EXTRACTING ACCURATE SINGULAR VALUES FROM APPROXIMATE SUBSPACES

Mathematical Institute

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Mathematical Institute - University of Oxford

Computational Mathematics Theme - STFC UKRI

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Oxford
Mathematics

PROBLEM SETTING

1

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

Given $\tilde{U}$ and/or $\tilde{V}$ (orthonormal) approximations of the leading singular subspaces of A

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

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

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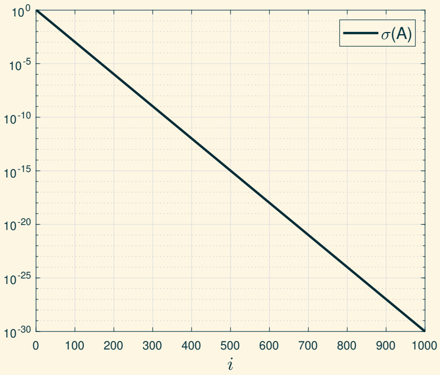

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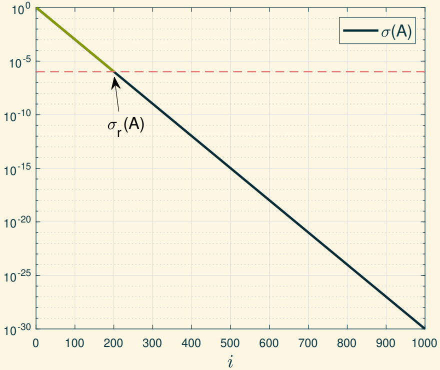

CLASSICAL APPROACHES

2

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)

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$$\bar{A} = Q_1^* A Q_2$$

$$\sigma_i(A_{RR,\tilde{V},\tilde{U}}) = \sigma_i(\bar{A}_{RR,\left[\begin{smallmatrix} I_r \\ 0 \end{smallmatrix}\right],\left[\begin{smallmatrix} I_{r+\ell} \\ 0 \end{smallmatrix}\right]})|$$

$$= \sigma_i(\bar{A}_{11}) = \sigma_i\left(\begin{bmatrix} \bar{A}_{11} & 0 \\ 0 & 0 \end{bmatrix}\right)$$

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$$\tilde{A} = AQ_2 = \begin{bmatrix} \tilde{A}_1 & \tilde{A}_2 \end{bmatrix}$$

$$\sigma_i(A_{SVD,\tilde{V}}) = \sigma_i(\tilde{A}_{SVD, \begin{bmatrix} I_r \\ 0 \end{bmatrix}})$$

$$= \sigma_i(\begin{bmatrix} \tilde{A}_1 & 0 \end{bmatrix})$$

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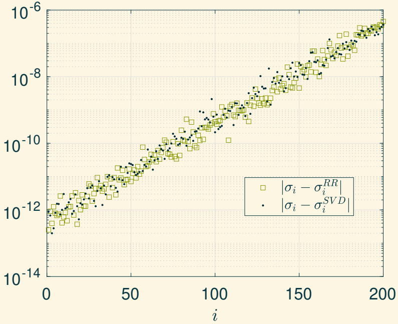

CLASSICAL APPROACHES > *Rayleigh Ritz and (one-sided) SVD approximations* > *Accuracy*

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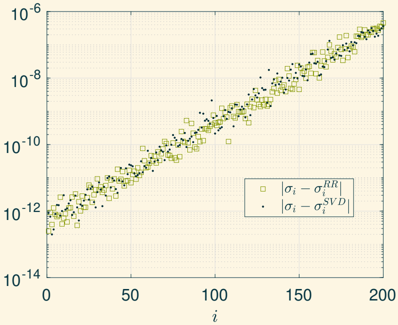

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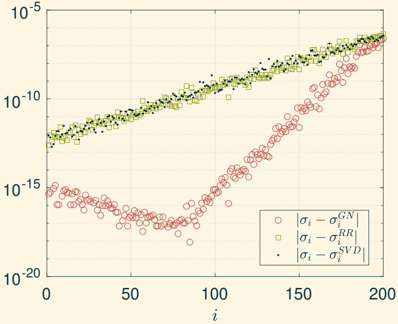

BUT,
what if we could have this?

