STAT 37797: Mathematics of Data Science

Matrix concentration inequalities



Cong Ma

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Let X_1, X_2, \ldots, X_n be i.i.d. random variables, law of large numbers tells us that

$$\frac{1}{n}\sum_{l=1}^{n}X_{l} - \mathbb{E}\left[\frac{1}{n}\sum_{l=1}^{n}X_{l}\right] \to 0, \quad \text{as } n \to \infty$$

Key message:

sum of independent random variables concentrate around its mean

— how fast does it concentrate?

Consider a sequence of independent random variables $\{X_l\} \in \mathbb{R}$

- $\mathbb{E}[X_l] = 0$ $|X_l| \le B$ for each l
- variance statistic:

$$v \coloneqq \mathbb{E}\big[\big(\sum_{l} X_{l}\big)^{2}\big] = \sum_{l=1}^{n} \mathbb{E}\big[X_{l}^{2}\big]$$

Theorem 4.1 (Bernstein's inequality)

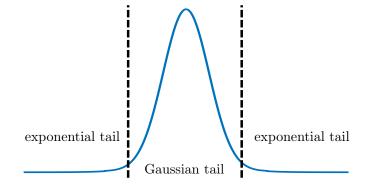
For all
$$\tau \ge 0$$
,
 $\mathbb{P}\left\{\left|\sum_{l} X_{l}\right| \ge \tau\right\} \le 2 \exp\left(\frac{-\tau^{2}/2}{v + B\tau/3}\right)$

Tail behavior

$$\mathbb{P}\left\{\left|\sum_{l} X_{l}\right| \geq \tau\right\} \leq 2\exp\left(\frac{-\tau^{2}/2}{v+B\tau/3}\right)$$

- moderate-deviation regime (τ is small): — sub-Gaussian tail behavior $\exp(-\tau^2/2v)$
- large-deviation regime (τ is large): — sub-exponential tail behavior $\exp(-3\tau/2B)$ (slower decay)
- user-friendly form (exercise): with prob. $1 O(n^{-10})$

$$\left|\sum_{l} X_{l}\right| \lesssim \sqrt{v \log n} + B \log n$$



There are exponential concentration inequalities for spectral norm of sum of independent random matrices

Matrix Bernstein inequality

Consider a sequence of independent random matrices $\{ \boldsymbol{X}_l \in \mathbb{R}^{d_1 imes d_2} \}$

- $\mathbb{E}[\mathbf{X}_l] = \mathbf{0}$ $\|\mathbf{X}_l\| \le B$ for each l
- variance statistic:

$$v := \max\left\{ \left\| \mathbb{E}\left[\sum_{l} \boldsymbol{X}_{l} \boldsymbol{X}_{l}^{\top}\right] \right\|, \left\| \mathbb{E}\left[\sum_{l} \boldsymbol{X}_{l}^{\top} \boldsymbol{X}_{l}\right] \right\| \right\}$$

Theorem 4.2 (Matrix Bernstein inequality)

For all
$$\tau \ge 0$$
,
 $\mathbb{P}\left\{\left\|\sum_{l} \mathbf{X}_{l}\right\| \ge \tau\right\} \le (d_{1} + d_{2}) \exp\left(\frac{-\tau^{2}/2}{v + B\tau/3}\right)$

Matrix Bernstein inequality

Consider a sequence of independent random matrices $\{ \boldsymbol{X}_l \in \mathbb{R}^{d_1 imes d_2} \}$

- $\mathbb{E}[\mathbf{X}_l] = \mathbf{0}$ $\|\mathbf{X}_l\| \le B$ for each l
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Theorem 4.2 (Matrix Bernstein inequality)

For all
$$\tau \ge 0$$
,
 $\mathbb{P}\left\{\left\|\sum_{l} \mathbf{X}_{l}\right\| \ge \tau\right\} \le (d_{1} + d_{2}) \exp\left(\frac{-\tau^{2}/2}{v + B\tau/3}\right)$

