Complex moment-based method with nonlinear transformation for computing large and sparse interior singular triplets

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Abstract

This paper considers computing interior singular triplets corresponding to the singular values in some interval. Based on the concept of the complex moment-based parallel eigensolvers, in this paper, we propose a novel complex moment-based method with a nonlinear transformation. We also analyse the error bounds of the proposed method and provide some practical techniques. Numerical experiments indicate that the proposed complex moment-based method with the nonlinear transformation computes accurate singular triplets for both exterior and interior problems within small computation time compared with existing methods.

1 Introduction

Given a rectangular matrix $A \in \mathbb{R}^{m \times n}$ ($m \geq n$), let

$$A = U \Sigma V^T = \sum_{i=1}^{n} \sigma_i u_i v_i^T$$

be a singular value decomposition of $A$, where $\sigma_i$ are singular values and $u_i$ and $v_i$ are the corresponding left and right singular vectors, respectively, and $U = [u_1, u_2, \ldots, u_n]$, $V = [v_1, v_2, \ldots, v_n]$ and $\Sigma = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_n)$. To compute partial singular triplets specifically corresponding to the larger part of singular values, there are several projection-type methods such as Golub-Kahan-Lanczos method [6], Jacobi-Davidson type method [8] and randomized SVD algorithm [22].

This paper considers computing interior singular triplets corresponding to the singular values in some interval,

$$\sigma_i, u_i, v_i, \quad \sigma_i \in \Omega := [a, b],$$

where $0 \leq a < b$. One of the simplest ideas to compute (1) is to apply some eigensolver for solving the corresponding symmetric eigenvalue problems,

$$A^T Av = \sigma^2 v \quad \text{or} \quad AA^T u = \sigma^2 u, \quad \sigma \in \Omega = [a, b].$$

One possible choice for solving interior eigenvalue problem (2) is complex moment-based parallel eigensolvers first proposed in [26] that are one of the hottest parallel methods for solving interior eigenvalue problems. However, as shown in Section 4, this simple strategy does not work well in some situation due to the numerical instability.
Based on the concept of the complex moment-based eigensolvers, in this paper, we propose a novel complex moment-based method to compute interior singular triplets (1). From the analysis of error bounds, we also show that the accuracy of the proposed method can be improved via a nonlinear problem although the target problem is a linear singular value problem. Some practical techniques are also provided.

The remainder of this paper is organized as follows. In Section 2, we briefly introduce the complex moment-based parallel eigensolvers. In Section 3, we propose a novel complex moment-based method for computing interior singular triplets and analyse its error bound. Here, we also propose an improvement technique using a nonlinear transformation. Numerical results are reported in Section 4. Section 5 concludes the paper.

Throughout the paper, the following notations are used. We define the range space of the matrix $V = [v_1, v_2, \ldots, v_L]$ by $R(V) := \text{span}\{v_1, v_2, \ldots, v_L\}$. We also use MATLAB notations.

### 2 Complex moment-based parallel eigensolvers

The proposed method in this paper is based on the concept of the complex moment-based parallel eigensolvers first proposed in [26] by Sakurai and Sugiura. Therefore, here, we briefly introduce the basic concepts of the complex moment-based eigensolvers for solving interior generalized eigenvalue problems of the form:

$$Ax_i = \lambda_i Bx_i, \quad A, B \in \mathbb{C}^{n \times n}, \quad x_i \in \mathbb{C}^n \setminus \{0\}, \quad \lambda_i \in \Omega \subset \mathbb{C},$$

where $zB - A$ is non-singular on a boundary $\Gamma$ of the target region $\Omega$.

The complex moment-based eigensolvers construct a special subspace using contour integral:

$$S_\Omega = \mathcal{R}(S), \quad S = [S_0, S_1, \ldots, S_{M-1}], \quad S_k := \frac{1}{2\pi i} \oint_\Gamma z^k(zB - A)^{-1}BV_{in}dz, \quad (3)$$

where $L, M \in \mathbb{N}_+$ are the input parameters and $V_{in} \in \mathbb{C}^{n \times L}$ is an input matrix. For this subspace $S_\Omega$, we have the following theorem; see e.g., [13].

**Theorem 1.** The complex moment-based subspace $S_\Omega$ is equivalent to an invariant subspace with respect to the eigenvectors corresponding to the eigenvalues in a given region $\Omega \subset \mathbb{C}$, that is,

$$S_\Omega = \text{span}\{x_i | \lambda_i \in \Omega\},$$

if and only if $\text{rank}(S) = d$, where $d$ is the number of target eigenvalues.