TECHNIQUES FROM (RANDOMIZED) LOW-RANK APPROXIMATIONS

3

RANDOMIZED SVD (HMT)

Randomized SVD

$$A \approx (A\Omega)(A\Omega)^\dagger A =: A_{HMT,\Omega}$$

(Clarkson, Woodruff, 2017)
(Halko, Martinsson, Tropp, 2011)
(Rokhlin, Szlam, Tygert, 2009)

1. Choose $\Omega \in \mathbb{R}^{n\times r}$ 2. Sketch: $X = A\Omega$ 3. $[\mathrm{Q},\sim] = \mathrm{qr}(X,0)$ 4. $A_{HMT,\Omega} = Q(Q^*A)$

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- $N_r + \mathcal{O}(mr^2) + \tilde{N}_r$
- Double-pass
- 2 multiplications by A

GENERALIZED NYSTRÖM APPROXIMATION

Generalized Nyström

$$A \approx A\Omega_1(\Omega_2^* A\Omega_1)^\dagger \Omega_2^* A =: A_{GN,\Omega_1,\Omega_2}$$

(Clarkson, Woodruff, 2009)
(Nakatsukasa, 2020)
(Woolfe, Liberty, Rokhlin, Tygert, 2008)

1. Choose $\Omega_1 \in \mathbb{R}^{n\times r}, \Omega_2 \in \mathbb{R}^{m\times(r+\ell)}$
2. Two-side Sketch: $X = A\Omega_1$ and $Y = \Omega_2^* A$
3. [Q,R] $=$ qr($Y\Omega_1$,0)
4. $A_{GN,\Omega_1,\Omega_2} = (XR^{-1})(Q^* Y)$

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- $N_{2r+\ell} + \mathcal{O}(r^3 + (m+n)r^2)$
- Single-pass
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EXTRACTING SINGULAR VALUES WITH GN

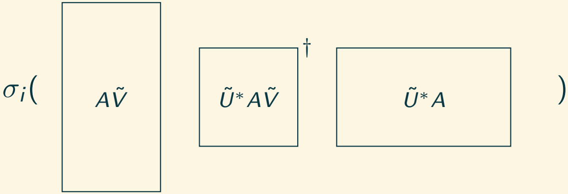
4

GN APPROXIMATION AND EXTRACTING SINGULAR VALUES

Generalized Nyström

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

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



$N_{2r+\ell}$

GN APPROXIMATION AND EXTRACTING SINGULAR VALUES

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$$\sigma_i\Big(Q_L \quad R_L \quad (\tilde{U}^*A\tilde{V})^\dagger \quad R_R^* \quad Q_R^* \Big)$$

$$N_{2r+\ell} + \mathcal{O}((m+n)r^2)$$

GN APPROXIMATION AND EXTRACTING SINGULAR VALUES

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$$\sigma_i\left(\boxed{R_L} \; \boxed{\tilde{U}^*A\tilde{V}}^{\dagger} \; \boxed{R_R^*} \right)$$

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GN APPROXIMATION AND EXTRACTING SINGULAR VALUES

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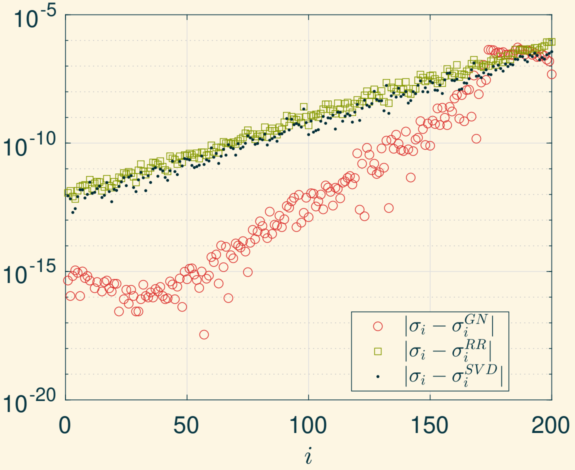
$$\sigma_i\Big(\boxed{R_L} \quad \boxed{R_p^\dagger} \quad \boxed{Q_p^*} \quad \boxed{R_R^*} \Big)$$

