

# Supp. 1 Random matrices and covariance estimation

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## 1 Preliminaries

Given any rectangular matrix  $\mathbf{A} \in \mathbb{R}^{n \times m}$  with  $n \geq m$ , its ordered singular values are written as

$$\sigma_{\max}(\mathbf{A}) = \sigma_1(\mathbf{A}) \geq \sigma_2(\mathbf{A}) \geq \dots \geq \sigma_m(\mathbf{A}) = \sigma_{\min}(\mathbf{A}) \geq 0$$

and we have

$$\sigma_{\max}(\mathbf{A}) = \max_{\mathbf{v} \in \mathbb{S}^{m-1}} \|\mathbf{A}\mathbf{v}\|_2 \quad \text{and} \quad \sigma_{\min}(\mathbf{A}) = \min_{\mathbf{v} \in \mathbb{S}^{m-1}} \|\mathbf{A}\mathbf{v}\|_2$$

where  $\mathbb{S}^{m-1} \triangleq \{\mathbf{v} \in \mathbb{R}^m \mid \|\mathbf{v}\|_2 = 1\}$  is the Euclidean unit sphere in  $\mathbb{R}^m$ . Note that  $\|\mathbf{A}\|_2 = \sigma_{\max}(\mathbf{A})$ .

Denote the set of symmetric matrices in  $\mathbb{R}^d$  as  $\mathcal{S}^{d \times d} = \{\mathbf{Q} \in \mathbb{R}^{d \times d} \mid \mathbf{Q}^T = \mathbf{Q}\}$  and the set of positive semi-definite matrices as  $\mathcal{S}_+^{d \times d} = \{\mathbf{Q} \in \mathcal{S}^{d \times d} \mid \mathbf{Q} \geq 0\}$ .

For any symmetric matrix  $\mathbf{Q} \in \mathbb{R}^{d \times d}$ , its ordered eigenvalues are written as

$$\gamma_{\max}(\mathbf{Q}) = \gamma_1(\mathbf{Q}) \geq \gamma_2(\mathbf{Q}) \geq \dots \geq \gamma_d(\mathbf{Q}) = \gamma_{\min}(\mathbf{Q}).$$

The Rayleigh-Ritz variational characterization of the min and max eigenvalues is defined as

$$\gamma_{\max}(\mathbf{Q}) = \max_{\mathbf{v} \in \mathbb{S}^{d-1}} \mathbf{v}^T \mathbf{Q} \mathbf{v} \quad \text{and} \quad \gamma_{\min}(\mathbf{Q}) = \min_{\mathbf{v} \in \mathbb{S}^{d-1}} \mathbf{v}^T \mathbf{Q} \mathbf{v}$$

For any symmetric matrix  $\mathbf{Q}$ , there are two equivalent forms of  $\ell_2$  operator norm of  $\mathbf{Q}$ , i.e.,

$$\|\mathbf{Q}\|_2 = \max\{\gamma_{\max}(\mathbf{Q}), |\gamma_{\min}(\mathbf{Q})|\} \iff \|\mathbf{Q}\|_2 = \max_{\mathbf{v} \in \mathbb{S}^{d-1}} |\mathbf{v}^T \mathbf{Q} \mathbf{v}|$$

( $\ell_2$ -operator norm in maximization)

For any rectangular matrix  $\mathbf{A} \in \mathbb{R}^{n \times m}$  with  $n \geq m$ , we define  $\mathbf{R} = \mathbf{A}^T \mathbf{A}$ . The following inequalities hold

$$\gamma_j(\mathbf{R}) = \sigma_j^2(\mathbf{A}), \quad j = 1, 2, \dots, m.$$

**Theorem 1.1 (Courant-Fisher min-max theorem):** For any  $Q \in \mathcal{S}^{d \times d}$ ,

$$\gamma_k = \max_{\substack{\dim(\mathbb{E})=k \\ \mathbb{E} \subseteq \mathbb{R}^d}} \min_{\substack{\mathbf{v} \in \mathbb{E} \\ \|\mathbf{v}\|=1}} \mathbf{v}^T Q \mathbf{v},$$

where  $\mathbb{E}$  is a subspace of  $\mathbb{R}^d$ .

## 2 Covariance Estimation

Let  $\{X_1, X_2, \dots, X_n\}$  be a collection of  $n$  independent and identically distributed samples from a distribution with zero mean and covariance  $\Sigma \in \mathbb{R}^{d \times d}$ . A unbiased estimator of  $\Sigma$  is the sample covariance matrix

$$\hat{\Sigma} = \frac{1}{n} \sum_{i=1}^n X_i X_i^T.$$

Since  $\mathbb{E}[X_i] = \mathbf{0}$ ,  $\mathbb{E}[\hat{\Sigma}] = \Sigma$ .

Our goal is to obtain bounds on the error  $\hat{\Sigma} - \Sigma$  measured in  $\ell_2$  operator norm. From ( $\ell_2$ -operator norm in maximization), we have

$$\|\hat{\Sigma} - \Sigma\|_2 \leq \epsilon \iff \max_{\mathbf{v} \in \mathbb{S}^{d-1}} \left| \frac{1}{n} \sum_{i=1}^n \langle X_i, \mathbf{v} \rangle^2 - \mathbf{v}^T \Sigma \mathbf{v} \right| \leq \epsilon$$

By the Weyl's theorem, we have the following corollary.

**Corollary 2.1:** For any symmetric matrices  $A, B \in \mathcal{S}^{d \times d}$ ,

$$\max_{k=1,2,\dots,d} |\gamma_k(A) - \gamma_k(B)| \leq \|A - B\|_2$$

holds.

Similar, for general rectangular matrices

$$|\sigma_k(A) - \sigma_k(B)| \leq \|A - B\|_2$$

holds, where  $\sigma_k(\cdot)$  is the  $k$ -largest singular value.

Hence, control in the operator norm guarantees the eigenvalues of  $\hat{\Sigma}$  are uniformly close to those of  $\Sigma$ .

