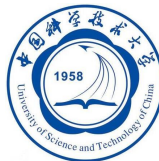


Random matrices and covariance estimation

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October 16, 2022



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Notation and basic facts

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

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

Note that $\sigma_{\min}(\mathbf{A}) = \min_{\mathbf{v} \in \mathbb{S}^{m-1}} \|\mathbf{A}\mathbf{v}\|_2$, and

$$\sigma_{\max}(\mathbf{A}) = \max_{\mathbf{v} \in \mathbb{S}^{m-1}} \|\mathbf{A}\mathbf{v}\|_2 =: \|\mathbf{A}\|_2$$

Denote $\mathcal{S}^{d \times d} := \{\mathbf{Q} \in \mathbb{R}^{d \times d} \mid \mathbf{Q} = \mathbf{Q}^T\}$, $\mathcal{S}_+^{d \times d} := \{\mathbf{Q} \in \mathcal{S}^{d \times d} \mid \mathbf{Q} \succeq 0\}$.

For a matrix $\mathbf{Q} \in \mathcal{S}^{d \times d}$, we write its eigenvalues as

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

Notation and basic facts

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

Then we have the relationship $\gamma_j(\mathbf{A}^T \mathbf{A}) = (\sigma_j(\mathbf{A}))^2$ for $j = 1, \dots, m$.

Let $\{x_1, \dots, x_n\}$ be a collection of n independent and identically distributed samples from a distribution in \mathbb{R}^d with zero mean, and covariance matrix $\mathbf{\Sigma} = \text{cov}(x_1) \in \mathcal{S}_+^{d \times d}$. A standard estimator of $\mathbf{\Sigma}$ is the sample covariance matrix

$$\widehat{\mathbf{\Sigma}} := \frac{1}{n} \sum_{i=1}^n x_i x_i^T = \frac{1}{n} \mathbf{X}^T \mathbf{X}$$

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Theorem

Let $\mathbf{X} \in \mathbb{R}^{n \times d}$ be drawn according to the Σ -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 lower deviation inequality

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

Proof

We can write $\mathbf{X} = \mathbf{W} \sqrt{\Sigma}$, where the random matrix $\mathbf{W} \in \mathbb{R}^{n \times d}$ has i.i.d. $\mathcal{N}(0, 1)$ entries. Let $\bar{\sigma}_{\max} = \gamma_{\max}(\sqrt{\Sigma})$, $\bar{\sigma}_{\min} = \gamma_{\min}(\sqrt{\Sigma})$. Consider the mapping $f : \mathbf{W} \mapsto \sigma_{\max}(\mathbf{W} \sqrt{\Sigma})$ as a real-valued function on \mathbb{R}^{nd} . Since we have

$$\|\mathbf{W} \sqrt{\Sigma}\|_2 = \max_{v \in \mathbb{S}^{d-1}} \|\mathbf{W} \sqrt{\Sigma} v\|_2 \leq \|\mathbf{W}\|_2 \max_{v \in \mathbb{S}^{d-1}} \|\sqrt{\Sigma} v\|_2 \leq \|\mathbf{W}\|_F \bar{\sigma}_{\max}$$

Then f is a $\bar{\sigma}_{\max}$ -Lipschitz function. According to Theorem 2.26, we conclude that

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

Proof

Consequently, it suffices to show that

$$\mathbb{E} [\sigma_{\max}(\mathbf{X})] \leq \sqrt{n} \bar{\sigma}_{\max} + \sqrt{\text{tr}(\mathbf{\Sigma})}$$

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

$$\sigma_{\max}(\mathbf{X}) = \max_{v \in \mathbb{S}^{d-1}(\mathbf{\Sigma}^{-1})} \|\mathbf{W}v\|_2 = \max_{u \in \mathbb{S}^{n-1}} \max_{v \in \mathbb{S}^{d-1}(\mathbf{\Sigma}^{-1})} \underbrace{u^T \mathbf{W}v}_{Z_{u,v}}$$

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

Proof

We try to apply the Sudakov–Fernique comparison (Theorem 5.27) to conclude that

$$\mathbb{E} [\sigma_{\max}(\mathbf{X})] = \mathbb{E} \left[\max_{(u,v) \in \mathbb{T}} Z_{u,v} \right] \leq \mathbb{E} \left[\max_{(u,v) \in \mathbb{T}} Y_{u,v} \right] \leq \sqrt{n} \bar{\sigma}_{\max} + \sqrt{\text{tr}(\mathbf{\Sigma})}$$

which means we need to construct another Gaussian process $\{Y_{u,v}, (u,v) \in \mathbb{T}\}$ such that

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

for all pairs (u,v) and (\tilde{u}, \tilde{v}) in $\mathbb{T} := \mathbb{S}^{n-1} \times \mathbb{S}^{d-1} (\mathbf{\Sigma}^{-1})$. Introducing the Gaussian process $Z_{u,v} := u^T \mathbf{W} v = \langle \langle \mathbf{W}, uv^T \rangle \rangle$, where we use $\langle \langle \mathbf{A}, \mathbf{B} \rangle \rangle := \sum_{j=1}^n \sum_{k=1}^d A_{jk} B_{jk}$ to denote the trace inner product.