$$N_{2r+\ell} + \mathcal{O}((m+n)r^2)$$

MOTIVATIONAL COMPARISON

Single-pass methods

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



GN AND MATRIX PERTURBATION THEORY

GN and Orthogonal Transformations

Consider T_1 and T_2 orthogonal matrices, then

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

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

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

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

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

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

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

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

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

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

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

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$$MM^{\dagger}M = M$$

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

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

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

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

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

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

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

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

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

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

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

No-oversample ($\ell = 0$)

→ $A_{12} - A_{11}A_{11}^{\dagger}A_{12} = 0$, but change of block sizes!

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

GN AND MATRIX PERTURBATION THEORY › *Weyl's bound*

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)

GN AND MATRIX PERTURBATION THEORY › *Weyl's bound*

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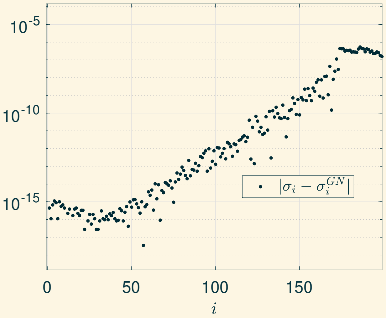
$$|\sigma_i(A) - \sigma_i(A_{GN,\tilde{V},\tilde{U}})|$$



GN AND MATRIX PERTURBATION THEORY › *Weyl's bound*

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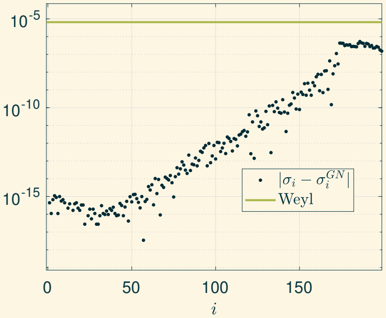

ANALYSIS AND COMPARISON

5

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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

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

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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 $\|E_{22}\|_2 \|H_{21}\|_2^2$

FROM THE SYMMETRIC TO THE GENERAL RESULT

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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 symmetric

↓

Obtain necessary structure

↓

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

$$\begin{bmatrix} 0 & M \\ M^* & 0 \end{bmatrix} \tag{1}$$

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

FROM THE SYMMETRIC TO THE GENERAL RESULT

General case

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$$\begin{bmatrix} 0 & M \\ M^* & 0 \end{bmatrix} \tag{1}$$

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

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

FROM THE SYMMETRIC TO THE GENERAL RESULT

General case

↓

Transform to symmetric

↓

Obtain necessary structure

↓

Apply symmetric 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

$$\begin{bmatrix} 0 & 0 & | & G_1 & B \\ 0 & 0 & | & C & G_2 \\ — & — & — & — & — \\ G_1^* & C^* & | & 0 & 0 \\ B^* & G_2^* & | & 0 & 0 \end{bmatrix}$$

FROM THE SYMMETRIC TO THE GENERAL RESULT

General case

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Transform to symmetric

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Apply symmetric Result

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

FROM THE SYMMETRIC TO THE GENERAL RESULT

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FROM THE SYMMETRIC TO THE GENERAL RESULT

General case

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Transform to symmetric

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$$\begin{bmatrix} 0 & 0 & | & G_1 & B \\ G_1^* & C^* & | & 0 & 0 \\ — & — & — & — & — \\ 0 & 0 & | & C & G_2 \\ B^* & G_2^* & | & 0 & 0 \end{bmatrix}$$

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FROM THE SYMMETRIC TO THE GENERAL RESULT

General case
↓
Transform to symmetric
↓
Obtain necessary structure
↓
Apply symmetric 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