Let  $\mathbf{X} \triangleq [X_1; X_2; \dots; X_n] \in \mathbb{R}^{n \times d}$  be a random matrix and  $\{\sigma_k(\mathbf{X})\}_{k=1}^{\min\{n,d\}}$  be the collection of singular values of  $\mathbf{X}$ , we have

$$\hat{\Sigma} = \frac{1}{n} \sum_{i=1}^n X_i X_i^T = \frac{1}{n} \mathbf{X}^T \mathbf{X}.$$

and hence it follows that

$$\gamma_k(\hat{\Sigma}) = \sigma_k^2(\mathbf{X}/\sqrt{n}) \quad k = 1, 2, \dots, \min\{n, d\}.$$

**Definition 2.1 ( $\Sigma$ -Gaussian ensemble):** Let  $X_i \stackrel{i.i.d.}{\sim} \mathcal{N}(0, \Sigma)$ . We say that the random matrix  $\mathbf{X} \triangleq [X_1; X_2; \dots, X_n] \in \mathbb{R}^{n \times d}$  is drawn from the  $\Sigma$ -Gaussian ensemble and the sample covariance matrix  $\hat{\Sigma} = \frac{1}{n} \mathbf{X}^T \mathbf{X}$  is said to follow a multivariate Wishart distribution.

**Theorem 2.1:** Let  $\mathbf{X} \in \mathbb{R}^{n \times d}$  be drawn according to the  $\Sigma$ -Gaussian ensemble. Then for all  $\delta > 0$ , the maximum singular value  $\sigma_{\max}(\mathbf{X})$  satisfies the upper deviation inequality

$$\mathbb{P} \left[ \frac{\sigma_{\max}(\mathbf{X})}{\sqrt{n}} \geq \gamma_{\max}(\sqrt{\Sigma})(1 + \delta) + \sqrt{\frac{\text{tr}(\Sigma)}{n}} \right] \leq e^{-n\delta^2/2}.$$

Moreover, for  $n \geq d$ , the minimum singular value  $\sigma_{\min}(\mathbf{X})$  satisfies the analogous low deviation inequality

$$\mathbb{P} \left[ \frac{\sigma_{\min}(\mathbf{X})}{n} \leq \gamma_{\min}(\sqrt{\Sigma})(1 - \delta) - \sqrt{\frac{\text{tr}(\Sigma)}{n}} \right] \leq e^{-n\delta^2/2}.$$

**Example 2.1 (Operator norm bounds for the standard Gaussian ensemble):** Consider a random matrix  $\mathbf{W} \in \mathbb{R}^{n \times d}$  drawn from  $\mathbf{I}_d$ -Gaussian ensemble, i.e.,  $\mathbf{W}$  has i.i.d  $\mathcal{N}(0, 1)$  entries. By specializing Theorem 2.1, we conclude that for  $n \geq d$ , we have

$$\frac{\sigma_{\max}(\mathbf{W})}{\sqrt{n}} \leq 1 + \delta + \sqrt{\frac{d}{n}} \quad \text{and} \quad \frac{\sigma_{\min}(\mathbf{W})}{\sqrt{n}} \geq 1 - \delta - \sqrt{\frac{d}{n}}$$

held with probability greater than  $1 - 2e^{-n\delta^2/2}$ , which implies

$$\left\| \frac{1}{n} \mathbf{W}^T \mathbf{W} - \mathbf{I}_d \right\|_2 \leq 2\epsilon + \epsilon^2 \quad \text{where } \epsilon = \sqrt{\frac{d}{n}} + \delta,$$

with the same probability. Consequently, the sample covariance  $\hat{\Sigma} = \frac{1}{n} \mathbf{W}^T \mathbf{W}$  is a consistent estimate of  $\mathbf{I}_d$  as  $d/n \rightarrow 0$ .

*Proof.* Let  $\mathbf{R} \triangleq \frac{1}{n} \mathbf{W}^T \mathbf{W}$ . Since

$$\gamma_k(\mathbf{R}) = \sigma_k^2(\mathbf{W}/\sqrt{n}) \quad \text{for } k = 1, 2, \dots, \min\{n, d\},$$

we have

$$\gamma_{\max}(\mathbf{R}) \leq \left( 1 + \delta + \sqrt{\frac{d}{n}} \right)^2 \quad \text{and} \quad \gamma_{\min}(\mathbf{R}) \geq \left( 1 - \delta - \sqrt{\frac{d}{n}} \right)^2$$

held with probability greater than  $1 - 2e^{-n\delta^2/2}$ .

By ( $\ell_2$ -operator norm in maximization)

$$\|\mathbf{R} - \mathbf{I}_d\|_2 = \max\{\gamma_{\max}(\mathbf{R}) - 1, |\gamma_{\min}(\mathbf{R}) - 1|\}.$$

Moreover,

$$\gamma_{\min} - 1 \leq \gamma_{\max} - 1 \leq 2 \left( \delta + \sqrt{\frac{d}{n}} \right) + \left( \delta + \sqrt{\frac{d}{n}} \right)^2,$$

and

$$\begin{aligned} \gamma_{\min} - 1 &\geq -2 \left( \delta + \sqrt{\frac{d}{n}} \right) + \left( \delta + \sqrt{\frac{d}{n}} \right)^2 \\ &\geq -2 \left( \delta + \sqrt{\frac{d}{n}} \right) - \left( \delta + \sqrt{\frac{d}{n}} \right)^2 \end{aligned}$$

