Verified error bounds for the singular values of structured matrices

Takeshi Terao
Kyushu University

Joint work with
Yoshitaka Watanabe (Kyushu University) and
Katsuhisa Ozaki (Shibaura Institute of Technology).

FJWNC 2025
2025/3/14

Introduction

- $A \in \mathbb{R}^{n\times n}$ is nonsingular and $B \in \mathbb{R}^{n\times n}$ is symmetric positive definite.
- The structured matrix is given by

$$RA^{-1}R^T, \tag{1}$$

  where $B = R^T R$.
- This study aims to compute bounds on the spectral norm of the structured matrix:

$$\underline{\rho} \leq \|RA^{-1}R^T\| \leq \overline{\rho}. \tag{2}$$

- This problem arises in the verified numerical computation of differential equations.

Previous Work

- Suppose $\mathtt{R}$ is an interval matrix enclosing R.
- $\mathtt{R}$ can be computed via interval Cholesky decomposition (e.g., the *verchol* function in VERSOFT[1]).
- Using INTLAB/MATLAB[2], we can compute an enclosure of $\rho = \|RA^{-1}R^T\|$ as follows:

```
X = A\R';            (3)
Y = R * X;           (4)
rho = norm(Y);       (5)
```

[1] G. Alefeld, G. Mayer, "The Cholesky method for interval data", Linear Algebra and its Applications, Vol. 194, 1993.

[2] S. M. Rump, "INTLAB - INTerval LABoratory", in: T. Csendes (Ed.), Developments in Reliable Computing, Kluwer Academic Publishers, Dordrecht, 1999, pp. 77–104

Proposed Method

Outline of the Proposed Method

- The proposed method considers the inverse of the structured matrix, defined as

$$S := R^{-T} A R^{-1}. \tag{6}$$

- Let σ_i be the ith largest singular value of S. We propose a method to verify σ_i:

$$\underline{\sigma}_i \leq \sigma_i \leq \overline{\sigma}_i, \quad i = 1, 2, \ldots, n. \tag{7}$$

- If an enclosure for σ_1 is obtained and $0 < \underline{\sigma}_1$ holds, then:

$$\frac{1}{\overline{\sigma}_1} \leq \|RA^{-1}R^T\| \leq \frac{1}{\underline{\sigma}_1}. \tag{8}$$

Variant Singular Value Decomposition

- Let A and B be given matrices.
- We consider the decomposition

$$U^T A V = \Sigma, \tag{9}$$

$$U^T B U = V^T B V = I, \tag{10}$$

where I is the identity matrix, and Σ is a diagonal matrix with nonnegative entries satisfying

$$\Sigma_{11} \geq \Sigma_{22} \geq \cdots \geq \Sigma_{nn} \geq 0. \tag{11}$$

- Then, we have $\Sigma_{ii} = \sigma_i$ for all i.

Variant Singular Value Decomposition

- Let $\widehat{U}$, $\widehat{V}$, and $\widehat{\Sigma}$ be approximations of U, V, and Σ, respectively.
- We expect the following approximations to hold:

$$\widehat{U}^T A \widehat{V} \approx \widehat{\Sigma}, \tag{12}$$

$$\widehat{U}^T B \widehat{U} \approx \widehat{V}^T B \widehat{V} \approx I. \tag{13}$$

- $\widehat{U}$, $\widehat{V}$, and $\widehat{\Sigma}$ can be computed using the following MATLAB code:

```
R = chol(B);                      (14)
[U, S, V] = svd(R'\A / R);        (15)
U = R\U; V = R\V;                 (16)
```

- Next, we present a verification method for the diagonal elements of Σ.