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

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

FROM THE SYMMETRIC TO THE GENERAL RESULT

Mathematical Institute

General case

↓

Transform to symmetric

↓

Obtain necessary structure

↓

Apply symmetric 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

$$G_p = \begin{bmatrix} 0 & G_1 & | & 0 & B \\ G_1^* & 0 & | & C^* & 0 \\ - & - & - & - & - \\ 0 & C & | & 0 & G_2 \\ B^* & 0 & | & G_2^* & 0 \end{bmatrix}$$

$$\hat{G}_p = G_p + \begin{bmatrix} 0 & F_{11} & | & 0 & F_{12} \\ F_{11}^* & 0 & | & F_{21}^* & 0 \\ - & - & - & - & - \\ 0 & F_{21} & | & 0 & F_{22} \\ F_{12}^* & 0 & | & F_{22}^* & 0 \end{bmatrix} =: G_p + F_p.$$

FROM THE SYMMETRIC TO THE GENERAL RESULT

Oxford Mathematical Institute

General case

↓

Transform to symmetric

↓

Obtain necessary structure

↓

Apply symmetric Result

↓

Transform back

↓

General Result

Define

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

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

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

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FROM THE SYMMETRIC TO THE GENERAL RESULT

General case

↓

Transform to symmetric

↓

Obtain necessary structure

↓

Apply symmetric Result

↓

Transform back

↓

General Result

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

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

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
↓
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↓
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)*

General case

↓

Transform to symmetric

↓

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General Result

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

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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 > *Derivation*

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

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

BOUND ON GN APPROXIMATION ERROR › *Derivation*

- $A, \tilde{V}, \tilde{U} \quad \to \quad A_{GN} = A\tilde{V}(\tilde{U}^* A\tilde{V})^\dagger \tilde{U}^* A$
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$$\implies \bar{A}_{GN} = \bar{A} - \begin{bmatrix} 0 & 0 \\ 0 & \bar{A}_{22} - \bar{A}_{21}\bar{A}_{11}^\dagger \bar{A}_{12} \end{bmatrix} =: \bar{A} - E_{GN}$$

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

Define

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

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

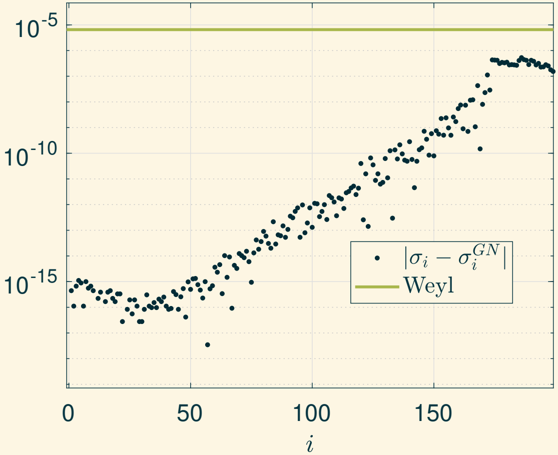
$$|\sigma_i(A) - \sigma_i(A_{GN})| = |\sigma_i(\bar{A}) - \sigma_i(\bar{A}_{GN})| \leq \left\|\bar{A}_{22} - \bar{A}_{21}\bar{A}_{11}^\dagger \bar{A}_{12}\right\|_2 \tau_i^2$$

- $\tau_i < 1$ 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
- $[\tilde{V}, \sim] = \texttt{qr}(A^*\Omega, 0)$
- $[\tilde{U}, \sim] = \texttt{qr}(A\Omega, 0)$
- $\tilde{V} \in \mathbb{R}^{1000\times 200}$
- $\tilde{U} \in \mathbb{R}^{1000\times 200}$
- 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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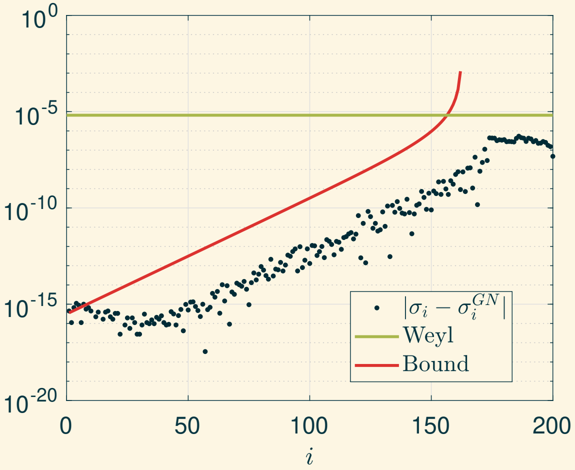

