

ERROR BOUND ON SINGULAR VALUES APPROXIMATIONS BY GENERALIZED NYSTRÖM (GN)

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$$A = U\Sigma V^*$$

Given \tilde{U} , \tilde{V} approximations of the leading singular vectors of A

$$n \begin{bmatrix} r \\ \tilde{V} \end{bmatrix}, \quad m \begin{bmatrix} r + \ell \\ \tilde{U} \end{bmatrix}$$

AIM: Approximate the leading singular values $\{\sigma_i(A)\}_{i=1}^r$

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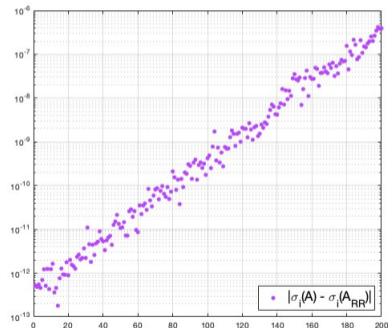
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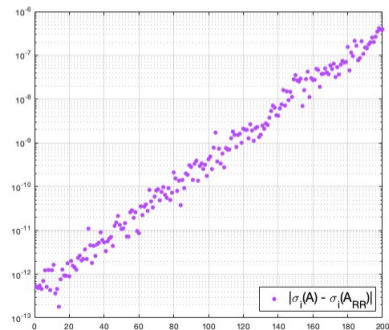
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$$\sigma_i(A) \approx \sigma_i(A_{GN, \tilde{V}, \tilde{U}}) = \sigma_i(A\tilde{V}(\tilde{U}^* A \tilde{V})^\dagger \tilde{U}^* A)$$



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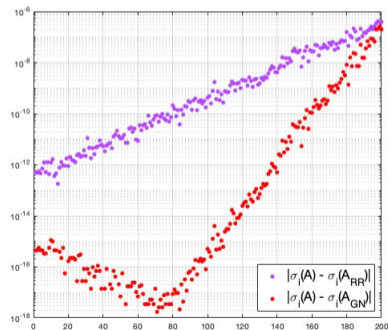
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- ① GN AS A PERTURBATION
- ② MATRIX PERTURBATION THEORY RESULT
- ③ BOUND ON GN APPROXIMATION ERROR
- ④ FUTURE WORK

GN AS A PERTURBATION

GN and Orthogonal Transformations

Consider T_1 and T_2 orthogonal matrices, then

$$T_1^*(M_{GN, \tilde{V}, \tilde{U}})T_2 = (T_1^*MT_2)_{GN, T_2^* \tilde{V}, T_1^* \tilde{U}}$$

For any orthonormal \tilde{V} and \tilde{U} , we can:

1. Define $Q_1 = \begin{bmatrix} \tilde{U} & \tilde{U}_\perp \end{bmatrix}$ $Q_2 = \begin{bmatrix} \tilde{V} & \tilde{V}_\perp \end{bmatrix}$;
2. Consider the transformed matrix: $Q_1^*AQ_2$;
3. Consider the transformed GN approximation:

$$Q_1^*A_{GN, \tilde{V}, \tilde{U}}Q_2 = (Q_1^*AQ_2)_{GN, Q_2^* \tilde{V}, Q_1^* \tilde{U}} = (Q_1^*AQ_2)_{GN, \begin{bmatrix} I_r \\ 0 \end{bmatrix}, \begin{bmatrix} I_{r+\ell} \\ 0 \end{bmatrix}}.$$

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$$\rightarrow |\sigma_i(A) - \sigma_i(A_{GN, \tilde{V}, \tilde{U}})| = |\sigma_i(Q_1^*AQ_2) - \sigma_i((Q_1^*AQ_2)_{GN, \begin{bmatrix} I_r \\ 0 \end{bmatrix}, \begin{bmatrix} I_{r+\ell} \\ 0 \end{bmatrix}})|$$

$$\tilde{V} := \begin{matrix} & r \\ r & \begin{bmatrix} I_r \\ - \\ 0 \end{bmatrix} \\ n-r & \end{matrix}, \quad \tilde{U} := \begin{matrix} & r+\ell \\ r+\ell & \begin{bmatrix} I_{r+\ell} \\ - \\ 0 \end{bmatrix} \\ m-(r+\ell) & \end{matrix}, \quad A := \begin{matrix} & r & n-r \\ r+\ell & \begin{bmatrix} A_{11} & | & A_{12} \\ - & - & - \end{bmatrix} \\ m-(r+\ell) & \begin{bmatrix} A_{21} & & A_{22} \end{bmatrix} \end{matrix}$$