Proof

We may assume without loss of generality that $\|v\|_2 \leq \|\tilde{v}\|_2$. Then

$$\begin{aligned}
 \mathbb{E}[(Z_{u,v} - Z_{\tilde{u},\tilde{v}})^2] &= \mathbb{E}\left[\left\langle \langle \mathbf{W}, uv^T - \tilde{u}\tilde{v}^T \rangle \right\rangle^2\right] = \|uv^T - \tilde{u}\tilde{v}^T\|_F^2 \\
 &= \|u(v - \tilde{v})^T + (u - \tilde{u})\tilde{v}^T\|_F^2 \\
 &= \|(u - \tilde{u})\tilde{v}^T\|_F^2 + \|u(v - \tilde{v})^T\|_F^2 + 2\left\langle \langle u(v - \tilde{v})^T, (u - \tilde{u})\tilde{v}^T \rangle \right\rangle \\
 &\leq \underbrace{\|\tilde{v}\|_2^2}_{\bar{\sigma}_{\max}^2} \|u - \tilde{u}\|_2^2 + \underbrace{\|u\|_2^2}_{=1} \|v - \tilde{v}\|_2^2 + 2 \underbrace{(\|u\|_2^2 - \langle u, \tilde{u} \rangle)}_{\geq 0} \underbrace{(\langle v, \tilde{v} \rangle - \|\tilde{v}\|_2^2)}_{\leq 0} \\
 &\leq \bar{\sigma}_{\max}^2 \|u - \tilde{u}\|_2^2 + \|v - \tilde{v}\|_2^2
 \end{aligned}$$

Proof

Motivated by this inequality, we define the Gaussian process $Y_{u,v} := \bar{\sigma}_{\max} \langle g, u \rangle + \langle h, v \rangle$, where $g \in \mathbb{R}^n$ and $h \in \mathbb{R}^d$ are both standard Gaussian random vectors and mutually independent. By construction, we have

$$\mathbb{E} \left[\left(Y_{\theta} - Y_{\tilde{\theta}} \right)^2 \right] = \bar{\sigma}_{\max}^2 \|u - \tilde{u}\|_2^2 + \|v - \tilde{v}\|_2^2.$$

Thus, we may apply the Sudakov-Fernique bound to conclude that

$$\begin{aligned} \mathbb{E} [\sigma_{\max}(\mathbf{X})] &\leq \mathbb{E} \left[\max_{(u,v) \in \mathbb{T}} Y_{u,v} \right] = \bar{\sigma}_{\max} \mathbb{E} \left[\max_{u \in \mathbb{S}^{n-1}} \langle g, u \rangle \right] + \mathbb{E} \left[\max_{v \in \mathbb{S}^{d-1}(\Sigma^{-1})} \langle h, v \rangle \right] \\ &= \bar{\sigma}_{\max} \mathbb{E} [\|g\|_2] + \mathbb{E} [\|\sqrt{\Sigma} h\|_2] \\ &\leq \sqrt{n} \bar{\sigma}_{\max} + \sqrt{\text{tr}(\Sigma)} \end{aligned}$$

which finishes the proof of the upper bound on $\sigma_{\max}(\mathbf{X})$.

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Assume that the random vector $x_i \in \mathbb{R}^d$ is zero-mean, and sub-Gaussian with parameter at most σ , by which we mean that, for each fixed $v \in \mathbb{S}^{d-1}$,

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

When the random matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$ is formed by drawing each row $x_i \in \mathbb{R}^d$ in an i.i.d. manner from a σ -sub-Gaussian distribution, then we say that \mathbf{X} is a sample from a row-wise σ -sub-Gaussian ensemble. For any such random matrix, we have the following result:

Theorem

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

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

and hence

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

Proof

We introduce the shorthand $\mathbf{Q} := \widehat{\Sigma} - \Sigma$. Let $\{v^1, \dots, v^N\}$ be a $\frac{1}{8}$ -covering of the sphere \mathbb{S}^{d-1} in the Euclidean norm; from Example 5.8, there exists such a covering with $N \leq 17^d$ vectors. Given any $v \in \mathbb{S}^{d-1}$, we can write $v = v^j + \Delta$ for some v^j in the cover, and an error vector Δ such that $\|\Delta\|_2 \leq \frac{1}{8}$, and hence

$$\begin{aligned} |\langle v, \mathbf{Q}v \rangle| &= |\langle v^j, \mathbf{Q}v^j \rangle + 2\langle \Delta, \mathbf{Q}v^j \rangle + \langle \Delta, \mathbf{Q}\Delta \rangle| \\ &\leq |\langle v^j, \mathbf{Q}v^j \rangle| + 2\|\Delta\|_2 \|\mathbf{Q}\|_2 \|v^j\|_2 + \|\mathbf{Q}\|_2 \|\Delta\|_2^2 \\ &\leq |\langle v^j, \mathbf{Q}v^j \rangle| + \frac{1}{4} \|\mathbf{Q}\|_2 + \frac{1}{64} \|\mathbf{Q}\|_2 \\ &\leq |\langle v^j, \mathbf{Q}v^j \rangle| + \frac{1}{2} \|\mathbf{Q}\|_2 \end{aligned}$$

Proof

$$\|\mathbf{Q}\|_2 = \max_{v \in \mathbb{S}^{d-1}} |\langle v, \mathbf{Q}v \rangle| \leq 2 \max_{j=1, \dots, N} |\langle v^j, \mathbf{Q}v^j \rangle|.$$

Consequently, we have

$$\begin{aligned} \mathbb{E} \left[e^{\lambda \|\mathbf{Q}\|_2} \right] &\leq \mathbb{E} \left[\exp \left(2\lambda \max_{j=1, \dots, N} |\langle v^j, \mathbf{Q}v^j \rangle| \right) \right] \\ &\leq \sum_{j=1}^N \left\{ \mathbb{E} \left[e^{2\lambda \langle v^j, \mathbf{Q}v^j \rangle} \right] + \mathbb{E} \left[e^{-2\lambda \langle v^j, \mathbf{Q}v^j \rangle} \right] \right\} \end{aligned}$$