COMPARISON OF METHODS > *Idea*

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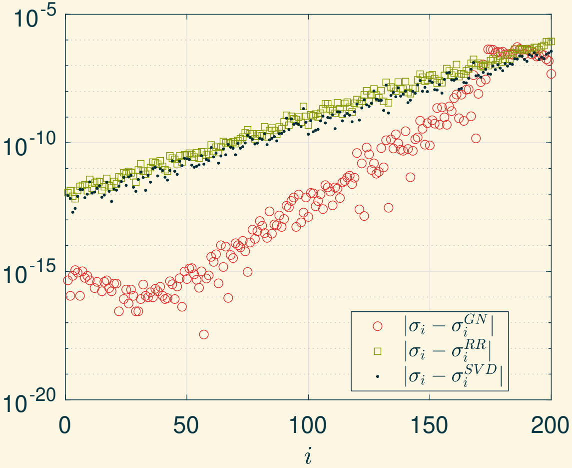
Single-pass methods

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



COMPARISON OF METHODS > *Idea*

Single-pass methods

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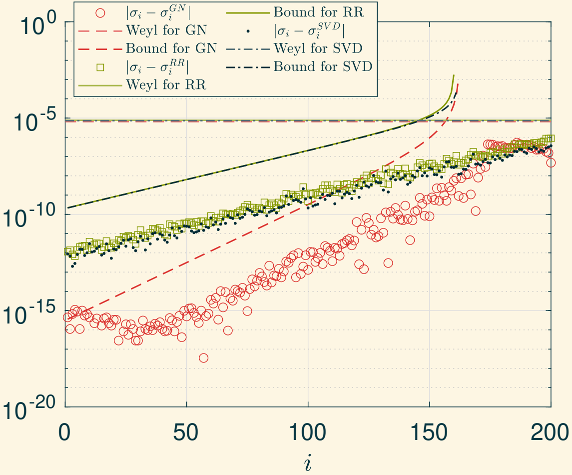

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- Similar results for oversampling case
- Different approximate singular subspaces
- Idea on how to modify bound to make it computable

Future work:

- More on the difference between oversampled and non-oversampled cases
- Use bounds to formally characterize the differences in behaviors of the different techniques: GN, HMT, Rayleigh-Ritz;

THANK YOU!

EXTRACTING ACCURATE SINGULAR VALUES FROM APPROXIMATE SUBSPACES

Lorenzo Lazzarino, Hussam Al Daas, Yuji Nakatsukasa

[1] Matrix perturbation analysis of methods for extracting singular values from approximate singular subspaces, L.L., H. Al Daas, Y. Nakatsukasa, 2024, Arxiv

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- $r + \ell = 1.5r$
- $A \in \mathbb{R}^{1000 \times 1000}$
- U_{ex}, V_{ex} Haar Matrices
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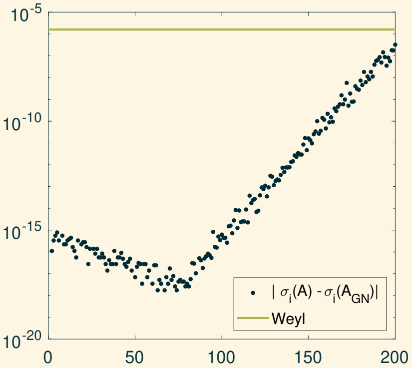
- $[\tilde{V}, \sim] = \mathtt{qr}(A^*\Omega, 0)$
- $[\tilde{U}, \sim] = \mathtt{qr}(A\Omega, 0)$
- $\tilde{V} \in \mathbb{R}^{1000 \times 200}$
- $\tilde{U} \in \mathbb{R}^{1000 \times 300}$
- Compute pseudoinverses by QR factorization