Express A_{GN} as a perturbation of the original matrix A

$$A_{GN, \tilde{V}, \tilde{U}} = A\tilde{V}(\tilde{U}^*A\tilde{V})^\dagger \tilde{U}^*A$$

$$\tilde{V} := \begin{matrix} & r \\ r & \begin{bmatrix} I_r \\ - \\ 0 \end{bmatrix} \\ n-r & \end{matrix}, \quad \tilde{U} := \begin{matrix} & r+\ell \\ r+\ell & \begin{bmatrix} I_{r+\ell} \\ - \\ 0 \end{bmatrix} \\ m-(r+\ell) & \end{matrix}, \quad A := \begin{matrix} & r & n-r \\ r+\ell & \begin{bmatrix} A_{11} & | & A_{12} \\ - & & - \end{bmatrix} \\ m-(r+\ell) & \begin{bmatrix} A_{21} & & A_{22} \end{bmatrix} \end{matrix}$$

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$$A_{GN, \tilde{V}, \tilde{U}} = \begin{bmatrix} A_{11} \\ - \\ A_{21} \end{bmatrix} (A_{11})^\dagger \left[\begin{array}{c|c} A_{11} & A_{12} \end{array} \right]$$

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Express A_{GN} as a perturbation of the original matrix A

$$MM^\dagger M = M$$

$$A_{GN, \tilde{V}, \tilde{U}} = \begin{bmatrix} A_{11} \\ - \\ A_{21} \end{bmatrix} (A_{11})^\dagger \left[\begin{array}{c|c} A_{11} & A_{12} \end{array} \right] = \left[\begin{array}{c|c} A_{11} A_{11}^\dagger A_{11} & A_{11} A_{11}^\dagger A_{12} \\ \hline A_{21} A_{11}^\dagger A_{11} & A_{21} A_{11}^\dagger A_{12} \end{array} \right]$$

$$\tilde{V} := \begin{matrix} r \\ n-r \end{matrix} \begin{bmatrix} r \\ l_r \\ - \\ 0 \end{bmatrix}, \quad \tilde{U} := \begin{matrix} r+\ell \\ m-(r+\ell) \end{matrix} \begin{bmatrix} r+\ell \\ l_{r+\ell} \\ - \\ 0 \end{bmatrix}, \quad A := \begin{matrix} r & n-r \\ r+\ell & \\ m-(r+\ell) & \end{matrix} \left[\begin{array}{c|c} A_{11} & A_{12} \\ \hline A_{21} & A_{22} \end{array} \right]$$

Express A_{GN} as a perturbation of the original matrix A

M has linearly independent columns
 $\implies M^\dagger M = M^{-1}M = M$

$$A_{GN, \tilde{V}, \tilde{U}} = \begin{bmatrix} A_{11} \\ - \\ A_{21} \end{bmatrix} (A_{11})^\dagger \left[A_{11} \mid A_{12} \right] = \left[\begin{array}{c|c} \overbrace{A_{11} A_{11}^\dagger A_{11}}^{= A_{11}} & A_{11} A_{11}^\dagger A_{12} \\ \hline A_{21} A_{11}^\dagger A_{11} & A_{21} A_{11}^\dagger A_{12} \end{array} \right]$$

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Express A_{GN} as a perturbation of the original matrix A

$$A_{GN, \tilde{V}, \tilde{U}} = A - \left[\begin{array}{c|c} 0 & A_{12} - A_{11}A_{11}^\dagger A_{12} \\ \hline - & - \\ 0 & A_{22} - A_{21}A_{11}^\dagger A_{12} \end{array} \right] =: A - E_{GN}$$

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Note: No-oversample ($\ell = 0$) $\rightarrow A_{12} - A_{11}A_{11}^\dagger A_{12} = 0$, but change of block sizes!

Weyl's Theorem

For any matrix M we have that

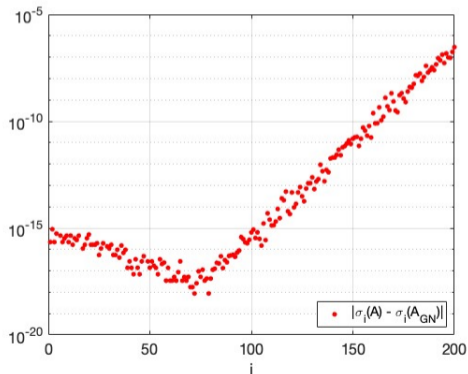
$$|\sigma_i(M) - \sigma_i(M + E)| \leq \|E\|_2$$

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$$|\sigma_i(A) - \sigma_i(A_{GN, \tilde{V}, \tilde{U}})|$$

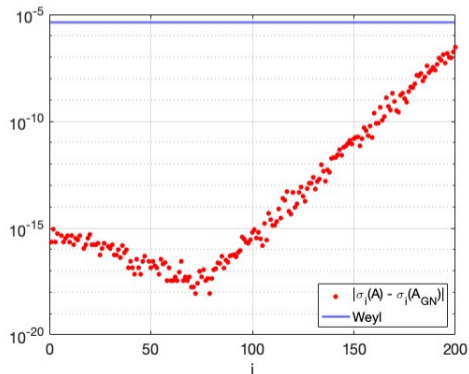


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$$|\sigma_i(A) - \sigma_i(A_{GN, \tilde{v}, \tilde{u}})| \leq \|E_{GN}\|_2$$