Based on this theorem, complex moment-based eigensolvers are mathematically designed on projection methods [13]. Practical algorithms are derived by approximating the contour integral (3) using the numerical integration rule:

$$\hat{S}_k := \sum_{j=1}^{N} \omega_j z_j^k(z_jB - A)^{-1}BV,$$  \quad (4)

where $z_j$ is a quadrature point and $\omega_j$ is its corresponding weight.
The most time-consuming part of using complex moment-based eigensolvers involves solving linear systems \[(4)\] at each quadrature point. Since these linear systems can be independently solved, the complex moment-based eigensolvers have a good scalability that was demonstrated in previous research \([18, 19]\).

Thanks to the high parallel efficiency, complex moment-based eigensolvers have attracted considerable attention. Currently, there are several methods including direct extensions of Sakurai and Sugiura’s approach \([9–11, 13, 14, 16, 27]\), the FEAST eigensolver \([23]\) developed by Polizzi and its improvements \([7, 19, 20, 29]\). High-performance parallel software based on the complex moment-based eigensolvers have been developed \([5, 33]\). Complex moment-based machine learning algorithms have also been developed \([15, 31]\). For details of these methods, refer to the study by \([25]\) and the references therein.

### 3 Complex moment-based method for computing interior singular triplets

Herein, we propose a complex moment-based method for computing interior singular triplets \([1]\) and analyse its error bound. Based on the analysis, we propose an improvement technique using a nonlinear transformation to improve accuracy of the proposed method. Some practical techniques are also provided.

#### 3.1 Derivation of the proposed method

Based on the concept of the complex moment-based parallel eigensolvers, now, we have the following theorem.

**Theorem 2.** Let \(L, M \in \mathbb{N}_+\) be the input parameters and \(V_{\text{in}} \in \mathbb{R}^{n \times L}\) be an input matrix. We define \(S \in \mathbb{R}^{n \times LM}\) and \(S_k \in \mathbb{R}^{n \times L}\) as follows:

\[
S := [S_0, S_1, \ldots, S_{M-1}], \quad S_k := \frac{1}{2\pi i} \oint_{\Gamma} z^{k} (zI - A^T A)^{-1} V_{\text{in}} d\zeta, \quad (5)
\]

where \(\Gamma\) is a positively oriented Jordan curve around \([a^2, b^2]\). Then, the subspaces \(R(AS)\) and \(R(S)\) are equivalent to subspaces with respect to the left and right singular vectors corresponding to the singular values in a given interval \(\Omega = [a, b]\), i.e.,

\[
R(AS) = \text{span}\{u_i|\sigma_i \in \Omega = [a, b]\}, \quad \text{and} \quad R(S) = \text{span}\{v_i|\sigma_i \in \Omega = [a, b]\},
\]

if and only if \(\text{rank}(S) = t\), where \(t\) is the number of target singular values.

**Proof.** Using the singular value decomposition of \(A, A = U\Sigma V^T\), and Cauchy’s integral formula, the matrix \(S_k\) can be decomposed as

\[
S_k = \frac{1}{2\pi i} \oint_{\Gamma} \sum_{i=1}^{n} \frac{z^{k}}{z - \sigma_i^2} v_i v_i^T V_{\text{in}} d\zeta = \sum_{\sigma_i \in \Omega} (\sigma_i^2)^k v_i v_i^T V_{\text{in}},
\]

that proves Theorem 2. \(\square\)
This theorem denotes that the target singular triplets (1) can be obtained by some projection method with \( R(AS) \) and/or \( R(S) \) constructed by contour integral (5). In practice, the contour integral (5) is approximated by a numerical integration rule such as the \( N \)-point trapezoidal rule, as follows:

\[
\tilde{S} := [\tilde{S}_0, \tilde{S}_1, \ldots, \tilde{S}_{M-1}], \quad \tilde{S}_k := \sum_{j=1}^{N} \omega_j z_j^k (z_j I - A^T A)^{-1} V_{\text{in}},
\]

where \((z_j, \omega_j), j = 1, 2, \ldots, N\), are the quadrature points and the corresponding weights, respectively. Then, the approximate singular triplets are computed by a projection method. Here, we consider using two-sided projection method with subspaces \( R(\tilde{A}S) \) and \( R(\tilde{S}) \). Note that one can also consider one-sided projection method.