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



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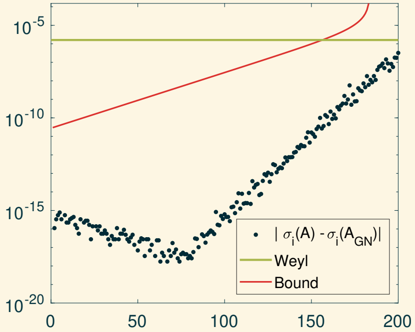
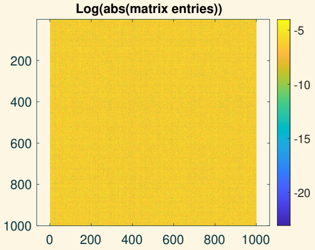
- $[\tilde{V}, \sim] = \mathtt{qr}(A^*\Omega, 0)$
- $[\tilde{U}, \sim] = \mathtt{qr}(A\Omega, 0)$
- $\tilde{V} \in \mathbb{R}^{1000 \times 200}$
- $\tilde{U} \in \mathbb{R}^{1000 \times 300}$
- Compute pseudoinverses by QR factorization

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



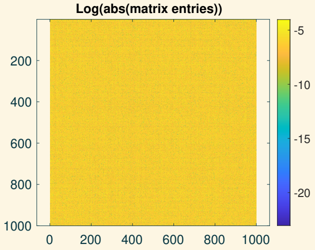
HEURISTIC BOUND FOR GN WITH OVERSAMPLE

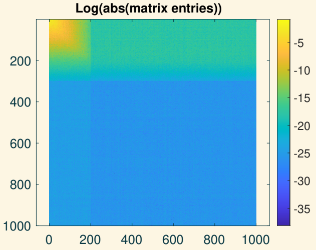
A



HEURISTIC BOUND FOR GN WITH OVERSAMPLE

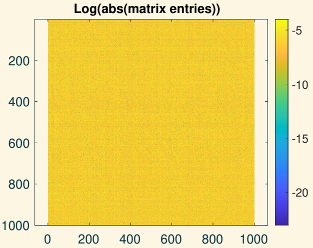
A $\rightarrow$ $\bar{A}$



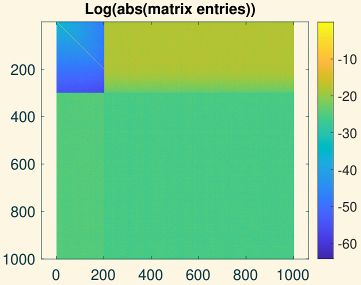


Oxford Mathematical Institute

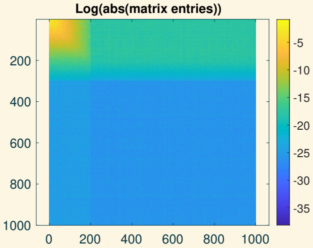
A



$\bar{\bar{A}}$

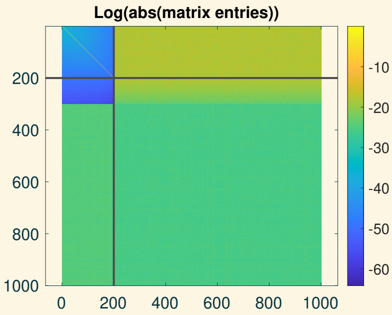


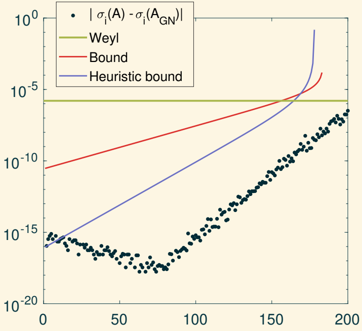
$\bar{A}$



$\tilde{V} \in \mathbb{R}^{1000 \times 200}$
$\tilde{U} \in \mathbb{R}^{1000 \times 300}$

Size of $\tilde{A}_{11}$: 200×200





Mathematical Institute

$$Q_1 = \begin{bmatrix} \tilde{U} & \tilde{U}_\perp \end{bmatrix}, \quad Q_2 = \begin{bmatrix} \tilde{V} & \tilde{V}_\perp \end{bmatrix}$$