MATRIX PERTURBATION THEORY RESULT

Consider the $n \times n$ Hermitian matrices

$$H := \begin{bmatrix} H_{11} & H_{21}^* \\ H_{21} & H_{22} \end{bmatrix}, \quad \hat{H} := H + \begin{bmatrix} E_{11} & E_{21}^* \\ E_{21} & E_{22} \end{bmatrix} =: H + E.$$

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Theorem 3.2 (Nakatsukasa, 2012)

Define

$$\tau_i = \left(\frac{\|H_{21}\|_2 + \|E_{21}\|_2}{\min_j |\lambda_i(H) - \lambda_j(H_{22})| - 2\|E\|_2} \right).$$

Then, for each i , if $\tau_i > 0$, then

$$|\lambda_i(H) - \lambda_i(\hat{H})| \leq \|E_{11}\|_2 + 2\|E_{21}\|_2\tau_i + \|E_{22}\|_2\tau_i^2,$$

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$$|\lambda_i(H) - \lambda_i(\hat{H})| \leq \|E_{11}\|_2 + 2\|E_{21}\|_2\tau_i + \|E_{22}\|_2\tau_i^2,$$

- $\tau_i < 1$ necessary to be better than Weyl
- If $\|E_{11}\|_2 \ll \|E\|_2$ and λ_i is far from the spectrum of H_{22} then $\tau_i \ll 1$
- If $E_{11} = E_{21} = 0$ and H_{21} is small, then λ_i is particularly insensitive to the perturbation E_{22}
 \rightarrow bound proportional to $\|E_{22}\|_2 \|H_{21}\|_2^2$

Generalize (Nakatsukasa, 2012) to the non-Hermitian/rectangular case:

General case



Transform to Hermitian



Obtain necessary
structure



Apply Hermitian Result



Transform back



General Result

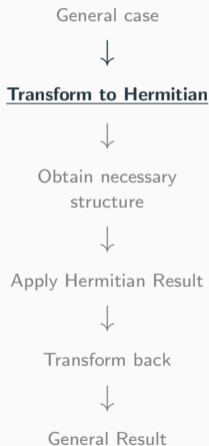
Consider the 2×2 block matrix:

$$G := \begin{bmatrix} G_1 & B \\ C & G_2 \end{bmatrix},$$

and its perturbation:

$$\hat{G} := G + \begin{bmatrix} F_{11} & F_{12} \\ F_{21} & F_{22} \end{bmatrix} =: G + F.$$

Strategy: Use a technique in (Li, Li, 2005)



Jordan-Wielandt (JW) Theorem

Let $\{\sigma_i(M)\}_{i=1}^n$ be the singular values of a matrix $M \in \mathbb{C}^{m \times n}$, with $m \geq n$. Then, the Hermitian matrix

$$\begin{bmatrix} 0 & M \\ M^* & 0 \end{bmatrix} \quad (1)$$

has eigenvalues $\pm\sigma_1(M), \dots, \pm\sigma_n(M)$ and $m - n$ zeros eigenvalues.



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$$G \rightarrow G_{JW} := \left[\begin{array}{c|c} 0 & G \\ \hline G^* & 0 \end{array} \right] = \left[\begin{array}{cc|cc} 0 & 0 & G_1 & B \\ 0 & 0 & C & G_2 \\ \hline - & - & - & - \\ G_1^* & C^* & 0 & 0 \\ B^* & G_2^* & 0 & 0 \end{array} \right]$$

General case



Transform to Hermitian



Obtain necessary structure



Apply Hermitian Result



Transform back



General Result

Obtain a matrix similar to G_{JW} suitable for (Nakatsukasa, 2012) and with blocks reasonably related to the blocks of G

$$\left[\begin{array}{cc|cc} 0 & 0 & G_1 & B \\ 0 & 0 & C & G_2 \\ \hline - & - & - & - \\ G_1^* & C^* & 0 & 0 \\ B^* & G_2^* & 0 & 0 \end{array} \right]$$

General case



Transform to Hermitian



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Apply Hermitian Result



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General case



Transform to Hermitian



Obtain necessary structure



Apply Hermitian Result



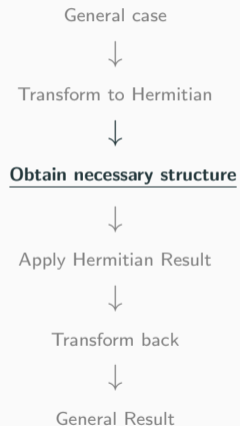
Transform back



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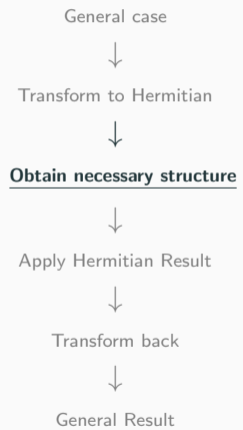
$$\left[\begin{array}{cc|cc} 0 & 0 & G_1 & B \\ G_1^* & C^* & 0 & 0 \\ \hline - & - & - & - \\ 0 & 0 & C & G_2 \\ B^* & G_2^* & 0 & 0 \end{array} \right]$$



