_n \geq 1$  be a sequence of real numbers possibly tending to infinity. In particular, we shall consider the following assumptions.

- (M.2)  $\mathbb{E}[|h_m(X, X')|^{2+\ell}] \leq B_n^\ell$  for  $\ell = 1, 2$  and for all  $m = 1, \dots, d$ .  
 (E.1)  $\|h_m(X, X')\|_{\psi_1} \leq B_n$  for all  $m = 1, \dots, d$ .  
 (E.2)  $\mathbb{E}[\max_{1 \leq m \leq d} (|h_m(X, X')|/B_n)^q] \leq 1$ .

In the high-dimensional context, the dimension  $d$  grows with the sample size  $n$  and the distribution function  $F$  may also depend on  $n$ . Therefore,  $B_n$  is allowed to increase with  $n$ . In particular, under (M.1) and (M.2),  $B_n$  can be interpreted as a uniform bound on the standardized absolute moments of  $g_m(X)$  for  $m = 1, \dots, d$ . For instance, the kurtosis parameter  $\kappa_m$  of  $g_m(X)$  obeys  $\kappa_m = [\mathbb{E}g_m^4(X)]/[\mathbb{E}g_m^2(X)]^2 - 3 \leq B_n^2/\underline{b}^2 - 3$ . Define

$$(4) \quad \varpi_{1,n} = \left( \frac{B_n^2 \log^7(nd)}{n} \right)^{1/6} \quad \text{and} \quad \varpi_{2,n} = \left( \frac{B_n^2 \log^3(nd)}{n^{1-2/q}} \right)^{1/3}.$$

**THEOREM 2.1 (Main result I:** Gaussian approximation for high-dimensional U-statistics for hyperrectangles). *Assume that (M.1) and (M.2)*

hold. Suppose that  $\log d \leq \bar{b}n$  for some constant  $\bar{b} > 0$ .

(i) If (E.1) holds, then there exists a constant  $C := C(\underline{b}, \bar{b}) > 0$  such that

$$(5) \quad \rho^{re}(T_n, Y) \leq C\varpi_{1,n}.$$

(ii) If (E.2) holds with  $q \geq 4$ , then there exists a constant  $C := C(\underline{b}, \bar{b}, q) > 0$  such that

$$(6) \quad \rho^{re}(T_n, Y) \leq C\{\varpi_{1,n} + \varpi_{2,n}\}.$$

The following Corollary is an immediate consequence of Theorem 2.1.

**COROLLARY 2.2.** *Assume that (M.1) and (M.2) hold. Let  $K \in (0, 1)$  and  $\bar{b} > 0$ . (i) If (E.1) holds and  $B_n^2 \log^7(dn) \leq \bar{b}n^{1-K}$ , then there exists a constant  $C := C(\underline{b}, \bar{b}) > 0$  such that*

$$(7) \quad \rho^{re}(T_n, Y) \leq Cn^{-K/6}.$$

*In particular,*

$$(8) \quad \rho(\bar{T}_n, \bar{Y}) \leq Cn^{-K/6},$$

*where  $\bar{T}_n = \max_{1 \leq m \leq d} T_{nm}$  and  $\bar{Y} = \max_{1 \leq m \leq d} Y_m$ .*

*(ii) If (E.2) holds with  $q = 4$  and  $B_n^4 \log^7(dn) \leq \bar{b}n^{1-K}$ , then there exists a constant  $C := C(\underline{b}, \bar{b}) > 0$  such that (7) and (8) hold.*

Theorem 2.1 and Corollary 2.2 are non-asymptotic, showing that the validity of the Gaussian approximation for centered non-degenerate U-statistics holds even if  $d$  can be much larger than  $n$  and no structural assumption on  $F$  is required. In particular, Theorem 2.1 applies to kernels with the sub-exponential distribution such that  $\|h_m\|_q \leq Cq$  for all  $q \geq 1$ , in which case  $B_n = O(1)$  and the dimension  $d$  is allowed to have a subexponential growth rate in the sample size  $n$ , i.e.  $d = O(\exp(n^{(1-K)/7}))$ . Condition (E.1) also covers bounded kernels  $\|h\|_\infty \leq B_n$ , where  $B_n$  may increase with  $n$ .

**REMARK 1** (Comments on the near-optimality of the convergence rate in Theorem 2.1). The rate of convergence  $n^{-K/6}$  obtained in (7) is slower than the Berry-Esseen rate  $n^{-1/2}$  when  $d$  is fixed. Similar observations have been made in the existing literature [55, 5] for the normalized sample mean vectors of iid mean-zero random vectors  $X_i \in \mathbb{R}^d$ , which corresponds to a U-statistic with the linear kernel  $h(x_1, x_2) = (x_1 + x_2)/2$ . Assuming  $\text{Cov}(X_i) = \text{Id}_d$ ,



[55] showed that  $\sqrt{n}\bar{X}_n$  has the asymptotic normality if  $d = o(\sqrt{n})$  and [5] showed that

$$\sup_{A \in \mathcal{A}} |\mathbb{P}(\sqrt{n}\bar{X}_n \in A) - \mathbb{P}(Y \in A)| \leq Cd^{1/4}\mathbb{E}|X_1|^3/n^{1/2},$$

where  $\mathcal{A}$  is the class of all convex subsets in  $\mathbb{R}^d$ ,  $Y \sim N(0, \text{Id}_d)$ , and  $C > 0$  is an absolute constant. In either case, the dependence of the CLT rate on the dimension  $d$  is polynomial ( $d/n^{1/2}$  and  $d^{7/4}/n^{1/2}$ , resp). On the contrary, our Theorem 2.1 allows  $d$  can be larger than  $n$  in order to obtain the CLT type results in much higher dimensions. Since the rate  $O(n^{-1/6})$  is minimax optimal in infinite-dimensional Banach spaces for the linear kernel case [4, 23], we argue that the rates derived in Theorem 2.1 for U-statistics seem un-improvable in  $n$  in the following sense. Let  $\{X_{ij}\}_{i=1, \dots, n; j=1, \dots, d}$  be an array of iid mean-zero random variables with the distribution  $F$  such that  $\mathbb{E}X_{ij}^2 = 1$  and  $\|X_{ij}\|_{\psi_1} \leq c$  for all  $i = 1, \dots, n$  and  $j = 1, \dots, d$ . Consider the linear kernel. Let  $Y \sim N(0, \text{Id}_d)$  and  $\bar{Y} = \max_{1 \leq j \leq d} Y_j$ . Denote  $\Phi(\cdot)$  and  $\phi(\cdot)$  as the cdf and pdf of the standard normal distribution, respectively. By the moderate deviation principle for sums of subexponential random variables (c.f. [16, equation (1.1)] or [54, Chapter 8, equation (2.41)]), there exist constants  $C_0, C_1 > 0$  depending only on  $c$  such that

$$\frac{\mathbb{P}(T_{nj} > x)}{1 - \Phi(x)} = 1 + \frac{\eta_1(1 + x^3)}{n^{1/2}}, \quad j = 1, \dots, d$$

for  $0 \leq x \leq C_0 n^{1/6}$  and  $|\eta_1| \leq C_1$ . Then, for all such  $x$  in the power zone of normal convergence, we have

$$\mathbb{P}(\bar{T}_n \leq x) - \mathbb{P}(\bar{Y} \leq x) = \mathbb{P}(\bar{Y} \leq x) \{ [1 + \eta_2(1 - \Phi(x))/\Phi(x)]^d - 1 \},$$

where  $\eta_2 = -\eta_1(1 + x^3)n^{-1/2}$ . Take a distribution  $F$  such that  $\eta_1 < 0$ . By the inequality  $(1 + x)^d \geq 1 + dx$  for  $x \geq 0$ ,

$$\mathbb{P}(\bar{T}_n \leq x) - \mathbb{P}(\bar{Y} \leq x) \geq |\eta_1|(1 + x^3)n^{-1/2}\mathbb{P}(\bar{Y} \leq x)d[1 - \Phi(x)].$$

Let  $x^*$  be the median of  $\bar{Y}$ ; i.e.  $\mathbb{P}(\bar{Y} \leq x^*) = 1/2$ . Then  $x^* \asymp \sqrt{2 \log d}$ . In fact, by [24, Corollary 3.1], we have  $x^* \leq \sqrt{2 \log d}$  for  $d \geq 31$ . Thus, if  $x^* \leq C_0 n^{1/6}$ , then using  $[1 - \Phi(x)]/[x^{-1}\phi(x)] \rightarrow 1$  as  $x \rightarrow \infty$  we have

$$\rho(\bar{T}_n, \bar{Y}) \geq C_2 n^{-1/2} x^{*2} d \exp(-x^{*2}/2) \geq C_2 n^{-1/2} x^{*2}.$$

Hence, there exist constants  $C$  and  $C'$  depending only on  $F$  such that if  $(\log d)^3 \leq C'n$ , then  $\rho(\bar{T}_n, \bar{Y}) \geq Cn^{-1/2} \log d$ . In particular, taking  $(\log d)^3 \asymp$

$n$ , we have  $\rho(\bar{T}_n, \bar{Y}) \geq Cn^{-1/6}$ . Therefore, in view of the upper bound in (5) and the lower bound in [4, 23], we conjecture that the optimal rate for  $\rho(\bar{T}_n, \bar{Y})$  in the high-dimensional setting is  $O((n^{-1}B_n^2 \log^a(nd))^{1/6})$  for some  $a > 0$ , based on which the rate of convergence in (5) is also nearly optimal in  $d$ . However, a rigorous lower bound for  $\rho(\bar{T}_n, \bar{Y})$  is still an open question. By the moderate deviations for self-normalized sums [60] and the argument above, we expect that similar comments apply for  $X_{ij}$  with weaker polynomial moment conditions.  $\square$

Theorem 2.1 and Corollary 2.2 can be viewed as nonlinear generalization of the results in [21, 23], which considered the Gaussian approximation for  $\max_{j \leq d} \sqrt{n} \bar{X}_{nj}$ . Therefore, for U-statistics with a nonlinear kernel  $h$  (possibly unbounded and discontinuous), the effect of higher-order terms than the Hájek projection to a linear subspace in the Hoeffding decomposition vanishes in the Gaussian approximation. For multivariate symmetric statistics of order two, to the best of our knowledge, the Gaussian approximation result (5), (6), (7), and (8) with the explicit convergence rate is new. When  $d$  is fixed, the rate of convergence and the Edgeworth expansion of such statistics can be found in [8, 32, 6]. In those papers, assuming the Cramér condition on  $g(X_1)$  and suitable moment conditions on  $h(X_1, X_2)$ , the Edgeworth expansion of U-statistics was established for the univariate case ( $d = 1$ ) with remainder  $o(n^{-1/2})$  or  $O(n^{-1})$  [8, 6] and the multivariate case ( $d > 1$  fixed) with remainder  $o(n^{-1/2})$  [32]. In the latter work [32], it is unclear that how the constant in the error bound depends on the dimensionality parameter  $d$ .

Theorem 2.1 and Corollary 2.2 allow us to approximate the probabilities of  $T_n$  belonging to the hyperrectangles in  $\mathbb{R}^d$  by those probabilities of  $Y$ , with the knowledge of  $\Gamma$ . Such results are useful for approximating the quantiles of  $\bar{T}_n$  by those of  $\bar{Y}$ . In practice, the covariance matrix  $\Gamma$  and the Hájek projection terms  $g(X_i), i = 1, \dots, n$ , depend on the underlying data distribution  $F$ , which is unknown. Thus, quantiles of  $\bar{Y}$  need to be estimated in real applications. However, we shall see in Section 3 that Theorem 2.1 can still be used to derive valid and computable (i.e. fully data-dependent) methods to approximate the quantiles of  $\bar{T}_n$ .

**3. Bootstrap approximations.** In this section, we consider *computable* approximations of the probabilities  $\mathbb{P}(T_n \in A)$  for  $A \in \mathcal{A}^{re}$ . Before proceeding to the rigorous results, we shall explain our general strategy. The validity of the bootstrap procedures is established by a series of approximations

$$(9) \quad \mathcal{L}(T_n) \approx_{(1)} \mathcal{L}(Y) \approx_{(2)} \mathcal{L}(Z^X | X_1^n) \approx_{(3)} \mathcal{L}(T_n^\sharp | X_1^n),$$

where  $Z^X$  is a conditionally mean-zero Gaussian random vector in  $\mathbb{R}^d$  given the observed sample  $X_1^n$ . The choice of  $Z^X$  and  $T_n^{\natural}$  depends on the specific bootstrap method such that the conditional covariance matrix of  $Z^X$  given  $X_1^n$  is a consistent estimator of  $\Gamma$  under the supremum norm. Step (1) follows from the GAR and CLT in Section 2. Step (2) relies on a (conditional) Gaussian comparison principle and the tail probability inequalities of maximal U-statistics to bound the probability of the events on which the Gaussian comparison can be applied. Those tail probability inequalities are developed in the SM (Section E), which are of independent interest and may be used for other high-dimensional problems. Step (3) is a conditional version of Step (1) given  $X_1^n$ .