Next we claim that for any fixed unit vector $u \in \mathbb{S}^{d-1}$,

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

Proof

Then we find that

$$\mathbb{E} \left[e^{\lambda \| \mathbf{Q} \|_2} \right] \leq 2Ne^{2048 \frac{\lambda^2}{n} e^4 \sigma^4} \leq e^{C_0 \frac{\lambda^2 \sigma^4}{n} + 4d},$$

valid for all $|\lambda| < \frac{n}{64e^2\sigma^2}$, where the final step uses the fact that $2(17^d) \leq e^{4d}$. Now we proof the claim. We have

$$\mathbb{E} \left[e^{t \langle u, Qu \rangle} \right] = \prod_{i=1}^n \mathbb{E} \left[e^{\frac{t}{n} \{ \langle x_i, u \rangle^2 - \langle u, \Sigma u \rangle \}} \right] = \left(\mathbb{E} \left[e^{\frac{t}{n} \{ \langle x_1, u \rangle^2 - \langle u, \Sigma u \rangle \}} \right] \right)^n.$$

Letting $\varepsilon \in \{-1, +1\}$ denote a Rademacher variable, independent of x_1 , a standard symmetrization argument (see Proposition 4.11) implies that

Proof

$$\begin{aligned}\mathbb{E}_{x_1} \left[e^{\frac{t}{n} \{ \langle x_1, u \rangle^2 - \langle u, \Sigma u \rangle \}} \right] &\leq \mathbb{E}_{x_1, \varepsilon} \left[e^{\frac{2t}{n} \varepsilon \langle x_1, u \rangle^2} \right] \\ &\stackrel{(i)}{=} \sum_{k=0}^{\infty} \frac{1}{k!} \left(\frac{2t}{n} \right)^k \mathbb{E} \left[\varepsilon^k \langle x_1, u \rangle^{2k} \right] \\ &\stackrel{(ii)}{=} 1 + \sum_{\ell=1}^{\infty} \frac{1}{(2\ell)!} \left(\frac{2t}{n} \right)^{2\ell} \mathbb{E} \left[\langle x_1, u \rangle^{4\ell} \right]\end{aligned}$$

where step (i) follows by the power-series expansion of the exponential, and step (ii) follows since ε and x_1 are independent, and all odd moments of the Rademacher term vanish. By property (III) in Theorem 2.6 on equivalent characterizations of sub-Gaussian variables, we are guaranteed that

Proof

$$\mathbb{E} \left[\langle x_1, u \rangle^{4\ell} \right] \leq \frac{(4\ell)!}{2^{2\ell}(2\ell)!} (\sqrt{8}e\sigma)^{4\ell} \quad \text{for all } \ell = 1, 2, \dots$$

and hence

$$\begin{aligned} \mathbb{E}_{x_1} \left[e^{\frac{t}{n} \{ \langle x_1, u \rangle^2 - \langle u, \Sigma u \rangle \}} \right] &\leq 1 + \sum_{\ell=1}^{\infty} \frac{1}{(2\ell)!} \left(\frac{2t}{n} \right)^{2\ell} \frac{(4\ell)!}{2^{2\ell}(2\ell)!} (\sqrt{8}e\sigma)^{4\ell} \\ &\leq 1 + \sum_{\ell=1}^{\infty} \underbrace{\left(\frac{16t}{n} e^2 \sigma^2 \right)^{2\ell}}_{f(t)} \end{aligned}$$

Proof

where we have used the fact that $(4\ell)! \leq 2^{2\ell}[(2\ell)!]^2$. As long as $f(t) := \frac{16t}{n}e^{2\sigma^2} < \frac{1}{2}$, we can write

$$1 + \sum_{\ell=1}^{\infty} [f^2(t)]^{\ell} \stackrel{(i)}{=} \frac{1}{1 - f^2(t)} \stackrel{(ii)}{\leq} \exp(2f^2(t))$$

where step (i) follows by summing the geometric series, and step (ii) follows because $\frac{1}{1-a} \leq e^{2a}$ for all $a \in [0, \frac{1}{2}]$. Putting together the pieces and combining with our earlier bound (6.23), we have shown that $\mathbb{E}[e^{t\langle u, Qu \rangle}] \leq e^{2nf^2(t)}$, valid for all $|t| < \frac{n}{32e^2\sigma^2}$, which establishes the claim.

Proof

$$\mathbb{E}_X [\Phi (\| \mathbb{P}_n - \mathbb{P} \|_{\mathcal{F}})] \leq \mathbb{E}_{X, \varepsilon} [\Phi (2 \| S_n \|_{\mathcal{F}})]$$

$$\| S_n \|_{\mathcal{F}} := \sup_{f \in \mathcal{F}} \left| \frac{1}{n} \sum_{i=1}^n \varepsilon_i f(X_i) \right|$$

$$\| \mathbb{P}_n - \mathbb{P} \|_{\mathcal{F}} := \sup_{f \in \mathcal{F}} \left| \frac{1}{n} \sum_{i=1}^n f(X_i) - \mathbb{E}[f(X)] \right|$$

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6.4.1 Background on matrix analysis