User-friendly form: with probability at least $1 - O((d_1 + d_2)^{-10})$

$$\left\|\sum_{l} \boldsymbol{X}_{l}\right\| \lesssim \sqrt{v \log(d_{1} + d_{2})} + B \log(d_{1} + d_{2})$$
(4.1)

This lecture: detailed introduction to matrix Bernstein

An introduction to matrix concentration inequalities — Joel Tropp '15

Outline

- Background on matrix functions
- Matrix Laplace transform method
- Matrix Bernstein inequality

Background on matrix functions

Suppose the eigendecomposition of a symmetric matrix $oldsymbol{A} \in \mathbb{R}^{d imes d}$ is

$$oldsymbol{A} = oldsymbol{U} \left[egin{array}{ccc} \lambda_1 & & & \ & \ddots & & \ & & \lambda_d \end{array}
ight] oldsymbol{U}^ op$$

Then we can define

$$f(\boldsymbol{A}) := \boldsymbol{U} \begin{bmatrix} f(\lambda_1) & & \\ & \ddots & \\ & & f(\lambda_d) \end{bmatrix} \boldsymbol{U}^\top$$

— align with our intuition about $oldsymbol{A}^k$

• Let
$$f(a) = c_0 + \sum_{k=1}^{\infty} c_k a^k$$
, then

$$f(\boldsymbol{A}) := c_0 \boldsymbol{I} + \sum_{k=1}^{\infty} c_k \boldsymbol{A}^k$$

- matrix exponential: e^A := I + ∑_{k=1}[∞] 1/k! A^k
 o monotonicity: if A ≺ H, then tr e^A H</sup>
- matrix logarithm: $\log(e^A) := A$
 - $\circ\;$ monotonicity: if $0 \preceq A \preceq H$, then $\log A \preceq \log(H)$ (does not hold for matrix exponential)

Let X be a random symmetric matrix. Then

• matrix moment generating function (MGF):

 $\boldsymbol{M}_{\boldsymbol{X}}(\boldsymbol{\theta}) := \mathbb{E}[\mathrm{e}^{\boldsymbol{\theta}\boldsymbol{X}}]$

• matrix cumulant generating function (CGF):

$$\boldsymbol{\Xi}_{\boldsymbol{X}}(\boldsymbol{\theta}) := \log \mathbb{E}[\mathrm{e}^{\boldsymbol{\theta}\boldsymbol{X}}]$$

— expectations may not exist for all θ

Matrix Laplace transform method

A key step for a scalar random variable Y: by Markov's inequality,

$$\mathbb{P}\left\{Y \ge t\right\} \le \inf_{\theta > 0} e^{-\theta t} \mathbb{E}\left[e^{\theta Y}\right]$$

This can be generalized to the matrix case

Matrix Laplace transform

Lemma 4.3

Let Y be a random symmetric matrix. For all $t \in \mathbb{R}$,

$$\mathbb{P}\left\{\lambda_{\max}(\boldsymbol{Y}) \geq t\right\} \leq \inf_{\theta > 0} e^{-\theta t} \mathbb{E}\left[\operatorname{tr} e^{\theta \boldsymbol{Y}}\right]$$

- can control the extreme eigenvalues of \boldsymbol{Y} via the trace of the matrix MGF
- similar result holds for minimum eigenvalue