Let \( \tilde{U} \) and \( \tilde{V} \) be the orthogonal matrices whose columns are orthonormal basis of \( R(\tilde{A}S) \) and \( R(\tilde{S}) \), respectively. From the definition of the subspace \( R(\tilde{A}S) \), the matrix \( \tilde{U} \) is obtained by a QR factorization of \( \tilde{A}V \),

\[
A\tilde{V} = \tilde{U}B.
\]

In a two-sided projection method, singular triplets are approximated as

\[
(\sigma_i, u_i, v_i) \approx (\tilde{\sigma}_i, \tilde{u}_i, \tilde{v}_i) = (\phi_i, \tilde{U}p_i, \tilde{V}q_i),
\]

and set \( P = [p_1, p_2, \ldots, p_{LM}], Q = [q_1, q_2, \ldots, q_{LM}] \) and \( \Phi = \text{diag}(\phi_1, \phi_2, \ldots, \phi_{LM}) \). Based on the Galerkin condition, the residual \( R = A - (\tilde{U}P)\Phi(\tilde{V}Q)^T \) is orthogonalized to the subspaces \( R(\tilde{A}S) \) and \( R(\tilde{S}) \), that is \( \tilde{U}^T R \tilde{V} = O \). From (6), we have \( \tilde{U}^T \tilde{A} \tilde{V} = B \), then the target singular triplets can be approximated by using a singular value decomposition of the matrix \( B \),

\[
B = P\Phi Q = \sum_{\sigma \in \Sigma} \phi_i p_i q_i^T.
\]

To improve the accuracy, we can use an iteration technique. The basic concept is that the matrix \( \tilde{S}_0^{(\ell - 1)} \) is iteratively calculated, from the initial matrix \( \tilde{S}_0^{(0)} = V_{\text{in}} \) as follows:

\[
\tilde{S}_0^{(\nu)} := \sum_{j=1}^{N} \omega_j z_j^\nu (z_j I - A^T A)^{-1} \tilde{S}_0^{(\nu - 1)}, \quad \nu = 1, 2, \ldots, \ell - 1.
\]

Then, \( \tilde{S}^{(\ell)} \) is constructed from \( \tilde{S}_0^{(\ell - 1)} \) by

\[
\tilde{S}^{(\ell)} := [\tilde{S}_0^{(\ell)}, \tilde{S}_1^{(\ell)}, \ldots, \tilde{S}_{M-1}^{(\ell)}], \quad \tilde{S}_k^{(\ell)} := \sum_{j=1}^{N} \omega_j z_j^k (z_j I - A^T A)^{-1} \tilde{S}_0^{(\ell - 1)}.
\]

Additionally, for improving the numerical stability, we use a low-rank approximation with a threshold \( \delta \) based on the singular value decomposition of \( \tilde{S}^{(\ell)} \):

\[
\tilde{S}^{(\ell)} = [U_{S1}, U_{S2}] \begin{bmatrix} \Sigma_{S1} & O \\ O & \Sigma_{S2} \end{bmatrix} \begin{bmatrix} W_{S1}^T \\ W_{S2}^T \end{bmatrix} \approx U_{S1} \Sigma_{S1} W_{S1}^T,
\]

where \( \Sigma_{S1} \) is a diagonal matrix whose diagonal entries are the larger part of the singular values, and the columns of \( U_{S1}, W_{S1} \) are the corresponding singular vectors. Then, \( U_{S1} \) is used for projection method instead of \( \tilde{S} \).
**Algorithm 1** A block SS–SVD method

**Input:** \( L, M, N, \ell \in \mathbb{N}_+, \delta \in \mathbb{R}, V_{in} \in \mathbb{R}^{n \times L}, (z_j, \omega_j) \) for \( j = 1, 2, \ldots, N/2 \)

**Output:** Approximate singular triplet \((\tilde{\sigma}_i, \tilde{\mu}_i, \tilde{v}_i)\) for \( i = 1, 2, \ldots, \ell \)

