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SUPPLEMENT TO "TESTING HIGH DIMENSIONAL COVARIANCE MATRICES, WITH APPLICATION TO DETECTING SCHIZOPHRENIA RISK GENES"

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This document provides supplementary material to the article "Testing High Dimensional Covariance Matrices, with Application to Detecting Schizophrenia Risk Genes" written by the same authors.

S1. Simulations. In this section, we present the remaining simulation results for comparing `sLED` with other existing methods, including `Sfrob` (Schott, 2007), `Ustat` (Li and Chen, 2012), `Max` (Cai, Liu and Xia, 2013), `MBoot` (Chang et al., 2016), and `RProj` (Wu and Li, 2015).

The samples are generated by $X_i = \Sigma_1^{1/2} Z_i$ for $i = 1, \cdots, n$, and $Y_l = \Sigma_2^{1/2} Z_{n+l}$ for $l = 1, \cdots, m$, where $\{Z_i\}_{i=1,n+m}$ are independent p-dimensional random variables with *i.i.d.* coordinates Z_{ij}, $j = 1, \cdots, p$. We let $\Sigma_2 = \Sigma_1$ under H_0 and $\Sigma_2 = \Sigma_1 + D$ under H_1. For the different choices of Σ_1 and D, please refer to the main manuscript (Zhu et al., 2017). We consider the following four distributions for Z_{ij}:

1. Standard Normal $N(0, 1)$, which leads to multinomial Gaussian samples X and Y.
2. Centralized Gamma distribution with $\alpha = 4, \beta = 0.5$ (i.e., the theoretical expectation $\alpha\beta = 2$ is subtracted from $\Gamma(4, 0.5)$ samples).
3. t-distribution with degrees of freedom 12 ($t(12)$).
4. Centralized Negative Binomial distribution with mean $\mu = 2$ and dispersion parameter $\phi = 2$ (i.e., the theoretical expectation $\mu = 2$ is subtracted from NB(2, 2) samples).

We compare the empirical power among different testing procedures, where 100 permutations are used to compute the p-values for all methods, except for `MBoot` where 100 bootstrap repetitions are used. Table S1 summarizes the empirical power under different covariance structures and differential matrices when Z_{ij}'s are sampled from t-distribution and centralized NB(2, 2). The results for standard Normal and centralized Gamma distributions are presented in the main manuscript. The smoothing parameter for sLED is set to be $\sqrt{R} = 0.3\sqrt{p}$, and 100 random projections are used for `Rproj`. We also examine the sensitivity of sLED to the smoothing parameter in Figure S1, where c is varied among $\{0.10, 0.12, \cdots, 0.30\}$ (recall that $\sqrt{R} = c\sqrt{p}$). We see that `sLED` achieves superior power to other approaches under most scenarios, and the results remain robust to many choices of c's. Finally, Figure S2 shows the distribution of the empirical size in 100 repetitions under all these scenarios, including 4 different choices of Σ_1, 3 different choices of p, and 4 different choices of the distribution of Z_{ij}. We see that for all of the 6 testing procedures, the empirical size is comparable and controlled around $\alpha = 0.05$. In addition, the empirical size of sLED is robust to the choice of c. We point out that only a small number of permutations is used in this simulation. In practice, more permutations will be conducted and the size will be more properly controlled.

S2. Proofs for consistency. In this section, we prove Theorems 1 to 3 for the asymptotic power of sLED.