Given a matrix $\mathbf{Q} \in \mathcal{S}^{d \times d}$, consider its eigendecomposition $\mathbf{Q} = \mathbf{U}^T \mathbf{\Gamma} \mathbf{U}$. Here the matrix $\mathbf{U} \in \mathbb{R}^{d \times d}$ is a unitary matrix, satisfying the relation $\mathbf{U}^T \mathbf{U} = \mathbf{I}_d$, whereas $\mathbf{\Gamma} := \text{diag}(\gamma(\mathbf{Q}))$ is a diagonal matrix specified by the vector of eigenvalues $\gamma(\mathbf{Q}) \in \mathbb{R}^d$.

$$\mathbf{Q} \mapsto f(\mathbf{Q}) := \mathbf{U}^T \text{diag}(f(\gamma_1(\mathbf{Q})), \dots, f(\gamma_d(\mathbf{Q}))) \mathbf{U}$$

By construction, this extension of f to $\mathcal{S}^{d \times d}$ is unitarily invariant, meaning that

$$f(\mathbf{V}^T \mathbf{Q} \mathbf{V}) = \mathbf{V}^T f(\mathbf{Q}) \mathbf{V} \quad \text{for all unitary matrices } \mathbf{V} \in \mathbb{R}^{d \times d},$$

$$\gamma(f(\mathbf{Q})) = \{f(\gamma_j(\mathbf{Q})), j = 1, \dots, d\}$$

The matrix exponential has the power-series expansion $e^{\mathbf{Q}} = \sum_{k=0}^{\infty} \frac{\mathbf{Q}^k}{k!}$. By the spectral mapping property, the eigenvalues of $e^{\mathbf{Q}}$ are positive.

6.4.2 Tail conditions for matrices

$\text{var}(\mathbf{Q}) := \mathbb{E}[\mathbf{Q}^2] - (\mathbb{E}[\mathbf{Q}])^2$. The moment generating function of a random matrix \mathbf{Q} is the matrix-valued mapping $\Psi_{\mathbf{Q}} : \mathbb{R} \rightarrow \mathcal{S}^{d \times d}$ given by

$$\Psi_{\mathbf{Q}}(\lambda) := \mathbb{E}[e^{\lambda \mathbf{Q}}] = \sum_{k=0}^{\infty} \frac{\lambda^k}{k!} \mathbb{E}[\mathbf{Q}^k].$$

Definition 6.6 A zero-mean symmetric random matrix $\mathbf{Q} \in \mathcal{S}^{d \times d}$ is sub-Gaussian with matrix parameter $\mathbf{V} \in \mathcal{S}_+^{d \times d}$ if

$$\Psi_{\mathbf{Q}}(\lambda) \leq e^{\frac{\lambda^2 \mathbf{V}}{2}} \quad \text{for all } \lambda \in \mathbb{R}.$$

Sub-exponential random matrices

- **Definition 6.9** (Sub-exponential random matrices) A zero-mean random matrix is sub-exponential with parameters (\mathbf{V}, α) if

$$\Psi_{\mathbf{Q}}(\lambda) \leq e^{\frac{\lambda^2 \mathbf{V}}{2}} \quad \text{for all } |\lambda| < \frac{1}{\alpha}.$$

- **Definition 6.10** (Bernstein's condition for matrices) A zero-mean symmetric random matrix \mathbf{Q} satisfies a Bernstein condition with parameter $b > 0$ if

$$\mathbb{E}[\mathbf{Q}^j] \leq \frac{1}{2} j! b^{j-2} \text{var}(\mathbf{Q}) \quad \text{for } j = 3, 4, \dots$$

- We note that (a stronger form of) Bernstein's condition holds whenever the matrix \mathbf{Q} has a bounded operator norm-say $\|\mathbf{Q}\|_2 \leq b$ almost surely.

$$\mathbb{E}[\mathbf{Q}^j] \leq b^{j-2} \text{var}(\mathbf{Q}) \quad \text{for all } j = 3, 4, \dots$$

Bernstein condition

Lemma 6.11 For any symmetric zero-mean random matrix satisfying the Bernstein condition, we have

$$\Psi_{\mathbf{Q}}(\lambda) \leq \exp\left(\frac{\lambda^2 \text{var}(\mathbf{Q})}{2(1 - b|\lambda|)}\right) \quad \text{for all } |\lambda| < \frac{1}{b}.$$

- **Proof:** Since $\mathbb{E}[\mathbf{Q}] = 0$, applying the definition of the matrix exponential for a suitably small $\lambda \in \mathbb{R}$ yields $(\mathbf{I}_d + \mathbf{A} \leq e^{\mathbf{A}})$

$$\begin{aligned} \mathbb{E}[e^{\lambda \mathbf{Q}}] &= \mathbf{I}_d + \frac{\lambda^2 \text{var}(\mathbf{Q})}{2} + \sum_{j=3}^{\infty} \frac{\lambda^j \mathbb{E}[\mathbf{Q}^j]}{j!} \\ &\stackrel{(i)}{\leq} \mathbf{I}_d + \frac{\lambda^2 \text{var}(\mathbf{Q})}{2} \left\{ \sum_{j=0}^{\infty} |\lambda|^j b^j \right\} \end{aligned}$$

Matrix Chernoff approach and independent decompositions

Lemma 6.12 (Matrix Chernoff technique) Let \mathbf{Q} be a zero-mean symmetric random matrix whose moment generating function $\Psi_{\mathbf{Q}}$ exists in an open interval $(-a, a)$. Then for any $\delta > 0$, we have

$$\mathbb{P} [\gamma_{\max}(\mathbf{Q}) \geq \delta] \leq \text{tr}(\Psi_{\mathbf{Q}}(\lambda)) e^{-\lambda\delta} \quad \text{for all } \lambda \in [0, a),$$

where $\text{tr}(\cdot)$ denotes the trace operator on matrices. Similarly, we have

$$\mathbb{P} [\|\mathbf{Q}\|_2 \geq \delta] \leq 2 \text{tr}(\Psi_{\mathbf{Q}}(\lambda)) e^{-\lambda\delta} \quad \text{for all } \lambda \in [0, a)$$

Proof:

- Applying Markov inequality.