3.1. *Empirical bootstrap.* Let  $X_1^*, \dots, X_n^*$  be a bootstrap sample independently drawn from the empirical distribution  $\hat{F}_n = n^{-1} \sum_{i=1}^n \delta_{X_i}$ , where  $\delta_x$  is the Dirac point mass at  $x$ . Define

$$(10) \quad U_n^* = \frac{1}{n(n-1)} \sum_{1 \leq i \neq j \leq n} h(X_i^*, X_j^*).$$

Then, the conditional distribution of  $T_n^* = \sqrt{n}(U_n^* - \mathbb{E}[U_n^* | X_1^n])/2$  given  $X_1^n$  is used to approximate the distribution of  $T_n$ . Here  $T_n^{\natural} = T_n^*$  in (9). Note that  $\mathbb{E}[U_n^* | X_1^n] = V_n$ , where  $V_n = n^{-2} \sum_{i,j=1}^n h(X_i, X_j)$  is a  $V$ -statistic. Let

$$\xi_i \stackrel{\text{iid}}{\sim} \text{multinomial}(1; 1/n, \dots, 1/n).$$

Denote  $\boldsymbol{\xi}_{n \times n} = (\xi_1, \dots, \xi_n)$  and  $\mathbf{X}_{p \times n} := X_1^n = (X_1, \dots, X_n)$ . Then we can write  $\mathbf{X}^* = (X_1^*, \dots, X_n^*) = \mathbf{X}\boldsymbol{\xi}$ . The key observation is that conditional on  $\mathbf{X}$ ,  $U_n^*$  is a U-statistic of  $\xi_1, \dots, \xi_n$  since

$$U_n^* = \frac{1}{n(n-1)} \sum_{1 \leq i \neq j \leq n} h(\mathbf{X}\xi_i, \mathbf{X}\xi_j).$$

Therefore, we can perform the conditional Hoeffding decomposition as follows. Let

$$\begin{aligned} g^X(\xi_1) &= \mathbb{E}[h(\mathbf{X}\xi_1, \mathbf{X}\xi_2) | \xi_1, X_1^n] - V_n \\ &= \frac{1}{n} \sum_{j=1}^n h(\mathbf{X}\xi_1, X_j) - \frac{1}{n^2} \sum_{i,j=1}^n h(X_i, X_j). \end{aligned}$$

Then,  $\mathbb{E}[g^X(\xi_1) | X_1^n] = 0$  and

(11)

$$\hat{\Gamma}_n := \text{Cov}(g^X(\xi_1) | X_1^n) = \frac{1}{n^3} \sum_{i=1}^n \sum_{j=1}^n \sum_{k=1}^n h(X_i, X_j) h(X_i, X_k)^\top - V_n V_n^\top.$$

For the special case  $d = 1$ , by the strong law of large numbers for U-statistics [59, Theorem A, page 190], we have with probability one

$$\lim_{n \rightarrow \infty} \text{Var}(g^X(\xi_1)|X_1^n) = \text{Var}(g(X_1)) = \mathbb{E}\{\mathbb{E}[h(X_1, X_2)|X_1]\}^2 - \{\mathbb{E}[h(X_1, X_2)]\}^2.$$

Therefore, we expect that  $T_n^*$  is a reasonable approximation of  $T_n$  and our goal is to bound the random quantity

$$\rho^B(T_n, T_n^*) = \sup_{A \in \mathcal{A}^{re}} |\mathbb{P}(T_n \in A) - \mathbb{P}(T_n^* \in A|X_1^n)|.$$

In addition to (M.2), (E.1) and (E.2), we shall also assume that

- (M.2')  $\mathbb{E}[|h_m(X, X)|^{2+\ell}] \leq B_n^\ell$  for  $\ell = 1, 2$  and for all  $m = 1, \dots, d$ .  
(E.1')  $\|h_m(X, X)\|_{\psi_1} \leq B_n$  for all  $m = 1, \dots, d$ .  
(E.2')  $\mathbb{E}[\max_{1 \leq m \leq d} (|h_m(X, X)|/B_n)^q] \leq 1$ .

(M.2'), (E.1') and (E.2') are the von Mises conditions on the empirical bootstrap of U-statistics [7], which require that the diagonal entries of the kernel  $h$  obey the same moment conditions as the off-diagonal ones (M.2), (E.1) and (E.2), respectively. Without (M.2'), (E.1') and (E.2'), the empirical bootstrap (Theorem 3.1) can fail and a counterexample was given in [7]; see also [45, Chapter 6.5]. For  $\gamma \in (0, e^{-1})$ , define

$$(12) \quad \varpi_{1,n}^B(\gamma) = \left( \frac{B_n^2 \log^5(nd) \log^2(1/\gamma)}{n} \right)^{1/6} \quad \text{and} \quad \varpi_{2,n}^B(\gamma) = \left( \frac{B_n^2 \log^3(nd)}{\gamma^{2/q} n^{1-2/q}} \right)^{1/3}.$$

**THEOREM 3.1 (Main result II: rate of convergence of the empirical bootstrap for U-statistics).** *Suppose that (M.1), (M.2) and (M.2') are satisfied. Assume that  $\log(1/\gamma) \leq K \log(dn)$  and  $\log d \leq \bar{b}n$  for some constants  $K, \bar{b} > 0$ .*

(i) *If (E.1) and (E.1') hold, then there exists a constant  $C := C(\bar{b}, \bar{b}, K) > 0$  such that we have with probability at least  $1 - \gamma$*

$$(13) \quad \rho^B(T_n, T_n^*) \leq C \varpi_{1,n}.$$

(ii) *If (E.2) and (E.2') hold with  $q \geq 4$ , then there exists a constant  $C := C(\bar{b}, \bar{b}, q, K) > 0$  such that we have with probability at least  $1 - \gamma$*

$$(14) \quad \rho^B(T_n, T_n^*) \leq C \{\varpi_{1,n} + \varpi_{2,n}^B(\gamma)\}.$$

Theorem 3.1 is non-asymptotic, which implies the asymptotic validity of the EB for U-statistics in the almost sure sense.

**COROLLARY 3.2** (Asymptotic validity of the empirical bootstrap for U-statistics in the almost sure sense). *Suppose that (M.1), (M.2) and (M.2') are satisfied and  $\log d \leq \bar{b}n$  for some constant  $\bar{b} > 0$ . (i) Under (E.1) and (E.1'), we have  $\mathbb{P}(\rho^B(T_n, T_n^*) \leq C\varpi_{1,n} \text{ for all but finitely many } n) = 1$ , where  $C > 0$  is a constant depending only on  $\underline{b}$  and  $\bar{b}$ . In particular, if  $B_n^2 \log^7(nd) = o(n)$ , then  $\rho^B(T_n, T_n^*) \rightarrow 0$  almost surely. (ii) Under (E.2) and (E.2') with  $q > 4$ , we have  $\mathbb{P}(\rho^B(T_n, T_n^*) \leq C\{\varpi_{1,n} + \varpi'_{2,n}\}) = 1$ , where*

$$\varpi'_{2,n} = \left( \frac{B_n^2 \log^3(nd) \log^{4/q}(n)}{n^{1-4/q}} \right)^{1/3}$$

and  $C > 0$  is a constant depending only on  $\underline{b}, \bar{b}$ , and  $q$ . In particular, if  $B_n^2 \log^7(nd) = o(n)$  and  $B_n^2 \log^3(nd) \log^{4/q}(n) = o(n^{1-4/q})$ , then  $\rho^B(T_n, T_n^*) \rightarrow 0$  almost surely.

**3.2. Randomly reweighted bootstrap with iid Gaussian weights.** Let  $w_1, \dots, w_n$  be iid  $N(1, 1)$  random variables that are also independent of  $X_1^n$  and  $Y$ . Consider

$$(15) \quad U_n^\diamond = \frac{1}{n(n-1)} \sum_{1 \leq i \neq j \leq n} w_i w_j h(X_i, X_j),$$

Then,  $U_n^\diamond$  is the stochastically reweighted version of  $U_n$  and it can also be viewed as a random quadratic form in  $w_1, \dots, w_n$ . Denote  $T^\diamond = \sqrt{n}(U_n^\diamond - U_n)/2$  and  $T_n^\diamond = T_n^\diamond$  in (9). Since the main focus of this paper is to approximate the distribution of the centered U-statistics; i.e  $\theta := \mathbb{E}h = 0$ , we first consider the bootstrap of the centered U-statistics of the random quadratic form (15) and discuss the effect of centering in the bootstraps in Remark 2.

**THEOREM 3.3 (Main result III: rate of convergence of the randomly reweighted bootstrap for centered U-statistics).** *Assume that  $\theta = 0$ . Suppose that (M.1) and (M.2) are satisfied. Assume that  $\log(1/\gamma) \leq K \log(dn)$  and  $\log d \leq \bar{b}n$  for some constants  $K, \bar{b} > 0$ . (i) If (E.1) holds, then there exists a constant  $C := C(\underline{b}, \bar{b}, K) > 0$  such that we have  $\rho^B(T_n, T_n^\diamond) \leq C\varpi_{1,n}$  holds with probability at least  $1 - \gamma$ . (ii) If (E.2) holds with  $q \geq 4$ , then there exists a constant  $C := C(\underline{b}, \bar{b}, q, K) > 0$  such that we have  $\rho^B(T_n, T_n^\diamond) \leq C\{\varpi_{1,n} + \varpi'_{2,n}(\gamma)\}$  holds with probability at least  $1 - \gamma$ .*

From Theorem 3.1 and 3.3, we see that the empirical and the randomly reweighted bootstraps are first-order equivalent, both achieving the same uniform rate of convergence for approximating the probabilities  $\mathbb{P}(T_n \in A)$

for  $A \in \mathcal{A}^{re}$ . However, unlike the EB, the randomly reweighted bootstrap does not assume the von Mises moment conditions on the diagonal entries.

REMARK 2 (Effect of centering in the randomly reweighted bootstrap). If  $\theta \neq 0$ , then we can show that the iid reweighted bootstrap  $T_n^\circ$  is not an asymptotically valid bootstrap approximation for  $T_n$ . The reason is that centering is a key structure to maintain in the conditional distribution of  $T_n^\circ$ . Therefore, in the case, we shall consider the following modified version

$$(16) \quad U_n^b = \frac{1}{n(n-1)} \sum_{1 \leq i \neq j \leq n} w_i w_j h(X_i, X_j) - 2(\bar{w} - 1)U_n$$

and  $T_n^b = \sqrt{n}(U_n^b - U_n)/2$ . Then,  $T_n^b = T_n^\circ - \sqrt{n}(\bar{w} - 1)U_n$ . Since  $w_i$  are iid  $N(1, 1)$ , we have  $\sqrt{n}(\bar{w} - 1)U_n | X_1^n \sim N(0, U_n U_n^\top)$ , which is not asymptotically vanishing for  $\theta \neq 0$ . Therefore, without the centering term  $2(\bar{w} - 1)U_n$  in  $U_n^b$ ,  $T_n^\circ$  is not an asymptotically tight sequence for approximating  $T_n$ .

THEOREM 3.4 (Rate of convergence of the randomly reweighted bootstrap for non-centered U-statistics). *Suppose that (M.1) and (M.2) are satisfied. Assume that  $\log(1/\gamma) \leq K \log(dn)$  and  $\log d \leq \bar{b}n$  for some constants  $K, \bar{b} > 0$ . (i) If (E.1) holds, then there exists a constant  $C := C(\underline{b}, \bar{b}, K) > 0$  such that we have  $\rho^B(T_n, T_n^b) \leq C\varpi_{1,n}$  holds with probability at least  $1 - \gamma$ . (ii) If (E.2) holds with  $q \geq 4$ , then there exists a constant  $C := C(\underline{b}, \bar{b}, q, K) > 0$  such that we have  $\rho^B(T_n, T_n^b) \leq C\{\varpi_{1,n} + \varpi_{2,n}^B(\gamma)\}$  holds with probability at least  $1 - \gamma$ .*

Theorem 3.4 is valid regardless  $\theta \neq 0$  and  $\theta = 0$  since in the latter case,  $\sqrt{n}(\bar{w} - 1)U_n$  is conditionally negligible compared with  $T_n^\circ$ . For the EB, centering in the empirical analog  $\hat{\Gamma}_n$  of the covariance matrix  $\Gamma$  is automatically fulfilled; see (11). Similar comments apply to the Gaussian multiplier bootstrap  $T_n^\sharp$  in Section 3.3.  $\square$

3.3. *Gaussian multiplier bootstrap with jackknife covariance matrix estimator.* The iid reweighted bootstrap is closely related to the Gaussian multiplier bootstrap with the jackknife estimator of the covariance matrix of  $T_n$ . Let  $e_1, \dots, e_n$  be iid  $N(0, 1)$  random variables that are independent of  $X_1^n$  and  $Y$  and

$$(17) \quad T_n^\sharp = \frac{1}{\sqrt{n}} \sum_{i=1}^n \left[ \frac{1}{n-1} \sum_{j \neq i} h(X_i, X_j) - U_n \right] e_i.$$

Define

$$(18) \quad \hat{\Gamma}_n^{JK} = \frac{1}{(n-1)(n-2)^2} \sum_{i=1}^n \sum_{j \neq i} \sum_{k \neq i} (h(X_i, X_j) - U_n)(h(X_i, X_k) - U_n)^\top.$$

Then,  $\hat{\Gamma}_n^{JK}$  is the jackknife estimator of the covariance matrix of  $T_n$  [14] and  $T_n^\# | X_1^n \sim N(0, \tilde{\Gamma}_n)$ , where

$$(19) \quad \tilde{\Gamma}_n = \frac{(n-2)^2}{n(n-1)} \hat{\Gamma}_n^{JK}.$$

Therefore, it is interesting to view the Gaussian multiplier bootstrap  $T_n^\#$  as a plug-in estimator of the distribution of  $T_n$  by its jackknife covariance matrix estimator. To distinguish the Gaussian wild bootstrap  $\hat{L}_0^*$  in (20) (c.f. Remark 3), we call  $T_n^\#$  the *jackknife Gaussian multiplier bootstrap*.