Notation. For a set $\mathcal{A}$, let $|\mathcal{A}|$ be its cardinality, and $\mathcal{A}^c$ be its complement. For $Z = (Z_1, \cdots Z_N) = (X_1, \cdots, X_n, Y_1, \cdots, Y_m)$, we denote Z_{ki} to be the i-th coordinate of the k-th sample Z_k, and

$$\hat{\Sigma} = \frac{1}{N}\sum_{k=1}^{N} Z_k Z_k^T\,,\ \bar{Z} = \frac{1}{N}\sum_{k=1}^{N} Z_k = (\bar{Z}_1, \cdots, \bar{Z}_p)^T\,,$$

$$m_z = ||Z||_\infty\,,\ \overline{m}_z = ||\bar{Z}||_\infty\,,\ \overline{m}_z^{(2q)} = \max_{1\le i,j\le p} \frac{1}{N}\sum_{k=1}^{N} Z_{ki}^q Z_{kj}^q\,,\ q = 1, 2\,.$$

Proof of Theorem 1. By Theorem 2 and Lemma 2, there exist some constants C', C'' depending on $(\underline{c}, \bar{c}, \nu^2, \delta)$, such that if (n, p) are sufficiently large, with probability at least $1 - \delta$,

$$||\hat{D}^*||_\infty \le C'\sqrt{\frac{\log p}{n}}\,,\ ||\hat{D} - D||_\infty \le C''\sqrt{\frac{\log p}{n}}\,.$$

Then we apply Theorem 3 on both $\hat{D}, -\hat{D}$ and $\hat{D}^*, -\hat{D}^*$, and this together with assumption (A4) imply the desired conclusion with $C = C' + C''$. □

Proof of Theorem 2. First, note that for $\forall\epsilon > 0$,

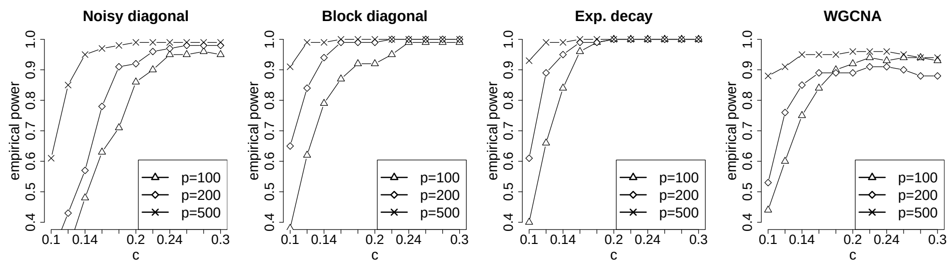
$$\mathbb{P}\left(||\hat{D}^*||_\infty > \epsilon\right) \le \mathbb{P}\left(||\hat{\Sigma}_1^* - \hat{\Sigma}||_\infty > \frac{\epsilon}{2}\right) + \mathbb{P}\left(||\hat{\Sigma}_2^* - \hat{\Sigma}||_\infty > \frac{\epsilon}{2}\right)\,. \tag{S2.1}$$

Now for any $\delta > 0$ and constants C_1, C_2, define

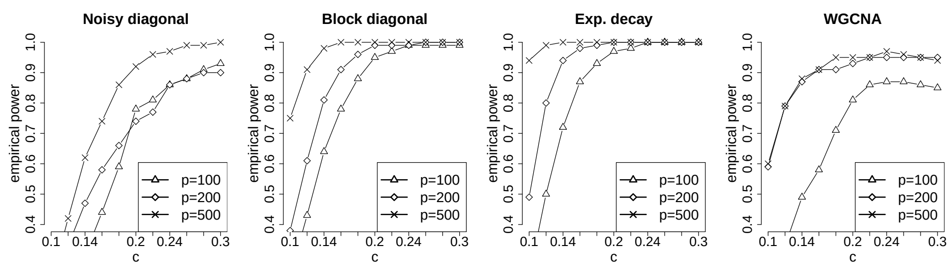
$$\mathcal{A} = \left\{Z : \, m_z \le C_2\sqrt{\log\left(\frac{C_1 np}{\delta}\right)}\,,\, \overline{m}_z \le C_2\sqrt{\frac{\log(C_1 p/\delta)}{n}}\,,\, \overline{m}_z^{(2q)} \le C_2\,,\, q = 1, 2\right\}.$$

Table S1
Empirical power in 100 repetitions, where $n = m = 100$, nominal level $\alpha = 0.05$, and Z_{ij}'s are sampled from centralized Negative Binomial $(2, 2)$ (top) and t-distribution with degrees of freedom 12 (bottom). Under each scenario, the largest power is highlighted.