Independent decompositions

Lemma 6.13 Let $\mathbf{Q}_1, \dots, \mathbf{Q}_n$ be independent symmetric random matrices whose moment generating functions exist for all $\lambda \in I$, and define the sum $\mathbf{S}_n := \sum_{i=1}^n \mathbf{Q}_i$. Then

$$\mathrm{tr}(\Psi_{\mathbf{S}_n}(\lambda)) \leq \mathrm{tr}\left(e^{\sum_{i=1}^n \log \Psi_{\mathbf{Q}_i}(\lambda)}\right) \quad \text{for all } \lambda \in I.$$

Independent decompositions

Proof: In order to prove this lemma, we require the following result due to Lieb (1973): for any fixed matrix $\mathbf{H} \in \mathcal{S}^{d \times d}$, the function $f : \mathcal{S}_+^{d \times d} \rightarrow \mathbb{R}$ given by

$$f(\mathbf{A}) := \text{tr} \left(e^{\mathbf{H} + \log(\mathbf{A})} \right)$$

is concave. Introducing the shorthand notation $G(\lambda) := \text{tr}(\Psi_{\mathbf{S}_n}(\lambda))$, we note that, by linearity of trace and expectation, we have

$$G(\lambda) = \text{tr} \left(\mathbb{E} \left[e^{\lambda \mathbf{S}_{n-1} + \log \exp(\lambda \mathbf{Q}_n)} \right] \right) = \mathbb{E}_{\mathbf{S}_{n-1}} \mathbb{E}_{\mathbf{Q}_n} \left[\text{tr} \left(e^{\lambda \mathbf{S}_{n-1} + \log \exp(\lambda \mathbf{Q}_n)} \right) \right]$$

Using concavity of the function f with $\mathbf{H} = \lambda \mathbf{S}_{n-1}$ and $\mathbf{A} = e^{\lambda \mathbf{Q}_n}$, Jensen's inequality implies that

$$\mathbb{E}_{\mathbf{Q}_n} \left[\text{tr} \left(e^{\lambda \mathbf{S}_{n-1} + \log \exp(\lambda \mathbf{Q}_n)} \right) \right] \leq \text{tr} \left(e^{\lambda \mathbf{S}_{n-1} + \log \mathbb{E}_{\mathbf{Q}_n} \exp(\lambda \mathbf{Q}_n)} \right),$$

so that we have shown that $G(\lambda) \leq \mathbb{E}_{\mathbf{S}_{n-1}} \left[\text{tr} \left(e^{\lambda \mathbf{S}_{n-1} + \log \Psi_{\mathbf{Q}_n}(\lambda)} \right) \right]$.

Symmetrization

Example 6.14 (Rademacher symmetrization for random matrices)

Let $\{\mathbf{A}_i\}_{i=1}^n$ be a sequence of independent symmetric random matrices, and suppose that our goal is to bound the maximum eigenvalue of the matrix sum $\sum_{i=1}^n (\mathbf{A}_i - \mathbb{E}[\mathbf{A}_i])$. $\tilde{\mathbf{Q}}_i = \varepsilon_i \mathbf{A}_i$, where ε_i is an independent Rademacher variable. Let us now work through this reduction. By Markov's inequality, we have

$$\mathbb{P} \left[\gamma_{\max} \left(\sum_{i=1}^n \{\mathbf{A}_i - \mathbb{E}[\mathbf{A}_i]\} \right) \geq \delta \right] \leq \mathbb{E} \left[e^{\lambda \gamma_{\max}(\sum_{i=1}^n [\mathbf{A}_i - \mathbb{E}[\mathbf{A}_i]])} \right] e^{-\lambda \delta}.$$

The proof of symmetrization

By the variational representation of the maximum eigenvalue, we have

$$\begin{aligned}
 \mathbb{E} \left[e^{\lambda \gamma_{\max}(\sum_{i=1}^n (\mathbf{A}_i - \mathbb{E}[\mathbf{A}_i]))} \right] &= \mathbb{E} \left[\exp \left(\lambda \sup_{\|u\|_2=1} \left\langle u, \left(\sum_{i=1}^n (\mathbf{A}_i - \mathbb{E}[\mathbf{A}_i]) \right) u \right\rangle \right) \right] \\
 &\leq \mathbb{E} \left[\exp \left(2\lambda \sup_{\|u\|_2=1} \left\langle u, \left(\sum_{i=1}^n \varepsilon_i \mathbf{A}_i \right) u \right\rangle \right) \right] \\
 &= \mathbb{E} \left[e^{2\lambda \gamma_{\max}(\sum_{i=1}^n \varepsilon_i \mathbf{A}_i)} \right] \\
 &= \mathbb{E} \left[\gamma_{\max} \left(e^{2\lambda \sum_{i=1}^n \varepsilon_i \mathbf{A}_i} \right) \right],
 \end{aligned}$$

So that

$$\mathbb{E} \left[\gamma_{\max} \left(e^{2\lambda \sum_{i=1}^n \varepsilon_i \mathbf{A}_i} \right) \right] \leq \text{tr} \left(\mathbb{E} \left[e^{2\lambda \sum_{i=1}^n \varepsilon_i \mathbf{A}_i} \right] \right) \leq \text{tr} \left(e^{\sum_{i=1}^n \log \Psi_{\tilde{\mathbf{A}}_i}(2\lambda)} \right)$$