**THEOREM 3.5 (Main result IV: rate of convergence of the jackknife Gaussian multiplier bootstrap for U-statistics).** *Suppose that (M.1) and (M.2) are satisfied. Assume that  $\log(1/\gamma) \leq K \log(dn)$  and  $\log d \leq \bar{b}n$  for some constants  $K, \bar{b} > 0$ . (i) If (E.1) holds, then there exists a constant  $C := C(\underline{b}, \bar{b}, K) > 0$  such that we have  $\rho^B(T_n, T_n^\#) \leq C\varpi_{1,n}$  holds with probability at least  $1 - \gamma$ . (ii) If (E.2) holds with  $q \geq 4$ , then there exists a constant  $C := C(\underline{b}, \bar{b}, q, K) > 0$  such that we have  $\rho^B(T_n, T_n^\#) \leq C\{\varpi_{1,n} + \varpi_{2,n}^B(\gamma)\}$  holds with probability at least  $1 - \gamma$ .*

In the special case  $h(x_1, x_2) = (x_1 + x_2)/2$  for  $x_1, x_2 \in \mathbb{R}^d$ , we have  $U_n = \bar{X}_n = n^{-1} \sum_{i=1}^n X_i$  is the sample mean vector and  $T_n = \sqrt{n}(\bar{X}_n - \theta)/2$  where  $\theta = \mathbb{E}(X_1)$ . Some algebra shows that  $\hat{\Gamma}_n^{JK} = [4(n-1)]^{-1} \sum_{i=1}^n (X_i - \bar{X}_n)(X_i - \bar{X}_n)^\top$ ,  $\hat{\Gamma}_n = n^{-1}(n-1)\hat{\Gamma}_n^{JK}$  in (11), and  $\tilde{\Gamma}_n = [(n-2)^2/(n(n-1))]\hat{\Gamma}_n^{JK}$  in (19). Then,  $T_n^\# \sim N(0, \tilde{\Gamma}_n)$  which is the equivalent to the multiplier bootstrap of [23]. Therefore, for iid samples, Theorem 3.1 and 3.5 are nonlinear generalizations of the empirical and Gaussian multiplier bootstraps considered in [23].

**REMARK 3 (Comparison with the Gaussian wild bootstrap of [18]).** In [18], a Gaussian wild bootstrap based on decoupling was proposed. Specifically, let  $X'_1, \dots, X'_n$  be an independent copy of  $X_1, \dots, X_n$ . The Hájek projection terms  $g(X_i), i = 1, \dots, n$ , are estimated by

$$\hat{g}_i = \frac{1}{n} \sum_{j=1}^n h(X_i, X'_j) - \frac{1}{n(n-1)} \sum_{1 \leq j \neq l \leq n} h(X'_j, X'_l).$$

Since  $g(X_i) = \mathbb{E}[h(X_i, X')|X_i] - \mathbb{E}[h(X, X')]$ ,  $\hat{g}_i$  can be viewed as an unbiased estimator of  $g(X_i)$  conditionally on  $X_i$  for  $i = 1, \dots, n$ . Then the Gaussian wild bootstrap procedure is defined as

$$(20) \quad \hat{L}_0^* = \max_{1 \leq m \leq d} \frac{1}{\sqrt{n}} \sum_{i=1}^n \hat{g}_{im} e_i,$$

where  $e_i$  are iid  $N(0, 1)$  random variables. Let  $a_{\hat{L}_0^*}(\alpha)$  be the  $\alpha$ -th conditional quantile of  $\hat{L}_0^*$  given  $X_1, \dots, X_n$  and  $X'_1, \dots, X'_n$ . Similarly, denote  $a_{\bar{T}_n^\sharp}(\alpha)$  as the  $\alpha$ -th conditional quantile of  $\bar{T}_n^\sharp$  given  $X_1, \dots, X_n$ . Let  $K \in (0, 1)$  be a constant. Assuming (M.1), (M.2), and in addition  $D_2 \leq 1$ , it was shown in [18] that: (i) if  $B_n^2 \log^7(dn) \leq n^{1-K}$  and (E.1) holds, then  $\sup_{\alpha \in (0,1)} |\mathbb{P}(\bar{T}_n \leq a_{\hat{L}_0^*}(\alpha)) - \alpha| \leq Cn^{-K/8}$ ; (ii) if  $B_n^4 \log^7(dn) \leq n^{1-K}$  and (E.2) holds with  $q = 4$ , then  $\sup_{\alpha \in (0,1)} |\mathbb{P}(\bar{T}_n \leq a_{\hat{L}_0^*}(\alpha)) - \alpha| \leq Cn^{-K/12}$ . Here, the constant  $C > 0$  depends only on  $\underline{b}$  in (M.1) in both cases. The following theorem shows that the jackknife Gaussian multiplier bootstrap improves the convergence rate of Gaussian wild bootstrap in [18].

**THEOREM 3.6.** *Suppose that (M.1) and (M.2) are satisfied. Let  $K \in (0, 1)$ . (i) Assume (E.1). If  $B_n^2 \log^7(dn) \leq n^{1-K}$ , then*

$$(21) \quad \sup_{\alpha \in (0,1)} |\mathbb{P}(\bar{T}_n \leq a_{\bar{T}_n^\sharp}(\alpha)) - \alpha| \leq Cn^{-K/6},$$

where  $\bar{T}_n^\sharp = \max_{1 \leq j \leq d} T_{n,j}^\sharp$  and  $C > 0$  is a constant depending only on  $\underline{b}$ .

(ii) Assume (E.2) with  $q \geq 4$ . If  $B_n^2 \log^7(dn) \leq n^{1-K}$  and  $B_n^4 \log^6(d) \leq n^{2-4(1+K/6)/q-K}$ , then we have (21) with the constant  $C$  depending only on  $\underline{b}$  and  $q$ .

In particular, for both subexponential and uniform polynomial kernels, the convergence rate of jackknife Gaussian multiplier bootstrap  $T_n^\sharp$  is  $O(n^{-K/6})$ . The improved dependence on  $n$  is due to two reasons. First, we established a GAR for high-dimensional U-statistics with sharper rate (Theorem 2.1). Second,  $T_n^\sharp$  does not estimate the individual terms  $g(X_i)$  in the Hájek projection which requires a strong control on the maximal deviation  $|\hat{g}_i - g(X_i)|_\infty$  over  $i = 1, \dots, n$ ; see Lemma C.4 in [18]. Instead,  $T_n^\sharp$  implicitly constructs an estimator  $\tilde{\Gamma}_n$  in (19) for the covariance matrix of the linear projection part in the Gaussian approximation. There is a slight trade-off between the moment and scaling limit for uniform polynomial kernels in Theorem 3.6 since the conditions  $B_n^2 \log^7(dn) \leq n^{1-K}$  and  $B_n^4 \log^6(d) \leq n^{2-4(1+K/6)/q-K}$  are



implied by either  $B_n^4 \log^7(dn) \leq n^{1-7K/6}$  for  $q = 4$  or  $B_n^4 \log^7(dn) \leq n^{1-K}$  for  $q \geq 4(1 + K/6)$ . However, in either case, Theorem 3.6 asymptotically permits  $d = O(e^{n^c})$  for some  $c \in (0, 1/7)$  when  $q \geq 4$  and  $B_n = O(1)$ .  $\square$

**4. Statistical applications.** In this section, we present two statistical applications for bootstrap methods in Section 3.1. For simplicity, we only present the results for the jackknife Gaussian multiplier bootstrap  $T_n^\sharp$  defined in (17). Similar results hold for other bootstraps in Section 3.1. Two additional examples can be found in the SM. Throughout the section, we consider the bootstrap of the sample covariance matrix (i.e.  $h(x_1, x_2) = (x_1 - x_2)(x_1 - x_2)^\top / 2$  and  $\mathbb{R}^d = \mathbb{R}^{p \times p}$ ). We define  $\bar{T}_n^\sharp = 2n^{-1/2} \max_{1 \leq m, k \leq p} |T_{n, mk}^\sharp|$  by rescaling and denote the  $\alpha$ -th conditional quantile of  $\bar{T}_n^\sharp$  given the data  $X_1^n$  as

$$(22) \quad a_{\bar{T}_n^\sharp}(\alpha) = \inf\{t \in \mathbb{R} : \mathbb{P}_e(\bar{T}_n^\sharp \leq t) \geq \alpha\}.$$

where  $\mathbb{P}_e$  is the probability taken w.r.t. the iid  $N(0, 1)$  random variables  $e_1, \dots, e_n$ . We can compute the conditional quantile  $a_{\bar{T}_n^\sharp}(\alpha)$  by repeatedly drawing independent samples of the standard Gaussian random variables  $e_1, \dots, e_n$ .

4.1. *Tuning parameter selection for the thresholded covariance matrix estimator.* Consider the problem of *sparse* covariance matrix estimation. Let  $r \in [0, 1)$  and

$$\mathcal{G}(r, \zeta_p) = \left\{ \Sigma \in \mathbb{R}^{p \times p} : \max_{1 \leq m \leq p} \sum_{k=1}^p |\sigma_{mk}|^r \leq \zeta_p \right\}$$

be the class of sparse covariance matrices in terms of the strong  $\ell^r$ -ball. Here,  $\zeta_p > 0$  may grow with  $p$ . Let  $\hat{S}_n = \{\hat{s}_{mk}\}_{m, k=1}^p$  be the sample covariance matrix and

$$\hat{\Sigma}(\tau) = \{\hat{s}_{mk} \mathbf{1}\{|\hat{s}_{mk}| > \tau\}\}_{m, k=1}^p, \quad \tau \geq 0,$$

be the thresholded sample covariance matrix estimator of  $\Sigma$ . A similar matrix class as  $\mathcal{G}(r, \zeta_p)$  was introduced in [10] by further requiring that  $\max_{1 \leq m \leq p} \sigma_{mm} \leq C_0$  for some constant  $C_0 > 0$ . Here, we do not assume the diagonal entries of  $\Sigma$  are bounded. Performance bounds of the thresholded estimator  $\hat{\Sigma}(\tau)$  critically depend on the tuning parameter  $\tau$ . The oracle choice of the threshold for establishing the rate of convergence under the spectral and Frobenius norms is  $\tau_\diamond = |\hat{S}_n - \Sigma|_\infty$ . Note that  $\tau_\diamond$  is a random variable and its distribution depends on the unknown underlying data distribution  $F$ . High probability bounds of  $\tau_\diamond$  were given in [10, 19] and asymptotic

properties of  $\hat{\Sigma}(\tau)$  were analyzed in [10, 13] for iid sub-Gaussian data and in [19, 20] for heavy-tailed time series with polynomial moments. In both scenarios, the rates of convergence were obtained with the Bonferroni (i.e. the union bound) technique and one-dimensional concentration inequalities. In the problem of the high-dimensional sparse covariance matrix estimation, data-dependent tuning parameter selection is often empirically done with the cross-validation (CV) and its theoretical properties when compared with  $\tau_\diamond$  largely remain unknown since the CV threshold does not approximate  $\tau_\diamond$ . Here, we provide a principled and fully data-dependent way to determine the threshold  $\tau$ . We first consider subgaussian observations.

DEFINITION 4.1 (Subgaussian random variable). A random variable  $X$  is said to be *subgaussian* with mean zero and *variance factor*  $\nu^2$ , if

$$(23) \quad \mathbb{E}[\exp(X^2/\nu^2)] \leq \sqrt{2}.$$

Denote  $X \sim \text{subgaussian}(\nu^2)$ . In particular, if  $X \sim N(0, \sigma^2)$ , then  $X \sim \text{subgaussian}(4\sigma^2)$ .

The upper bound  $\sqrt{2}$  in (23) is not essential and it is chosen for conveniently comparing with  $\|X\|_{\psi_2}$ : if  $X \sim \text{subgaussian}(\nu^2)$ , then  $\nu^2 \geq \|X\|_{\psi_2}$ . Clearly, bounded random variables are subgaussian. In addition, random variables with the mixture of subgaussian distributions are also subgaussian. Let  $K$  be a positive integer and  $\{\pi_k\}_{k=1}^K$  be subgaussian distributions with the variance factors  $\{\nu_k^2\}_{k=1}^K$ . If a random variable  $X$  follows a mixture of  $K$  subgaussian distributions  $\sum_{k=1}^K \varepsilon_k \pi_k$  with  $0 \leq \varepsilon_k \leq 1$  and  $\sum_{k=1}^K \varepsilon_k = 1$ , then  $X \sim \text{subgaussian}(\bar{\nu}^2)$ , where  $\bar{\nu}^2 = \max\{\nu_1^2, \dots, \nu_K^2\}$ . In general, the variance factor for a subgaussian random variable is *not* equivalent to the variance. For a sequence of random variables  $X_n, n = 1, 2, \dots$ , if  $X_n \sim \text{subgaussian}(\nu_n^2)$  and  $\sigma_n^2 = \text{Var}(X_n)$ , then by Markov's inequality, we always have  $\sigma_n^2 \leq \sqrt{2}\nu_n^2$ , while  $\nu_n^2$  may diverge at faster rate than  $\sigma_n^2$  as  $n \rightarrow \infty$ . Below we shall give two such examples.

EXAMPLE 4.1 (Mixture of two Gaussian distributions). Let  $\{X_n\}_{n=1}^\infty$  be a sequence of random variables with the distribution  $F_n = (1 - \varepsilon_n)N(0, 1) + \varepsilon_n N(0, a_n^2)$ . Suppose that  $a_n \geq 1$ ,  $a_n \rightarrow \infty$  as  $n \rightarrow \infty$ , and consider  $\varepsilon_n = a_n^{-4}$ . Then, we have  $X_n \sim \text{subgaussian}(4a_n^2)$ ,  $\text{Var}(X_n) \asymp 1$ ,  $\|X_n\|_4 \asymp 1$ ,  $\|X_n\|_6 \asymp a_n^{1/3}$ , and  $\|X_n\|_8 \asymp a_n^{1/2}$ . The distribution  $F_n$  can be viewed as a  $\varepsilon_n$ -contaminated one-dimensional normal distribution given by (38) in the Supplemental Materials.