Obtain a matrix similar to G_{JW} suitable for (Nakatsukasa, 2012) and with blocks reasonably related to the blocks of G

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Obtain a matrix similar to G_{JW} suitable for (Nakatsukasa, 2012) and with blocks reasonably related to the blocks of G



$$\left[\begin{array}{cc|cc} 0 & G_1 & 0 & B \\ G_1^* & 0 & C^* & 0 \\ \hline - & - & - & - \\ 0 & C & 0 & G_2 \\ B^* & 0 & G_2^* & 0 \end{array} \right] =: G_p$$

Note: $\lambda_i(G_p) = \lambda_i(G_{JW})^{JW} = \pm \sigma_i(G)$

General case



Transform to Hermitian



Obtain necessary structure



Apply Hermitian Result



Transform back

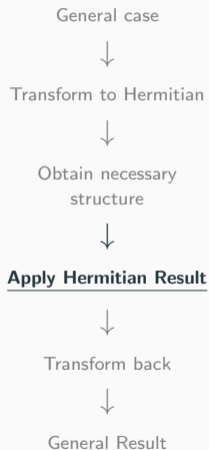


General Result

Obtain a matrix similar to G_{JW} suitable for (Nakatsukasa, 2012) and with blocks reasonably related to the blocks of G

$$G_p = \left[\begin{array}{cc|cc} 0 & G_1 & 0 & B \\ G_1^* & 0 & C^* & 0 \\ \hline 0 & C & 0 & G_2 \\ B^* & 0 & G_2^* & 0 \end{array} \right]$$

$$\hat{G}_p = G_p + \left[\begin{array}{cc|cc} 0 & F_{11} & 0 & F_{12} \\ F_{11}^* & 0 & F_{21}^* & 0 \\ \hline 0 & F_{21} & 0 & F_{22} \\ F_{12}^* & 0 & F_{22}^* & 0 \end{array} \right] =: G_p + F_p.$$

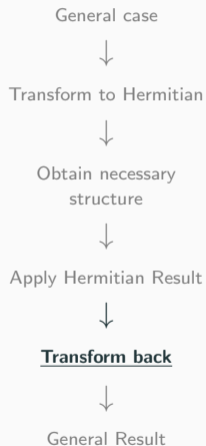


Define

$$\tau_i = \left(\frac{\left\| \begin{bmatrix} 0 & C \\ B^* & 0 \end{bmatrix} \right\|_2 + \left\| \begin{bmatrix} 0 & F_{21} \\ F_{12}^* & 0 \end{bmatrix} \right\|_2}{\min_j |\lambda_i - \lambda_j| \left(\left\| \begin{bmatrix} 0 & G_2 \\ G_2^* & 0 \end{bmatrix} \right\| - 2 \|F_p\|_2 \right)} \right).$$

Then, for each i , if $\tau_i > 0$:

$$|\lambda_i(G_p) - \lambda_i(\hat{G}_p)| \leq \left\| \begin{bmatrix} 0 & F_{11} \\ F_{11}^* & 0 \end{bmatrix} \right\|_2 + 2 \left\| \begin{bmatrix} 0 & F_{21} \\ F_{12}^* & 0 \end{bmatrix} \right\|_2 \tau_i + \left\| \begin{bmatrix} 0 & F_{22} \\ F_{22}^* & 0 \end{bmatrix} \right\|_2 \tau_i^2,$$



- $\left\| \begin{bmatrix} 0 & M_1 \\ M_2 & 0 \end{bmatrix} \right\|_2 = \max\{\|M_1\|_2, \|M_2\|_2\};$

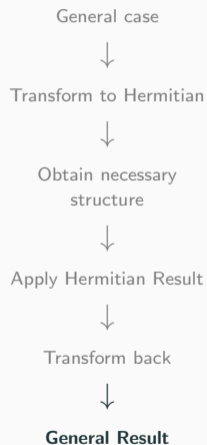
- Jordan-Wielandt theorem

$$\implies |\lambda_i(G_p) - \lambda_i(\hat{G}_p)| = |\sigma_i(G) - \sigma_i(\hat{G})|,$$

for $i = 1, \dots, n$;

- By Jordan-Wielandt theorem and by construction of F_p :

$$\|F_p\|_2 = \|F\|_2$$



Generalization of result in (Nakatsukasa, 2012)

Theorem (Al Daas, Lazzarino, Nakatsukasa)