Putting all these inequalities together, we conclude that

$$\|\mathbf{R} - \mathbf{I}_d\|_2 = \max\{\gamma_{\max}(\mathbf{R}) - 1, |\gamma_{\min}(\mathbf{R}) - 1|\} \leq 2 \left( \delta + \sqrt{\frac{d}{n}} \right) + \left( \delta + \sqrt{\frac{d}{n}} \right)^2$$

holds with the probability greater than  $1 - 2e^{-n\delta^2/2}$ . □

**Example 2.2 (Gaussian covariance estimation):** Let  $\mathbf{X} \in \mathbb{R}^{n \times d}$  be a random matrix from the  $\Sigma$ -Gaussian ensemble. By standard properties of the multivariate Gaussian, we can write  $\mathbf{X} = \mathbf{W} \sqrt{\Sigma}$ , where  $\mathbf{W}$  is a standard Gaussian random matrix, and hence

$$\left\| \frac{1}{n} \mathbf{X}^T \mathbf{X} - \Sigma \right\|_2 = \left\| \sqrt{\Sigma} \left( \frac{1}{n} \mathbf{W}^T \mathbf{W} - \mathbf{I}_d \right) \sqrt{\Sigma} \right\|_2 \leq \|\Sigma\|_2 \left\| \frac{1}{n} \mathbf{W}^T \mathbf{W} - \mathbf{I}_d \right\|_2.$$

Consequently, from Example 2.1 we conclude that, for  $n \geq d$

$$\frac{\|\hat{\Sigma} - \Sigma\|_2}{\|\Sigma\|_2} \leq 2\sqrt{\frac{d}{n}} + 2\delta + \left( \sqrt{\frac{d}{n}} + \delta \right)$$

with probability at least  $1 - e^{-n\delta^2/2}$  for all  $\delta > 0$ , which implies the relative error  $\frac{\|\hat{\Sigma} - \Sigma\|_2}{\|\Sigma\|_2}$  converges to zero as long the ratio  $d/n$  converges to zero.

**Example 2.3 (Faster rates under trace constraints):** Let  $\{\gamma_j(\boldsymbol{\Sigma})\}_{j=1}^d$  be the ordered eigenvalues of  $\boldsymbol{\Sigma}$ , with  $\gamma_1(\boldsymbol{\Sigma})$  being the maximum eigenvalue. Now consider a non-zero covariance matrix  $\boldsymbol{\Sigma}$  that satisfies a “trace constraint” of the form

$$\frac{\text{tr}(\boldsymbol{\Sigma})}{\|\boldsymbol{\Sigma}\|_2} = \frac{\sum_{j=1}^d \gamma_j(\boldsymbol{\Sigma})}{\gamma_1(\boldsymbol{\Sigma})} \leq C,$$

where  $C$  is some constant independent of dimension. The above inequality always holds with  $C = \text{rank}(\boldsymbol{\Sigma})$ , providing a lower bound of the matrix rank.

For any matrix be drawn according to the  $\boldsymbol{\Sigma}$ -Gaussian ensemble with its covariance matrix satisfied the “trace constraint”, Theorem 2.1 guarantees that, with high probability, the maximum singular value is bounded above as

$$\frac{\sigma_{\mathbf{X}}}{\sqrt{n}} \leq \gamma_{\max}(\sqrt{\boldsymbol{\Sigma}}) \left( 1 + \delta + \sqrt{\frac{C}{n}} \right).$$

By comparison to the earlier bound for  $\boldsymbol{\Sigma} = \mathbf{I}_d$  in Example 2.1, we know that the parameter  $C$  acts as the *effective dimension*.

A more general of the “trace constraint” is the Schatten  $q$ -“balls” of matrices, which take the form

$$\mathbb{B}_q(R_q) := \left\{ \boldsymbol{\Sigma} \in \mathcal{S}^{d \times d} \mid \sum_{j=1}^d |\gamma_j(\boldsymbol{\Sigma})|^q \leq R_q \right\},$$

with  $q \in [0, 1]$  is a given parameter, and  $R_q > 0$  is the radius. **These matrices exhibit a relatively fast eigendecay.**

Before justifying Theorem 2.1, we present the Sudakov-Fernique inequality

**Theorem 2.2 (Sudakov-Fernique Inequality):** Given a pair of zero-mean  $N$ -dimensional Gaussian vectors  $(X_1, \dots, X_N)$  and  $(Y_1, \dots, Y_N)$ , suppose that

$$\mathbb{E}[(X_i - X_j)^2] \leq \mathbb{E}[(Y_j - Y_i)^2] \quad \text{for all } (i, j) \in [N] \times [N].$$

Then

$$\mathbb{E}[\max_{j \in [N]} X_j] \leq \mathbb{E}[\max_{j \in [N]} Y_j].$$

**Q: Does Sudakov-Fernique inequality hold in infinite dimension? A:Yes!**

**Proof of Theorem 2.1.** For brevity, Let  $\bar{\sigma}$  denote  $\gamma_{\max}(\sqrt{\boldsymbol{\Sigma}})$ . We rewrite  $\mathbf{X}$  as  $\mathbf{W}\sqrt{\boldsymbol{\Sigma}}$ , where the random matrix  $\mathbf{W} \in \mathbb{R}^{n \times d}$  has  $\mathcal{N}(0, 1)$  entries.

Viewing the mapping  $\mathbf{W} \mapsto \frac{\sigma_{\max}(\mathbf{W}\sqrt{\boldsymbol{\Sigma}})}{\sqrt{n}}$  as a function of matrices. By Corollary 2.1, we have

$$\left| \frac{\sigma_{\max}(\mathbf{P}\sqrt{\boldsymbol{\Sigma}})}{\sqrt{n}} - \frac{\sigma_{\max}(\mathbf{Q}\sqrt{\boldsymbol{\Sigma}})}{\sqrt{n}} \right| \leq \frac{1}{\sqrt{n}} \|\mathbf{P} - \mathbf{Q}\|_2 \leq \frac{\bar{\sigma}}{\sqrt{n}} \|\mathbf{P} - \mathbf{Q}\|_2 \leq \frac{\bar{\sigma}}{\sqrt{n}} \|\mathbf{P} - \mathbf{Q}\|_F.$$

Hence, such function is Lipschitz continuous with constant  $\frac{\bar{\sigma}}{\sqrt{n}}$ . By concentration measure for Lipschitz functions Gaussian random vectors, we conclude that

$$\mathbb{P}[\sigma_{\max}(\mathbf{X}) \geq \mathbb{E}[\sigma_{\max}(\mathbf{X})] + \sqrt{n}\bar{\sigma}\delta] \leq e^{-n\bar{\sigma}^2/2} (e^{-n^2\delta^2/2?}),$$