For any $\theta > 0$,

$$\begin{split} \mathbb{P}\left\{\lambda_{\max}(\boldsymbol{Y}) \geq t\right\} &= \mathbb{P}\left\{e^{\theta\lambda_{\max}(\boldsymbol{Y})} \geq e^{\theta t}\right\} \\ &\leq \frac{\mathbb{E}[e^{\theta\lambda_{\max}(\boldsymbol{Y})}]}{e^{\theta t}} \qquad (\mathsf{Markov's inequality}) \\ &= \frac{\mathbb{E}[e^{\lambda_{\max}(\theta\boldsymbol{Y})}]}{e^{\theta t}} \\ &= \frac{\mathbb{E}[\lambda_{\max}(e^{\theta\boldsymbol{Y}})]}{e^{\theta t}} \qquad (e^{\lambda_{\max}(\boldsymbol{Z})} = \lambda_{\max}(e^{\boldsymbol{Z}})) \\ &\leq \frac{\mathbb{E}[\operatorname{tr} e^{\theta\boldsymbol{Y}}]}{e^{\theta t}} \end{split}$$

This completes the proof since it holds for any $\theta > 0$

The Laplace transform method is effective for controlling an independent sum when MGF decomposes

• in the scalar case where $X = X_1 + \dots + X_n$ with independent $\{X_l\}$:

$$M_X(\theta) = \mathbb{E}[e^{\theta X_1 + \dots + \theta X_n}] = \mathbb{E}[e^{\theta X_1}] \cdots \mathbb{E}[e^{\theta X_n}] = \prod_{l=1}^n M_{X_l}(\theta)$$

Issues in the matrix settings:

$$e^{X_1+X_2} \neq e^{X_1}e^{X_2}$$
 unless X_1 and X_2 commute
 $\operatorname{tr} e^{X_1+\dots+X_n} \nleq \operatorname{tr} e^{X_1}e^{X_1}\dots e^{X_n}$ for $n \ge 3$

• in the scalar case where $X = X_1 + \dots + X_n$ with independent $\{X_l\}$:

$$\Xi_X(\theta) = \log M_X(\theta) = \sum_{\substack{l=1 \\ \text{look at each } X_l \text{ separately}}}^n \log M_{X_l}(\theta) = \sum_{\substack{l \\ look \text{ at each } X_l \text{ separately}}}^n \Xi_{X_l}(\theta)$$

In matrix case, can we hope for

$$\boldsymbol{\Xi}_{\sum_{l}\boldsymbol{X}_{l}}(\boldsymbol{\theta}) = \sum_{l} \boldsymbol{\Xi}_{\boldsymbol{X}_{l}}(\boldsymbol{\theta}) \quad ?$$

- Nope; But...

Fortunately, the matrix CGF satisfies certain subadditivity rules, allowing us to decompose independent matrix components

Lemma 4.4

Consider a finite sequence $\{X_l\}_{1 \le l \le n}$ of independent random symmetric matrices. Then for any $\theta \in \mathbb{R}$,

$$\underbrace{\mathbb{E}\left[\operatorname{tr} e^{\theta \sum_{l} \boldsymbol{X}_{l}}\right]}_{\operatorname{tr} \exp\left(\boldsymbol{\Xi}_{\Sigma_{l} \boldsymbol{X}_{l}}(\theta)\right)} \leq \underbrace{\operatorname{tr} \exp\left(\sum_{l} \log \mathbb{E}\left[e^{\theta \boldsymbol{X}_{l}}\right]\right)}_{\operatorname{tr} \exp\left(\sum_{l} \boldsymbol{\Xi}_{\boldsymbol{X}_{l}}(\theta)\right)}$$

• this is a deep result — based on Lieb's Theorem!

Lieb's Theorem



Elliott Lieb

Theorem 4.5 (Lieb '73)

Fix a symmetric matrix H. Then

 $\boldsymbol{A} \mapsto \operatorname{tr} \exp(\boldsymbol{H} + \log \boldsymbol{A})$

is concave on positive-definite cone

Lieb's Theorem immediately implies (exercise: Jensen's inequality) $\mathbb{E}[\operatorname{tr}\exp(\boldsymbol{H} + \boldsymbol{X})] \leq \operatorname{tr}\exp(\boldsymbol{H} + \log \mathbb{E}[\mathrm{e}^{\boldsymbol{X}}]) \tag{4.2}$

