

EXTRACTING ACCURATE SINGULAR VALUES FROM APPROXIMATE SUBSPACES



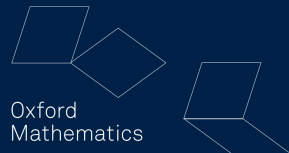
Mathematical
Institute

LORENZO LAZZARINO, HUSSAM AL DAAS, YUJI NAKATSUKASA

Mathematical Institute - University of Oxford

Computational Mathematics Theme - STFC UKRI

DUE GIORNI DI ALGEBRA LINEARE NUMERICA E APPLICAZIONI,
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EXTRACTING ACCURATE SINGULAR VALUES FROM APPROXIMATE SUBSPACES

- 1 PROBLEM SETTING AND CLASSICAL APPROACHES
- 2 GENERALIZED NYSTRÖM
- 3 MATRIX PERTURBATION THEORY RESULT
- 4 APPLICATION TO GN AND COMPARISON

PROBLEM SETTING AND CLASSICAL APPROACHES

1

PROBLEM SETTING

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

Given \tilde{U} and/or \tilde{V} approximations of the leading singular subspaces 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 $\{\sigma_i(A)\}_{i=1}^r$

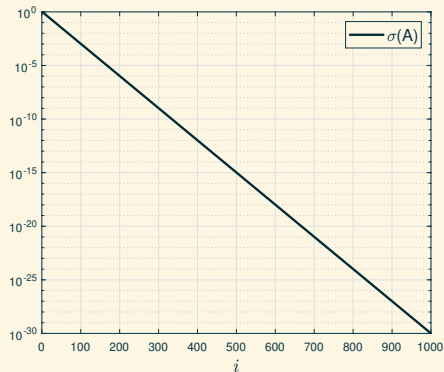
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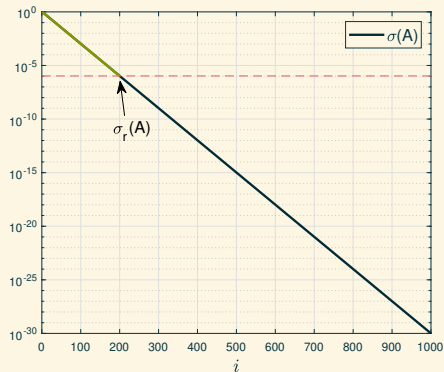
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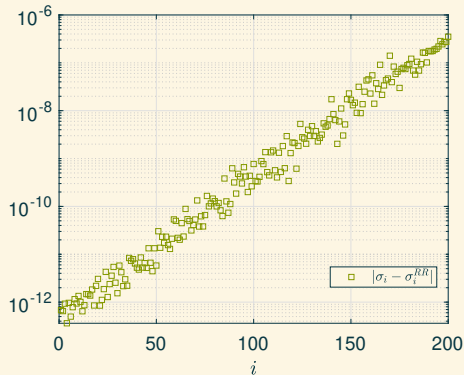
CLASSICAL APPROACHES > Rayleigh Ritz and (one-sided) SVD approximations

Rayleigh Ritz (RR)

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



(Dax, 2012)
(Saad, 2011)
(Xin-guo, 1992)



CLASSICAL APPROACHES > Rayleigh Ritz and (one-sided) SVD approximations

Rayleigh Ritz (RR)

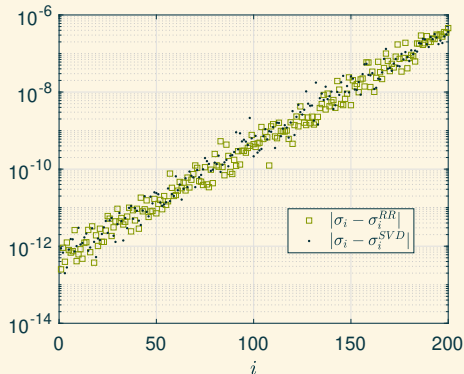
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(Dax, 2012)
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(one-sided) SVD approximations