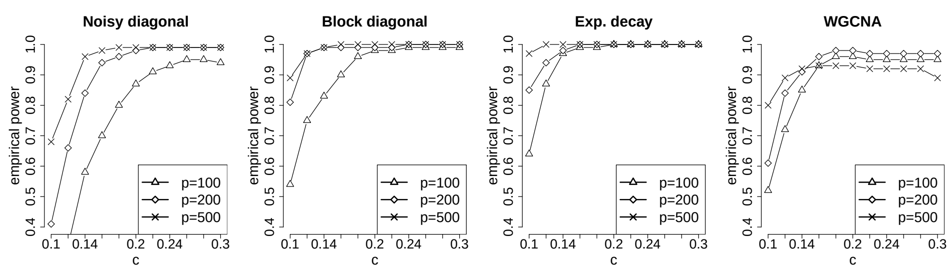
D	$\mathbf{\Sigma_1}$	**Noisy diagonal**			**Block diagonal**			**Exp. decay**			**WGCNA**		
	p	**100**	**200**	**500**	**100**	**200**	**500**	**100**	**200**	**500**	**100**	**200**	**500**
							Centralized Negative Binomial						
Block	Max	0.59	0.18	0.11	0.87	0.69	0.25	**1.00**	0.94	0.50	0.80	0.84	0.28
	MBoot	0.47	0.12	0.07	0.80	0.60	0.16	0.99	0.82	0.33	0.72	0.73	0.17
	Ustat	0.69	0.62	0.68	0.89	0.93	0.94	0.99	0.99	**1.00**	0.57	0.78	0.74
	Sfrob	0.66	0.63	0.69	0.91	0.91	0.94	0.98	0.99	**1.00**	0.58	0.79	0.80
	RProj	0.11	0.13	0.06	0.18	0.13	0.11	0.21	0.21	0.10	0.15	0.10	0.16
	sLED	**0.91**	**0.90**	**0.99**	**0.99**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**0.86**	**0.95**	**0.95**
Spiked	Max	0.04	0.07	0.06	0.60	0.20	0.10	0.93	0.82	0.25	0.93	0.41	0.06
	MBoot	0.03	0.04	0.03	0.51	0.20	0.02	0.92	0.76	0.18	0.89	0.33	0.05
	Ustat	**0.25**	**0.12**	0.03	0.82	0.35	0.13	0.98	0.94	0.72	0.36	0.12	0.03
	Sfrob	**0.25**	0.11	0.03	0.85	0.35	0.12	0.98	0.96	0.69	0.40	0.12	0.06
	RProj	0.08	0.07	0.02	0.31	0.17	0.10	0.35	0.17	0.06	0.58	0.17	**0.13**
	sLED	0.22	0.04	**0.08**	**0.97**	**0.68**	**0.16**	**0.99**	**1.00**	**1.00**	**0.96**	**0.48**	**0.13**
							T-distribution						
Block	Max	0.22	0.15	0.12	0.88	0.73	0.23	**1.00**	0.85	0.27	**0.97**	0.40	0.15
	MBoot	0.23	0.14	0.13	0.88	0.68	0.20	**1.00**	0.84	0.23	0.91	0.37	0.13
	Ustat	0.53	0.63	0.74	0.97	0.93	0.96	**1.00**	0.99	**1.00**	0.75	0.67	0.84
	Sfrob	0.52	0.63	0.71	0.97	0.93	0.97	**1.00**	0.99	0.99	0.74	0.67	0.76
	RProj	0.08	0.13	0.11	0.28	0.12	0.02	0.28	0.19	0.08	0.17	0.13	0.06
	sLED	**0.95**	**0.99**	**0.99**	**0.99**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	0.95	**0.97**	**0.92**
Spiked	Max	0.13	0.08	0.05	0.78	0.50	0.08	0.96	0.79	0.18	0.85	0.27	0.10
	MBoot	0.12	0.07	0.03	0.78	0.49	0.07	0.97	0.77	0.11	0.83	0.32	0.13
	Ustat	0.14	0.07	**0.10**	0.79	0.36	0.07	**1.00**	0.91	0.68	0.30	0.06	0.05
	Sfrob	0.12	**0.10**	**0.10**	0.80	0.36	0.07	**1.00**	0.91	0.66	0.29	0.09	0.05
	RProj	0.07	0.06	0.06	0.34	0.20	0.08	0.36	0.16	0.07	0.57	0.27	**0.14**
	sLED	**0.40**	0.09	0.03	**0.96**	**0.76**	**0.14**	**1.00**	**1.00**	**1.00**	**0.95**	**0.55**	0.08