Therefore, it suffices to show that

$$\mathbb{E}[\sigma_{\max}(\mathbf{X})] \leq \sqrt{n}\bar{\sigma} + \sqrt{\text{tr}(\boldsymbol{\Sigma})}. \quad (\text{Upper Bound of Max Singular Value})$$

Since  $\sigma_{\max}(\mathbf{X}) = \max_{\mathbf{v}' \in \mathbb{S}^{d-1}} \|\mathbf{X}\mathbf{v}'\|_2$ , making the substitution  $\mathbf{v} = \sqrt{\boldsymbol{\Sigma}}\mathbf{v}'$ , we can write

$$\sigma_{\max}(\mathbf{X}) = \max_{\mathbf{v} \in \mathbb{S}^{d-1}(\boldsymbol{\Sigma}^{-1})} \|\mathbf{W}\mathbf{v}\| = \max_{\mathbf{u} \in \mathbb{S}^{d-1}} \max_{\mathbf{v} \in \mathbb{S}^{d-1}(\boldsymbol{\Sigma}^{-1})} \underbrace{\mathbf{u}^T \mathbf{W} \mathbf{v}}_{Z_{\mathbf{u},\mathbf{v}}}$$

where  $\mathbb{S}^{d-1}(\boldsymbol{\Sigma}^{-1}) = \{\mathbf{v} \in \mathbb{R}^d \mid \|\boldsymbol{\Sigma}^{-\frac{1}{2}}\mathbf{v}\|_2 = 1\}$  is an ellipse.

Let  $\mathbb{T} = \mathbb{S}^{n-1} \times \mathbb{S}^{d-1}(\boldsymbol{\Sigma}^{-1})$ . To proof (Upper Bound of Max Singular Value), we construct another Gaussian process  $\{Y_{\mathbf{u},\mathbf{v}} : (\mathbf{u}, \mathbf{v}) \in \mathbb{T}\}$  such that

$$\mathbb{E} \left[ (Z_{(\mathbf{u},\mathbf{v})} - Z_{(\tilde{\mathbf{u}},\tilde{\mathbf{v}})})^2 \right] \leq \mathbb{E} \left[ (Y_{(\mathbf{u},\mathbf{v})} - Y_{(\tilde{\mathbf{u}},\tilde{\mathbf{v}})})^2 \right],$$

and subsequently applying the Sudakov-Fernique inequality, we have

$$\mathbb{E}[\sigma_{\max}(\mathbf{X})] = \mathbb{E} \left[ \max_{(\mathbf{u},\mathbf{v}) \in \mathbb{T}} Z_{\mathbf{u},\mathbf{v}} \right] \leq \mathbb{E} \left[ \max_{(\mathbf{u},\mathbf{v}) \in \mathbb{T}} Y_{\mathbf{u},\mathbf{v}} \right].$$

By the symmetry of  $(Z_{(\mathbf{u},\mathbf{v})} - Z_{(\tilde{\mathbf{u}},\tilde{\mathbf{v}})})^2$  w.r.t the argument pairs  $(\mathbf{u}, \mathbf{v})$  and  $(\tilde{\mathbf{u}}, \tilde{\mathbf{v}})$ , we assume that  $\|\mathbf{v}\|_2 \leq \|\tilde{\mathbf{v}}\|_2$ .

$$\begin{aligned} \mathbb{E} \left[ (Z_{(\mathbf{u},\mathbf{v})} - Z_{(\tilde{\mathbf{u}},\tilde{\mathbf{v}})})^2 \right] &= \mathbb{E} \left[ \langle \mathbf{u}^T \mathbf{W} \mathbf{v} - \tilde{\mathbf{u}}^T \mathbf{W} \tilde{\mathbf{v}} \rangle^2 \right] \\ &= \mathbb{E} \left[ (\langle \mathbf{W}, \mathbf{u} \mathbf{v}^T \rangle - \langle \mathbf{W}, \tilde{\mathbf{u}} \tilde{\mathbf{v}}^T \rangle)^2 \right] \\ &= \mathbb{E} \left[ \langle \mathbf{W}, \mathbf{u} \mathbf{v}^T - \tilde{\mathbf{u}} \tilde{\mathbf{v}}^T \rangle^2 \right] \end{aligned}$$

Since the matrix  $\mathbf{W}$  has i.i.d.  $\mathcal{N}(0, 1)$  entries, and by the expansion of inner produce  $\langle \mathbf{A}, \mathbf{B} \rangle = \sum_{i,j=1} \mathbf{A}_{ij} \mathbf{B}_{ij}$ , we show that

$$\mathbb{E} \left[ (Z_{(\mathbf{u},\mathbf{v})} - Z_{(\tilde{\mathbf{u}},\tilde{\mathbf{v}})})^2 \right] = \mathbb{E} \left[ \langle \mathbf{W}, \mathbf{u} \mathbf{v}^T - \tilde{\mathbf{u}} \tilde{\mathbf{v}}^T \rangle^2 \right] = \|\mathbf{u} \mathbf{v}^T - \tilde{\mathbf{u}} \tilde{\mathbf{v}}^T\|_F^2$$