Consider the matrices

$$G := \begin{bmatrix} G_1 & B \\ C & G_2 \end{bmatrix}, \quad \hat{G} := G + \begin{bmatrix} F_{11} & F_{12} \\ F_{21} & F_{22} \end{bmatrix} =: G + F,$$

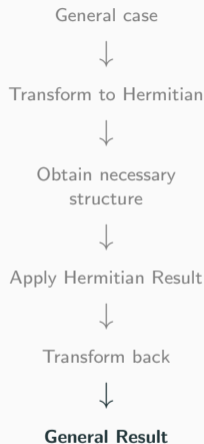
and define

$$\tau_i = \left(\frac{\max\{\|B\|_2, \|C\|_2\} + \max\{\|F_{12}\|_2, \|F_{21}\|_2\}}{\min_j |\sigma_i(G) - \sigma_j(G_2)| - 2\|F\|_2} \right).$$

Then, for each i , if $\tau_i > 0$, then

$$|\sigma_i(G) - \sigma_i(\hat{G})| \leq \|F_{11}\|_2 + 2 \max\{\|F_{12}\|_2, \|F_{21}\|_2\} \tau_i + \|F_{22}\|_2 \tau_i^2,$$

Generalization of result in (Nakatsukasa, 2012)



Theorem (Al Daas, Lazzarino, Nakatsukasa)

Consider the matrices

$$G := \begin{bmatrix} G_1 & B \\ C & G_2 \end{bmatrix}, \quad \hat{G} := G + \begin{bmatrix} F_{11} & F_{12} \\ F_{21} & F_{22} \end{bmatrix} =: G + F,$$

and define

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- **Generalization to Block Tridiagonal:** A Singular Value is insensitive to blockwise perturbation if it is well-separated from the spectrum of the diagonal blocks near the perturbed blocks.

BOUND ON GN APPROXIMATION ERROR

Use previous results to obtain a bound on GN singular values approximation error

- $A, \tilde{V}, \tilde{U} \rightarrow A_{GN} = A\tilde{V}(\tilde{U}^*A\tilde{V})^\dagger\tilde{U}^*A$

- Define $\bar{A} = [\tilde{U} \ \tilde{U}_\perp]^*A[\tilde{V} \ \tilde{V}_\perp]$, $\bar{A}_{GN} = \left([\tilde{U} \ \tilde{U}_\perp]^*A[\tilde{V} \ \tilde{V}_\perp]\right)_{GN, \begin{bmatrix} l_r \\ 0 \end{bmatrix}, \begin{bmatrix} l_{r+\ell} \\ 0 \end{bmatrix}}$

$$\Rightarrow \bar{A}_{GN} = \bar{A} - \begin{bmatrix} 0 & \bar{A}_{12} - \bar{A}_{11}\bar{A}_{11}^\dagger\bar{A}_{12} \\ 0 & \bar{A}_{22} - \bar{A}_{21}\bar{A}_{11}^\dagger\bar{A}_{12} \end{bmatrix} =: \bar{A} - E_{GN}$$

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Theorem, Bound on GN Singular Values Approximation Error (Al Daas, Lazzarino, Nakatsukasa)

Define

$$\tau_i = \frac{\max\{\|\bar{A}_{12}\|_2, \|\bar{A}_{21}\|_2\} + \left\|\bar{A}_{12} - \bar{A}_{11}\bar{A}_{11}^\dagger\bar{A}_{12}\right\|_2}{\min_j |\sigma_i(\bar{A}) - \sigma_j(\bar{A}_{22})| - 2\|E_{GN}\|_2}.$$

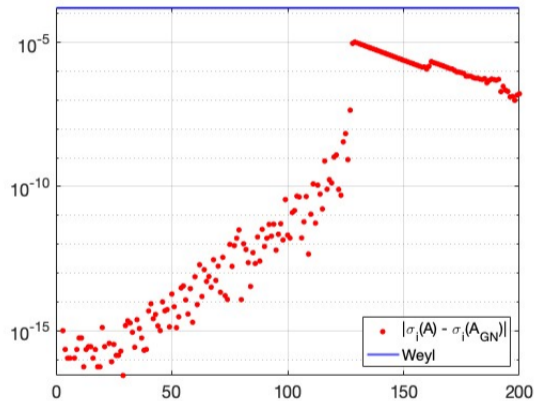
Then, for each i , if $\tau_i > 0$

$$|\sigma_i(A) - \sigma_i(A_{GN})| = |\sigma_i(\bar{A}) - \sigma_i(\bar{A}_{GN})| \leq 2 \left\|\bar{A}_{12} - \bar{A}_{11}\bar{A}_{11}^\dagger\bar{A}_{12}\right\|_2 \tau_i + \left\|\bar{A}_{22} - \bar{A}_{21}\bar{A}_{11}^\dagger\bar{A}_{12}\right\|_2 \tau_i^2$$