1. Compute \( \hat{S}_0^{(\nu)} = 2 \sum_{j=1}^{N/2} \text{Re} \left( \omega_j (z_j I - A^T A)^{-1} \hat{S}_0^{(\nu-1)} \right) \) for \( \nu = 1, 2, \ldots, \ell - 1 \)
2. Compute \( \hat{S}_k^{(\ell)} = 2 \sum_{j=1}^{N/2} \text{Re} \left( \omega_j z_j^k (z_j I - A^T A)^{-1} \hat{S}_0^{(\ell-1)} \right) \) for \( k = 0, 1, \ldots, M - 1 \), and set \( \hat{S}^{(\ell)} = [\hat{S}_0^{(\ell)}, \hat{S}_1^{(\ell)}, \ldots, \hat{S}_{M-1}^{(\ell)}] \)
3. Compute low-rank approx. of \( \hat{S}^{(\ell)} \) using the threshold \( \delta \):
   \( \hat{S}^{(\ell)} = [U_{S1}, U_{S2}] [\Sigma_{S1}, O; O, \Sigma_{S2}][W_{S1}, W_{S2}]^T \approx U_{S1} \Sigma_{S1} W_{S1}^T \), and set \( \tilde{V} = U_{S1} \)
4. Compute QR factorization of \( AU_{S1} : [\tilde{U}, B] = qr(A \tilde{V}) \)
5. Compute singular triplets \((\phi_i, p_i, q_i)\) of the matrix \( B \) and set \((\tilde{\sigma}_i, \tilde{\mu}_i, \tilde{v}_i) = (\phi_i, \tilde{U} p_i, \tilde{V} q_i)\)

Because of the symmetric property of \( A^T A \), if quadrature points and the corresponding weights are symmetric about the real axis,

\[
(z_j, \omega_j) = (\overline{z}_{j+N/2}, \overline{\omega}_{j+N/2}), \quad j = 1, 2, \ldots, N/2,
\]

we can reduce the number of linear systems as

\[
\hat{S}_k = 2 \sum_{j=1}^{N/2} \text{Re} \left( \omega_j z_j^k (z_j I - A^T A)^{-1} V_{in} \right).
\]

The practical algorithm of the proposed method is shown in Algorithm 1. One of the most time-consuming part of the complex moment-based parallel eigensolvers. solved, the proposed method is expected to exhibit good scalability in the same manner as the complex moment-based parallel eigensolvers.

### 3.2 Error analysis of the proposed method

Assume that \((z_j, \omega_j)\) satisfy

\[
\sum_{j=1}^{N} \omega_j z_j^k \begin{cases} 
0, & k = 0, 1, \ldots, N - 2 \\
\neq 0, & k = -1
\end{cases}.
\]

(11)

Here, we have the following proposition for \( \hat{S} \); see, e.g., [12].

**Proposition 1.** Let \((z_j, \omega_j)\) satisfy (11), then we have the following relationship,

\[
\hat{S}_k = \sum_{j=1}^{N} \sum_{i=1}^{n} \frac{\omega_j z_j^k}{z_j - \sigma_i} v_i v_i^T V_{in} = \sum_{i=1}^{n} \sigma_i^{2k} \left( \sum_{j=1}^{N} \frac{\omega_j}{z_j - \sigma_i^2} \right) v_i v_i^T V_{in} = (A^T A)^k \hat{S}_0,
\]

for \( k = 0, 1, \ldots, N - 1 \).

Let \( f(\sigma_i) \) be a filter function

\[
f(\sigma_i) := \sum_{j=1}^{N} \frac{\omega_j}{z_j - \sigma_i^2},
\]

5
commonly used in the analyses of some eigensolvers [7, 12, 13, 28, 29]. Then, the matrix \( \hat{S}_k^{(\ell)} \) can be rewritten as

\[
\hat{S}_k^{(\ell)} = \sum_{i=1}^{n} \left( \sum_{j=1}^{N} \frac{\omega_j z_j^k}{\sigma_i^2} \right) \left( \sum_{j=1}^{N} \frac{\omega_j}{z_j - \sigma_i^2} \right)^{\ell-1} v_i v_i^T V_n
\]

\[
= \sum_{i=1}^{n} (\sigma_i^2)^k \left( \sum_{j=1}^{N} \frac{\omega_j}{z_j - \sigma_i^2} \right)^{\ell} v_i v_i^T V_n
\]

\[
= \sum_{i=1}^{n} \sigma_i^{2k} (f(\sigma_i))^\ell v_i v_i^T V_n
\]

\[
= V \Sigma^{2k} V^T V (f(\Sigma))^\ell V V_n
\]

where \( f(\Sigma) = \text{diag}(f(\sigma_1), f(\sigma_2), \ldots, f(\sigma_n)) \) that provides

\[
S^{(\ell)} = F^\ell K
\]

with

\[
F = V f(\Sigma^2) V^T, \quad K = [V_n, (A^T A) V_n, \ldots, (A^T A)^{M-1} V_n].
\]

Using (12), we have the following theorem for the error bound of the proposed method in the same manner as an error analysis of the subspace iteration method, see, e.g., Lemma 6.2.1 of [4] and Theorem 5.2 of [24].