Moreover,

$$\begin{aligned} \|\mathbf{u} \mathbf{v}^T - \tilde{\mathbf{u}} \tilde{\mathbf{v}}^T\|_F^2 &= \|\mathbf{u} \mathbf{v}^T - \mathbf{u} \tilde{\mathbf{v}}^T + \mathbf{u} \tilde{\mathbf{v}}^T - \tilde{\mathbf{u}} \tilde{\mathbf{v}}^T\|_F^2 \\ &= \|(\mathbf{u} - \tilde{\mathbf{u}}) \tilde{\mathbf{v}}^T + \mathbf{u}(\mathbf{v} - \tilde{\mathbf{v}})^T\|_F^2 \\ &= \|(\mathbf{u} - \tilde{\mathbf{u}}) \tilde{\mathbf{v}}^T\|_F^2 + \|\mathbf{u}(\mathbf{v} - \tilde{\mathbf{v}})^T\|_F^2 + 2\langle (\mathbf{u} - \tilde{\mathbf{u}}) \tilde{\mathbf{v}}^T, \mathbf{u}(\mathbf{v} - \tilde{\mathbf{v}})^T \rangle \\ &\leq \|\mathbf{u} - \tilde{\mathbf{u}}\|_2^2 \|\tilde{\mathbf{v}}\|_2^2 + \|\mathbf{v} - \tilde{\mathbf{v}}\|_2^2 \|\mathbf{u}\|_2^2 + 2\langle (\mathbf{u} - \tilde{\mathbf{u}}) \tilde{\mathbf{v}}^T, \mathbf{u}(\mathbf{v} - \tilde{\mathbf{v}})^T \rangle \end{aligned}$$

and

$$\begin{aligned} \langle (\mathbf{u} - \tilde{\mathbf{u}}) \tilde{\mathbf{v}}^T, \mathbf{u}(\mathbf{v} - \tilde{\mathbf{v}})^T \rangle &= \mathbf{u}^T (\mathbf{u} - \tilde{\mathbf{u}}) \tilde{\mathbf{v}}^T (\mathbf{v} - \tilde{\mathbf{v}}) \\ &= (\|\mathbf{u}\|_2^2 - \mathbf{u}^T \tilde{\mathbf{u}}) \cdot (\tilde{\mathbf{v}}^T \mathbf{v} - \|\tilde{\mathbf{v}}\|_2^2) \end{aligned}$$

Note that  $\|\mathbf{u}\|_2 = \|\tilde{\mathbf{u}}\|_2 = 1$ ,  $\|\mathbf{u}\|_2^2 - \mathbf{u}^T \tilde{\mathbf{u}}^T \geq 0$ . By the Cauchy-Schwartz inequality and  $\|\mathbf{v}\|_2 \leq \|\tilde{\mathbf{v}}\|_2$ , we obtain

$$\langle \tilde{\mathbf{v}}, \mathbf{v} \rangle \leq \|\tilde{\mathbf{v}}\|_2 \cdot \|\mathbf{v}\|_2 \leq \|\tilde{\mathbf{v}}\|_2^2$$

Since  $\mathbf{v} \in \mathbb{S}^{d-1}(\Sigma)$  and  $\bar{\sigma} = \|\Sigma^{\frac{1}{2}}\|_2 = \max_{\|\Sigma^{-\frac{1}{2}}\mathbf{v}\|_2=1} \|\Sigma^{\frac{1}{2}}\Sigma^{-\frac{1}{2}}\mathbf{v}\|$ , we have  $\|\mathbf{v}\|_2 \leq \bar{\sigma}$ .

Putting together, we have

$$\mathbb{E}[(Z_{(\mathbf{u},\mathbf{v})} - Z_{\tilde{\mathbf{u}},\tilde{\mathbf{v}}})^2] \leq \bar{\sigma}^2 \|\mathbf{u} - \tilde{\mathbf{u}}\|_2^2 + \|\mathbf{v} - \tilde{\mathbf{v}}\|_2^2$$

Define the Gaussian process  $Y_{\mathbf{u},\mathbf{v}} := \bar{\sigma} \langle \mathbf{g}, \mathbf{u} \rangle + \langle \mathbf{h}, \mathbf{v} \rangle$ , where  $\mathbf{g} \in \mathbb{R}^n$  and  $\mathbf{h} \in \mathbb{R}^d$  are both standard Gaussian random vectors, and mutually independent.

Computing the expectation directly, we have

$$\mathbb{E}[(Y_{(\mathbf{u},\mathbf{v})} - Y_{\tilde{\mathbf{u}},\tilde{\mathbf{v}}})^2] = \bar{\sigma}^2 \|\mathbf{u} - \tilde{\mathbf{u}}\|_2^2 + \|\mathbf{v} - \tilde{\mathbf{v}}\|_2^2.$$

Recalling the Sudakov-Fernique inequality, we obtain

$$\begin{aligned} \mathbb{E}[\sigma_{\max}(\mathbf{X})] &= \mathbb{E} \left[ \max_{(\mathbf{u},\mathbf{v}) \in \mathbb{T}} Z_{\mathbf{u},\mathbf{v}} \right] \leq \mathbb{E} \left[ \max_{(\mathbf{u},\mathbf{v}) \in \mathbb{T}} Y_{\mathbf{u},\mathbf{v}} \right] \\ &= \bar{\sigma} \mathbb{E}[\|\mathbf{g}\|_2] + \mathbb{E}[\|\sqrt{\Sigma} \mathbf{h}\|_2] \\ &\stackrel{(i)}{\leq} \bar{\sigma} \sqrt{n} + \mathbb{E}[\|\sqrt{\Sigma} \mathbf{h}\|_2] \\ &\stackrel{(ii)}{\leq} \bar{\sigma} \sqrt{n} + \sqrt{\text{tr}(\Sigma)} \end{aligned}$$

where both (i) and (ii) are results of the Jensen's inequality. □

### 3 Covariance matrices from sub-Gaussian ensembles

**Definition 3.1:** A zero-mean random vector  $\mathbf{x} \in \mathbb{R}^d$  is said to be sub-Gaussian with parameter at most  $\sigma$ , if for each fixed  $\mathbf{v} \in \mathbb{S}^{d-1}$ , we have

$$\mathbb{E}[e^{\lambda \langle \mathbf{v}, \mathbf{x} \rangle}] \leq e^{\frac{\lambda^2 \sigma^2}{2}} \quad \text{for all } \lambda \in \mathbb{R}.$$