- $\tau_i < 1$ necessary to be better than Weyl. If $\sigma_i(\bar{A})$ is far from the spectrum of \bar{A}_{22} then $\tau_i \ll 1$

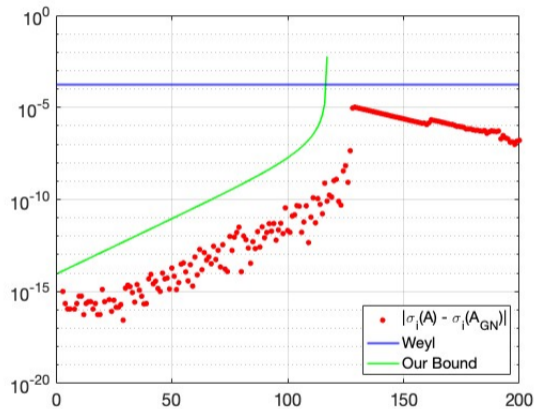
- $A \in \mathbb{R}^{1000 \times 1000}$
- U_{ex}, V_{ex} Haar Matrices
- $\sigma_i(A)$ exponentially decaying
- $[\tilde{V}, \sim] = \text{qr}(A^* \Omega, 0)$
- $[\tilde{U}, \sim] = \text{qr}(A \Omega, 0)$
- $\tilde{V} \in \mathbb{R}^{1000 \times 200}$
- $\tilde{U} \in \mathbb{R}^{1000 \times 200}$
- Compute pseudoinverses by QR factorization

$$\sigma_i(A_{GN, \tilde{V}, \tilde{U}}) = \sigma_i(A \tilde{V} (\tilde{U}^* A \tilde{V})^\dagger \tilde{U}^* A)$$



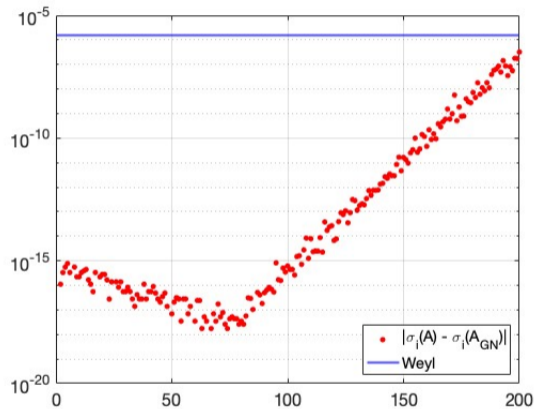
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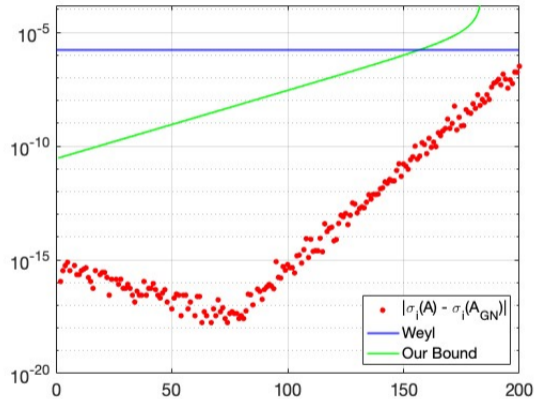
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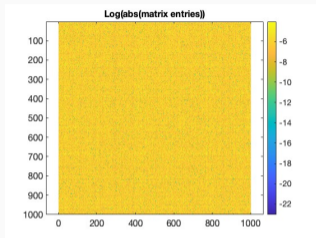


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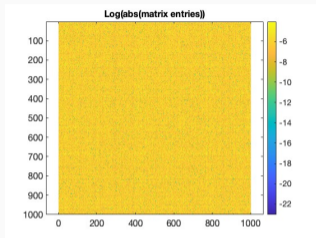
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A