6.4.4 Upper tail bounds for random matrices

(Theorem 6.15) (Hoeffding bound for random matrices) Let $\{\mathbf{Q}_i\}_{i=1}^n$ be a sequence of zero-mean independent symmetric random matrices that satisfy the sub-Gaussian condition with parameters $\{\mathbf{V}_i\}_{i=1}^n$. Then for all $\delta > 0$, we have the upper tail bound

$$\mathbb{P}\left[\left\|\frac{1}{n}\sum_{i=1}^n \mathbf{Q}_i\right\|_2 \geq \delta\right] \leq 2 \operatorname{rank}\left(\sum_{i=1}^n \mathbf{V}_i\right) e^{-\frac{n\sigma^2}{2\sigma^2}} \leq 2de^{-\frac{n\sigma^2}{2\sigma^2}},$$

where $\sigma^2 = \left\|\frac{1}{n}\sum_{i=1}^n \mathbf{V}_i\right\|_2$.

Proof: Lemma 6.13 and $\operatorname{tr}(e^{\mathbf{R}}) \leq de^{\|\mathbf{R}\|_2}$.

Bernstein bound for random matrices

Theorem 6.17 (Bernstein bound for random matrices) Let $\{\mathbf{Q}_i\}_{i=1}^n$ be a sequence of independent, zero-mean, symmetric random matrices that satisfy the Bernstein condition with parameter $b > 0$. Then for all $\delta \geq 0$, the operator norm satisfies the tail bound

$$\mathbb{P} \left[\frac{1}{n} \left\| \sum_{i=1}^n \mathbf{Q}_i \right\|_2 \geq \delta \right] \leq 2 \operatorname{rank} \left(\sum_{i=1}^n \operatorname{var}(\mathbf{Q}_i) \right) \exp \left\{ -\frac{n\delta^2}{2(\sigma^2 + b\delta)} \right\},$$

where $\sigma^2 := \frac{1}{n} \left\| \sum_{j=1}^n \operatorname{var}(\mathbf{Q}_j) \right\|_2$.

Proof: Lemma 6.13 and $\log \Psi_{\mathbf{Q}_i}(\lambda) \leq \frac{\lambda^2 \operatorname{var}(\mathbf{Q}_i)}{1-b|\lambda|}$

symmetrization

With d replaced by $(d_1 + d_2)$, a problem involving general zero-mean random matrices $\mathbf{A}_i \in \mathbb{R}^{d_1 \times d_2}$ can be transformed to a symmetric version by defining the $(d_1 + d_2)$ -dimensional square matrices

$$\mathbf{Q}_i := \begin{bmatrix} \mathbf{0}_{d_1 \times d_1} & \mathbf{A}_i \\ \mathbf{A}_i^T & \mathbf{0}_{d_2 \times d_2} \end{bmatrix},$$

and imposing some form of moment generating function bound-for instance, the sub-Gaussian condition on the symmetric matrices \mathbf{Q}_i .

The condition of **Theorem 6.17** is the quantity

$$\sigma^2 := \max \left\{ \left\| \frac{1}{n} \sum_{i=1}^n \mathbb{E} [\mathbf{A}_i \mathbf{A}_i^T] \right\|_2, \left\| \frac{1}{n} \sum_{i=1}^n \mathbb{E} [\mathbf{A}_i^T \mathbf{A}_i] \right\|_2 \right\}$$

Bernstein bounds with sharpened dimension dependence

(Example 6.19) Consider a sequence of independent zero-mean random matrices \mathbf{Q}_i bounded as $\|\mathbf{Q}_i\|_2 \leq 1$ almost surely, and suppose that our goal is to upper bound the maximum eigenvalue $\gamma_{\max}(\mathbf{S}_n)$ of the sum $\mathbf{S}_n := \sum_{i=1}^n \mathbf{Q}_i$. Defining the function $\phi(\lambda) := e^\lambda - \lambda - 1$. For any pair $\delta > 0$, we have

$$\mathbb{P}[\gamma_{\max}(\mathbf{S}_n) \geq \delta] \leq \frac{\text{tr}(\bar{\mathbf{V}})}{\|\bar{\mathbf{V}}\|_2} \inf_{\lambda > 0} \left\{ \frac{e^{\phi(\lambda)\|\bar{\mathbf{V}}\|_2}}{\phi(\lambda\delta)} \right\}.$$

where $\bar{\mathbf{V}} := \sum_{i=1}^n \text{var}(\mathbf{Q}_i)$.

Proof:

- $\mathbb{P}[\gamma_{\max}(\mathbf{S}_n) \geq \delta] \leq \inf_{\lambda > 0} \frac{\text{tr}(\mathbb{E}[\phi(\lambda\mathbf{S}_n)])}{\phi(\lambda\delta)}.$
- $\log \Psi_{\mathbf{Q}_i}(\lambda) \leq \phi(\lambda) \text{var}(\mathbf{Q}_i)$
- $\text{tr}(\mathbb{E}[\phi(\lambda\mathbf{S}_n)]) \leq \frac{\text{tr}(\bar{\mathbf{V}})}{\|\bar{\mathbf{V}}\|_2} e^{\phi(\lambda)\|\bar{\mathbf{V}}\|_2}$