- Suppose that the matrix  $\mathbf{X} \in \mathbb{R}^{n \times d}$  has i.i.d.  $\mathcal{N}(0,1)$  entries. Hence each entry  $x_{ij}$  is zero-mean and sub-Gaussian with parameter  $\sigma = 1$ . In all of rows  $\mathbf{x}_i$  of  $\mathbf{X}$ , for any vector  $\mathbf{v} \in \mathbb{S}^{d-1}$ ,  $\langle \mathbf{v}, \mathbf{x}_i \rangle \sim \mathcal{N}(0,1)$  and therefore is sub-Gaussian with parameter at most  $\sigma$ .
- Suppose that  $\mathbf{x} \sim \mathcal{N}(0, \Sigma)$ . For any  $\mathbf{v} \in \mathbb{S}^{d-1}$ , we have  $\langle \mathbf{v}, \mathbf{x} \rangle \sim \mathcal{N}(0, \mathbf{v}^T \Sigma \mathbf{v})$ . By definition of operator norm for positive semi-definite matrices, we have  $\mathbf{v}^T \Sigma \mathbf{v} \leq \|\Sigma\|$ . Hence,  $\mathbf{x}$  is sub-Gaussian with parameter at most  $\sigma^2 = \|\Sigma\|$ .

**Definition 3.2 (Row-wise  $\sigma$ -sub-Gaussian ensemble):** If a random matrix  $\mathbf{X} \in \mathbb{R}^{n \times d}$  is formed by drawing each row  $\mathbf{x}_i \in \mathbb{R}^d$  in an i.i.d. manner from a  $\sigma$ -sub-Gaussian distribution, then we say that  $\mathbf{X}$  is a sample from a row-wise  $\sigma$ -sub-Gaussian ensemble.

**Theorem 3.1:** There are universal constants  $\{c_j\}_{j=0}^3$  such that, for any row-wise  $\sigma$ -sub-Gaussian random matrix  $\mathbf{X} \in \mathbb{R}^{n \times d}$ , the sample covariance  $\widehat{\Sigma} = \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i \mathbf{x}_i^T$  satisfies the bounds

$$\mathbb{E} \left[ e^{\lambda \|\widehat{\Sigma} - \Sigma\|_2} \right] \leq e^{c_0 \frac{\lambda^2 \sigma^4}{n} + 4d} \quad \text{for all } |\lambda| < \frac{n}{64e^2 \sigma^2},$$

and hence

$$\mathbb{P} \left[ \frac{\|\widehat{\Sigma} - \Sigma\|_2}{\sigma^2} \geq c_1 \left\{ \sqrt{\frac{d}{n}} + \frac{d}{n} \right\} + \delta \right] \leq c_2 e^{c_3 n \min\{\delta, \delta^2\}} \quad \text{for all } \delta \geq 0.$$

- Suppose  $\Sigma = I_d$  and each  $\mathbf{x}_i$  is sub-Gaussian with parameter  $\sigma = 1$ , the second tail bound in Theorem 3.1 implies that

$$\|\widehat{\Sigma} - I_d\|_2 \lesssim \sqrt{\frac{d}{n}} + \frac{d}{n}$$

with high probability.

Since

$$\|\widehat{\Sigma} - I_d\|_2 = \max\{\gamma_{\max}(\widehat{\Sigma}) - 1, |\gamma_{\min}(\widehat{\Sigma}) - 1|\}$$

and note that  $\gamma_k(\widehat{\Sigma}) = \sigma_k^2(\mathbf{X}/\sqrt{n})$  for  $k = 1, 2, \dots, \min\{n, d\}$ , we have

$$1 - \sqrt{\frac{d}{n}} - \frac{d}{n} \leq \sigma_{\min}^2(\mathbf{X}/\sqrt{n}) \leq \sigma_{\max}^2(\mathbf{X}/\sqrt{n}) \leq 1 + \sqrt{\frac{d}{n}} + \frac{d}{n}.$$

If  $n \geq c'^2 d$  for some  $c' > 1$ , we can conclude that

$$1 - c' \sqrt{\frac{d}{n}} \lesssim \frac{\sigma_{\min}(\mathbf{X})}{\sqrt{n}} \lesssim \frac{\sigma_{\max}(\mathbf{X})}{\sqrt{n}} \lesssim 1 + c' \sqrt{\frac{d}{n}}.$$

This result is similar to Example 2.1, except that the constant  $c'$  is larger than one.

**Proof of Theorem 3.1.** For brevity, let  $\mathbf{Q} := \widehat{\Sigma} - \Sigma$  and note that  $\|\mathbf{Q}\|_2 = \max_{\mathbf{v} \in \mathbb{S}^{d-1}} |\langle \mathbf{v}, \mathbf{Q}\mathbf{v} \rangle|$ .

There exists a collection of vectors  $\mathcal{C} \triangleq \{\mathbf{v}_1, \dots, \mathbf{v}_N\}$  as an  $\frac{1}{8}$ -cover of  $\mathbb{S}^{d-1}$  in the Euclidean norm, where the size of the collection  $N \leq 17^d$ . For any  $\mathbf{v} \in \mathbb{S}^{d-1}$ , there exists  $\mathbf{v}_i \in \mathcal{C}$  such that  $\|\mathbf{v} - \mathbf{v}_i\|_2 \leq \frac{1}{8}$ , which implies  $\mathbf{v}$  can be represented as  $\mathbf{v} = \mathbf{v}_i + \Delta$  with  $\|\Delta\|_2 \leq \frac{1}{8}$ .