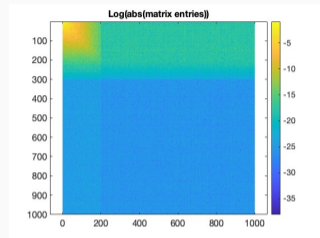


A

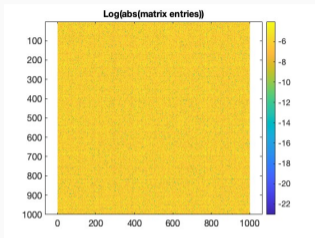


\rightarrow

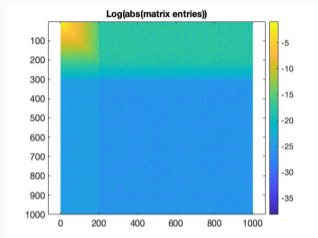
\bar{A}



A

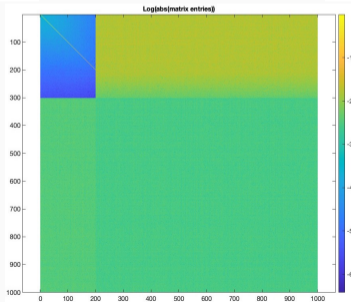


\bar{A}



\rightarrow

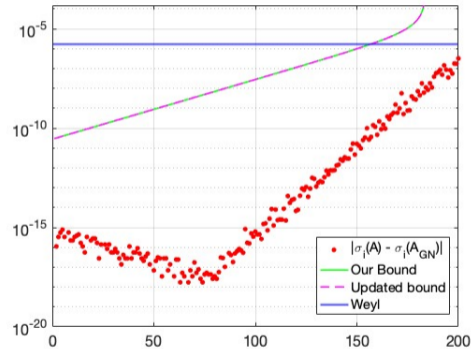
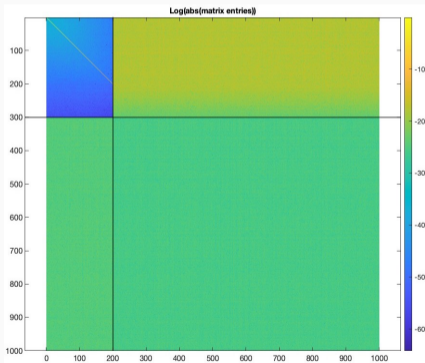
\tilde{A}



$$\tilde{V} \in \mathbb{R}^{1000 \times 200}$$

$$\tilde{U} \in \mathbb{R}^{1000 \times 300}$$

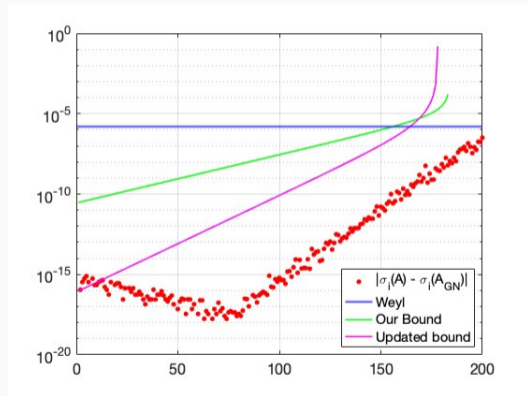
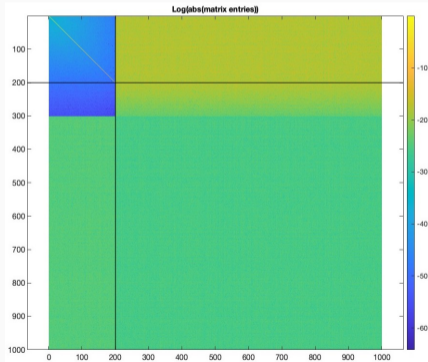
Size of \tilde{A}_{11} : 300×200



$$\tilde{V} \in \mathbb{R}^{1000 \times 200}$$

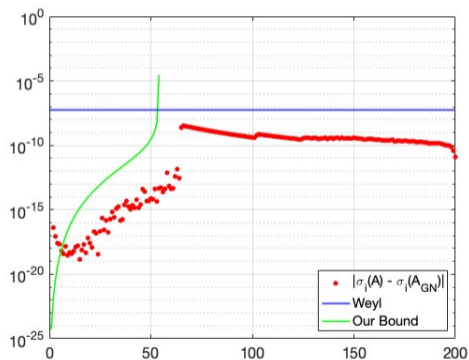
$$\tilde{U} \in \mathbb{R}^{1000 \times 300}$$

Size of \tilde{A}_{11} : 200×200

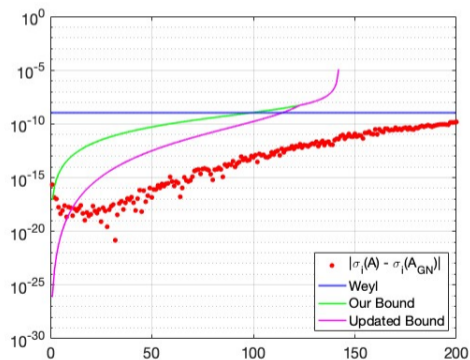


$$\sigma_i(A) = \left(\frac{1}{i}\right)^4$$

Without oversample ($\ell = 0$)



With oversample ($r + \ell = 1.5r$)



Rayleigh Ritz (RR)

$$\sigma_i(A) \approx \sigma_i(\tilde{U}^* A \tilde{V}) =: \sigma_i(A_{RR, \tilde{V}, \tilde{U}})$$

- $\bar{A} = [\tilde{U} \ \tilde{U}_\perp]^* A [\tilde{V} \ \tilde{V}_\perp]$
- $|\sigma_i(\bar{A}) - \sigma_i(\bar{A}_{RR, \begin{bmatrix} l_r \\ 0 \end{bmatrix}, \begin{bmatrix} l_r + \ell \\ 0 \end{bmatrix}})|$
- $\sigma_i(\bar{A}_{RR}) \stackrel{nnz}{=} \sigma_i\left(\bar{A} - \begin{bmatrix} 0 & \bar{A}_{12} \\ \bar{A}_{21} & \bar{A}_{22} \end{bmatrix}\right)$

\implies Perform the same analysis and derive a similar bound!