EXAMPLE 4.2 (Mixture of two symmetric discrete distributions). Let  $\pi_1$  be the distribution of a Rademacher random variable  $Y$  (i.e.  $\mathbb{P}(Y = \pm 1) = 1/2$ ) and  $\pi_2$  be the distribution of a discrete random variable  $Z_n$  such that  $\mathbb{P}(Z_n = \pm a_n) = (2a_n^2)^{-1}$  and  $\mathbb{P}(Z_n = 0) = 1 - a_n^{-2}$ . Let  $\{X_n\}_{n=1}^\infty$  be a sequence of random variables with the distribution  $F_n = (1 - \varepsilon_n)\pi_1 + \varepsilon_n\pi_2$ , where  $\varepsilon_n = 2/(a_n^2 - 1)$ ,  $a_n > \sqrt{3}$ , and  $a_n \rightarrow \infty$  as  $n \rightarrow \infty$ . Then  $X_n \sim$  subgaussian( $Ca_n^2$ ) for some large enough constant  $C > 0$  and elementary calculations show that  $\text{Var}(X_n) = 1$ ,  $\|X_n\|_4 = 3^{1/4}$ ,  $\|X_n\|_6 \asymp a_n^{1/3}$ , and  $\|X_n\|_8 \asymp a_n^{1/2}$ .

Therefore, in the statistical applications for subgaussian data, we allow  $\nu_n^2 \rightarrow \infty$  as  $n \rightarrow \infty$ . Let  $\xi_q = \max_{1 \leq k \leq p} \|X_{1k}\|_q$  and recall  $\Gamma = \text{Cov}(g(X_1))$ .

THEOREM 4.1 (**Main result V**: data-driven threshold selection: subgaussian observations). *Let  $\nu_n \geq 1$  and  $X_i$  be iid mean zero random vectors in  $\mathbb{R}^p$  such that  $X_{ik} \sim$  subgaussian( $\nu_n^2$ ) for all  $k = 1, \dots, p$  and  $\Sigma \in \mathcal{G}(r, \zeta_p)$ . Suppose that there exist constants  $C_i > 0, i = 1, \dots, 3$ , such that  $\Gamma_{(j,k),(j,k)} \geq C_1$ ,  $\xi_6 \leq C_2\nu_n^{1/3}$  and  $\xi_8 \leq C_3\nu_n^{1/2}$  for all  $j, k = 1, \dots, p$ . Let  $\alpha, \beta, K \in (0, 1)$  and  $\tau_* = \beta^{-1}a_{T_n^\#}(1 - \alpha)$ . If  $\nu_n^4 \log^7(np) \leq C_4n^{1-K}$ , then we have*

$$(24) \quad \|\hat{\Sigma}(\tau_*) - \Sigma\|_2 \leq \left[ \frac{3 + 2\beta}{\beta^{1-r}} + \left( \frac{\beta}{1 - \beta} \right)^r \right] \zeta_p a_{T_n^\#}^{1-r} (1 - \alpha),$$

$$(25) \quad \frac{1}{p} |\hat{\Sigma}(\tau_*) - \Sigma|_F^2 \leq 2 \left[ \frac{4 + 3\beta^2}{\beta^{2-r}} + 2 \left( \frac{\beta}{1 - \beta} \right)^r \right] \zeta_p a_{T_n^\#}^{2-r} (1 - \alpha),$$

with probability at least  $1 - \alpha - Cn^{-K/6}$  for some constant  $C > 0$  depending only on  $C_1, \dots, C_4$ . In addition,  $\mathbb{E}[a_{T_n^\#}(1 - \alpha)] \leq C'\xi_4^2(\log(p)/n)^{1/2}$  and

$$(26) \quad \mathbb{E}[\tau_*] \leq C'\beta^{-1}\xi_4^2(\log(p)/n)^{1/2},$$

where  $C' > 0$  is a constant depending only on  $\alpha$  and  $C_1, \dots, C_4$ .

REMARK 4 (Comments on the conditions in Theorem 4.1). **Conditions on the growth rate  $\xi_6 \leq C_2\nu_n^{1/3}$  and  $\xi_8 \leq C_3\nu_n^{1/2}$  are satisfied by Example 4.1 and 4.2.** The non-degeneracy condition  $\Gamma_{(j,k),(j,k)} \geq C_1$  is quite mild. Consider the multivariate cumulants of the joint distribution of the random vector  $X = (X_1, \dots, X_p)^\top$  following a distribution  $F$  in  $\mathbb{R}^p$ . Let  $\chi(t) = \mathbb{E}[\exp(it^\top X)]$  be the characteristic function of  $X$ , where  $t = (t_1, \dots, t_p)^\top \in$

$\mathbb{R}^p$  and  $\iota = \sqrt{-1}$ . Then, the *multivariate cumulants*  $\kappa_{r_1 r_2 \dots r_p}^{12 \dots p}$  of the joint distribution of  $X$  are the coefficients in the expansion

$$\log \chi(t) = \sum_{r_1, r_2, \dots, r_p=0}^{\infty} \kappa_{r_1 r_2 \dots r_p}^{12 \dots p} \frac{(\iota t_1)^{r_1} (\iota t_2)^{r_2} \dots (\iota t_p)^{r_p}}{r_1! r_2! \dots r_p!}.$$

For the covariance matrix kernel, we have

$$(27) \quad \Gamma_{(j,k),(m,l)} = (\kappa_{1111}^{jkm l} + \sigma_{jm} \sigma_{kl} + \sigma_{jl} \sigma_{km})/4,$$

where  $\kappa_{1111}^{jkm l}$  is the joint fourth-order cumulants of  $F$ . Therefore, if  $\kappa_{1111}^{jkm l} \geq 4C_1$ , then  $\Gamma_{(j,k),(j,k)} \geq C_1$ .

If the data follow a distribution in the elliptic family [51, Chapter 1], then the condition  $\Gamma_{(j,k),(j,k)} \geq C_1$  is equivalent to  $\min_{1 \leq j \leq p} \sigma_{jj} \geq C$  for some constant  $C > 0$  depending only on  $C_1$ . To see this, for  $F$  in the elliptic family, it is known that  $\kappa_{1111}^{jkm l} = \kappa(\sigma_{jk} \sigma_{ml} + \sigma_{jm} \sigma_{kl} + \sigma_{jl} \sigma_{km})$ , where  $\kappa$  is the kurtosis of  $F$ . Therefore,  $\Gamma_{(j,k),(j,k)} = [(2\kappa + 1)\sigma_{jk}^2 + (\kappa + 1)\sigma_{jj} \sigma_{kk}]/4$  and  $\Gamma_{(j,k),(j,k)} \geq C_1$  if and only if there exists a constant  $C > 0$  such that  $\sigma_{jj} \geq C$  for all  $j = 1, \dots, p$ .  $\square$

There are a number of interesting features of Theorem 4.1. Consider  $r = 0$ ; i.e.  $\Sigma$  is truly sparse such that  $\max_{1 \leq m \leq p} \sum_{k=1}^p \mathbf{1}\{\sigma_{mk} \neq 0\} \leq \zeta_p$  for  $\Sigma \in \mathcal{G}(0, \zeta_p)$ . Then we can take  $\beta = 1$  (i.e.  $\tau_* = a_{T_n^\#}(1 - \alpha)$ ) and the convergence rates are

$$\|\hat{\Sigma}(\tau_*) - \Sigma\|_2 \leq 6\zeta_p \tau_* \quad \text{and} \quad p^{-1} |\hat{\Sigma}(\tau_*) - \Sigma|_F^2 \leq 18\zeta_p \tau_*^2.$$

Hence, the tuning parameter can be adaptively selected by bootstrap samples while the rate of convergence is *nearly optimal* in the following sense. Since the distribution of  $\tau_*$  mimics that of  $\tau_\diamond$ ,  $\hat{\Sigma}(\tau_*)$  achieves the same convergence rate as the thresholded estimator  $\hat{\Sigma}(\tau_\diamond)$  for the oracle choice of the threshold  $\tau_\diamond$  with probability at least  $1 - \alpha - Cn^{-K/6}$ . On the other hand, the bootstrap method is not fully equivalent to the oracle procedure in terms of the constants in the estimation error bounds. Suppose that we know the support  $\Theta$  of  $\Sigma$ , i.e. locations of the nonzero entries in  $\Sigma$ . Then, the *oracle estimator* is simply  $\check{\Sigma} = \{\hat{\sigma}_{mk} \mathbf{1}\{(m, k) \in \Theta\}\}_{m,k=1}^p$  and we have

$$\begin{aligned} \|\check{\Sigma} - \Sigma\|_2 &\leq \max_{1 \leq m \leq p} \sum_{k=1}^p |\hat{\sigma}_{mk} - \sigma_{mk}| \mathbf{1}\{(m, k) \in \Theta\} \\ &\leq |\hat{S}_n - \Sigma|_\infty \max_{1 \leq m \leq p} \sum_{k=1}^p \mathbf{1}\{(m, k) \in \Theta\} \leq \tau_\diamond \zeta_p. \end{aligned}$$

Therefore, the constant of the convergence rate for the bootstrap method does not attain the oracle estimator. However, we shall comment that  $\beta$  is not a tuning parameter since it does not depend on  $F$  and the effect of  $\beta$  only appears in the constants in front of the convergence rates (24) and (25).

Assuming that the observations are subgaussian( $\nu^2$ ) and the variance factor  $\nu^2$  is a *fixed* constant, it is known that the threshold value  $\tau_\Delta = C(\nu)\sqrt{\log(p)/n}$  achieves the minimax rate for estimating the sparse covariance matrix [13]. Compared with the minimax optimal tuning parameter  $\tau_\Delta$ , our bootstrap threshold  $\tau_*$  exhibits several advantages for certain subgaussian distributions which we shall highlight (with stronger side conditions).

First, the bootstrap threshold  $\tau_*$  does not need the knowledge of  $\nu_n^2$  and it allows  $\nu_n^2 \rightarrow \infty$  as  $n \rightarrow \infty$ . In this case, from (26), the bootstrap threshold  $\tau_* = O_{\mathbb{P}}(\xi_4^2 \sqrt{\log(p)/n})$ , where the constant of  $O_{\mathbb{P}}(\cdot)$  depends only on  $\alpha, \beta, C_1, \dots, C_4$  in Theorem 4.1, while the universal thresholding rule  $\tau_\Delta = C'\nu_n^2 \sqrt{\log(p)/n}$ . Therefore, if  $\xi_4 = o(\nu_n)$ , then  $\tau_* = o_{\mathbb{P}}(\tau_\Delta)$  and the bootstrap threshold  $\tau_*$  is less conservative than the minimax threshold. For instance, suppose that  $X_{im}, i = 1, \dots, n; m = 1, \dots, p$  have the same marginal distribution in Example 4.1 (continuous case) or Example 4.2 (discrete case). Then we have  $\mathbb{E}[\tau_*] = O(\sqrt{\log(p)/n})$  by (26) and  $\tau_\Delta = Ca_n^2 \sqrt{\log(p)/n}$ . Thus  $\tau_* = o_{\mathbb{P}}(\tau_\Delta)$  for  $a_n \rightarrow \infty$ .

Second,  $\tau_\Delta$  is non-adaptive to the observations  $X_1^n$  since the minimax lower bound is based on the worst case analysis and the matching upper bound is obtained by the Bonferroni inequality which ignores the dependence structures in  $F$ . On the contrary,  $\tau_*$  takes into account the dependence information of  $F$  by conditioning on the observations. Therefore, the bootstrap threshold may better adjust to the dependence structure for some designs of  $X_i$ .

**EXAMPLE 4.3** (A block diagonal covariance matrix example with reduced rank). Let  $L, m$  be two positive integers and  $p = Lm$ . Let  $Z_{il}, i = 1, \dots, n; l = 1, \dots, L$ , be iid mean zero subgaussian( $\nu_n^2$ ) random variables with unit variance and  $Y_{il} = \mathbf{1}_m Z_{il}$ , where  $\mathbf{1}_m$  is the  $m \times 1$  vector containing all ones. Let  $X_i = (Y_{i1}^\top, \dots, Y_{iL}^\top)^\top$ . Under the assumptions in Theorem 4.1, we can show that  $\mathbb{E}[\tau_*] \leq C'\beta^{-1}\xi_4^2(\log(L)/n)^{1/2}$ . If  $\log L = o(\log p)$ , then  $\tau_* = o_{\mathbb{P}}(\tau_\Delta)$  and  $\hat{\Sigma}(\tau_*)$  can gain much tighter performance bounds in (24) and (25) than  $\hat{\Sigma}(\tau_\Delta)$ . Note that the covariance matrix  $\Sigma = \text{Cov}(X_i)$  in this example is block diagonal such that the diagonal blocks of  $\Sigma$  are rank-one matrices  $\mathbf{1}_m \mathbf{1}_m^\top$ . Therefore,  $\Sigma$  has the simultaneous sparsity (i.e.  $\zeta_p = m$ ) and reduced rank (i.e.  $\text{rank}(\Sigma) = L$ ).

Third, as we shall demonstrate in Theorem 4.2, the Gaussian type convergence rate of the bootstrap method in Theorem 4.1 can be achieved even for heavy-tailed data with polynomial moments.