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

$$\bar{A} = Q_1^* A Q_2$$

$$\sigma_i(A_{RR,\tilde{V},\tilde{U}}) = \sigma_i(\bar{A}_{RR, \begin{bmatrix} I_r \\ 0 \end{bmatrix}, \begin{bmatrix} I_{r+\ell} \\ 0 \end{bmatrix}})| = \sigma_i(\bar{A}_{11}) = \sigma_i\left(\begin{bmatrix} \bar{A}_{11} & 0 \\ 0 & 0 \end{bmatrix}\right)$$

$$Q_1 = \begin{bmatrix} \tilde{U} & \tilde{U}_\perp \end{bmatrix}, \quad Q_2 = \begin{bmatrix} \tilde{V} & \tilde{V}_\perp \end{bmatrix}$$

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

$$\bar{A} = Q_1^* A Q_2$$

$$\sigma_i(A_{RR,\tilde{V},\tilde{U}}) = \sigma_i(\bar{A}_{RR, \begin{bmatrix} I_r \\ 0 \end{bmatrix}, \begin{bmatrix} I_{r+\ell} \\ 0 \end{bmatrix}})| = \sigma_i(\bar{A}_{11}) = \sigma_i\left(\begin{bmatrix} \bar{A}_{11} & 0 \\ 0 & 0 \end{bmatrix}\right)$$

Define

$$\tau_i^{RR} := \frac{2\max\{\|\bar{A}_{12}\|_2, \|\bar{A}_{21}\|_2\}}{(\min_k |\sigma_i - \sigma_k(\bar{A}_{22})| - 2\|E_{RR}\|_2)} > 0$$

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

$$|\sigma_i - \sigma_i^{RR}| \leq 4 \frac{\max\{\|\bar{A}_{12}\|_2, \|\bar{A}_{21}\|_2\}^2}{\min_k |\sigma_i - \sigma_k(\bar{A}_{22})| - 2\|E_{RR}\|_2} + \|\bar{A}_{22}\|_2 \frac{4\max\{\|\bar{A}_{12}\|_2, \|\bar{A}_{21}\|_2\}^2}{(\min_k |\sigma_i - \sigma_k(\bar{A}_{22})| - 2\|E_{RR}\|_2)^2}$$

Mathematical Institute

$$Q_1 = \begin{bmatrix} \tilde{U} & \tilde{U}_\perp \end{bmatrix}, \quad Q_2 = \begin{bmatrix} \tilde{V} & \tilde{V}_\perp \end{bmatrix}$$

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

$$\bar{A} = Q_1^* A Q_2$$

$$\sigma_i(A_{RR,\tilde{V},\tilde{U}}) = \sigma_i(\bar{A}_{RR, \begin{bmatrix} I_r \\ 0 \end{bmatrix}, \begin{bmatrix} I_{r+\ell} \\ 0 \end{bmatrix}})| = \sigma_i(\bar{A}_{11}) = \sigma_i\left(\begin{bmatrix} \bar{A}_{11} & 0 \\ 0 & 0 \end{bmatrix}\right)$$

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

$$\tilde{A} = AQ_2 = \begin{bmatrix} \tilde{A}_1 & \tilde{A}_2 \end{bmatrix}$$

$$\sigma_i(A_{SVD,\tilde{V}}) = \sigma_i(\tilde{A}_{SVD, \begin{bmatrix} I_r \\ 0 \end{bmatrix}}) = \sigma_i(\begin{bmatrix} \tilde{A}_1 & 0 \end{bmatrix})$$

Define

$$\tau_i^{RR} := \frac{2\max\{\|\bar{A}_{12}\|_2, \|\bar{A}_{21}\|_2\}}{(\min_k |\sigma_i - \sigma_k(\bar{A}_{22})| - 2\|E_{RR}\|_2)} > 0$$