**Theorem 3.** Let \((\sigma_i, u_i, v_i)\) be exact singular triplets of \(A\). Assume that \(f(\sigma_i)\) are ordered by decreasing magnitude \(|f(\sigma_i)| \geq |f(\sigma_{i+1})|\). Define \(P_U^{(\ell)}\) and \(P_V^{(\ell)}\) as orthogonal projectors onto the subspaces \(\mathcal{R}(A \hat{S}_k^{(\ell)})\) and \(\mathcal{R}(\hat{S}_k^{(\ell)})\), respectively. We also define \(P_{LM}\) as the spectral projector with an invariant subspace \(\text{span}\{v_1, v_2, \ldots, v_{LM}\}\). Assume that the matrix \(P_{LM} K\) is full rank. Then, for each right singular vector \(v_i, i = 1, 2, \ldots, LM\), there exists a unique vector \(s_i \in \mathcal{R}(K)\) such that \(P_{LM} s_i = v_i\). Here, we have

\[
\| (I - P_U^{(\ell)}) u_i \|_2 \leq \alpha_i \beta_i \left| \frac{f(\sigma_{LM+1})}{f(\sigma_i)} \right|^{\ell}, \quad i = 1, 2, \ldots, LM,
\]

and

\[
\| (I - P_V^{(\ell)}) v_i \|_2 \leq \beta_i \left| \frac{f(\sigma_{LM+1})}{f(\sigma_i)} \right|^{\ell}, \quad i = 1, 2, \ldots, LM,
\]

where \(\alpha_i = \max_{j \geq LM+1} \sigma_j / \sigma_i\) and \(\beta_i = \|v_i - s_i\|_2\).

**Proof.** Since \(P_{LM} K\) is full rank, there exists a unique vector \(s_i \in \mathcal{R}(K)\) as

\[
v_i = \sum_{j=1}^{LM} \alpha_j P_{LM} k_j = P_{LM} \left( \sum_{j=1}^{LM} \alpha_j k_j \right) =: P_{LM} s_i,
\]

where \(K = [k_1, k_2, \ldots, k_{LM}]\). Then, using \(w_i = (I - P_{LM}) s_i\), we have

\[
s_i = P_{LM} s_i + (I - P_{LM}) s_i = v_i + w_i.
\]
Let \( y_i = \frac{1}{\sigma_i} A (1/f(\sigma_i))^\ell F^\ell s_i \in \mathcal{R}(A \tilde{S}(i)) \). Then, multiplying the matrix \( (1/\sigma_i) A (1/f(\sigma_i))^\ell F^\ell \) to \((13)\) from the left-side and considering \( u_i = (1/\sigma_i) A (1/f(\sigma_i))^\ell F^\ell v_i \) and \( w_i = (I - \mathcal{P}_{LM}) s_i = \mathcal{P}_{LM}^\perp s_i \), we have

\[
y_i - u_i = \frac{1}{\sigma_i} A \left( \frac{1}{f(\sigma_i)} F \right)^\ell \ w_i = \frac{1}{\sigma_i} A \mathcal{P}_{LM}^\perp \left( \frac{1}{f(\sigma_i)} F \mathcal{P}_{LM}^\perp \right)^\ell \ w_i,
\]

that provides

\[
\|y_i - u_i\|_2 \leq \frac{1}{\sigma_i} \|A \mathcal{P}_{LM}^\perp\|_2 \left\| \left( \frac{1}{f(\sigma_i)} F \mathcal{P}_{LM}^\perp \right)^\ell \right\| \|w_i\|_2.
\]

Here, using the relationship

\[
\min_{y_i \in \mathcal{R}(A \tilde{S}(i))} \|y_i - u_i\|_2 = \|(I - \mathcal{P}_{U}(i)) u_i\|_2,
\]

we thus have

\[
\|(I - \mathcal{P}_{U}(i)) u_i\|_2 \leq \|y_i - u_i\|_2 \leq \alpha_i \beta_i \left| \frac{f(\sigma_{LM+1})}{f(\sigma_i)} \right|^{\ell}.
\]

In the same manner, letting \( z_i = (1/f(\sigma_i))^\ell F^\ell s_i \in \mathcal{R}(\tilde{S}(i)) \) and considering \( v_i = (1/f(\sigma_i))^\ell F^\ell v_i \), we have

\[
\|(I - \mathcal{P}_{V}(i)) v_i\|_2 \leq \|z_i - v_i\|_2 \leq \beta_i \left| \frac{f(\sigma_{LM+1})}{f(\sigma_i)} \right|^{\ell},
\]

that proves Theorem 3.