**THEOREM 4.2** (Data-driven threshold selection: uniform polynomial moment observations). *Let  $X_i$  be iid mean zero random vectors such that  $\|\max_{1 \leq k \leq p} |X_{1k}|\|_8 \leq \nu_n$  and  $\Sigma \in \mathcal{G}(r, \zeta_p)$ . Suppose that there exist constants  $C_i > 0, i = 1, \dots, 3$ , such that  $\Gamma_{(j,k),(j,k)} \geq C_1$ ,  $\xi_6 \leq C_2 \nu_n^{1/3}$  and  $\xi_8 \leq C_3 \nu_n^{1/2}$  for all  $j, k = 1, \dots, p$ . Let  $\alpha, \beta, K \in (0, 1)$  and  $\tau_* = \beta^{-1} a_{T_n^\#}(1 - \alpha)$ . If  $\nu_n^8 \log^7(np) \leq C_4 n^{1-7K/6}$ , then (24) and (25) hold with probability at least  $1 - \alpha - Cn^{-K/6}$  for some constant  $C > 0$  depending only on  $C_1, \dots, C_4$ . In addition, (26) holds for some constant  $C' > 0$  depending only on  $\alpha$  and  $C_1, \dots, C_4$ .*

We compare Theorem 4.2 with the threshold obtained by the union bound approach. Assume that  $\max_{1 \leq k \leq p} \mathbb{E}|X_{1k}|^q < \infty$  for  $q \geq 8$ . By the Nagaev inequality [52] applied to the split sample in Remark 5, one can show that

$$\tau_{\#} = C(q) \left\{ \frac{p^{4/q}}{n^{1-2/q}} \xi_q^2 + \left( \frac{\log p}{n} \right)^{1/2} \xi_4^2 \right\}$$

is the right threshold that gives a large probability bound for  $\tau_\circ = |\hat{S}_n - \Sigma|_\infty$ . Consider  $q = 8$ ,  $\xi_8 = O(1)$ , and the scaling limit  $p = n^A$  for  $A > 0$ . Then the universal threshold  $\tau_{\#} = o(1)$  if  $0 < A < 3/2$ . In contrast, since  $\|\max_{1 \leq k \leq p} |X_{1k}|\|_8 \leq p^{1/8} \xi_8 = O(p^{1/8})$ , it follows from Theorem 4.2 that the bootstrap threshold  $\tau_*$  is asymptotically valid if  $0 < A < 1$  and by (26),  $\mathbb{E}[\tau_*] = O(\sqrt{(\log p)/n})$ . Therefore, in the least favorable case for the bootstrap, we conclude that: (i) if  $A \in (0, 1/2]$ , then  $\mathbb{E}[\tau_*] \asymp \tau_{\#}$ ; (ii) if  $A \in (1/2, 1)$ , then  $\mathbb{E}[\tau_*] = o(\tau_{\#})$  and  $\tau_{\#} = o(1)$ ; (iii) if  $A \in [1, 3/2)$ , then  $\tau_{\#} = o(1)$  while the bootstrap threshold  $\tau_*$  is not asymptotically valid; (iv) if  $A \in [3/2, \infty)$ , then neither  $\hat{\Sigma}(\tau_*)$  or  $\hat{\Sigma}(\tau_{\#})$  is consistent for estimating  $\Sigma$ . Hence, the bootstrap method gives better convergence rate than the universal thresholding method under the spectral and Frobenius norms when  $A \in (1/2, 1)$ . On the other hand, since  $\tau_{\#} = o(1)$  when  $A \in (0, 3/2)$ , the cost of the bootstrap to achieve the Gaussian-like convergence rate  $\tau_* = O_{\mathbb{P}}(\sqrt{(\log p)/n})$  for the heavy-tailed distribution  $F$  is a stronger requirement on the scaling limit for  $A \in (0, 1)$ . Moreover, to the best of our knowledge, the minimax lower bound is currently not available to justify  $\tau_{\#}$  for observations with polynomial moments. Finally, we remark that bootstrap can adapt to the dependency structure in  $F$ . For Example 4.3 with a block diagonal covariance matrix, we only need  $L \log^7(nL) = o(n)$ , where  $L$  can be much

smaller than  $p$  and the dimension  $p$  may still be allowed to be larger or even much larger than the sample size  $n$ .

4.2. *Simultaneous inference for covariance and rank correlation matrices.*

Another related important problem of estimating the sparse covariance matrix  $\Sigma$  is the consistent recovery of its support, i.e. non-zero off-diagonal entries in  $\Sigma$  [42]. Towards this end, a lower bound of the minimum signal strength ( $\Sigma$ -min condition) is a necessary condition to separate the weak signals and true zeros. Yet, the  $\Sigma$ -min condition is never verifiable. To avoid this undesirable condition, we can alternatively formulate the recovery problem as a more general hypothesis testing problem

$$(28) \quad H_0 : \Sigma = \Sigma_0 \quad \text{versus} \quad H_1 : \Sigma \neq \Sigma_0,$$

where  $\Sigma_0$  is a known  $p \times p$  matrix. In particular, if  $\Sigma_0 = \text{Id}_{p \times p}$ , then the support recovery can be re-stated as the following simultaneously testing problem: for all  $m, k \in \{1, \dots, p\}$  and  $m \neq k$ ,

$$(29) \quad H_{0,mk} : \sigma_{mk} = 0 \quad \text{versus} \quad H_{1,mk} : \sigma_{mk} \neq 0.$$

The test statistic we construct is  $\bar{T}_0 = |\hat{S}_n - \Sigma_0|_{\infty, \text{off}}$ , which is an  $\ell^\infty$  statistic by taking the maximum magnitudes on the off-diagonal entries. Then  $H_0$  is rejected if  $\bar{T}_0 \geq a_{\bar{T}_n^\#}(1 - \alpha)$ .

**COROLLARY 4.3** (Asymptotic size of the simultaneous test: subgaussian observations). *Let  $\nu_n \geq 1$  and  $X_i$  be iid mean zero random vectors in  $\mathbb{R}^p$  such that  $X_{ik} \sim \text{subgaussian}(\nu_n^2)$  for all  $k = 1, \dots, p$ . Suppose that there exist constants  $C_i > 0, i = 1, \dots, 3$ , such that  $\Gamma_{(j,k),(j,k)} \geq C_1$ ,  $\xi_6 \leq C_2 \nu_n^{1/3}$  and  $\xi_8 \leq C_3 \nu_n^{1/2}$  for all  $j, k = 1, \dots, p$ . Let  $\alpha, \beta, K \in (0, 1)$  and  $\tau_* = \beta^{-1} a_{\bar{T}_n^\#}(1 - \alpha)$ . If  $\nu_n^4 \log^7(np) \leq C_4 n^{1-K}$ , then the above test based on  $\bar{T}_0$  for (28) has the size  $\alpha + O(n^{-K/6})$ ; i.e. the family-wise error rate of the simultaneous test problem (29) is asymptotically controlled at the level  $\alpha$ .*

From Corollary 4.3, the test based on  $\bar{T}_0$  is asymptotically exact of size  $\alpha$  for subgaussian data. A similar result can be established for observations with polynomial moments. Due to the space limit, details are omitted. [15] proposed a similar test statistic for comparing the two-sample large covariance matrices. Their results (Theorem 1 in [15]) are analogous to Corollary 4.3 in this paper in that no structural assumptions in  $\Sigma$  are needed in order to obtain the asymptotic validity of both tests. However, we shall note that their assumptions (C.1), (C.2), and (C.3) on the non-degeneracy are

stronger than our condition  $\Gamma_{(j,k),(j,k)} \geq C_1$ . For subgaussian observations  $X_{ik} \sim \text{subgaussian}(\nu_n^2)$ , (C.3) in [15] assumed that  $\min_{1 \leq j \leq k \leq p} \gamma_{jk}/\nu_n^4 \geq c$  for some constant  $c > 0$ , where  $\gamma_{jk} = \text{Var}(X_{1j}X_{1k})$ . If  $\nu_n^2 \rightarrow \infty$ , then [15, Theorem 1] requires that  $\gamma_{jk}$  for all  $j, k = 1, \dots, p$  have to obey a uniform lower bound that diverges to infinity. For the covariance matrix kernel, since  $g(x) = (xx^\top - \Sigma)/2$ , we only need that  $\min_{j,k} \gamma_{jk} \geq c$  for some fixed lower bound.

Next, we comment that a distinguishing feature of our bootstrap test from the  $\ell^2$  test statistic [17] is that no structural assumptions are made on  $F$  and we allow for the strong dependence in  $\Sigma$ . For example, consider again the elliptic distributions [51, Chapter 1] with the positive-definite  $V = \varrho \mathbf{1}_p \mathbf{1}_p^\top + (1 - \varrho) \text{Id}_{p \times p}$  such that the covariance matrix  $\Sigma$  is proportion to  $V$ . Then, we have

$$\begin{aligned} \text{tr}(V^4) &= p[1 + (p-1)\varrho^2]^2 + p(p-1)[2\varrho + (p-2)\varrho^2]^2, \\ \text{tr}(V^2) &= \varrho^2 p^2 + (1 - \varrho^2)p. \end{aligned}$$

For any  $\varrho \in (0, 1)$ ,  $\text{tr}(V^4)/\text{tr}^2(V^2) \rightarrow 1$  as  $p \rightarrow \infty$ . Therefore, the limiting distribution of the  $\ell^2$  test statistic in [17] is no longer normal and its asymptotic distribution remains unclear.

Finally, the covariance matrix testing problem (28) can be generalized further to nonparametric forms which can gain more robustness to outliers and the nonlinearity in the dependency structures. Let  $U_\diamond = \mathbb{E}[h(X_1, X_2)]$  be the expectation of the random matrix associated with  $h$  and  $U_0$  be a known  $p \times p$  matrix. Consider the testing problem

$$H_0 : U_\diamond = U_0 \quad \text{versus} \quad H_1 : U_\diamond \neq U_0.$$

Then, the test statistic can be constructed as  $\bar{T}_0 = |U_n - U_0|_\infty$  (or  $\bar{T}'_0 = |U_n - U_0|_{\infty, \text{off}}$ ) and  $H_0$  is rejected if  $\bar{T}_0 \geq a_{\bar{T}'_n} (1 - \alpha)$  (or  $\bar{T}'_0 \geq a_{\bar{T}'_n} (1 - \alpha)$ ), where the bootstrap samples are generated w.r.t. the kernel  $h$ . The above test covers Kendall's tau rank correlation matrix as a special case where  $h$  is the bounded kernel.

**COROLLARY 4.4** (Asymptotic size of the simultaneous test for Kendall's tau rank correlation matrix). *Let  $X_i$  be iid random vectors with a distribution  $F$  in  $\mathbb{R}^p$ . Suppose that there exists a constant  $C_1 > 0$  such that  $\Gamma_{(j,k),(j,k)} \geq C_1$  for all  $j, k = 1, \dots, p$ . Let  $\alpha, \beta, K \in (0, 1)$  and  $\tau_* = \beta^{-1} a_{\bar{T}'_n} (1 - \alpha)$ , where the bootstrap samples are generated with Kendall's tau rank correlation coefficient matrix kernel. If  $\log^7(np) \leq C_2 n^{1-K}$ , then the test based on  $\bar{T}'_0$  has the size  $\alpha + O(n^{-K/6})$ .*



Therefore, the asymptotic validity of the bootstrap test for large Kendall's tau rank correlation matrix is obtained when  $\log p = o(n^{1/7})$  without imposing structural and moment assumptions on  $F$ .

**5. Proof of the main results.** The rest of the paper is organized as follows. In Section 5.1, we first present a useful inequality for bounding the expectation of the sup-norm of the *canonical* U-statistics and then compare with an alternative simple data splitting bound by reducing to the moment bounding exercise for the sup-norm of sums of iid random vectors. We shall discuss several advantages of using the U-statistics approach by exploring the degeneracy structure. Section 5.2 contains the proof of the Gaussian approximation result and Section 5.3 proves the convergence rate of the bootstrap validity. Proofs of the statistical applications are given in Section 5.4. Additional proofs and technical lemmas are given in the SM.

5.1. *A maximal inequality for canonical U-statistics.* Before proving our main results, we first establish a maximal inequality of the canonical U-statistics of order two. The derived expectation bound is useful in controlling the size of the nonlinear and completely degenerate error term in the Gaussian approximation.

**THEOREM 5.1** (A maximal inequality for canonical U-statistics). *Let  $X_1^n$  be a sample of iid random variables in a separable and measurable space  $(S, \mathcal{S})$ . Let  $f : S \times S \rightarrow \mathbb{R}^d$  be an  $\mathcal{S} \otimes \mathcal{S}$ -measurable, symmetric and canonical kernel such that  $\mathbb{E}|f_m(X_1, X_2)| < \infty$  for all  $m = 1, \dots, d$ . Let  $V_n = [n(n-1)]^{-1} \sum_{1 \leq i \neq j \leq n} f(X_i, X_j)$ ,  $M = \max_{1 \leq i \neq j \leq n} \max_{1 \leq m \leq d} |f_m(X_i, X_j)|$ ,  $D_q = \max_{1 \leq m \leq d} (\mathbb{E}|f_m(X_1, X_2)|^q)^{1/q}$  for  $q > 0$ . If  $2 \leq d \leq \exp(bn)$  for some constant  $b > 0$ , then there exists an absolute constant  $K > 0$  such that*

$$(30) \quad \mathbb{E}[|V_n|_\infty] \leq K(1 + b^{1/2}) \left\{ \left( \frac{\log d}{n} \right)^{3/2} \|M\|_4 + \frac{\log d}{n} D_2 + \left( \frac{\log d}{n} \right)^{5/4} D_4 \right\}.$$

Note that Theorem 5.1 is non-asymptotic. As immediate consequences of Theorem 5.1, we can derive the rate of convergence of  $\mathbb{E}[|V_n|_\infty]$  with kernels under the subexponential and uniform polynomial moment conditions.