Verification Theory

- Define

$$\alpha := \|\widehat{U}^T B \widehat{U} - I\|, \tag{17}$$

$$\beta := \|\widehat{V}^T B \widehat{V} - I\|, \tag{18}$$

$$\gamma := \|\widehat{U}^T A \widehat{V} - \widehat{\Sigma}\|. \tag{19}$$

- If $\alpha, \beta < 1$, then the following inequality holds:

$$\frac{(\widehat{\Sigma})_{ii} - \gamma}{\sqrt{(1+\alpha)(1+\beta)}} \le \sigma_i(S) \le \frac{(\widehat{\Sigma})_{ii} + \gamma}{\sqrt{(1-\alpha)(1-\beta)}}. \tag{20}$$

- If $(\widehat{\Sigma})_{nn} > \gamma$, we obtain the following enclosure for $\rho = \|RA^{-1}R^T\|$:

$$\frac{\sqrt{(1-\alpha)(1-\beta)}}{(\widehat{\Sigma})_{nn} + \gamma} \le \rho \le \frac{\sqrt{(1+\alpha)(1+\beta)}}{(\widehat{\Sigma})_{nn} - \gamma}. \tag{21}$$

For Complex Matrices

- Consider complex matrices $A, B \in \mathbb{C}^{n\times n}$. We define their real representations as

$$A_r := \begin{pmatrix} \mathrm{Re}(A) & -\mathrm{Im}(A) \\ \mathrm{Im}(A) & \mathrm{Re}(A) \end{pmatrix}, \tag{22}$$

$$B_r := \begin{pmatrix} \mathrm{Re}(B) & -\mathrm{Im}(B) \\ \mathrm{Im}(B) & \mathrm{Re}(B) \end{pmatrix}. \tag{23}$$

- If $B_r = R_r^T R_r$, then the following relation holds:

$$\sigma_n(R^{-T} A R^{-1}) = \sigma_{2n}(R_r^{-T} A_r R_r^{-1}). \tag{24}$$

Summary of SVD-Based Method

- The proposed method does not require interval Cholesky decomposition.
- As a result, the proposed method achieves high numerical stability and computational efficiency.
- However, even if A and B are sparse, the computed matrices $\widehat{U}$ and $\widehat{V}$ tend to be dense.
- To address this issue, we propose a verification method that does not rely on singular value decomposition.

For sparse matrices

Sylvester's Law of Inertia

- Consider a symmetric matrix A and a nonsingular matrix L.
- Then, A and $S^T AS$ have the same inertia, meaning that they have the same number of negative, zero, and positive eigenvalues.
- Moreover, a symmetric matrix A can be factorized as

$$A = LDL^T, \tag{25}$$

  where L is unit lower triangular and D is diagonal.
- A and D have the same inertia.
- Based on this theorem, N. Yamamoto proposed an efficient and simple verification method for the eigenvalue problem. [3]

---

[3] N. Yamamoto: A simple method for error bounds of eigenvalues of symmetric matrices, Linear Alg. Appl., 324 (2001), 227–234.

Verification for Symmetric Eigenvalue Problem

- Let $A \in \mathbb{R}^{n \times n}$ be a given symmetric matrix ($A = A^T$).
- Let $\lambda_{\min}$ denote the smallest eigenvalue of A in absolute value.
- For α_1, α_2 satisfying $\alpha_1 < \alpha_2$, assume that

$$A + \alpha_1 I \approx \widehat{L}_1 \widehat{D}_1 \widehat{L}_1^T, \quad \delta_1 = \|A + \alpha_1 I - \widehat{L}_1 \widehat{D}_1 \widehat{L}_1^T\|, \tag{26}$$

$$A + \alpha_2 I \approx \widehat{L}_2 \widehat{D}_2 \widehat{L}_2^T, \quad \delta_2 = \|A + \alpha_2 I - \widehat{L}_2 \widehat{D}_2 \widehat{L}_2^T\|. \tag{27}$$

- If $\widehat{D}_1, \widehat{D}_2$, and A have the same inertia, then:

$$\lambda_{\min} \geq \min(|\alpha_1| - \delta_1, |\alpha_2| - \delta_2). \tag{28}$$