(a) $Z_{ij} \sim$ centralized $\Gamma(4, 0.5)$.

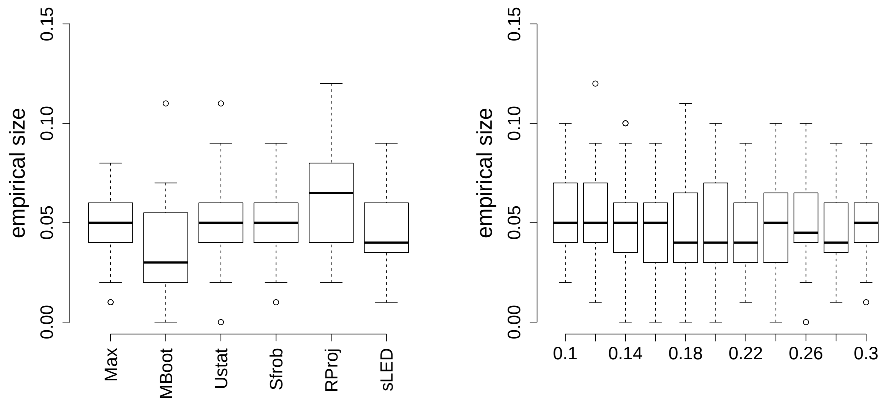


(b) $Z_{ij} \sim$ centralized NB(2, 2).



(c) $Z_{ij} \sim t(12)$.

FIG. S1. *Empirical power of sLED in 100 repetitions using different smoothing parameters* $\sqrt{R} = c\sqrt{p}$ *for* $c \in \{0.10, 0.12, \cdots, 0.30\}$*, where* D *has sparse block difference and* Z_{ij}*'s are sampled from different distributions.*



(a) 6 testing procedures

(b) sLED with $c \in \{0.10, \cdots, 0.30\}$

FIG. S2. **(a)** *Boxplot of the empirical size in 100 repetitions of the 6 testing procedures under different scenarios, where the smoothing parameter for sLED is chosen to be* $c = 0.3$. **(b)** *Boxplot of the empirical size in 100 repetitions of sLED under different scenarios, using different smoothing parameters* $c \in \{0.10, 0.12, \cdots, 0.30\}$.