**COROLLARY 5.2** (Kernels with subexponential and uniform polynomial moments). *Let  $B_n, B'_n$  be two sequences of positive reals and  $f$  be a symmetric and canonical kernel. Suppose that  $2 \leq d \leq \exp(bn)$  for some constant  $b > 0$ . (i) If*

$$(31) \quad \max_{1 \leq m \leq d} \mathbb{E}[\exp(|f_m|/B_n)] \leq 2,$$

then there exists a constant  $C(b) > 0$  such that

$$(32) \quad \mathbb{E}[|V|_\infty] \leq C(b)B_n\{(n^{-1}\log d)^{3/2}\log(nd) + n^{-1}\log d\}.$$

(ii) Let  $q \geq 4$ . If

$$(33) \quad \mathbb{E}\left(\max_{1 \leq m \leq d} |f_m|/B_n\right)^q \vee \max_{1 \leq m \leq d} \mathbb{E}(|f_m|/B'_n)^4 \leq 1,$$

then there exists a constant  $C(b) > 0$  such that

$$(34) \quad \mathbb{E}[|V|_\infty] \leq C(b)\{B_n n^{-3/2+2/q}(\log d)^{3/2} + B'_n n^{-1}\log d\}.$$

REMARK 5 (Comparison of Theorem 5.1 with sums of iid random vectors by data splitting). We can also bound the expected norm of a  $U$ -statistic by the expected norm of sums of iid random vectors. Assume that  $\mathbb{E}|f_k(X_1, X_2)| < \infty$  for all  $k = 1, \dots, d$  and let  $m = \lfloor n/2 \rfloor$  be the largest integer no greater than  $n/2$ . As noted in [35], we can write

$$(35) \quad m(V_n - \mathbb{E}V_n) = \frac{1}{n!} \sum_{\text{all } \pi_n} S(X_{\pi_n(1)}, \dots, X_{\pi_n(n)}),$$

where  $S(X_1^n) = \sum_{i=1}^m [f(X_{2i-1}, X_{2i}) - \mathbb{E}f]$  and the summation  $\sum_{\text{all } \pi_n}$  is taken over all possible permutations  $\pi_n : \{1, \dots, n\} \rightarrow \{1, \dots, n\}$ . By Jensen's inequality and the iid assumption of  $X_i$ , we have

$$(36) \quad \mathbb{E}|V_n - \mathbb{E}V_n|_\infty \leq \frac{1}{m} \mathbb{E} \left| \sum_{i=1}^m [f(X_i, X_{i+m}) - \mathbb{E}f] \right|_\infty,$$

which can be viewed as a data splitting method into two halves. Assuming (31), it follows from Bernstein's inequality [63, Proposition 5.16] that

$$(37) \quad \mathbb{E}|V_n - \mathbb{E}V_n|_\infty \leq K_1 B_n (\sqrt{\log(d)/n} + \log(d)/n)$$

for some absolute constant  $K_1 > 0$ . So if  $\log d \leq bn^{1-\varepsilon}$  for some  $\varepsilon \in (0, 1)$ , then  $\mathbb{E}|V_n - \mathbb{E}V_n|_\infty \leq C(b)B_n(\log(d)/n)^{1/2} \leq C(b)B_n n^{-\varepsilon/2}$ . For the canonical kernel where  $\mathbb{E}V_n = 0$ , there are two advantages of using the  $U$ -statistics approach in Theorem 5.1 over the data splitting method into iid summands (36) and (37).

First, we can obtain from (32) that  $\mathbb{E}|V_n|_\infty \leq C(b)B_n\{n^{1-5\varepsilon/2} + n^{-\varepsilon}\}$ . Therefore, sharper rate is obtained by (32) when  $\varepsilon \in (1/2, 1)$  which covers the regime of valid Gaussian approximation and bootstrap. Under the scaling limit for the Gaussian approximation validity, i.e.  $B_n^a \log^7(np)/n \leq Cn^{-K_2}$

for some  $K_2 \in (0, 1)$ , where  $a = 2$  for the subexponential moment kernel and  $a = 4$  for the uniform polynomial moment kernel, it is easy to see that  $\log d \leq \log(nd) \leq Cn^{(1-K_2)/7}$  so we can take  $\varepsilon = (6 + K_2)/7$ .

Second and more importantly, the rate of convergence obtained by the Bernstein bound (37) does not lead to a convergence rate for the Gaussian and bootstrap approximations. The reason is that, although (37) is rate-exact for *non-degenerate* U-statistics, where the dependence of the rate in (37) on the sample size is  $O(B_n n^{-1/2})$ , it is not strong enough to control the size of the nonlinear remainder term  $\mathbb{E}[|n^{1/2}V_n|_\infty]$  when  $d \rightarrow \infty$  (recall that  $R_n = n^{1/2}V_n/2$ ); c.f. Proposition 5.3. On the contrary, our bound in Theorem 5.1 exploits the degeneracy structure of  $V$  and the dependence of the rate in (30) on the sample size is  $O(B_n n^{-1} + \|M\|_4 n^{-3/2})$ . Therefore, Theorem 5.1 is more mathematically appealing in the degenerate case.

For non-degenerate U-statistics  $U_n = [n(n-1)]^{-1} \sum_{1 \leq i \neq j \leq n} h(X_i, X_j)$ , the reduction to sums of iid random vectors in (36) does not give tight asymptotic distributions. To illustrate this point, we consider the case  $d = 1$  and let  $X_i$  be iid mean zero random variables with variance  $\sigma^2$ . Let  $\zeta_1^2 = \text{Var}(g(X_1))$  and  $\zeta_2^2 = \text{Var}(h(X_1, X_2))$ . Assume that  $\zeta_1^2 > 0$ . So  $\zeta_1^2$  is the variance of the leading projection term used in the Gaussian approximation and by Jensen's inequality  $\zeta_1^2 \leq \zeta_2^2$ . Note that  $\sqrt{n}(U_n - \mathbb{E}U_n) \xrightarrow{D} N(0, 4\zeta_1^2)$  [59, Theorem A, page 192] and by the CLT  $\sqrt{2/m} \sum_{i=1}^m [f(X_i, X_{i+m}) - \mathbb{E}f] \xrightarrow{D} N(0, 2\zeta_2^2)$ . Since in general  $\zeta_2^2 \neq 2\zeta_1^2$ , the limiting distribution of the U-statistic is not the same as that in the data splitting method. For example, consider the non-degenerate covariance kernel  $h(x_1, x_2) = (x_1 - x_2)^2/2$ . Denote  $\mu_4 = \mathbb{E}X_1^4$  and  $g(x_1) = (x_1^2 - \sigma^2)/2$ . Then,  $\zeta_2^2 = (\mu_4 + \sigma^4)/2$  and  $\zeta_1^2 = (\mu_4 - \sigma^4)/4$  so that  $\zeta_2^2 > 2\zeta_1^2$  when  $\sigma^2 > 0$ . In particular, if  $X_i$  are iid  $N(0, \sigma^2)$ , then  $\mu_4 = 3\sigma^4$ ,  $4\zeta_1^2 = 2\sigma^4$ , and  $2\zeta_2^2 = 4\sigma^4$ . Therefore, even though (37) gives better rate in the non-degenerate case, the reduction by splitting the data into the iid summands is not optimal for the Gaussian approximation purpose, which is the main motivation of this paper. In fact,  $\zeta_2^2$  serves no purpose in the limiting distribution of  $\sqrt{n}(U_n - \mathbb{E}U_n)$ .  $\square$

5.2. *Proof of results in Section 2.* For  $q > 0$  and  $\phi \geq 1$ , we define

$$\begin{aligned} D_{g,q} &= \max_{1 \leq m \leq d} \mathbb{E}|g_m(X)|^q, \\ M_{g,q}(\phi) &= \mathbb{E} \left[ \max_{1 \leq m \leq d} |g_m(X)|^q \mathbf{1} \left( \max_{1 \leq m \leq d} |g_m(X)| > \frac{\sqrt{n}}{4\phi \log d} \right) \right], \\ M_{Y,q}(\phi) &= \mathbb{E} \left[ \max_{1 \leq m \leq d} |Y_m|^q \mathbf{1} \left( \max_{1 \leq m \leq d} |Y_m| > \frac{\sqrt{n}}{4\phi \log d} \right) \right]. \end{aligned}$$

and  $M_q(\phi) = M_{g,q}(\phi) + M_{Y,q}(\phi)$ . The Gaussian approximation result (GAR) in Proposition 5.3 below relies on the control of  $D_{g,3}$  and  $M_3(\phi)$ . Interestingly, the quantity  $M_{g,3}(\phi)$  can be viewed as a stronger version of the Lindeberg condition that allows us to derive the explicit convergence rate of the Gaussian approximation when  $d \rightarrow \infty$ . Denote  $\chi_{\tau,ij} = \mathbf{1}(\max_{1 \leq m \leq d} |h_m(X_i, X_j)| > \tau)$  for  $\tau \geq 0$ . Let

$$\begin{aligned} D_q &= \max_{1 \leq m \leq d} \mathbb{E}|h_m(X_1, X_2)|^q, \\ M_{h,q}(\tau) &= \mathbb{E} \left[ \max_{1 \leq i \neq j \leq n} \max_{1 \leq m \leq d} |h_m(X_i, X_j)|^q \chi_{\tau,ij} \right]. \end{aligned}$$

For two random vectors  $X$  and  $Y$  in  $\mathbb{R}^d$ , we denote

$$\tilde{\rho}^{re}(X, Y) = \sup_{y \in \mathbb{R}^d} |\mathbb{P}(X \leq y) - \mathbb{P}(Y \leq y)|.$$

PROPOSITION 5.3 (A general Gaussian approximation result for U-statistics). *Assume that (M.1) holds and  $\log d \leq \bar{b}n$  for some constant  $\bar{b} > 0$ . Then there exist constants  $C_i := C_i(\underline{b}, \bar{b}) > 0, i = 1, 2$  such that for any real sequence  $\bar{D}_{g,3}$  satisfying  $D_{g,3} \leq \bar{D}_{g,3}$ , we have*

$$\begin{aligned} \tilde{\rho}^{re}(T_n, Y) &\leq C_1 \left\{ \left( \frac{\bar{D}_{g,3}^2 \log^7 d}{n} \right)^{1/6} + \frac{M_3(\phi_n)}{\bar{D}_{g,3}} \right. \\ (38) \quad &\left. + \phi_n \left( \frac{\log^{3/2} d}{n} (M_{h,4}(\tau))^{1/4} + \tau \right) + \frac{\log d}{n^{1/2}} D_2^{1/2} + \frac{\log^{5/4} d}{n^{3/4}} D_4^{1/4} \right\}, \end{aligned}$$

where

$$(39) \quad \phi_n = C_2 \left( \frac{\bar{D}_{g,3}^2 \log^4 d}{n} \right)^{-1/6}.$$

In addition,  $\rho^{re}(T_n, Y)$  obeys the same bound in (38).

With the help of Proposition 5.3, we are now ready to prove Theorem 2.1.

PROOF OF THEOREM 2.1. We may assume that  $\varpi_{1,n} \leq 1$ ; otherwise the proof is trivial. Let  $\ell_n = \log(nd) > 1$ . By (M.2) and Jensen's inequality, we have  $D_2 \leq B_n^{2/3}$ ,  $D_{g,3} \leq D_3 \leq B_n$ , and  $D_4 \leq B_n^2$ . Write  $M_{h,q} = M_{h,q}(0)$ . By

Proposition 5.3 with  $\tau = 0$  and  $\phi_n$  is given by (39), we have

$$(40) \quad \rho^{re}(T_n, Y) \leq C_1 \left\{ \left( \frac{\bar{D}_{g,3}^2 \log^7 d}{n} \right)^{1/6} + \frac{M_3(\phi_n)}{\bar{D}_{g,3}} + \phi_n \left( \frac{\log^{3/2} d}{n} M_{h,4}^{1/4} + \frac{\log d}{n^{1/2}} D_2^{1/2} + \frac{\log^{5/4} d}{n^{3/4}} D_4^{1/4} \right) \right\},$$

where  $C_1 > 0$  is a constant only depending on  $\underline{b}$  and  $\bar{b}$ .

**Case (E.1).** By [62, Lemma 2.2.2],  $M_{h,4}^{1/4} \leq K_1 B_n \ell_n$ . Then, we have

$$\begin{aligned} \phi_n \frac{\log^{3/2} d}{n} M_{h,4}^{1/4} &\leq C_2 \frac{B_n^{2/3} \ell_n^{11/6}}{n^{5/6}} \leq C_2 \varpi_{1,n}, \\ \phi_n \frac{\log d}{n^{1/2}} D_2^{1/2} &\leq C_3 \frac{(\log d)^{1/3}}{n^{1/3}} \leq C_3 \varpi_{1,n}, \\ \phi_n \frac{\log^{5/4} d}{n^{3/4}} D_4^{1/4} &\leq C_4 \frac{B_n^{1/6} (\log d)^{7/12}}{n^{7/12}} \leq C_4 \varpi_{1,n}. \end{aligned}$$

Choosing  $\bar{D}_{g,3} = B_n$  and following the proof of [23, Proposition 2.1], we can show that

$$\left( \frac{\bar{D}_{g,3}^2 \log^7 d}{n} \right)^{1/6} + \frac{M_3(\phi_n)}{\bar{D}_{g,3}} \leq C_5 \varpi_{1,n}.$$

Then, (5) follows from (40). Here, all constants  $C_i$  for  $i = 2, \dots, 5$  depend only on  $\underline{b}$  and  $\bar{b}$ .

**Case (E.2).**  $D_2$  and  $D_4$  obey the same bounds as case (E.1). Assuming (E.2),  $M_{h,4}^{1/4} \leq n^{1/2} B_n$ . Then,

$$\phi_n \frac{\log^{3/2} d}{n} M_{h,4}^{1/4} \leq C_6 \frac{B_n^{2/3} \ell_n^{5/6}}{n^{1/3}} \leq C_6 \varpi_{1,n}.$$

Choosing  $\bar{D}_{g,3} = B_n + B_n^2 n^{-1/2+2/q} (\log d)^{-1/2}$  and following the proof of [23, Proposition 2.1], we can show that

$$\left( \frac{\bar{D}_{g,3}^2 \log^7 d}{n} \right)^{1/6} + \frac{M_3(\phi_n)}{\bar{D}_{g,3}} \leq C_7 \{ \varpi_{1,n} + \varpi_{2,n} \}.$$

Here,  $C_6, C_7$  are constants depending only on  $\underline{b}, \bar{b}$ , and  $q$ . Then, (5) is immediate.  $\square$

5.3. *Proof of results in Section 3.* In view of the approximation diagram (9), our first task is to control the random quantity

$$\sup_{A \in \mathcal{A}^{re}} |\mathbb{P}(Y \in A) - \mathbb{P}(Z^X \in A \mid X_1^n)|$$

on an event occurring with large probability, which is Step (2) in the approximation diagram (9).