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

$$|\sigma_i - \sigma_i^{RR}| \leq 4 \frac{\max\{\|\bar{A}_{12}\|_2, \|\bar{A}_{21}\|_2\}^2}{\min_k |\sigma_i - \sigma_k(\bar{A}_{22})| - 2\|E_{RR}\|_2} + \|\bar{A}_{22}\|_2 \frac{4\max\{\|\bar{A}_{12}\|_2, \|\bar{A}_{21}\|_2\}^2}{(\min_k |\sigma_i - \sigma_k(\bar{A}_{22})| - 2\|E_{RR}\|_2)^2}$$

$$Q_1 = \begin{bmatrix} \tilde{U} & \tilde{U}_\perp \end{bmatrix}, \quad Q_2 = \begin{bmatrix} \tilde{V} & \tilde{V}_\perp \end{bmatrix}$$

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

$$\bar{A} = Q_1^* A Q_2$$

$$\sigma_i(A_{RR,\tilde{V},\tilde{U}}) = \sigma_i(\bar{A}_{RR, \begin{bmatrix} I_r \\ 0 \end{bmatrix}, \begin{bmatrix} I_{r+\ell} \\ 0 \end{bmatrix}})| = \sigma_i(\bar{A}_{11}) = \sigma_i\left(\begin{bmatrix} \bar{A}_{11} & 0 \\ 0 & 0 \end{bmatrix}\right)$$

Define

$$\tau_i^{RR} := \frac{2\max\{\|\bar{A}_{12}\|_2, \|\bar{A}_{21}\|_2\}}{(\min_k |\sigma_i - \sigma_k(\bar{A}_{22})| - 2\|E_{RR}\|_2)} > 0$$

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

$$|\sigma_i - \sigma_i^{RR}| \le 4 \frac{\max\{\|\bar{A}_{12}\|_2, \|\bar{A}_{21}\|_2\}^2}{\min_k |\sigma_i - \sigma_k(\bar{A}_{22})| - 2\|E_{RR}\|_2} + \|\bar{A}_{22}\|_2 \frac{4\max\{\|\bar{A}_{12}\|_2, \|\bar{A}_{21}\|_2\}^2}{(\min_k |\sigma_i - \sigma_k(\bar{A}_{22})| - 2\|E_{RR}\|_2)^2}$$

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

$$\tilde{A} = AQ_2 = \begin{bmatrix} \tilde{A}_1 & \tilde{A}_2 \end{bmatrix}$$

$$\sigma_i(A_{SVD,\tilde{V}}) = \sigma_i(\tilde{A}_{SVD, \begin{bmatrix} I_r \\ 0 \end{bmatrix}}) = \sigma_i(\begin{bmatrix} \tilde{A}_1 & 0 \end{bmatrix})$$

Define

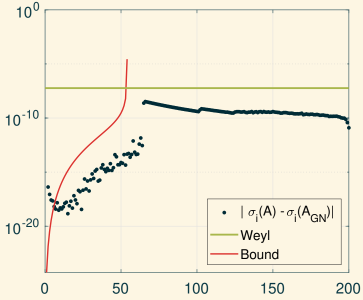
$$\tau_i^{SVD} := \frac{2\|\tilde{A}_2\|_2}{\sigma_i - 2\|E_{SVD}\|_2} > 0$$

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

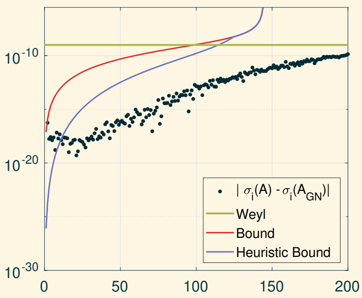
$$|\sigma_i - \sigma_i^{SVD}| \le 4 \frac{\|\tilde{A}_2\|_2^2}{\sigma_i - 2\|E_{SVD}\|_2}$$

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

Without oversample ($\ell = 0$)



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



Provide ideas on how to make the bound computable in practice

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

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

Provide ideas on how to make the bound computable in practice

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

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

Provide ideas on how to make the bound computable in practice

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

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

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

Provide ideas on how to make the bound computable in practice

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

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

Provide ideas on how to make the bound computable in practice

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

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