Hence

$$\langle \mathbf{v}, \mathbf{Q}\mathbf{v} \rangle = \langle \mathbf{v}_i, \mathbf{Q}\mathbf{v}_i \rangle + 2\langle \mathbf{v}_i, \mathbf{Q}\Delta \rangle + \langle \Delta, \mathbf{Q}\Delta \rangle.$$

From the triangle inequality, we get

$$\begin{aligned} |\langle \mathbf{v}, \mathbf{Q}\mathbf{v} \rangle| &= |\langle \mathbf{v}_i, \mathbf{Q}\mathbf{v}_i \rangle + 2\langle \mathbf{v}_i, \mathbf{Q}\Delta \rangle + \langle \Delta, \mathbf{Q}\Delta \rangle| \\ &\leq |\langle \mathbf{v}_i, \mathbf{Q}\mathbf{v}_i \rangle| + 2|\langle \mathbf{v}_i, \mathbf{Q}\Delta \rangle| + |\langle \Delta, \mathbf{Q}\Delta \rangle| \\ &\leq |\langle \mathbf{v}_i, \mathbf{Q}\mathbf{v}_i \rangle| + 2\|\mathbf{Q}\|_2 \|\Delta\|_2 + \|\Delta\|_2^2 \|\mathbf{Q}\|_2 \\ &\leq |\langle \mathbf{v}_i, \mathbf{Q}\mathbf{v}_i \rangle| + 2 \cdot \frac{1}{8} \|\mathbf{Q}\|_2 + \left(\frac{1}{8}\right)^2 \|\mathbf{Q}\|_2 \\ &\leq |\langle \mathbf{v}_i, \mathbf{Q}\mathbf{v}_i \rangle| + \frac{1}{2} \|\mathbf{Q}\|_2 \end{aligned}$$

We conclude that, for any  $\mathbf{v} \in \mathbb{S}^{d-1}$ ,

$$\|\mathbf{Q}\|_2 \triangleq \max_{\mathbf{v} \in \mathbb{S}^{d-1}} |\langle \mathbf{v}, \mathbf{Q}\mathbf{v} \rangle| \leq 2 \max_{\mathbf{v}_i \in \mathcal{C}} |\langle \mathbf{v}_i, \mathbf{Q}\mathbf{v}_i \rangle|.$$

And therefore, for  $\lambda \geq 0$ ,

$$\mathbb{E} \left[ e^{\lambda \|\mathbf{Q}\|_2} \right] \leq \mathbb{E} \left[ e^{2\lambda \max_{\mathbf{v}_i \in \mathcal{C}} |\langle \mathbf{v}_i, \mathbf{Q}\mathbf{v}_i \rangle|} \right] \leq \sum_{i=1}^N \left( \mathbb{E} \left[ e^{2\lambda \langle \mathbf{v}_i, \mathbf{Q}\mathbf{v}_i \rangle} \right] + \mathbb{E} \left[ e^{-2\lambda \langle \mathbf{v}_i, \mathbf{Q}\mathbf{v}_i \rangle} \right] \right).$$

By the symmetry of  $\lambda$  in the last inequality, we have

$$\mathbb{E} \left[ e^{\lambda \|\mathbf{Q}\|_2} \right] \leq \sum_{i=1}^N \left( \mathbb{E} \left[ e^{2\lambda \langle \mathbf{v}_i, \mathbf{Q}\mathbf{v}_i \rangle} \right] + \mathbb{E} \left[ e^{-2\lambda \langle \mathbf{v}_i, \mathbf{Q}\mathbf{v}_i \rangle} \right] \right) \quad \text{for all } \lambda \in \mathbb{R}.$$

We claim that for any fixed  $\mathbf{u} \in \mathbb{S}^{d-1}$ ,

$$\mathbb{E} \left[ e^{t \langle \mathbf{u}, \mathbf{Q}\mathbf{u} \rangle} \right] \leq e^{512 \frac{t^2}{n} e^4 \sigma^4} \quad \text{for all } |t| \leq \frac{n}{32e^2 \sigma^2} \quad (\spadesuit)$$

Applying the inequality  $(\spadesuit)$  twice with  $t = 2\lambda$  and  $t = -2\lambda$ , respectively, we obtain

$$\mathbb{E} \left[ e^{\lambda \|\mathbf{Q}\|_2} \right] \leq 2Ne^{2048 \frac{\lambda^2}{n} e^4 \sigma^4} \quad \text{for all } |\lambda| \leq \frac{n}{64e^2 \sigma^2}.$$

Since  $2N \leq 2(17)^d \leq e^{4d}$ ,

$$\mathbb{E} \left[ e^{\lambda \|\mathbf{Q}\|_2} \right] \leq e^{2048 \frac{\lambda^2}{n} e^4 \sigma^4 + 4d} \quad \text{for all } |\lambda| \leq \frac{n}{64e^2 \sigma^2}.$$

Let  $c_0 = 2048e^4$ , we prove the first inequality in the theorem. The second inequality is a result of the Chernoff trick.

The remaining detail is to prove the bound  $(\spadesuit)$ .

By the definition of  $\mathbf{Q}$  and the i.i.d

$$\begin{aligned} \mathbb{E} \left[ e^{t \langle \mathbf{u}, \mathbf{Q}\mathbf{u} \rangle} \right] &= \mathbb{E} \left[ e^{\frac{t}{n} \sum_{i=1}^n (\langle \mathbf{x}_i, \mathbf{u} \rangle^2 - \langle \mathbf{u}, \Sigma \mathbf{u} \rangle)} \right] \\ &= \prod_{i=1}^n \mathbb{E} \left[ e^{\frac{t}{n} \{\langle \mathbf{x}_i, \mathbf{u} \rangle^2 - \langle \mathbf{u}, \Sigma \mathbf{u} \rangle\}} \right] \\ &= \left( \mathbb{E} \left[ e^{\frac{t}{n} \{\langle \mathbf{x}_1, \mathbf{u} \rangle^2 - \langle \mathbf{u}, \Sigma \mathbf{u} \rangle\}} \right] \right)^n \end{aligned}$$