Main observation: $\mathrm{tr}(\cdot)$ admits a variational formula

Lemma 4.6

For any $M \succeq 0$, one has $\operatorname{tr} M = \sup_{\substack{T \succ 0 \\ relative \text{ entropy is } -T \log M + T \log T - T + M}} \left[\underbrace{T \log M - T \log T + T}_{relative \text{ entropy is } -T \log M + T \log T - T + M} \right]$

$$\begin{split} \mathbb{E}[\operatorname{tr} e^{\theta \sum_{l} \boldsymbol{X}_{l}}] &= \mathbb{E}[\operatorname{tr} \exp\left(\theta \sum_{l=1}^{n-1} \boldsymbol{X}_{l} + \theta \boldsymbol{X}_{n}\right)] \\ &\leq \mathbb{E}\left[\operatorname{tr} \exp\left(\theta \sum_{l=1}^{n-1} \boldsymbol{X}_{l} + \log \mathbb{E}[e^{\theta \boldsymbol{X}_{n}}]\right)\right] \quad (\text{by (4.2)}) \\ &\leq \mathbb{E}\left[\operatorname{tr} \exp\left(\theta \sum_{l=1}^{n-2} \boldsymbol{X}_{l} + \log \mathbb{E}[e^{\theta \boldsymbol{X}_{n-1}}] + \log \mathbb{E}[e^{\theta \boldsymbol{X}_{n}}]\right)\right] \\ &\leq \cdots \\ &\leq \operatorname{tr} \exp\left(\sum_{l=1}^{n} \log \mathbb{E}[e^{\theta \boldsymbol{X}_{l}}]\right) \end{split}$$

Combining the Laplace transform method with the subadditivity of CGF yields:

Theorem 4.7 (Master bounds for sum of independent matrices)

Consider a finite sequence $\{X_l\}$ of independent random symmetric matrices. Then

$$\mathbb{P}\left\{\lambda_{\max}\left(\sum_{l} \boldsymbol{X}_{l}\right) \geq t\right\} \leq \inf_{\theta > 0} \frac{\operatorname{tr} \exp\left(\sum_{l} \log \mathbb{E}[e^{\theta \boldsymbol{X}_{l}}]\right)}{e^{\theta t}}$$

• this is a general result underlying the proofs of the matrix Bernstein inequality and beyond (e.g., matrix Chernoff)

Matrix Bernstein inequality

$$\mathbb{P}\left\{\lambda_{\max}\left(\sum_{l} \boldsymbol{X}_{l}\right) \geq t\right\} \leq \inf_{\theta > 0} \frac{\operatorname{tr}\exp\left(\sum_{l} \log \mathbb{E}[e^{\theta \boldsymbol{X}_{l}}]\right)}{e^{\theta t}}$$

To invoke the master bound, one needs to <u>control the matrix CGF</u> main step for proving matrix Bernstein Consider a sequence of independent random symmetric matrices $\{ \mathbf{X}_l \in \mathbb{R}^{d imes d} \}$

- $\mathbb{E}[\boldsymbol{X}_l] = \boldsymbol{0}$ $\lambda_{\max}(\boldsymbol{X}_l) \leq B$ for each l
- variance statistic: $v := \left\| \mathbb{E}\left[\sum_{l} X_{l}^{2} \right] \right\|$

Theorem 4.8 (Matrix Bernstein inequality: symmetric case)

For all
$$\tau \ge 0$$
,
 $\mathbb{P}\left\{\lambda_{\max}\left(\sum_{l} \mathbf{X}_{l}\right) \ge \tau\right\} \le d \exp\left(\frac{-\tau^{2}/2}{v + B\tau/3}\right)$

- left as exercise to prove extension to rectangular case

For bounded random matrices, one can control the matrix CGF as follows:

