Leave-one-out Analysis: An Illustrative Example

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1 Introduction

Consider the following toy example

$$M = M^* + E = U^* \Lambda^* U^{*\top} + E \in \mathbb{R}^{n \times n}.$$

Assume that M^* is a rank-r matrix, and E is symmetric, with $E_{ij} \overset{i.i.d.}{\sim} \mathcal{N}(0, \sigma^2)$. We first show how to establish ℓ_2 bound for the subspace, using $\operatorname{dist}(U, U^*) := \min_{R \in \mathcal{O}^{r \times r}} \|UR - U^*\|$.

By truncated matrix Bernstein inequality, we have with probability at least $1 - O(n^{-8})$,

$$||E|| \le 5\sigma\sqrt{n}.\tag{1}$$

Now by **Davis-Kahan** $\sin \Theta$ **Theorem**, which is

Theorem 1.1. If $||E|| \le (1 - 1/\sqrt{2}) (|\lambda_r^{\star}| - |\lambda_{r+1}^{\star}|)$, then

$$\operatorname{dist}(U, U^{\star}) \le \frac{2 \|EU^{\star}\|}{|\lambda_r^{\star}| - |\lambda_{r+1}^{\star}|} \le \frac{2 \|E\|}{|\lambda_r^{\star}| - |\lambda_{r+1}^{\star}|}.$$

Thus, if we assume that $\sigma\sqrt{n} \leq \frac{1-1/\sqrt{2}}{5}|\lambda_r^{\star}|$, then one has with high probability,

$$\operatorname{dist}(U, U^{\star}) \le \frac{2\|E\|}{|\lambda_r^{\star}|} \le \frac{10\sigma\sqrt{n}}{\lambda_r^{\star}}.$$

From Weyl's inequality, the bound (1) also implies that

$$|\lambda_i| \le ||E|| \le 5\sigma\sqrt{n}$$
, for all $i \ge r + 1$,

and

$$|\lambda_i - \lambda_i^{\star}| \le ||E|| \le 5\sigma\sqrt{n}$$
, for all $i \le r$.

$2 \quad \ell_{\infty} \text{ Performance Guarantees}$

Now we focus on the case r = 1. Our goal is to obtain bound for

$$\operatorname{dist}_{\infty}(u, u^{\star}) := \min\{\|u - u^{\star}\|_{\infty}, \|u + u^{\star}\|_{\infty}\}.$$

Let us first construct an auxiliary matrix

$$M^{(l)} := \lambda^* u^* u^{*\top} + E^{(l)}.$$

where the noise matrix $E^{(l)}$ is generated according to

$$E_{i,j}^{(l)} := \begin{cases} E_{i,j}, & \text{if } i \neq l \text{ and } j \neq l, \\ 0, & \text{else.} \end{cases}$$

Assume that $C\sigma\sqrt{n} < \lambda^*$, for sufficiently large C. For simplicity, we also assume that

$$||u - u^*||_2 = \operatorname{dist}(u, u^*),$$

 $||u^{(l)} - u^*||_2 = \operatorname{dist}(u^{(l)}, u^*), \quad 1 \le l \le n$

otherwise we simply change the sign of u or $u^{(l)}$. We claim that

$$||u - u^{(l)}||_2 = \operatorname{dist}(u, u^{(l)}).$$

To see this, we have

$$||u - u^{(l)}||_2 \le ||u - u^*||_2 + ||u^{(l)} - u^*||_2 \le \frac{20\sigma\sqrt{n}}{\lambda^*} < 1.$$

And it follows that

$$\|u + u^{(l)}\|_{2}^{2} = 2\|u\|_{2}^{2} + 2\|u^{(l)}\|_{2}^{2} - \|u - u^{(l)}\|_{2}^{2} > 1 > \|u - u^{(l)}\|_{2}^{2}$$

After the previous preparations, we state the ideas here. Since $M^{(l)}$ is very close to M, we expect that u and $u^{(l)}$ are also quite close. By the previous result, this can be shown by establishing a bound for $\operatorname{dist}(u, u^{(l)})$. Now observe that

$$u_l^{(l)} = u^{(l)\top} u^{(l)} u_l^{(l)\top} = \frac{1}{\lambda^{(l)}} u^{(l)\top} M_{\cdot l}^{(l)} = \frac{1}{\lambda^{(l)}} u^{(l)\top} M_{\cdot l}^{\star} = \frac{\lambda^{\star}}{\lambda^{(l)}} u^{(l)\top} u^{\star} u_l^{\star},$$

if $\lambda^{(l)} \approx \lambda^*$ and $u^{(l)\top}u^* \approx 1$, we have $u_l^{(l)} \approx u_l^*$. This is not hard to achieve as we already have

$$\frac{|\lambda^{(l)} - \lambda^{\star}|}{\lambda^{\star}} \le ||E||/\lambda^{\star} \le \frac{5\sigma\sqrt{n}}{\lambda^{\star}},$$

and

$$||u^{(l)} - u^{\star}||_2 \le \frac{10\sigma\sqrt{n}}{\lambda^{\star}}.$$

So we proceed as follows.