$$\sigma_i(A) \approx \sigma_i(A \tilde{V}) =: \sigma_i(A_{SVD, \tilde{V}})$$



GENERALIZED NYSTRÖM APPROXIMATION > Motivational Comparison

Generalized Nyström

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



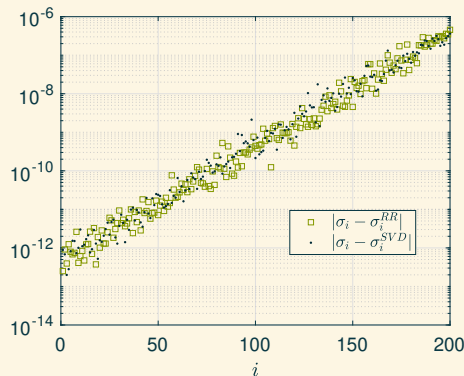
(Clarkson, Woodruff, 2009)

(Nakatsukasa, 2020)

(Woolfe, Liberty, Rokhlin, Tygert, 2008)

$$\triangleright \sigma_i^{SVD} = \sigma_i(A\tilde{V})$$

$$\triangleright \sigma_i^{RR} = \sigma_i(\tilde{U}^*A\tilde{V})$$



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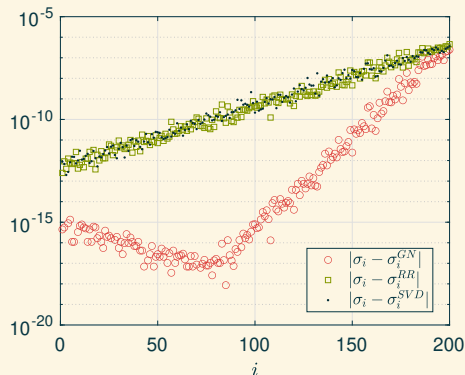
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$$\triangleright \sigma_i^{SVD} = \sigma_i(A\tilde{V})$$

$$\triangleright \sigma_i^{RR} = \sigma_i(\tilde{U}^*A\tilde{V})$$

$$\triangleright \sigma_i^{GN} = \sigma_i\left(A\tilde{V}(\tilde{U}^*A\tilde{V})^\dagger\tilde{U}^*A\right)$$



GENERALIZED NYSTRÖM

2

GN APPROXIMATION AND EXTRACTING SINGULAR VALUES

Generalized Nyström

Given approximations \tilde{U} and \tilde{V} to the leading singular subspaces,

$$\sigma_i(A) \approx \sigma_i \left(A\tilde{V}(\tilde{U}^*A\tilde{V})^\dagger \tilde{U}^*A \right) =: \sigma_i^{GN}$$

$$\sigma_i \left(\begin{array}{|c|} \hline A\tilde{V} \\ \hline \end{array} \begin{array}{|c|} \hline \tilde{U}^*A\tilde{V} \\ \hline \end{array}^\dagger \begin{array}{|c|} \hline \tilde{U}^*A \\ \hline \end{array} \right)$$

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$$\sigma_i \left(\begin{array}{c} Q_L \\ \\ \\ \end{array} \begin{array}{c} R_L \\ \\ \\ \end{array} \begin{array}{c} \tilde{U}^* A \tilde{V} \\ \\ \\ \end{array}^\dagger \begin{array}{c} R_R^* \\ \\ \\ \end{array} \begin{array}{c} Q_R^* \\ \\ \\ \end{array} \right)$$

GN APPROXIMATION AND EXTRACTING SINGULAR VALUES

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GN AND MATRIX PERTURBATION THEORY

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 $Q_1 = [\tilde{U} \quad \tilde{U}_\perp]$ $Q_2 = [\tilde{V} \quad \tilde{V}_\perp]$;
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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$$\rightarrow |\sigma_i(A) - \sigma_i(A_{GN, \tilde{V}, \tilde{U}})| = |\sigma_i(Q_1^*AQ_2) - \sigma_i((Q_1^*AQ_2)_{GN, \begin{bmatrix} I_r \\ 0 \end{bmatrix}, \begin{bmatrix} I_{r+\ell} \\ 0 \end{bmatrix}})|$$