6.4.5 Consequences for covariance matrices

(Corollary 6.20) Let x_1, \dots, x_n be i.i.d. zero-mean random vectors with covariance Σ such that $\|x_j\|_2 \leq \sqrt{b}$ almost surely. Then for all $\delta > 0$, the sample covariance matrix $\widehat{\Sigma} = \frac{1}{n} \sum_{i=1}^n x_i x_i^T$ satisfies

$$\mathbb{P} \left[\|\widehat{\Sigma} - \Sigma\|_2 \geq \delta \right] \leq 2d \exp \left(-\frac{n\delta^2}{2b(\|\Sigma\|_2 + \delta)} \right).$$

Proof: $Q_i := x_i x_i^T - \Sigma$

- $\|Q_i\|_2 \leq \|x_i\|_2^2 + \|\Sigma\|_2 \leq b + \|\Sigma\|_2 \leq 2b$
- $\text{var}(Q_i) = \mathbb{E} \left[(x_i x_i^T)^2 \right] - \Sigma^2 \leq \mathbb{E} \left[\|x_i\|_2^2 x_i x_i^T \right] \leq b \Sigma$
- **Theorem 6.17** (Bernstein bound for random matrices)

Example 6.21 (Random vectors uniform on a sphere) Suppose that the random vectors x_i are chosen uniformly from the sphere $\mathbb{S}^{d-1}(\sqrt{d})$, so that $\|x_i\|_2 = \sqrt{d}$ for all $i = 1, \dots, n$. By construction, we have $\mathbb{E}[x_i x_i^T] = \Sigma = \mathbf{I}_d$, and hence $\|\Sigma\|_2 = 1$.

$$\mathbb{P}\left[\left\|\widehat{\Sigma} - \mathbf{I}_d\right\|_2 \geq \delta\right] \leq 2de^{-\frac{n\delta^2}{2d+2d\delta}}$$

for all $\delta \geq 0$. This bound implies that

$$\left\|\widehat{\Sigma} - \mathbf{I}_d\right\|_2 \lesssim \sqrt{\frac{d \log d}{n}} + \frac{d \log d}{n}$$

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Sparsity:6.5.1

- Suppose that the covariance matrix Σ is known to be relatively sparse, but that the positions of the non-zero entries are no longer known. Its zero pattern is captured by the adjacency matrix $\mathbf{A} \in \mathbb{R}^{d \times d}$ with entries $A_{j\ell} = \mathbb{I}[\Sigma_{j\ell} \neq 0]$. This adjacency matrix defines the edge structure of an undirected graph G on the vertices $\{1, 2, \dots, d\}$, with edge (j, ℓ) included in the graph if and only if $\Sigma_{j\ell} \neq 0$, along with the self-edges (j, j) for each of the diagonal entries.

Sparsity

- The operator norm $\|\mathbf{A}\|_2$ of the adjacency matrix provides a natural measure of sparsity. In particular, it can be verified that $\|\mathbf{A}\|_2 \leq d$, with equality holding when G is fully connected, meaning that Σ has no zero entries. More generally, we have $\|\mathbf{A}\|_2 \leq s$ whenever Σ has at most s non-zero entries per row, or equivalently when the graph G has maximum degree at most $s - 1$.

6.5.1 Unknown sparsity and thresholding

Given a parameter $\lambda > 0$, the hard-thresholding operator is given by

$$T_\lambda(u) := u\mathbb{I}[|u| > \lambda] = \begin{cases} u & \text{if } |u| > \lambda \\ 0 & \text{otherwise} \end{cases}$$

- With a minor abuse of notation, for a matrix \mathbf{M} , we write $T_\lambda(\mathbf{M})$ for the matrix obtained by applying the thresholding operator to each element of \mathbf{M} .

Thresholding-based covariance estimation

Theorem 6.23 Let $\{x_i\}_{i=1}^n$ be an i.i.d. sequence of zero-mean random vectors with covariance matrix Σ , and suppose that each component x_{ij} is sub-Gaussian with parameter at most σ . If $n > \log d$, then for any $\delta > 0$, the thresholded sample covariance matrix $T_{\lambda_n}(\widehat{\Sigma})$ with $\lambda_n/\sigma^2 = 8\sqrt{\frac{\log d}{n}} + \delta$ satisfies

$$\mathbb{P}\left[\left\|T_{\lambda_n}(\widehat{\Sigma}) - \Sigma\right\|_2 \geq 2\|\mathbf{A}\|_2\lambda_n\right] \leq 8e^{-\frac{n}{16}\min\{\delta, \delta^2\}}.$$

Proof:

- For any choice of λ_n such that $\|\Sigma - \widehat{\Sigma}\|_{\max} \leq \lambda_n$, we have
$$\left\|T_{\lambda_n}(\widehat{\Sigma}) - \Sigma\right\|_2 \leq 2\|\mathbf{A}\|_2\lambda_n$$
- $\mathbf{B} := \left|T_{\lambda_n}(\widehat{\Sigma}) - \Sigma\right| \Rightarrow \mathbf{B} \leq 2\lambda_n\mathbf{A} \Rightarrow \|\mathbf{B}\|_2 \leq 2\lambda_n\|\mathbf{A}\|_2$

The proof of the remainder of Theorem 6.23

The error matrix $\widehat{\Delta} := \widehat{\Sigma} - \Sigma$.