PROPOSITION 5.4 (Gaussian comparison bound for the linear part in U-statistic and its EB version). *Let  $Z^X \mid X_1^n \sim N(0, \hat{\Gamma}_n)$ , where  $\hat{\Gamma}_n$  is defined in (11). Suppose that (M.1), (M.2) and (M.2') are satisfied.*

(i) *If (E.1) and (E.1') hold, then there exists a constant  $C(\underline{b}) > 0$  such that with probability at least  $1 - \gamma$  we have*

$$(41) \quad \sup_{A \in \mathcal{A}^{re}} |\mathbb{P}(Y \in A) - \mathbb{P}(Z^X \in A \mid X_1^n)| \leq C(\underline{b}) \varpi_{1,n}^B(\gamma).$$

(ii) *If (E.2) and (E.2') hold with  $q \geq 4$ , then there exists a constant  $C(\underline{b}, q) > 0$  such that with probability at least  $1 - \gamma$  we have*

$$(42) \quad \sup_{A \in \mathcal{A}^{re}} |\mathbb{P}(Y \in A) - \mathbb{P}(Z^X \in A \mid X_1^n)| \leq C(\underline{b}, q) \{\varpi_{1,n}^B(\gamma) + \varpi_{2,n}^B(\gamma)\}.$$

From Proposition 5.4, we are now ready to establish the rate of convergence of the empirical bootstrap for U-statistics. Let  $W_{jk} = |n^{-1} \sum_{i=1}^n h_j(X_k, X_i) - V_{nj}|$  for  $j = 1, \dots, d$  and  $k = 1, \dots, n$ . For  $q, \tau > 0$ , and  $\phi \geq 1$ , we define

$$\begin{aligned} \hat{D}_{g,q} &= \max_{1 \leq j \leq d} n^{-1} \sum_{k=1}^n W_{jk}^q, \\ \hat{D}_q &= \max_{1 \leq j \leq d} n^{-2} \sum_{k,l=1}^n |h_j(X_k, X_l)|^q, \\ \hat{M}_{h,q}(\tau) &= n^{-2} \sum_{i,k=1}^n \max_{1 \leq j \leq d} |h_j(X_i, X_k)|^q \mathbf{1}(\max_{1 \leq j \leq d} |h_j(X_i, X_k)| > \tau), \\ \hat{M}_{g,q}(\phi) &= n^{-1} \sum_{k=1}^n \max_{1 \leq j \leq d} W_{jk}^q \mathbf{1}\left(\max_{1 \leq j \leq d} W_{jk} > \frac{\sqrt{n}}{4\phi \log d}\right), \\ \hat{M}_{Z,q}(\phi) &= \mathbb{E} \left[ \max_{1 \leq j \leq d} |Z_j^X|^q \mathbf{1}\left(\max_{1 \leq j \leq d} |Z_j^X| > \frac{\sqrt{n}}{4\phi \log d}\right) \mid X_1^n \right], \end{aligned}$$

$$\hat{M}_q(\phi) = \hat{M}_{g,q}(\phi) + \hat{M}_{Z,q}(\phi), \text{ and } Z^X \mid X_1^n \sim N(0, \hat{\Gamma}_n).$$

PROOF OF THEOREM 3.1. In this proof, the constants  $C_1, C_2, \dots$  depend only on  $\underline{b}, \bar{b}, K$  in case (i) and  $\underline{b}, \bar{b}, q, K$  in case (ii). First, we may assume that

$$(43) \quad n^{-1}B_n^2 \log^7(nd) \leq c_1 \leq 1$$

for some sufficiently small constant  $c_1 > 0$ , where  $c_1$  depends only on  $\underline{b}, \bar{b}, K$  in case (i) and on  $\underline{b}, \bar{b}, q, K$  in case (ii), since otherwise the proof is trivial by setting the constants  $C(\underline{b}, \bar{b}, K)$  in (i) and  $C(\underline{b}, \bar{b}, q, K)$  in (ii) large enough. By (9) and the triangle inequality,

$$(44) \quad \begin{aligned} \rho^B(T_n, T_n^*) &\leq \rho^{re}(T_n, Y) + \sup_{A \in \mathcal{A}^{re}} |\mathbb{P}(Y \in A) - \mathbb{P}(Z^X \in A \mid X_1^n)| \\ &\quad + \rho^{re}(Z^X, T_n^* \mid X_1^n), \end{aligned}$$

where  $\rho^{re}(Z^X, T_n^* \mid X_1^n) = \sup_{A \in \mathcal{A}^{re}} |\mathbb{P}(Z^X \in A \mid X_1^n) - \mathbb{P}(T_n^* \in A \mid X_1^n)|$ . Since  $\log(1/\gamma) \leq K \log(dn)$ , we have  $\varpi_{1,n}^B(\gamma) \leq K^{1/3} \varpi_{1,n}$  and  $\varpi_{2,n} \leq \varpi_{2,n}^B(\gamma)$  for  $\gamma \in (0, e^{-1})$ . By Theorem 2.1 and Proposition 5.4, we have: (i) if (E.1) and (E.1') hold, then with probability at least  $1 - 2\gamma/9$  we have

$$\rho^{re}(T_n, Y) + \sup_{A \in \mathcal{A}^{re}} |\mathbb{P}(Y \in A) - \mathbb{P}(Z^X \in A \mid X_1^n)| \leq C(\underline{b}, \bar{b}, K) \varpi_{1,n};$$

(ii) if (E.2) and (E.2') hold, then with probability at least  $1 - 2\gamma/9$  we have

$$\rho^{re}(T_n, Y) + \sup_{A \in \mathcal{A}^{re}} |\mathbb{P}(Y \in A) - \mathbb{P}(Z^X \in A \mid X_1^n)| \leq C(\underline{b}, \bar{b}, q, K) \{\varpi_{1,n} + \varpi_{2,n}^B(\gamma)\}.$$

To deal with the third term on the right-hand side of (44), we observe that conditionally on  $X_1^n$ ,  $U_n^*$  is a U-statistics of  $\xi_1, \dots, \xi_n$  and  $Z^X$  has the conditional covariance matrix  $\hat{\Gamma}_n$ ; c.f. (11). So we can apply Proposition 5.3 conditionally.

**Case (i).** As in the proof of Proposition 5.4, we have with probability at least  $1 - \gamma/9$

$$(45) \quad |\hat{\Gamma}_n - \Gamma|_\infty \leq C_1(K) [n^{-1}B_n^2 \log(nd) \log^2(1/\gamma)]^{1/2}.$$

By (43), (M.1), (M.2) and (M.2'), there exists a constant  $C_2 > 0$  such that  $\underline{b}/2 \leq \hat{\Gamma}_{n,jj} \leq C_2 B_n^{2/3} \leq C_2 B_n$  for all  $j = 1, \dots, d$  holds with probability at least  $1 - \gamma/9$ . Let  $\bar{D}_{g,3} = C_3 B_n$ ,  $\bar{D}_2 = C_4 B_n^{2/3}$ , and  $\bar{D}_4 = C_5 B_n^2 \log(dn)$ . By Lemma C.2, each of the three events  $\{\hat{D}_{g,3} \geq \bar{D}_{g,3}\}$ ,  $\{\hat{D}_2 \geq \bar{D}_2\}$ , and  $\{\hat{D}_4 \geq \bar{D}_4\}$  occur with probability at most  $\gamma/9$ . Let  $\phi_n = C_6 (n^{-1} \bar{D}_{g,3}^2 \log^4 d)^{-1/6}$  for some  $C_6 > 0$  such that  $\phi_n \geq 1$ . By Jensen's

inequality,  $\max_{k,j} W_{kj} \leq 2n^{-1} \max_{k,j} \sum_{i=1}^n |h_j(X_k, X_i)|$ . Then, by the union bound and the assumptions (E.1) and (E.1'), we have

$$\begin{aligned}
\mathbb{P}(\hat{M}_{g,3}(\phi_n) > 0) &= \mathbb{P}\left(\max_{1 \leq j \leq d, 1 \leq k \leq n} W_{jk} > \sqrt{n}/(4\phi_n \log d)\right) \\
&\leq (dn) \max_{1 \leq j \leq d, 1 \leq k \leq n} \mathbb{P}\left(\frac{1}{n} \sum_{i=1}^n |h_j(X_k, X_i)| > \frac{\sqrt{n}}{8\phi_n \log d}\right) \\
(46) \quad &\leq (2dn) \exp\left(-\frac{\sqrt{n}}{8\phi_n(\log d)B_n}\right),
\end{aligned}$$

where the last step (46) follows from the triangle inequality on the Orlicz space with the  $\psi_1$  norm  $\|n^{-1} \sum_{i=1}^n |h_j(X_k, X_i)|\|_{\psi_1} \leq n^{-1} \sum_{i=1}^n \|h_j(X_k, X_i)\|_{\psi_1} \leq B_n$ . Substituting the value of  $\phi_n$  and using (43), we have

$$(47) \quad \frac{\sqrt{n}}{8\phi_n(\log d)B_n} \geq \frac{C_3^{1/3} \log(nd)}{8C_6c_1^{1/3}} \geq \frac{C_3^{1/3}}{16C_6c_1^{1/3}} \left[\log(nd) + \frac{1}{K} \log(1/\gamma)\right].$$

Therefore  $\mathbb{P}(\hat{M}_{g,3}(\phi_n) > 0) \leq \gamma/9$  by choosing  $c_1 > 0$  small enough. Next, we deal with  $\hat{M}_{Z,3}(\phi_n)$ . Since conditional on  $X_1^n$ ,  $Z^X \sim N(0, \hat{\Gamma}_n)$ . On the event  $\{\hat{\Gamma}_{n,jj} \leq C_2B_n, \forall j = 1, \dots, d\}$ , we have  $\|Z_j^X\|_{\psi_2} \leq \sqrt{8C_2B_n/3B_n^{1/2}}$  and  $\|Z_j^X\|_{\psi_1} \leq C_7B_n^{1/2}$  for all  $j = 1, \dots, d$ , where  $C_7 = \sqrt{8C_2/(3 \log 2)}$ . Integration-by-parts yields

$$\hat{M}_{Z,3}(\phi_n) = \int_t^\infty \mathbb{P}(\max_j |Z_j^X| > u^{1/3} | X_1^n) du + t \mathbb{P}(\max_j |Z_j^X| > t^{1/3} | X_1^n),$$

where  $t = (\sqrt{n}/4\phi_n \log d)^3$ . Since for any  $u > 0$

$$\mathbb{P}(\max_j |Z_j^X| > u^{1/3} | X_1^n) \leq (2d) \exp(-u^{1/3}/(C_7B_n^{1/2})),$$

we have by elementary calculations that

$$\int_t^\infty \mathbb{P}(\max_j |Z_j^X| > u^{1/3} | X_1^n) du \leq C_8 dt \left[ \sum_{\ell=1}^3 (B_n^{1/2} t^{-1/3})^\ell \right] \exp\left(-\frac{t^{1/3}}{C_7B_n^{1/2}}\right).$$

Since  $B_n^{1/2} t^{-1/3} \log(nd) \leq 4C_6C_3^{-1/3} [n^{-1} B_n^2 \log^4(nd)]^{1/3} \leq 4C_6C_3^{-1/3} c_1^{1/3}$ , it follows from (46) and (47) that

$$\hat{M}_{Z,3}(\phi_n) \leq C_9 dt \exp\left(-\frac{t^{1/3}}{C_7B_n^{1/2}}\right) \leq C_9 dn^{3/2} \exp\left(-\frac{\log(nd)}{4C_7C_6C_3^{-1/3}c_1^{1/3}}\right) \leq C_9 n^{-1/2}$$



for  $c_1 > 0$  small enough. For the term  $\hat{M}_{h,4}(\tau)$ , we note that

$$\mathbb{P}(\hat{M}_{h,4}(\tau) > 0) = \mathbb{P}\left(\max_{1 \leq i, k \leq n} \max_{1 \leq j \leq d} |h_j(X_i, X_k)| > \tau\right)$$

and by (E.1) and (E.1')  $\|h_j(X_j, X_k)\|_{\psi_1} \leq B_n$ . So we have

$$\mathbb{P}(\hat{M}_{h,4}(\tau) > 0) \leq (2dn^2) \exp(-\tau/B_n).$$

Choose  $\tau = C_{10}n^{1/2}/[\phi_n \log d]$ . Then, by (46) and (47), we have  $\mathbb{P}(\hat{M}_{h,4}(\tau) > 0) \leq \gamma/9$ . Now, by Proposition 5.3 conditional on  $X_1^n$  with  $M_{h,4}(\tau) \leq n^2 \mathbb{E}[\max_{1 \leq j \leq d} |h_j(X, X')|^4 \mathbf{1}(\max_{1 \leq j \leq d} |h_j(X, X')| > \tau)]$ , we conclude that

$$\begin{aligned} \rho^{re}(Z^X, T_n^* | X_1^n) &\leq C_{11} \left\{ \left( \frac{B_n^2 \log^7 d}{n} \right)^{1/6} + \frac{1}{n^{1/2} B_n} + \phi_n \frac{\log d}{n^{1/2}} B_n^{1/3} \right. \\ &\quad \left. + \phi_n \frac{\log^{5/4} d}{n^{3/4}} B_n^{1/2} \log^{1/4}(dn) + \frac{\log^{1/2} d}{n^{1/2}} \right\} \\ &\leq C_{12} \varpi_{1,n} \end{aligned}$$

holds with probability at least  $1 - 7\gamma/9$ . So (13) follows.