- Conversely, if $\widehat{D}_i$ ($i \in \{1, 2\}$) and A do not have the same inertia, then:

$$\lambda_{\min} \leq |\alpha_i| + \delta_i. \tag{29}$$

Augmented Matrix

- For a square matrix A, consider the augmented matrix:

$$\bar{A} = \begin{pmatrix} O & A^T \\ A & O \end{pmatrix}. \tag{30}$$

- Let $\lambda_i(\bar{A})$ be the eigenvalues of $\bar{A}$, and let $\sigma_i(A)$ be the singular values of A.
- Then, the following relation holds:

$$\{\lambda_i(\bar{A}) \mid 1 \leq i \leq 2n\} = \{\pm\sigma_j(A) \mid 1 \leq j \leq n\}. \tag{31}$$

- The inertia of $\bar{A}$ is $(n, 0, n)$ for nonsingular A.

Verification for Generalized Eigenvalue Problem

- Define

$$\bar{A} = \begin{pmatrix} O & A^T \\ A & O \end{pmatrix}, \quad \bar{B} = \begin{pmatrix} B & O \\ O & B \end{pmatrix}. \tag{32}$$

- The matrix $\bar{A}$ is symmetric, and $\bar{B}$ is symmetric positive definite.
- For the generalized eigenvalue problem $\bar{A}x_i = \lambda_i \bar{B} x_i$, we have the following relation:

$$\{\lambda_i\}_{1 \le i \le 2n} = \{\pm \sigma_j\}_{1 \le j \le n}, \tag{33}$$

where σ_j denotes the singular values of $R^{-T} A R^{-1}$.

Proposed Method

- Consider

$$G(\theta) = \begin{pmatrix} \theta B & A^T \\ A & \theta B \end{pmatrix} \approx \widehat{L}\widehat{D}\widehat{L}^T. \tag{34}$$

- If the inertia of $G(\theta)$ is $(n, 0, n)$, then we have:

$$\sigma_n \geq |\theta| - \|G(\theta) - \widehat{L}\widehat{D}\widehat{L}^T\|. \tag{35}$$

- This follows from the factorization:

$$\begin{pmatrix} \theta B & A^T \\ A & \theta B \end{pmatrix} = \begin{pmatrix} R^T & O \\ O & R^T \end{pmatrix} \begin{pmatrix} \theta I & (R^{-T}AR^{-1})^T \\ R^{-T}AR^{-1} & \theta I \end{pmatrix} \begin{pmatrix} R & O \\ O & R \end{pmatrix}. \tag{36}$$

Numerical results
(random matrices)

Computer environment

- CPU: Intel Xeon Platinum 8490H (60 cores, 1.90 GHz - 3.50 GHz) $\times$ 2 sockets
- Memory: 512 GiB
- Software: MATLAB 2024a, INTLAB V13, VERSOFT

Numerical experiment

表 **1:** Comparison of relative errors and elapsed times [sec] of the verification methods

	Relative error of ρ		Elapsed times [sec]		
n	Previous	Proposed	Previous	Proposed	Speedup
2,500	5.12e-06	3.85e-07	26.46	1.34	18.80
5,000	5.13e-06	3.80e-06	202.33	7.44	24.93
10,000	5.13e-06	4.54e-06	3,285.43	45.48	48.20
20,000	5.13e-06	4.84e-05	26,964.60	237.38	65.79

- $\mathtt{A} = \mathtt{randn}(\mathtt{n}); \mathtt{C} = \mathtt{randn}(\mathtt{n}); \mathtt{B} = \mathtt{n} * \mathtt{eye}(\mathtt{n}) + (\mathtt{C} + \mathtt{C}') * 0.5;$

Numerical experiment

表 **2:** Comparison of relative errors of the verification methods ($n = 1000$)

$\kappa_2(B)$	Relative error of ρ Previous	Relative error of ρ Proposed
10^1	2.11e-02	5.26e-08
10^3	failed	3.14e-07
10^6	failed	4.69e-04
10^9	failed	1.15e-01
10^{12}	failed	inf

- $\mathtt{A} = \mathtt{randn(n)}; \mathtt{B} = \mathtt{gallery('randsvd', n, -cnd, 3, n-1, n-1, 1)};$