GN AND MATRIX PERTURBATION THEORY > Express A_{GN} as a perturbation of the original matrix A

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



(Tropp, Webber, 2023)

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

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

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$$MM^\dagger M = M$$

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

GN AND MATRIX PERTURBATION THEORY > Express A_{GN} as a perturbation of the original matrix A

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

$$A_{GN, \tilde{V}, \tilde{U}} = \begin{bmatrix} A_{11} \\ - \\ A_{21} \end{bmatrix} (A_{11})^\dagger \begin{bmatrix} A_{11} & A_{12} \end{bmatrix} = \begin{bmatrix} \overbrace{A_{11} A_{11}^\dagger A_{11}}^{= A_{11}} & A_{11} A_{11}^\dagger A_{12} \\ \hline A_{21} A_{11}^\dagger A_{11} & A_{21} A_{11}^\dagger A_{12} \end{bmatrix}$$

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

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$$A_{GN, \tilde{V}, \tilde{U}} = A - \begin{bmatrix} 0 & | & A_{12} - A_{11}A_{11}^\dagger A_{12} \\ \hline & | & \\ 0 & | & A_{22} - A_{21}A_{11}^\dagger A_{12} \\ & | & \end{bmatrix} =: A - E_{GN}$$

GN AND MATRIX PERTURBATION THEORY > Express A_{GN} as a perturbation of the original matrix A

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

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

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

Weyl's Theorem

For any matrix M we have that

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



Cor. 7.3.5 (Horn, Johnson, 2012)

Cor. I.4.31 (Stewart, 1998)

Weyl's Theorem

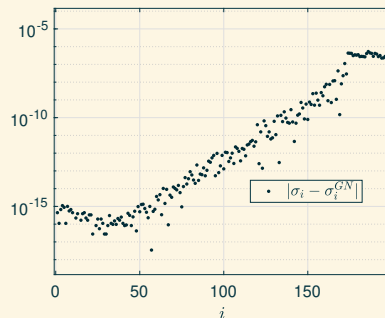
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Cor. 7.3.5 (Horn, Johnson, 2012)
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$$|\sigma_i(A) - \sigma_i(A_{GN, \tilde{V}, \tilde{U}})|$$



Weyl's Theorem

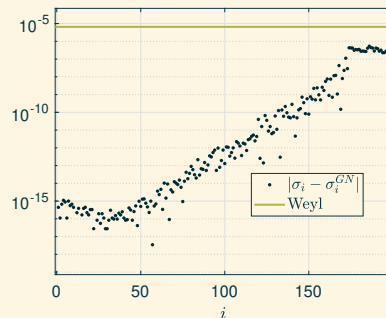
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$$|\sigma_i(A) - \sigma_i(A_{GN, \tilde{V}, \tilde{U}})| \leq \|E_{GN}\|_2$$



MATRIX PERTURBATION THEORY RESULT

3

RESULT ON SYMMETRIC MATRICES

Consider the $n \times n$ symmetric matrices

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



Theorem 3.2 (Nakatsukasa, 2012)

RESULT ON SYMMETRIC MATRICES

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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

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

RESULT ON SYMMETRIC MATRICES

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Theorem 3.2 (Nakatsukasa, 2012)

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

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

- ▶ $\tau_i < 1$ 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}
 → bound proportional to $\|E_{22}\|_2 \|H_{21}\|_2^2$

FROM THE SYMMETRIC TO THE GENERAL RESULT

General case



Transform to symmetric



Obtain necessary
structure



Apply symmetric Result



Transform back



General Result

Generalize (Nakatsukasa, 2012) to 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)

FROM THE SYMMETRIC TO THE GENERAL RESULT

General case

Transform to symmetricObtain necessary
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Apply symmetric Result



Transform back



General Result



Thm. 7.3.3 (Horn, Johnson, 2012)

Thm. I.4.2 (Stewart, Sun, 1990)

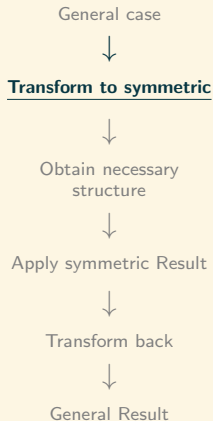
Jordan-Wielandt (JW) Theorem

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 symmetric 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.