Theorem 3 indicates that the accuracy of the proposed method depends on the subspace dimension \( LM \). Given a sufficiently large subspace, i.e.,

\[
|\frac{f(\sigma_{LM+1})}{f(\sigma_i)}|^{\ell} \approx 0,
\]

the target singular triplets can be obtained accurately, even if some singular values exist outside but near the region.

### 3.3 An improvement technique using a nonlinear transformation

Theorem 3 also indicates that if there is a cluster of singular values outside but near the region, then, to obtain accurate singular triplets, we have to use huge \( LM \) that takes into account the number of the clustered singular values even though these are not the target. This becomes huge computational costs. Such a situation happens in the case that the singular values are uniformly distributed on the logarithmic scale.

To overcome this difficulty, in this paper, inspired by complex moment-based nonlinear eigensolvers [1–3, 17, 30, 32], we consider introducing a nonlinear transformation, \( z = g(t) \), with an analytic monotonic increasing function \( g \). Then, we reset

\[
S_k = \frac{1}{2\pi i} \oint_{\Gamma_t} t^k (g(t) I - A^T A)^{-1} V_{in} dt,
\]
where $\Gamma_t$ is a Jordan curve around $[g^{-1}(a^2), g^{-1}(b^2)]$. Note that this also holds Theorem 2. The matrix $\hat{S}_k$ is approximated by using contour integral as

$$\hat{S}_k = \sum_{j=1}^{N} \psi_j t_j^k (g(t_j)I - A^T A)^{-1} V_{\text{in}},$$

where $(t_j, \psi_j), j = 1, 2, \ldots, N$ are the quadrature points and the corresponding weights, respectively.

Although Proposition 1 usually does not hold in the case using the nonlinear transform, since we have

$$S_k = \frac{1}{2\pi i} \oint_{\Gamma} \sum_{i=1}^{n} t_i^k g(t)^{-1} v_i v_i^T V_{\text{in}} dt = \sum_{\sigma_i \in \Omega} (g^{-1}(\sigma_i^2))^k v_i v_i^T V_{\text{in}} = (g^{-1}(A^T A))^k S_0,$$

we expect

$$\hat{S}_k = \sum_{j=1}^{N} \sum_{i=1}^{n} \psi_j t_j^k g(t_j) - \sigma_i^2 v_i v_i^T V_{\text{in}}$$

$$\approx \sum_{i=1}^{n} (g^{-1}(\sigma_i))^2 k \left( \sum_{j=1}^{N} \frac{\psi_j g(t_j)}{g(t_j) - \sigma_i^2} \right) v_i v_i^T V_{\text{in}}$$

$$= (g^{-1}(A^T A))^k \hat{S}_0.$$

(14)

Therefore, letting $f_g(\sigma)$ be a filter function

$$f_g(\sigma) := \sum_{j=1}^{N} \frac{\psi_j}{g(t_j) - \sigma_i^2},$$

then $\hat{S}_k^{(t)}$ can be rewritten as

$$\hat{S}_k^{(t)} \approx V (g^{-1}(\Sigma))^2 k V^T V (f_g(\Sigma))^k V^T V_{\text{in}},$$

that provides

$$\hat{S}_k \approx F_g^T K_g$$

with

$$F_g = V f_g(\Sigma) V^T, \quad K_g = [V_{\text{in}}, g^{-1}(A^T A) V_{\text{in}}, \ldots, (g^{-1}(A^T A))^{M-1} V_{\text{in}}].$$

Thus, we have approximately the same error bounds as Theorem 3 with $f_g(\sigma)$ instead of $f(\sigma)$ as the filter function.