By Lemma 2, there exist some constants C_1, C_2 depending on $(\underline{c}, \bar{c}, \nu^2)$, such that if (n, p) are sufficiently large, $\mathbb{P}(Z \notin \mathcal{A}) \le \delta/4$. Therefore, in order to show that

$$\mathbb{P}\left(||\hat{\Sigma}_1^* - \hat{\Sigma}||_\infty > \frac{\epsilon}{2}\right) \le \mathbb{P}\left(||\hat{\Sigma}_1^* - \hat{\Sigma}||_\infty > \frac{\epsilon}{2}\Big| Z \in \mathcal{A}\right) + \mathbb{P}(Z \notin \mathcal{A}) \le \frac{\delta}{2},$$

it suffices to show that given any $Z \in \mathcal{A}$, the conditional probability satisfies

$$\mathbb{P}_Z\left(||\hat{\Sigma}_1^* - \hat{\Sigma}||_\infty > \frac{\epsilon}{2}\right) \le \frac{\delta}{4}. \tag{S2.2}$$

For any $1 \le i, j \le p$, we first bound the (i, j)-th entry:

$$\mathbb{P}_Z\left(|\hat{\Sigma}_{1,ij}^* - \hat{\Sigma}_{ij}| > \frac{\epsilon}{2}\right) \le \underbrace{\mathbb{P}_Z\left(\left|\frac{1}{n}\sum_{k=1}^{n} Z_{ki}^* Z_{kj}^* - \frac{1}{N}\sum_{k=1}^{N} Z_{ki} Z_{kj}\right| > \frac{\epsilon}{4}\right)}_{\Delta_1} + \underbrace{\mathbb{P}_Z\left(\left|\bar{X}_i^* \bar{X}_j^* - \bar{Z}_i \bar{Z}_j\right| > \frac{\epsilon}{4}\right)}_{\Delta_2},$$

where $\bar{X}_i^* = \frac{1}{n}\sum_{k=1}^{n} Z_{ki}^*$. Now we bound Δ_1 and Δ_2 separately.

(i) Δ_1: Note that for any (k,i,j),

$$\left|Z^*_{ki}Z^*_{kj}\right| \le (m_z)^2\,,\ \mathrm{var}_Z\left(Z^*_{ki}Z^*_{kj}\right) \le \frac{1}{N}\sum_{l=1}^{N} Z_{li}^2 Z_{lj}^2 \le \overline{m}_z^{(4)}\,.$$

By Lemma 1, there exists a constant C_2' depending on (C_2,ν^2), such that if (n,p) are sufficiently large,

$$\Delta_1 \le 2\exp\left\{-\frac{n\epsilon^2/C_2'}{1+\log(C_1 np/\delta)\epsilon}\right\}. \tag{S2.3}$$

(ii) Δ_2: Note that

$$\bar{X}^*_i\bar{X}^*_j - \bar{Z}_i\bar{Z}_j = (\bar{X}^*_i-\bar{Z}_i)(\bar{X}^*_j-\bar{Z}_j) + \bar{Z}_j(\bar{X}^*_i-\bar{Z}_i) + \bar{Z}_i(\bar{X}^*_j-\bar{Z}_j)\,,$$

and for any (k,i,j),

$$|\bar{Z}_i| \le \overline{m}_z\,,\ |Z^*_{ki}| \le m_z\,,\ \mathrm{var}_Z(Z^*_{ki}) \le \frac{1}{N}\sum_{l=1}^{N} Z_{li}^2 \le \overline{m}_z^{(2)}\,.$$

Therefore,

$$\Delta_2 \le 2\max_i\left[\mathbb{P}_Z\left(\left|\frac{1}{n}\sum_{k=1}^{n} Z^*_{ki}-\bar{Z}_i\right| > \sqrt{\frac{\epsilon}{8}}\right) + \mathbb{P}_Z\left(\left|\frac{1}{n}\sum_{k=1}^{n} Z^*_{ki}-\bar{Z}_i\right| > \frac{\epsilon}{16\overline{m}_z}\right)\right].$$

Applying Lemma 1 on both terms, we know that there exists a constant C_2'' depending on (C_2,ν^2), such that if (n,p) are sufficiently large,

$$\begin{aligned}\Delta_2 \le & 4\exp\left\{-\frac{n\epsilon/C_2''}{1+\sqrt{\log(C_1np/\delta)}\sqrt{\epsilon}}\right\} + \\ & 4\exp\left\{-\frac{n\epsilon^2/C_2''}{\frac{\log(C_1p/\delta)}{n}+\sqrt{\frac{\log(C_1p/\delta)\log(C_1np/\delta)}{n}}\epsilon}\right\}.\end{aligned} \tag{S2.4}$$