Lemma 4.9

Suppose $\mathbb{E}[\mathbf{X}] = \mathbf{0}$ and $\lambda_{\max}(\mathbf{X}) \leq B$. Then for $0 < \theta < 3/B$, $\log \mathbb{E}[e^{\theta \mathbf{X}}] \preceq \frac{\theta^2/2}{1 - \theta B/3} \mathbb{E}[\mathbf{X}^2]$

Let $g(\theta) := \frac{\theta^2/2}{1-\theta B/3}$, then it follows from the master bound that

$$\mathbb{P}\left\{\lambda_{\max}\left(\sum_{i} \mathbf{X}_{i}\right) \geq t\right\} \leq \inf_{\theta > 0} \frac{\operatorname{tr}\exp\left(\sum_{i=1}^{n} \log \mathbb{E}[e^{\theta \mathbf{X}_{i}}]\right)}{e^{\theta t}}$$

$$\stackrel{\text{Lemma 4.9}}{\leq} \inf_{0 < \theta < 3/B} \frac{\operatorname{tr}\exp\left(g(\theta)\sum_{i=1}^{n} \mathbb{E}[\mathbf{X}_{i}^{2}]\right)}{e^{\theta t}}$$

$$\leq \inf_{0 < \theta < 3/B} \frac{d \exp\left(g(\theta)v\right)}{e^{\theta t}}$$

Taking $\theta = \frac{t}{v+Bt/3}$ and simplifying the above expression, we establish matrix Bernstein

Proof of Lemma 4.9

Define $f(x) = \frac{e^{\theta x} - 1 - \theta x}{x^2}$, then for any X with $\lambda_{\max}(X) \leq B$: $e^{\theta X} = I + \theta X + (e^{\theta X} - I - \theta X) = I + \theta X + X \cdot f(X) \cdot X$ $\leq I + \theta X + f(B) \cdot X^2$

In addition, we note an elementary inequality: for any $0 < \theta < 3/B$,

$$f(B) = \frac{\mathrm{e}^{\theta B} - 1 - \theta B}{B^2} = \frac{1}{B^2} \sum_{k=2}^{\infty} \frac{(\theta B)^k}{k!} \le \frac{\theta^2}{2} \sum_{k=2}^{\infty} \frac{(\theta B)^{k-2}}{3^{k-2}} = \frac{\theta^2/2}{1 - \theta B/3}$$

$$\implies \qquad \mathrm{e}^{\theta \boldsymbol{X}} \preceq \boldsymbol{I} + \theta \boldsymbol{X} + \frac{\theta^2/2}{1 - \theta B/3} \cdot \boldsymbol{X}^2$$

Since X is zero-mean, one further has

$$\mathbb{E}\left[\mathrm{e}^{\theta \boldsymbol{X}}\right] \preceq \boldsymbol{I} + \frac{\theta^2/2}{1 - \theta B/3} \mathbb{E}[\boldsymbol{X}^2] \preceq \exp\left(\frac{\theta^2/2}{1 - \theta B/3} \mathbb{E}[\boldsymbol{X}^2]\right)$$

Finish by observing \log is monotone

Matrix concentration

Appendix: asymptotic notation

• $f(n) \lesssim g(n)$ or f(n) = O(g(n)) means

$$\limsup_{n \to \infty} \frac{|f(n)|}{|g(n)|} \leq \text{ const}$$

 $\bullet \ f(n)\gtrsim g(n) \text{ or } f(n)=\Omega(g(n)) \text{ means}$

$$\liminf_{n \to \infty} \frac{|f(n)|}{|g(n)|} \geq \text{ const}$$

$$\bullet \ f(n) \asymp g(n) \text{ or } f(n) = \Theta(g(n)) \text{ means}$$

$$f(n) \lesssim g(n) \quad \text{and} f(n) \gtrsim g(n)$$

• f(n) = o(g(n)) means

$$\lim_{n \to \infty} \frac{|f(n)|}{|g(n)|} = 0$$