To set the function $g$ as $|f_g(\sigma_{LM+1})/f_g(\sigma_i)| \ll |f(\sigma_{LM+1})/f(\sigma_i)|$, the obtained accuracy is expected to be improved. For example, if the singular values are uniformly distributed on the logarithmic scale, $g(t) = \exp(t)$ is a good choice to achieve small $|f_g(\sigma_{LM+1})/f_g(\sigma_i)|$. The algorithm of the proposed method with a nonlinear transform is shown in Algorithm 2.
Algorithm 2 A block SS–SVD method with nonlinear transformation

**Input:** $L, M, N, \ell \in \mathbb{N}_+, \delta \in \mathbb{R}, V_m \in \mathbb{R}^{n \times L}, (t_j, \psi_j)$ for $j = 1, 2, \ldots, N/2$

**Output:** Approximate singular triplet $(\hat{S}_{\iota}, \hat{U}_{\iota}, \hat{V}_{\iota})$ for $i = 1, 2, \ldots, \ell$

1. Compute $S_{\iota} = 2 \sum_{j=1}^{N/2} \text{Re} \left( \psi_j (g(t_j)I - A^T A)^{-1} S_{\nu} \right)$ for $\nu = 1, 2, \ldots, \ell - 1$
2. Compute $S_{\ell} = 2 \sum_{j=1}^{N/2} \text{Re} \left( \psi_j \left(g(t_j)I - A^T A\right)^{-1} S_{\nu} \right)$ for $k = 0, 1, \ldots, M - 1$, and set $S_{\nu} = [S_{\iota}, S_1, \ldots, S_{M-1}]
3. Compute low-rank approx. of $S_{\iota}$ using the threshold $\delta$: $S_{\iota} = [U_{\iota}, S_{\iota}][\Sigma_{\iota}, O; O, \Sigma_{\iota}][W_{\iota}, W_{\iota}] = U_{\iota} \Sigma_{\iota} W_{\iota}^T$, and set $\tilde{V} = U_{\iota}$
4. Compute QR factorization of $A U_{\iota} = [\tilde{U}, B] = \text{qr}(A \tilde{V})$
5. Compute singular triplets $(\phi_{\iota}, p_{\iota}, q_{\iota})$ of the matrix $B$ and set $(\hat{S}_{\iota}, \hat{U}_{\iota}, \hat{V}_{\iota}) = (\phi_{\iota}, \tilde{U} p_{\iota}, \tilde{V} q_{\iota})$

### 3.4 Practical techniques

Here, we introduce two practical techniques: an efficient residual norm computation and a spurious singular value detection.

#### 3.4.1 Efficient residual norm computation

Computation of the residual norms for obtained singular triplets is computationally costly when the problem size is large. Here, we consider an efficient computation of the residual 2-norm $\|r_{\iota}\|_2 = \|A^T \hat{U}_{\iota} - \hat{\sigma}_{\iota} \hat{V}_{\iota}\|_2$.

Since the proposed method based on the Galerkin-type two-sided projection provides $B = P \Phi Q^T (1)$ and $A \tilde{V} = \tilde{U} B (6)$, we have $A \tilde{V} q_{\iota} = \tilde{U} P \Phi$, i.e., we have $A \tilde{V}_{\iota} = \hat{S}_{\iota} \hat{V}_{\iota}$ for all $i$. Therefore, the residual 2-norm $\|r_{\iota}\|_2$ can be replaced as

$$\|r_{\iota}\|_2 = \left\| \frac{\sigma_{\iota}}{\sigma_{\iota}} A^T A \tilde{V}_{\iota} - \hat{\sigma}_{\iota} \hat{V}_{\iota} \right\|_2 = \left\| \frac{\sigma_{\iota}}{\sigma_{\iota}} A^T A \tilde{V}_{\iota} - \hat{\sigma}_{\iota}^2 \hat{V}_{\iota} \right\|_2.$$

Let $\tilde{S}_{\iota} = [\tilde{S}_{\iota}, \tilde{S}_1, \ldots, \tilde{S}_{M}].$ For the case of Algorithm 1, from Proposition 1, we have $\tilde{S}_{\iota} = (A^T A) \tilde{S}_{\iota}$. Therefore, the residual 2-norm $\|r_{\iota}\|_2$ is rewritten as

$$\|r_{\iota}\|_2 = \left\| \frac{\sigma_{\iota}}{\sigma_{\iota}} A^T A U_{\iota} q_{\iota} - \hat{\sigma}_{\iota}^2 U_{\iota} q_{\iota} \right\|_2 = \left\| \frac{\sigma_{\iota}}{\sigma_{\iota}} A^T A \tilde{S}_{\iota} V_{\iota} \Sigma_{\iota}^{-1} q_{\iota} - \hat{\sigma}_{\iota}^2 U_{\iota} q_{\iota} \right\|_2 = \left\| \frac{\sigma_{\iota}}{\sigma_{\iota}} A^T A \tilde{S}_{\iota} V_{\iota} \Sigma_{\iota}^{-1} q_{\iota} - \hat{\sigma}_{\iota}^2 U_{\iota} q_{\iota} \right\|_2,$$

that achieves an efficient residual 2-norm computation without a matrix product for $A$, since the matrix $\tilde{B}_{\iota}$ is efficiently obtained by contour integral as well as (8) and (9).