Combining the results in (S2.3) and (S2.4), and note that $(\log p)^3 = O(n)$ by assumption (A3), we have $\Delta_1\,,\Delta_2 \le \frac{\delta}{8}p^{-2}$ if (n,p) are sufficiently large, as long as

$$\epsilon \ge C'\sqrt{\frac{\log(C_1p^2/\delta)}{n}}$$

for some constant C' depending on C_2' and C_2''. Finally, (S2.2) follows from a union bound over $1 \le i,j \le p$. Similar statement also holds for $||\hat{\Sigma}^*_2 - \hat{\Sigma}||_\infty$ with sample size m, and the final result follows from (S2.1) and the fact that $\underline{c}n \le m \le \bar{c}n$. $\square$

Proof of Theorem 3. (i) Note that a feasible solution of (2.12) or (2.14) in the main manuscript always satisfies $||H||_1 \leq R$, where $H = vv^T$ if using (2.14). Then the result directly follows from the Hölder's inequality:

$$\mathrm{tr}\left(\hat{D}H\right) \leq ||\hat{D}||_\infty ||H||_1 \, .$$

(ii) Let v^* be the R-sparse leading eigenvector of D, then $||v^*||_2 = 1$ and $||v^*(v^*)^T||_1 = ||v^*||_1^2 \leq ||v^*||_0 = R$, so $v^*(v^*)^T$ is feasible for (2.12) and (2.14). The result follows from

$$\tilde{\lambda}_1^R(\hat{D}) - \lambda_1^R(D) \geq (v^*)^T \hat{D} v^* - (v^*)^T D v^*$$

and $\left|(v^*)^T(\hat{D} - D)v^*\right| \leq ||\hat{D} - D||_\infty ||v^*(v^*)^T||_1$.

□

S3. Lemmas. In this section, we state and prove the lemmas that are used in Section S2.

Lemma 1 (Bernstein inequality for sampling without replacement). *Let $\mathcal{Z} = \{z_1, ..., z_N\}$ be a finite set containing N real numbers, and $(z_1^*, ..., z_n^*)$ be i.i.d. random variables that are drawn without replacement from $\mathcal{Z}$. Let*

$$\bar{z} = \max_{1 \leq i \leq N} |z_i| \, , \; \mu_z = \frac{1}{N}\sum_{i=1}^N z_i \, , \; \sigma_z^2 = \frac{1}{N}\sum_{i=1}^N (z_i - \mu_z)^2 \, ,$$

then for any $\epsilon > 0$,

$$\mathbb{P}\left(\left|\frac{1}{n}\sum_{i=1}^n z_i^* - \mu_z\right| \geq \epsilon\right) \leq 2\exp\left\{-\frac{n\epsilon^2}{2\sigma_z^2 + \frac{4}{3}\bar{z}\epsilon}\right\} \, .$$

As a consequence, for any $t > 0$,

$$\mathbb{P}\left(\left|\frac{1}{n}\sum_{i=1}^n z_i^* - \mu_z\right| > \frac{4\bar{z}}{3}\frac{t}{n} + \sqrt{2\sigma_z^2 \frac{t}{n}}\right) \leq 2e^{-t} \, .$$