Lemma 6.26 Under the conditions of Theorem 6.23, we have

$$\mathbb{P} \left[\|\widehat{\Delta}\|_{\max} / \sigma^2 \geq t \right] \leq 8e^{-\frac{n}{16} \min\{t, t^2\} + 2 \log d} \quad \text{for all } t > 0.$$

Setting $t = \lambda_n / \sigma^2 = 8 \sqrt{\frac{\log d}{n}} + \delta$

Proof:

- $\frac{1}{n} \sum_{i=1}^n x_{ij}^2$ is sub-exponential so that there are universal positive constants c_1, c_2 such that

$$\mathbb{P} \left[\left| \widehat{\Delta}_{jj} \right| \geq c_1 \delta \right] \leq 2e^{-c_2 n \delta^2} \quad \text{for all } \delta \in (0, 1)$$

- $2\widehat{\Delta}_{j\ell} = \frac{2}{n} \sum_{i=1}^n x_{ij}x_{i\ell} - 2\Sigma_{j\ell} =$
 $\frac{1}{n} \sum_{i=1}^n (x_{ij} + x_{i\ell})^2 - (\Sigma_{jj} + \Sigma_{\ell\ell} + 2\Sigma_{j\ell}) - \widehat{\Delta}_{jj} - \widehat{\Delta}_{\ell\ell}$
- $\mathbb{P} \left[\left| \frac{1}{n} \sum_{i=1}^n (x_{ij} + x_{i\ell})^2 - (\Sigma_{jj} + \Sigma_{\ell\ell} + 2\Sigma_{j\ell}) \right| \geq c_3 \delta \right] \leq 2e^{-c_2 n \delta^2}$

- **Corollary 6.24** Suppose that, in addition to the conditions of Theorem 6.23, the covariance matrix Σ has at most s non-zero entries per row. Then with $\lambda_n/\sigma^2 = 8\sqrt{\frac{\log d}{n}} + \delta$ for some $\delta > 0$, we have

$$\mathbb{P}\left[\left\|T_{\lambda_n}(\widehat{\Sigma}) - \Sigma\right\|_2 \geq 2s\lambda_n\right] \leq 8e^{-\frac{n}{16}\min\{\delta, \delta^2\}}.$$

Sparsity:6.5.2

More specifically, given a parameter $q \in [0, 1]$ and a radius R_q , we impose the constraint

$$\max_{j=1,\dots,d} \sum_{\ell=1}^d |\Sigma_{j\ell}|^q \leq R_q$$

In the special case $q = 0$, this constraint is equivalent to requiring that each row of Σ have at most R_0 nonzero entries. For intermediate values $q \in (0, 1]$, it allows for many non-zero entries but requires that their absolute magnitudes (if ordered from largest to smallest) drop off relatively quickly.

Theorem 6.27 (Covariance estimation under ℓ_q -sparsity)

Suppose that the covariance matrix Σ satisfies the ℓ_q -sparsity constraint (6.58). Then for any λ_n such that $\|\widehat{\Sigma} - \Sigma\|_{\max} \leq \lambda_n/2$, we are guaranteed that

$$\left\| T_{\lambda_n}(\widehat{\Sigma}) - \Sigma \right\|_2 \leq 4R_q \lambda_n^{1-q}.$$

Consequently, if the sample covariance is formed using i.i.d. samples $\{x_i\}_{i=1}^n$ that are zero-mean with sub-Gaussian parameter at most σ , then with $\lambda_n/\sigma^2 = 8\sqrt{\frac{\log d}{n}} + \delta$, we have

$$\mathbb{P} \left[\left\| T_{\lambda_n}(\widehat{\Sigma}) - \Sigma \right\|_2 \geq 4R_q \lambda_n^{1-q} \right] \leq 8e^{-\frac{n}{16} \min\{\delta, \delta^2\}} \quad \text{for all } \delta > 0$$

Proof: Fixing an index $j \in \{1, 2, \dots, d\}$, define the set

$$S_j(\lambda_n/2) = \{\ell \in \{1, \dots, d\} \mid |\Sigma_{j\ell}| > \lambda_n/2\}.$$

- $\left\| T_{\lambda_n}(\widehat{\Sigma}) - \Sigma \right\|_2 \leq \max_{j=1, \dots, d} \sum_{\ell=1}^d \left| T_{\lambda_n}(\widehat{\Sigma}_{j\ell}) - \Sigma_{j\ell} \right|$
- $\sum_{\ell=1}^d \left| T_{\lambda_n}(\widehat{\Sigma}_{j\ell}) - \Sigma_{j\ell} \right| = \sum_{\ell \in S_j(\lambda_n)} \left| T_{\lambda_n}(\widehat{\Sigma}_{j\ell}) - \Sigma_{j\ell} \right| + \sum_{\ell \notin S_j(\lambda_n)} \left| T_{\lambda_n}(\widehat{\Sigma}_{j\ell}) - \Sigma_{j\ell} \right| \leq |S_j(\lambda_n/2)| \frac{3}{2} \lambda_n + \sum_{\ell \notin S_j(\lambda_n)} |\Sigma_{j\ell}|$
- $\sum_{\ell \notin S_j(\lambda_n/2)} |\Sigma_{j\ell}| = \frac{\lambda_n}{2} \sum_{\ell \notin S_j(\lambda_n/2)} \frac{|\Sigma_{j\ell}|}{\lambda_n/2} \stackrel{(i)}{\leq} \frac{\lambda_n}{2} \sum_{\ell \notin S_j(\lambda_n/2)} \left(\frac{|\Sigma_{j\ell}|}{\lambda_n/2} \right)^q \stackrel{(ii)}{\leq} \lambda_n^{1-q} R_q$
- $R_q \geq \sum_{\ell=1}^d |\Sigma_{j\ell}|^q \geq |S_j(\lambda_n/2)| \left(\frac{\lambda_n}{2} \right)^q$