Numerical experiment

表 **3:** Comparison of the relative errors of the verification methods ($n = 1000$)

$\kappa_2(A)$	Relative error of $\sigma_{\min}^{-1}$ Previous	Proposed
10^1	5.34e-06	7.71e-11
10^3	5.22e-06	4.09e-09
10^6	5.17e-06	2.87e-06
10^9	5.16e-06	2.34e-03
10^{12}	1.34e-05	inf

- $\mathtt{A = gallery('randsvd', n, cnd, mode, n-1, n-1, 1);}$
- $\mathtt{C = randn(n); B = n * eye(n) + (C + C') * 0.5;}$

Numerical results
(sparse matrices)

Finite Element Approximation for an Elliptic Operator

- Consider a convex bounded polygonal domain $\Omega \subset \mathbb{R}^d$ $(d = 1, 2)$.
- Define the Sobolev space $H_0^1(\Omega) := \{u \in H^1(\Omega) \mid u = 0$ on $\partial\Omega\}$.
- Define the linear elliptic operator:

$$\mathscr{L}u := -\Delta u + b \cdot \nabla u + cu : \quad H^2(\Omega) \cap H_0^1(\Omega) \to L^2(\Omega) \tag{37}$$

  for $b \in L^\infty(\Omega)^d$, $c \in L^\infty(\Omega)$.
- The invertibility and norm bound of $\mathscr{L}^{-1}$ are crucial for computer-assisted proofs.

Takeshi Terao, Yoshitaka Watanabe, and Katsuhisa Ozaki.“Verified error bounds for the singular values of structured matrices with applications to computer-assisted proofs for differential equations.” arXiv preprint arXiv:2502.09984 (2025).

Finite Element Approximation

- Let S_h be a finite element subspace of $H_0^1(\Omega)$ with basis functions $\phi_i i = 1^N$, where $N = \dim S_h$.
- Define $N \times N$ matrices A and B:

$$[A]_{ij} = (\nabla\phi_j, \nabla\phi_i)_{L^2} + (b \cdot \nabla\phi_j + c\phi_j, \phi_i)_{L^2}, \; [B]_{ij} \quad = (\nabla\phi_j, \nabla\phi_i)_{L^2}. \tag{38}$$

- The matrix B is positive definite.
- Results for $(R, c) = (5, -15)$ and $(R, c) = (6.75, -1 - 1.5i)$ from a convection-diffusion equation.

Numerical experiment

表 **4:** Upper bounds of $\sigma_{\min}^{-1}$ and the computation times of the verification methods. The matrices are real.

n	Upper bounds $\sigma_{\min}^{-1}$			Elapsed times [sec]		
	Previous	SVD	LDL^T	Previous	SVD	LDL^T
841	4.1234	4.1233	4.1233	6.79	0.98	1.08
9,801	4.1555	4.1555	4.1555	298.92	100.94	0.98
89,401	-	-	4.1625	-	-	10.65
998,001	-	-	4.1628	-	-	1408.68

Numerical experiment

表 **5:** Upper bounds of $\sigma_{\min}^{-1}$ and the computation times of the verification methods. The matrices are complex.

n	Upper bounds $\sigma_{\min}^{-1}$			Elapsed times [sec]		
	Previous	SVD	LDL^T	Previous	SVD	LDL^T
841	1.0496	1.0495	1.0496	29.65	4.28	1.12
9,801	1.0497	1.0497	1.0497	983.32	339.53	3.08
89,401	-	-	1.0497	-	-	46.79
998,001	-	-	1.0500	-	-	2340.33

Summary

- We proposed two verification methods.
- Compared to previous studies, the proposed method does not use interval Cholesky decomposition, which improves numerical stability.
- The SVD-based method is highly numerically stable, but difficult to apply to large-scale problems.
- The LDL^T-based method has some numerical stability issues but is potentially applicable to large-scale sparse matrices.
- However, equilibration can potentially mitigate the numerical instability of the LDL^T decomposition.