Step 1. A bound for $dist(\mathbf{u}, \mathbf{u}^{(1)})$. This kind of bound is usually established by Davis-Kahan $\sin \Theta$ Theorem. For the moment, assume the condition for Davis-Kahan holds. Since

$$\operatorname{dist}(u, u^{(l)}) \le \frac{2\|(M - M^{(l)})u^{(l)}\|_2}{\lambda^{(l)} - \max_{j \ge 2} |\lambda_j(M^{(l)})|},$$

and

$$\lambda^{(l)} - \max_{j \ge 2} |\lambda_j(M^{(l)})| \ge (\lambda^* - 5\sigma\sqrt{n}) - 5\sigma\sqrt{n} \ge \lambda^*/2,$$

we have

$$\operatorname{dist}(u, u^{(l)}) \le \frac{4\|(M - M^{(l)})u^{(l)}\|_2}{\lambda^*}$$

Now observe that

$$||(M - M^{(l)})u^{(l)}||_2 = ||(E - E^{(l)})u^{(l)}||_2$$
$$= ||e_l E_{l \cdot} u^{(l)} + u_l^{(l)} (E_{\cdot l} - E_{ll} e_l)||_2,$$

where e_l is the l-th standard basis vector. By construction, $u^{(l)}$ is **independent** of E_l , which is the key observation in leave-one-out analysis. We have

$$E_{l}.u^{(l)} \sim \mathcal{N}(0, \sigma^2 ||u^{(l)}||_2^2) = \mathcal{N}(0, \sigma^2)$$

conditioned on $u^{(l)}$. Hence, with probability at least $1 - n^{-10}$,

$$|E_l.u^{(l)}| \le 5\sigma\sqrt{\log n}, \quad 1 \le l \le n.$$

In addition, $||E_{\cdot l} - E_{ll}e_l||_2 \le ||E_{\cdot l}||_2 = ||Ee_l||_2 \le ||E||_2 ||e_l||_2 = ||E||_2 \le 5\sigma\sqrt{n}$. Consequently,

$$\begin{split} \|(M - M^{(l)})u^{(l)}\|_{2} &\leq 5\sigma\sqrt{\log n} + 5\sigma\sqrt{n}|u_{l}^{(l)}| \\ &\leq 5\sigma\sqrt{\log n} + 5\sigma\sqrt{n}\left(\|u\|_{\infty} + \|u - u^{(l)}\|_{\infty}\right) \\ &\leq 5\sigma\sqrt{\log n} + 5\sigma\sqrt{n}\left(\|u\|_{\infty} + \|u - u^{(l)}\|_{2}\right). \end{split}$$

Thus,

$$\operatorname{dist}(u, u^{(l)}) \le \frac{20\sigma\sqrt{\log n} + 20\sigma\sqrt{n}\left(\|u\|_{\infty} + \|u - u^{(l)}\|_{2}\right)}{\lambda^{\star}}$$

which implies that

$$||u - u^{(l)}||_2 \le \frac{40\sigma\sqrt{\log n} + 40\sigma\sqrt{n}||u||_{\infty}}{\lambda^*}, \quad 1 \le l \le n.$$

Now we verify the condition for Davis-Kahan, which is

$$||M - M^{(l)}|| \le (1 - 1/\sqrt{2}) \left(\lambda^{(l)} - \max_{j \ge 2} \left|\lambda_j \left(M^{(l)}\right)\right|\right).$$

It follows that

$$||M - M^{(l)}|| \le ||M - M^*|| + ||M^{(l)} - M^*||$$

$$= ||E||_2 + ||E^{(l)}||_2$$

$$\le 10\sigma\sqrt{n} \le c\lambda^* \le (1 - 1/\sqrt{2}) \left(\lambda^{(l)} - \max_{j \ge 2} \left|\lambda_j \left(M^{(l)}\right)\right|\right).$$

Step 2. Show that $\mathbf{u}_1^{(1)} \approx \mathbf{u}_1^{\star}$. It follows that

$$\begin{split} |u_l^{(l)} - u_l^\star| &= |\frac{\lambda^\star}{\lambda^{(l)}} u^{(l)\top} u^\star u_l^\star - u^{\star\top} u^\star u_l^\star| \\ &\leq \left| u_l^\star \left(\frac{\lambda^\star - \lambda^{(l)}}{\lambda^{(l)}} u^{\star\top} u^{(l)} \right) \right| + \left| u_l^\star u^{\star\top} (u^{(l)} - u^\star) \right| \\ &\leq |u_l^\star| \frac{10\sigma\sqrt{n}}{\lambda^\star} + |u_l^\star| \frac{10\sigma\sqrt{n}}{\lambda^\star} \\ &\leq \frac{20\sigma\sqrt{n}}{\lambda^\star} \|u^\star\|_\infty. \end{split}$$

Step 3. Now it is time to put everything together.

$$||u - u^{\star}||_{\infty} = \max_{l} |u_{l} - u_{l}^{\star}| \le \max_{l} \left\{ |u_{l}^{(l)} - u_{l}^{\star}| + ||u - u^{(l)}||_{2} \right\}$$

$$\le \frac{20\sigma\sqrt{n}}{\lambda^{\star}} ||u^{\star}||_{\infty} + \frac{40\sigma\sqrt{\log n} + 40\sigma\sqrt{n} ||u||_{\infty}}{\lambda^{\star}}$$

$$\le \frac{40\sigma\sqrt{\log n} + 60\sigma\sqrt{n} ||u^{\star}||_{\infty}}{\lambda^{\star}} + \frac{1}{2}||u - u^{\star}||_{\infty}.$$

Thus,

$$\|u - u^*\|_{\infty} \le \frac{80\sigma\sqrt{\log n} + 120\sigma\sqrt{n} \|u^*\|_{\infty}}{\lambda^*}.$$

This gives an entry level control.