FROM THE SYMMETRIC TO THE GENERAL RESULT



Thm. 7.3.3 (Horn, Johnson, 2012)
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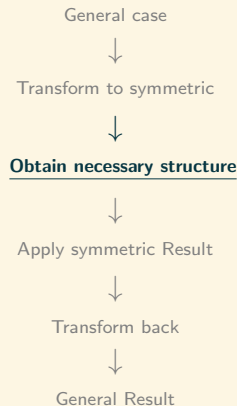
$$\begin{bmatrix} 0 & M \\ M^* & 0 \end{bmatrix} \quad (1)$$

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

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

FROM THE SYMMETRIC TO THE GENERAL RESULT

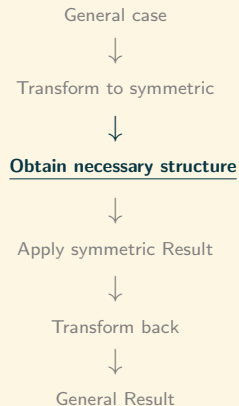
Obtain a matrix similar to G_{JW} suitable for (Nakatsukasa, 2012) and with blocks reasonably related to the blocks of G



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

FROM THE SYMMETRIC TO THE GENERAL RESULT

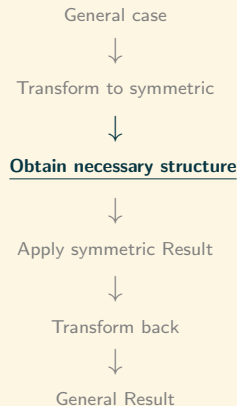
Obtain a matrix similar to G_{JW} suitable for (Nakatsukasa, 2012) and with blocks reasonably related to the blocks of G



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

FROM THE SYMMETRIC TO THE GENERAL RESULT

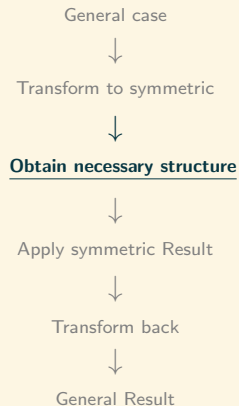
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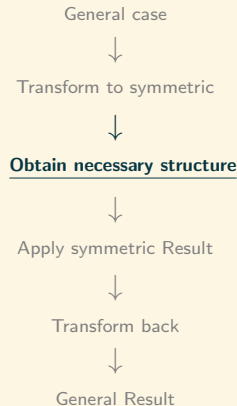
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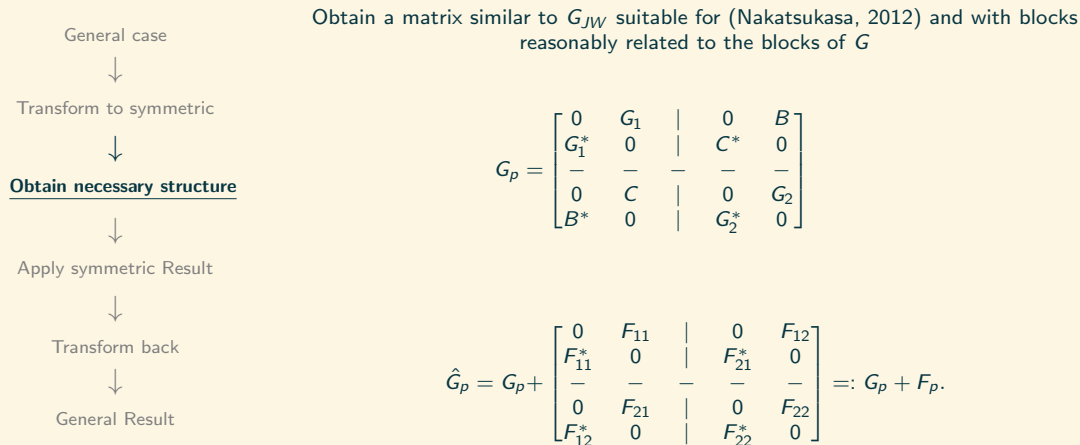
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Note: $\lambda_i(G_p) = \lambda_i(G_{JW}) \stackrel{JW}{=} \pm \sigma_i(G)$