Letting  $\epsilon \in \{-1, +1\}$  denote a Rademacher variable, independent of  $x_1$ . By the symmetrization technique, we have

$$\begin{aligned} \mathbb{E}_{\mathbf{x}_1} \left[ e^{\frac{t}{n} \{\langle \mathbf{x}_1, \mathbf{u} \rangle^2 - \langle \mathbf{u}, \Sigma \mathbf{u} \rangle\}} \right] &= \mathbb{E}_{\mathbf{x}_1} \left[ e^{\frac{t}{n} \mathbb{E}_{\mathbf{x}'} \{\langle \mathbf{x}_1, \mathbf{u} \rangle^2 - \langle \mathbf{x}', \mathbf{u} \rangle^2\}} \right] \\ &\leq \mathbb{E}_{\mathbf{x}_1, \mathbf{x}'} \left[ e^{\frac{t}{n} (\langle \mathbf{x}_1, \mathbf{u} \rangle^2 - \langle \mathbf{x}', \mathbf{u} \rangle^2)} \right] \\ &= \mathbb{E}_{\mathbf{x}_1} \left[ e^{\frac{t}{n} \langle \mathbf{x}_1, \mathbf{u} \rangle^2} \right] \cdot \mathbb{E}_{\mathbf{x}_1} \left[ e^{-\frac{t}{n} \langle \mathbf{x}_1, \mathbf{u} \rangle^2} \right] \\ &\leq \sqrt{\mathbb{E}_{\mathbf{x}_1} \left[ e^{\frac{2t}{n} \langle \mathbf{x}_1, \mathbf{u} \rangle^2} \right]} \cdot \sqrt{\mathbb{E}_{\mathbf{x}_1} \left[ e^{-\frac{2t}{n} \langle \mathbf{x}_1, \mathbf{u} \rangle^2} \right]} \\ &\leq \frac{\mathbb{E}_{\mathbf{x}_1} \left[ e^{\frac{2t}{n} \langle \mathbf{x}_1, \mathbf{u} \rangle^2} \right] + \mathbb{E}_{\mathbf{x}_1} \left[ e^{-\frac{2t}{n} \langle \mathbf{x}_1, \mathbf{u} \rangle^2} \right]}{2}. \end{aligned}$$

By the Taylor series of  $e^x$ , we show that

$$\begin{aligned}
\mathbb{E}_{\mathbf{x}_1} \left[ e^{\frac{t}{n} \{\langle \mathbf{x}_1, \mathbf{u} \rangle^2 - \langle \mathbf{u}, \Sigma \mathbf{u} \rangle\}} \right] &\leq \frac{\mathbb{E}_{\mathbf{x}_1} \left[ e^{\frac{2t}{n} \langle \mathbf{x}_1, \mathbf{u} \rangle^2} \right] + \mathbb{E}_{\mathbf{x}_1} \left[ e^{-\frac{2t}{n} \langle \mathbf{x}_1, \mathbf{u} \rangle^2} \right]}{2} \\
&\leq \frac{1}{2} e^{\frac{2t}{n} \mathbb{E} \langle \mathbf{x}_1, \mathbf{u} \rangle^2} + \frac{1}{2} e^{-\frac{2t}{n} \mathbb{E} \langle \mathbf{x}_1, \mathbf{u} \rangle^2} \\
&= \frac{1}{2} \left( \sum_{k=0}^{\infty} \frac{1}{k!} \left( \frac{2t}{n} \right)^k [\mathbb{E} \langle \mathbf{x}_1, \mathbf{u} \rangle^2]^k + \sum_{k=0}^{\infty} \frac{1}{k!} \left( -\frac{2t}{n} \right)^k [\mathbb{E} \langle \mathbf{x}_1, \mathbf{u} \rangle^2]^k \right) \\
&= 1 + \sum_{\ell=1}^{\infty} \frac{1}{(2\ell)!} \left( \frac{2t}{n} \right)^{2\ell} \mathbb{E} [\langle \mathbf{x}_1, \mathbf{u} \rangle^2]^{2\ell} \\
&\leq 1 + \sum_{\ell=1}^{\infty} \frac{1}{(2\ell)!} \left( \frac{2t}{n} \right)^{2\ell} \mathbb{E} [\langle \mathbf{x}_1, \mathbf{u} \rangle^{4\ell}]
\end{aligned}$$

Using the equivalent characterization of sub-Gaussian variables, we have

$$\mathbb{E} [\langle \mathbf{x}_1, \mathbf{u} \rangle^{4\ell}] \leq \frac{(4\ell)!}{2^{2\ell} (2\ell)!} (\sqrt{8e}\sigma)^{4\ell} \quad \ell = 1, 2, \dots.$$

Hence

$$\begin{aligned}
\mathbb{E}_{\mathbf{x}_1} \left[ e^{\frac{t}{n} \{\langle \mathbf{x}_1, \mathbf{u} \rangle^2 - \langle \mathbf{u}, \Sigma \mathbf{u} \rangle\}} \right] &\leq 1 + \sum_{\ell=1}^{\infty} \frac{1}{(2\ell)!} \left( \frac{2t}{n} \right)^{2\ell} \frac{(4\ell)!}{2^{2\ell} (2\ell)!} (\sqrt{8e}\sigma)^{4\ell} \\
&\leq 1 + \sum_{\ell=1}^{\infty} \left( \underbrace{\frac{16t}{n} e^2 \sigma^2}_{f(t)} \right)^{2\ell}
\end{aligned}$$

by the fact that  $(4\ell)! \leq 2^{2\ell} [(2\ell)!]^2$  ( $\ell = 1, 2, \dots$ ).

By the Taylor series of  $\frac{1}{1-x}$  and the inequality  $\frac{1}{1-a} \leq e^{2a}$  for  $a \in [0, \frac{1}{2}]$ , we have

$$1 + \sum_{\ell=1}^{\infty} \frac{16t}{n} e^2 \sigma^2 = \frac{1}{1 - f^2(t)} \leq e^{2f^2(t)} \quad \text{if } \left| \frac{16t}{n} e^2 \sigma^2 \right| < \frac{\sqrt{2}}{2}.$$

Putting together, we conclude that

$$\mathbb{E} \left[ e^{t \langle \mathbf{u}, \mathbf{Q} \mathbf{u} \rangle} \right] \leq 2e^{nf^2(t)} \quad \text{if } |t| < \frac{\sqrt{2}n}{32e^2\sigma^2}.$$

which of course holds when  $|t| \leq \frac{n}{32e^2\sigma^2}$ . □