Rayleigh Ritz (RR)

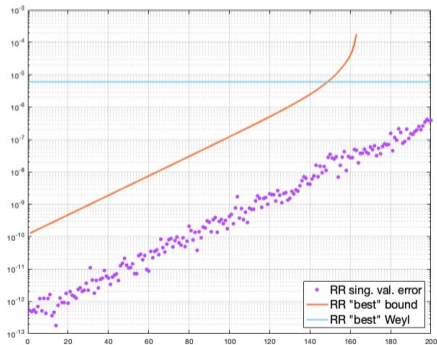
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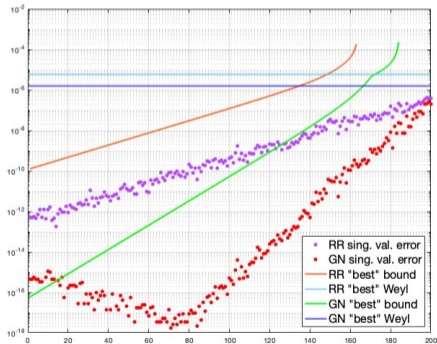
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⇒ Perform the same analysis and derive a similar bound!



Provide ideas on how to make the bound computable in practice

$$\text{For } \tau_i > 0, \quad |\sigma_i(A) - \sigma_i(A_{GN})| \leq 2 \left\| \bar{A}_{12} - \bar{A}_{11} \bar{A}_{11}^\dagger \bar{A}_{12} \right\|_2 \tau_i + \left\| \bar{A}_{22} - \bar{A}_{21} \bar{A}_{11}^\dagger \bar{A}_{12} \right\|_2 \tau_i^2$$

$$\tau_i = \frac{\max\{\|\bar{A}_{12}\|_2, \|\bar{A}_{21}\|_2\} + \left\| \bar{A}_{12} - \bar{A}_{11} \bar{A}_{11}^\dagger \bar{A}_{12} \right\|_2}{\min_j |\sigma_i(\bar{A}) - \sigma_j(\bar{A}_{22})| - 2 \|\bar{E}_{GN}\|_2}$$

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$$\text{(Backward Bound)} \quad \bar{A} = \bar{A}_{GN} + E_{GN} \implies \tau_i = \frac{\max\{\|\bar{A}_{11} \bar{A}_{11}^\dagger \bar{A}_{12}\|_2, \|\bar{A}_{12}\|_2\} + \left\| \bar{A}_{12} - \bar{A}_{11} \bar{A}_{11}^\dagger \bar{A}_{12} \right\|_2}{\min_j |\sigma_i(\bar{A}_{GN}) - \sigma_j(\bar{A}_{21} \bar{A}_{11}^\dagger \bar{A}_{12})| - 2 \|E_{GN}\|_2}$$

Provide ideas on how to make the bound computable in practice

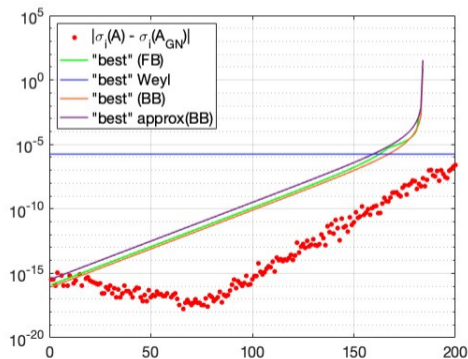
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$$\tau_i = \frac{\overbrace{\max\{\|\bar{A}_{11} \bar{A}_{11}^\dagger \bar{A}_{12}\|_2, \|\bar{A}_{12}\|_2\}}^{\leq \|\bar{A}_{12}\|_2} + \overbrace{\|\bar{A}_{12} - \bar{A}_{11} \bar{A}_{11}^\dagger \bar{A}_{12}\|_2}^{\leq \|\bar{A}_{12}\|_2}}{\min_j |\sigma_j(\bar{A}_{GN}) - \sigma_j(\bar{A}_{21} \bar{A}_{11}^\dagger \bar{A}_{12})| - 2 \|E_{GN}\|_2}$$

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FUTURE WORK

- More on the difference between oversampled and non-oversampled cases
- More on the strategy to improve the bound;
- Use bounds to formally characterize the differences in behaviors of the different techniques: GN, HMT, Rayleigh-Ritz;
- Use norm estimation strategies to make the bound fully computable.

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- More on the strategy to improve the bound;
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Thank You!

$$\tilde{V} = \text{qr}(A' * \text{randn}(1000, 200));$$

$$\tilde{U} = \text{qr}(A * \text{randn}(1000, 300));$$

Size of \tilde{A}_{11} : 180×175