FROM THE SYMMETRIC TO THE GENERAL RESULT



FROM THE SYMMETRIC TO THE GENERAL RESULT

General case



Transform to symmetric

Obtain necessary
structureApply symmetric Result

Transform back



General Result

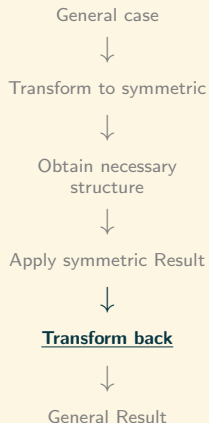
Define

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

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

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

FROM THE SYMMETRIC TO THE GENERAL RESULT



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

▶ 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 :

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

FROM THE SYMMETRIC TO THE GENERAL RESULT > Generalization of (Nakatsukasa, 2012)

General case



Transform to symmetric



Obtain necessary
structure



Apply symmetric Result



Transform back



General Result



Theorem 4.1 (L., Al Daas, Nakatsukasa, 2024)

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

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

FROM THE SYMMETRIC TO THE GENERAL RESULT > Generalization of (Nakatsukasa, 2012)

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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.

APPLICATION TO GN AND COMPARISON

4

BOUND ON GN APPROXIMATION ERROR \triangleright Derivation

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

- Define

$$\bar{A} = [\tilde{U} \ \tilde{U}_\perp]^* A [\tilde{V} \ \tilde{V}_\perp], \quad \bar{A}_{GN} = \left([\tilde{U} \ \tilde{U}_\perp]^* A [\tilde{V} \ \tilde{V}_\perp] \right)_{GN, \begin{bmatrix} I_r \\ 0 \end{bmatrix}, \begin{bmatrix} I_r \\ 0 \end{bmatrix}}$$

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

BOUND ON GN APPROXIMATION ERROR > Derivation

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Corollary 5.1
(L., Al Daas, Nakatsukasa, 2024)

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

Define

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

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

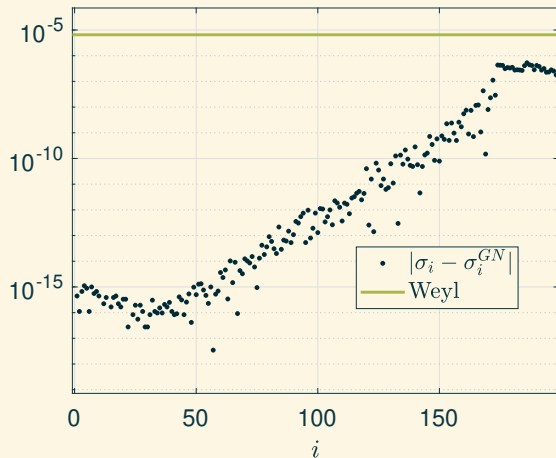
$$|\sigma_i(A) - \sigma_i(A_{GN})| = |\sigma_i(\bar{A}) - \sigma_i(\bar{A}_{GN})| \leq \left\| \bar{A}_{22} - \bar{A}_{21} \bar{A}_{11}^\dagger \bar{A}_{12} \right\|_2 \tau_i^2$$

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

BOUND ON GN APPROXIMATION ERROR > Numerical illustration

- $\ell = 0$
- $A \in \mathbb{R}^{1000 \times 1000}$
- 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