**Case (ii).** In addition to (43), we may assume that

$$(48) \quad \frac{B_n^2 \log^3(nd)}{\gamma^{2/q} n^{1-2/q}} \leq c_2 \leq 1$$

for some small enough constant  $c_2 > 0$ . As in Case (i), there exists a constant  $C_1 > 0$  such that  $\underline{b}/2 \leq \hat{\Gamma}_{n,jj} \leq C_1 B_n$  for all  $j = 1, \dots, d$  holds with probability at least  $1 - \gamma/9$ . Let  $\bar{D}_{g,3} = C_2[B_n + n^{-1+3/q} B_n^3 \gamma^{-3/q} (\log d)]$ ,  $\bar{D}_2 = C_3[B_n^{2/3} + n^{-1+2/q} B_n^2 \gamma^{-2/q} (\log d)]$ , and  $\bar{D}_4 = C_4[B_n^2 + n^{-1+4/q} B_n^2 \gamma^{-4/q} (\log d)]$ . By Lemma C.2, each of the three events  $\{\hat{D}_{g,3} \geq \bar{D}_{g,3}\}$ ,  $\{\hat{D}_2 \geq \bar{D}_2\}$ , and  $\{\hat{D}_4 \geq \bar{D}_4\}$  occur with probability at most  $\gamma/9$ . Note that

$$(49) \quad \begin{aligned} \phi_n &:= C_5(n^{-1} \bar{D}_{g,3}^2 \log^4 d)^{-1/6} \\ &\leq C_5 C_2^{-1/3} \min\{n^{1/6} B_n^{-1/3} \log^{-2/3} d, n^{1/2-1/q} B_n^{-1} \gamma^{1/q} \log^{-1} d\}. \end{aligned}$$

By (46), the union bound, (49), and choosing  $C_2$  large enough we have

$$\begin{aligned} \mathbb{P}(\hat{M}_{g,3}(\phi_n) > 0) &\leq n \max_{1 \leq k \leq n} \mathbb{P}\left(\frac{1}{n} \sum_{i=1}^n \max_j |h_j(X_k, X_i)| > \frac{\sqrt{n}}{8\phi_n \log d}\right) \\ &\leq \frac{(8B_n \phi_n \log d)^q}{n^{q/2-1}} \leq \frac{\gamma}{9}, \end{aligned}$$

where the second last step follows from (E.2), (E.2') and the triangle inequality  $\|n^{-1} \sum_{i=1}^n \max_j |h_j(X_k, X_i)|\|_q \leq n^{-1} \sum_{i=1}^n \|\max_j |h_j(X_k, X_i)|\|_q \leq B_n$ . Bound on the term  $\hat{M}_{Z,3}(\phi_n)$  is the same as in Case (i). Choose  $\tau = C_6 n^{1/2+1/q} / [\phi_n \log d]$  for some  $C_6 > 0$ . Then we have

$$\mathbb{P}(\hat{M}_{h,4}(\tau) > 0) \leq C_6^{-q} n^2 \frac{(3B_n \phi_n \log d)^q}{n^{q/2+1}} \leq \frac{\gamma}{9}.$$

Then, we have by elementary calculations that

$$\begin{aligned} \rho^{re}(Z^X, T_n^* | X_1^n) &\leq C_7 \left\{ \left( \frac{\bar{D}_{g,3}^2 \log^7 d}{n} \right)^{1/6} + \frac{1}{n^{1/2} B_n} + \phi_n \frac{\log d}{n^{1/2}} \bar{D}_2^{1/2} \right. \\ &\quad \left. + \phi_n \frac{\log^{5/4} d}{n^{3/4}} \bar{D}_4^{1/4} + \frac{\log^{1/2} d}{n^{1/2-1/q}} \right\} \\ &\leq C_8 \{ \varpi_{1,n} + \varpi_{2,n}^B(\gamma) \} \end{aligned}$$

with probability at least  $1 - 7\gamma/9$ . The proof is now complete.  $\square$

**PROOF OF COROLLARY 3.2.** Let  $\gamma_n = [n \log^2(n)]^{-1}$ . Then  $\sum_{n=4}^{\infty} \gamma_n \leq \int_3^{\infty} [x \log^2(x)]^{-1} dx = \log^{-1}(3) < \infty$ . Applying Theorem 3.1 with  $\gamma = \gamma_n$  and by the Borel-Cantelli lemma, we have  $\mathbb{P}(\rho^B(T_n, T_n^*) > C \varpi_{1,n} \text{ i.o.}) = 0$  for part (i) and  $\mathbb{P}(\rho^B(T_n, T_n^*) > C \{ \varpi_{1,n} + \varpi_{2,n}^B(\gamma) \} \text{ i.o.}) = 0$  for part (ii), from which the Corollary follows.  $\square$

The proof of the validity of the randomly reweighted bootstrap with iid Gaussian weights (Section 3.2) and Gaussian multiplier bootstrap with the jackknife covariance matrix estimator (Section 3.3) can be found in Section C in the SM.

#### 5.4. Proof of results in Section 4.

**PROOF OF THEOREM 4.1.** Let  $\tau_{\diamond} = \beta^{-1} |\hat{S}_n - \Sigma|_{\infty}$ . By the subgaussian assumption and Lemma F.1, it is easy to verify that there is a large enough constant  $C > 0$  depending only on  $C_2, C_3$  such that

$$(50) \quad \max_{\ell=1,2} \mathbb{E}[|h_{mk}|^{2+\ell} / (C \nu_n^{2\ell})] \vee \mathbb{E}[\exp(|h_{mk}| / \nu_n^2)] \leq 2,$$

where  $h$  is the covariance matrix kernel. Since  $\Gamma_{(j,k),(j,k)} \geq C_1$  for all  $j, k = 1, \dots, p$  and  $\nu_n^4 \log^7(np) \leq C_4 n^{1-K}$ , we have by Theorem 3.6 that  $|\hat{S}_n - \Sigma|_{\infty} \leq a_{T_n^{\#}}(1 - \alpha)$  with probability at least  $1 - \alpha - C n^{-K/6}$ , where  $C > 0$  is a constant depending only on  $C_i, i = 1, \dots, 4$ . Therefore,  $\mathbb{P}(\tau_{\diamond} \leq \tau_*) \geq$

$1 - \alpha - Cn^{-K/6}$  and the rest of the proof is restricted to the event  $\{\tau_\diamond \leq \tau_*\}$ . By the decomposition,

$$\begin{aligned} \|\hat{\Sigma}(\tau_*) - \Sigma\|_2 &\leq \|\hat{\Sigma}(\tau_*) - T_{\tau_*}(\Sigma)\|_2 + \|T_{\tau_*}(\Sigma) - \Sigma\|_2 \\ &\leq I + II + III + \tau_*^{1-r} \zeta_p, \end{aligned}$$

where  $T_\tau(\Sigma) = \{\sigma_{mk} \mathbf{1}\{|\sigma_{mk}| > \tau\}\}_{m,k=1}^p$  is the resulting matrix of the thresholding operator on  $\Sigma$  at the level  $\tau$  and

$$\begin{aligned} I &= \max_m \sum_k |\hat{s}_{mk}| \mathbf{1}\{|\hat{s}_{mk}| > \tau_*, |\sigma_{mk}| \leq \tau_*\}, \\ II &= \max_m \sum_k |\sigma_{mk}| \mathbf{1}\{|\hat{s}_{mk}| \leq \tau_*, |\sigma_{mk}| > \tau_*\}, \\ III &= \max_m \sum_k |\hat{s}_{mk} - \sigma_{mk}| \mathbf{1}\{|\hat{s}_{mk}| > \tau_*, |\sigma_{mk}| > \tau_*\}. \end{aligned}$$

Note that on the event  $\{\tau_\diamond \leq \tau_*\}$ ,  $\max_{m,k} |\hat{s}_{mk} - \sigma_{mk}| \leq \beta\tau_*$ . Since  $\Sigma \in \mathcal{G}(r, \zeta_p)$ , we can bound

$$III \leq (\beta\tau_*)(\tau_*^{-r} \zeta_p) = \beta\tau_*^{1-r} \zeta_p.$$

By triangle inequality,

$$\begin{aligned} II &\leq \max_m \sum_k |\hat{s}_{mk} - \sigma_{mk}| \mathbf{1}\{|\sigma_{mk}| > \tau_*\} + \max_m \sum_k |\hat{s}_{mk}| \mathbf{1}\{|\hat{s}_{mk}| \leq \tau_*, |\sigma_{mk}| > \tau_*\} \\ &\leq (\beta\tau_*)(\tau_*^{-r} \zeta_p) + \tau_*(\tau_*^{-r} \zeta_p) = (1 + \beta)\tau_*^{1-r} \zeta_p. \end{aligned}$$

Let  $\eta \in (0, 1)$ . We have  $I \leq IV + V + VI$ , where

$$\begin{aligned} IV &= \max_m \sum_k |\sigma_{mk}| \mathbf{1}\{|\hat{s}_{mk}| > \tau_*, |\sigma_{mk}| \leq \tau_*\}, \\ V &= \max_m \sum_k |\hat{s}_{mk} - \sigma_{mk}| \mathbf{1}\{|\hat{s}_{mk}| > \tau_*, |\sigma_{mk}| \leq \eta\tau_*\}, \\ VI &= \max_m \sum_k |\hat{s}_{mk} - \sigma_{mk}| \mathbf{1}\{|\hat{s}_{mk}| > \tau_*, \eta\tau_* < |\sigma_{mk}| \leq \tau_*\}. \end{aligned}$$

Clearly,  $IV \leq \tau_*^{1-r} \zeta_p$ . On the indicator event of  $V$ , we observe that

$$\beta\tau_* \geq |\hat{s}_{mk} - \sigma_{mk}| \geq |\hat{s}_{mk}| - |\sigma_{mk}| > (1 - \eta)\tau_*.$$

Therefore,  $V = 0$  if  $\eta + \beta \leq 1$ . For  $VI$ , we have

$$VI \leq (\beta\tau_*)(\eta\tau_*)^{-r} \zeta_p.$$

Collecting all terms, we conclude that

$$\|\hat{\Sigma}(\tau_*) - \Sigma\|_2 \leq (3 + 2\beta + \eta^{-r}\beta)\zeta_p\tau_*^{1-r} + V.$$

Then (24) follows from the choice  $\eta = 1 - \beta$ . The Frobenius norm rate (25) can be established similarly. Details are omitted.

Next, we prove (26). Let  $\hat{g}_i = (n-1)^{-1} \sum_{j \neq i} h(X_i, X_j) - U_n$  and denote  $\Phi(\cdot)$  as the cdf of the standard Gaussian random variable. By the union bound, we have for all  $t > 0$

$$\mathbb{P}_e \left( \frac{2}{\sqrt{n}} \left| \sum_{i=1}^n \hat{g}_i e_i \right|_\infty \geq t \right) \leq 2p^2 \left[ 1 - \Phi \left( \frac{t}{\bar{\psi}} \right) \right],$$

where  $\bar{\psi} = \max_{1 \leq m, k \leq p} |\psi_{mk}|$  and  $\psi_{mk}^2 = 4n^{-1} \sum_{i=1}^n \hat{g}_{i, mk}^2$ . Let  $\tilde{\tau} = n^{-1/2} \beta^{-1} \bar{\psi} \Phi^{-1}(1 - \alpha/(2p^2))$ ; then  $\tau_* \leq \tilde{\tau}$ . Since  $\Phi^{-1}(1 - \alpha/(2p^2)) \asymp (\log p)^{1/2}$ , we have  $\mathbb{E}[\tau_*] \leq C' \beta^{-1} \mathbb{E}[\bar{\psi}] (\log(p)/n)^{1/2}$ , where  $C' > 0$  is a constant only depending on  $\alpha$ . Now, we bound  $\mathbb{E}[\bar{\psi}]$ . By Jensen's inequality,

$$\psi_{mk}^2 \leq \frac{16}{n(n-1)} \sum_{1 \leq i \neq j \leq n} h_{mk}^2(X_i, X_j).$$

Let  $\ell = \lceil n/2 \rceil$ . By the data splitting argument in (36), [22, Lemma 9] and Jensen's inequality, we have

$$\begin{aligned} \mathbb{E} \left\{ \max_{m,k} \frac{1}{n(n-1)} \left| \sum_{1 \leq i \neq j \leq n} [h_{mk}^2(X_i, X_j) - \mathbb{E}h_{mk}^2] \right| \right\} &\leq \frac{1}{\ell} \mathbb{E} \left\{ \max_{m,k} \left| \sum_{i=1}^{\ell} [h_{mk}^2(X_i, X_{i+\ell}) - \mathbb{E}h_{mk}^2] \right| \right\} \\ &\leq \frac{K_1}{\ell} \left\{ (\log p)^{1/2} \left[ \max_{m,k} \sum_{i=1}^{\ell} \mathbb{E}h_{mk}^4(X_i, X_{i+\ell}) \right]^{1/2} + (\log p) \left[ \mathbb{E} \max_{m,k} \max_{1 \leq i \leq \ell} h_{mk}^4(X_i, X_{i+\ell}) \right]^{1/2} \right\}. \end{aligned}$$

By Pisier's inequality [62, Lemma 2.2.2], we have

$$\left\| \max_{m,k} \max_{i \leq \ell} |h_{mk}(X_i, X_{i+\ell})| \right\|_4 \leq K_2 \nu_n^2 \log(np).$$

Hence it follows from (50) that

$$\mathbb{E}[\bar{\psi}^2] \leq C \left\{ \xi_4^4 + \xi_8^4 \left( \frac{\log p}{n} \right)^{1/2} + \nu_n^4 \frac{\log^3(np)}{n} \right\}.$$

Since  $\nu_n^4 \log^7(np) \leq C_4 n^{1-K}$  and  $\xi_8 \leq C_3 \nu_n^{1/2}$ , we have  $\mathbb{E}[\bar{\psi}] \leq C \xi_4^2$ , where  $C > 0$  is constant depending only on  $C_i, i = 1, \dots, 4$ . Then, we conclude that  $\mathbb{E}[\tau_*] \leq C(\alpha, C_1, \dots, C_4) \beta^{-1} \xi_4^2 (\log(p)/n)^{1/2}$ .  $\square$

**Acknowledgments.** The author would like to thank two anonymous referees, an Associate Editor, and the Co-Editor Tailen Hsing for their careful readings and many constructive comments that lead to significant improvements of this paper. The author is also grateful to Stephen Portnoy (UIUC), Xiaofeng Shao (UIUC), and Wei Biao Wu (University of Chicago) for their helpful discussions.

## SUPPLEMENTARY MATERIAL

**Supplemental Materials to: “Gaussian and bootstrap approximations for high-dimensional U-statistics and their applications”** (). This supplemental file contains additional proofs, technical lemmas, and simulation results.

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