Proof. See Proposition 1.4 in Bardenet et al. (2015). □

Lemma 2 (Sub-gaussian tail bound). *Under assumptions (A1)-(A2), for $\forall \delta > 0$, there exist constants C_1, C_2 depending on $(\underline{c}, \bar{c}, \nu^2)$, such that if (n, p) are sufficiently large, with probability at least $1 - \delta$,* *(i)* $||\hat{\Sigma}_q - \Sigma_q||_\infty \le C_2\sqrt{\frac{\log(C_1p^2/\delta)}{N}}$ *for* $q = 1, 2$. *As a consequence,*

$$||\hat{D} - D||_\infty \le 2C_2\sqrt{\frac{\log(C_1p^2/\delta)}{N}}\,.$$

(ii) $\overline{m}_z \le C_2\sqrt{\frac{\log(C_1p/\delta)}{N}}$. *This together with (i) imply that*

$$\overline{m}_z^{(2)} \le 2\nu^2 + 2C_2\sqrt{\frac{\log(C_1p^2/\delta)}{N}}\,.$$

(iii) $m_z \le C_2\sqrt{\log(C_1Np/\delta)}$.
(iv) $\overline{m}_z^{(4)} \le C_2\left[1 + \frac{\log(C_1p^2/\delta)}{N}\right]$.

Proof. (i) See for example, Lemma 12 in Yuan (2010).
(ii) The first part is standard Hoeffding's bound on $\frac{1}{N}\sum_{k=1}^N Z_{ki}$, with a union bound over $1 \le i \le p$. The second part follows from

$$\overline{m}_z^{(2)} \le \max\{||\hat{\Sigma}_1||_\infty, ||\hat{\Sigma}_2||_\infty\} + (\overline{m}_z)^2\,.$$

(iii) By Markov inequality, $\forall \epsilon, t > 0$,

$$\mathbb{P}\left(\max_{k,i} Z_{ki} > \epsilon\right) \le e^{-t\epsilon}\mathbb{E}\left[e^{t\max_{k,i} Z_{ki}}\right] = e^{-t\epsilon}\mathbb{E}\left[\max_{k,i} e^{tZ_{ki}}\right]$$
$$\le e^{-t\epsilon}\sum_{k=1}^N\sum_{i=1}^p \mathbb{E}\left[e^{tZ_{ki}}\right] \le Np\cdot e^{-t\epsilon+\frac{t^2\nu^2}{2}}\,.$$

Finally, take $t = \frac{\epsilon}{\nu^2}$, and note that similar arguments hold for $-Z_{ki}$.
(iv) For any given (i, j), let $W_k = Z_{ki}^2 Z_{kj}^2$, and define its cumulant generating function

$$\Psi_k(\theta) = \log\mathbb{E}\left[e^{\theta(W_k - \mathbb{E}(W_k))}\right]\,.$$

Note that $\Psi_1 = \cdots = \Psi_n$ and $\Psi_{n+1} = \cdots = \Psi_{n+m}$. By Markov inequality, for any $t, \theta > 0$,

$$\mathbb{P}\left(\left|\frac{1}{n}\sum_{k=1}^n W_k - \mathbb{E}(W_1)\right| > t\right) \le 2\exp\left\{-n\theta t + n\Psi(\theta)\right\}\,, \tag{S3.1}$$

where $\Psi(\theta) = \max\{\Psi_1(\theta), \Psi_{n+1}(\theta)\}$ is an upper bound of the cumulant generating functions. Since Z_{ki}, Z_{kj} are sub-gaussian, there exists a small constant $\theta_0 \neq 0$, such that $\Psi(\theta_0) < \infty$. Plugging in θ_0 to (S3.1), we know that with probability at least $1 - \frac{\delta}{2} p^{-2}$,

$$\frac{1}{n} \sum_{k=1}^{n} W_k - \mathbb{E}(W_1) \leq \frac{\log(4p^2/\delta)}{n\theta_0} + \frac{\Psi(\theta_0)}{\theta_0} .$$

The same arguments also hold for $\frac{1}{m} \sum_{k=(n+1)}^{n+m} W_k - \mathbb{E}(W_{n+1})$. Then the final result follows from a union bound over (i, j) and the fact that $\mathbb{E}(W_k) \leq C\nu^4$ for some constant C.

□

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