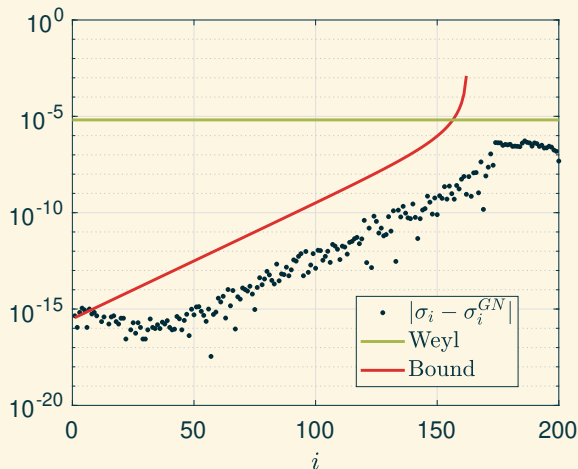
$$\sigma_i(A_{GN, \tilde{V}, \tilde{U}}) = \sigma_i(A \tilde{V} (\tilde{U}^* A \tilde{V})^\dagger \tilde{U}^* A)$$



BOUND ON GN APPROXIMATION ERROR > Numerical illustration

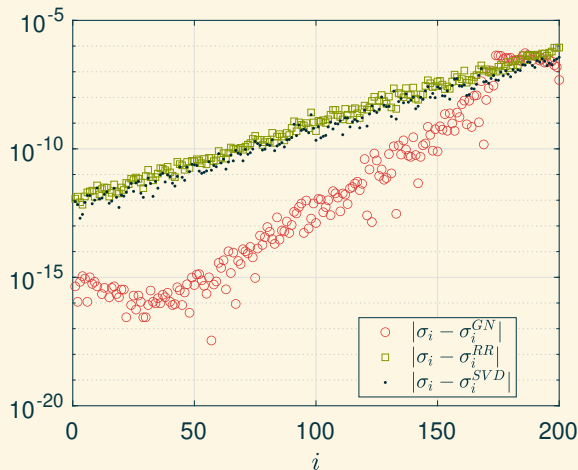
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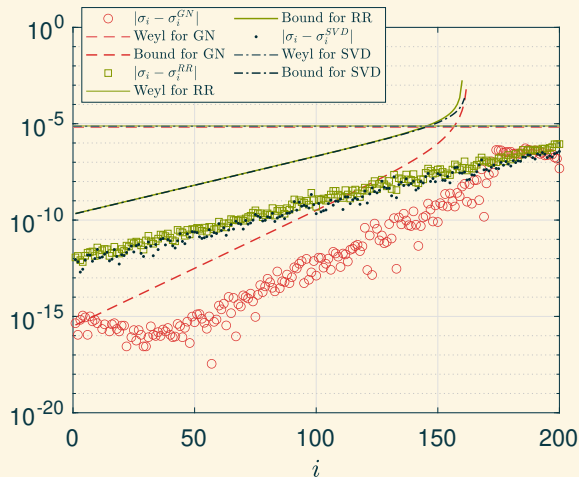
COMPARISON OF METHODS > Idea

- ▶ $\sigma_i^{SVD} = \sigma_i(A\tilde{V})$
- ▶ $\sigma_i^{RR} = \sigma_i(\tilde{U}^* A \tilde{V})$
- ▶ $\sigma_i^{GN} = \sigma_i\left(A\tilde{V}(\tilde{U}^* A \tilde{V})^\dagger \tilde{U}^* A\right)$



COMPARISON OF METHODS > Idea

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- ▶ $\sigma_i^{GN} = \sigma_i\left(A\tilde{V}(\tilde{U}^* A \tilde{V})^\dagger \tilde{U}^* A\right)$



THANK YOU!



EXTRACTING ACCURATE SINGULAR VALUES FROM APPROXIMATE SUBSPACES

LORENZO LAZZARINO, HUSSAM AL DAAS, YUJI NAKATSUKASA