Next, we consider the case of using the nonlinear transformation. Assuming that the relative residual of symmetric eigenvalue problem is almost invariant to nonlinear transform,

$$\frac{\|A^T A \tilde{V}_{\iota} - \hat{\sigma}_{\iota}^2 \tilde{V}_{\iota}\|_2}{\|A^T A\|_2} \approx \frac{\|g^{-1}(A^T A) \tilde{V}_{\iota} - g^{-1}(\hat{\sigma}_{\iota}^2) \tilde{V}_{\iota}\|_2}{\|g^{-1}(A^T A)\|_2},$$
we have
\[ \|r_i\|_2 \approx \frac{1}{\sigma_i} \|g^{-1}(A^T A)\hat{v}_i - g^{-1}(\hat{\sigma}_i^2)\hat{v}_i\|_2 \|A^T A\|_2. \] (16)

Here, from (14), we have \( \hat{S}_i(\cdot) \approx g^{-1}(A^T A)\hat{S}(\cdot) \). Then, the 1st part of (16) can be approximated as
\[
\frac{1}{\sigma_i} \|g^{-1}(A^T A)\hat{v}_i - g^{-1}(\hat{\sigma}_i^2)\hat{v}_i\|_2 \\
= \frac{1}{\sigma_i} \|g^{-1}(A^T A)US_1 q_i - g^{-1}(\hat{\sigma}_i^2)US_1 q_i\|_2 \\
= \frac{1}{\sigma_i} \|g^{-1}(A^T A)\hat{S}_i(\cdot)VS_1 \Sigma_{S_1}^{-1} q_i - g^{-1}(\hat{\sigma}_i^2)US_1 q_i\|_2 \\
\approx \frac{1}{\sigma_i} \|\hat{S}_i(\cdot)VS_1 \Sigma_{S_1}^{-1} q_i - g^{-1}(\hat{\sigma}_i^2)US_1 q_i\|_2 \\
=: \|\tilde{r}_i\|_2.
\]

Since the 2nd part of (16) is constant for \( i \), we have
\[
\frac{\|A^T A\|_2}{\|g^{-1}(A^T A)\|_2} \approx \frac{\|r_i\|_2}{\|\tilde{r}_i\|_2}, \quad i' \in \{1, 2, \ldots, \hat{i}\}.
\]
As a result, we can efficiently approximate all \( \|r_i\|_2 \) by
\[
\|r_i\|_2 \approx \mu \|\tilde{r}_i\|_2, \quad \mu = \frac{\|r_i\|_2}{\|\tilde{r}_i\|_2}
\] (17)
with only one exact residual 2-norm \( \|r_i\|_2 = \|A^T \hat{u}_i - \hat{\sigma}_i \hat{v}_i\|_2 \).

### 3.4.2 Spurious singular value detection

Similarly to other methods, the proposed method may compute spurious singular values in the target region. In the proposed method, both subspaces \( \mathcal{R}(AU_{S_1}) \) and \( \mathcal{R}(U_{S_1}) \) are constructed from the matrix \( U_{S_1} \) obtained by a low-rank approximation (10) of \( \hat{S} \). Here, we focus on this low-rank approximation and introduce a technique for spurious singular value detection.

Let \( U_{S_1} \) be split as \( U_{S_1} = [U_{S_1}^{(1)}, U_{S_1}^{(2)}] \), where \( U_{S_1}^{(1)} \) and \( U_{S_1}^{(2)} \) correspond to large and small singular values in \( \Sigma_{S_1} \), respectively. Then, since \( \hat{V} = U_{S_1} \), the approximation of right singular vectors \( v_i = \hat{V} q_i \) is replaced as
\[
v_i = U_{S_1} q_i = [U_{S_1}^{(1)}, U_{S_1}^{(2)}] \begin{bmatrix} q_i^{(1)} \\ q_i^{(2)} \end{bmatrix}.
\]

From Theorem 2, we expect \( \text{span}\{v_i | \sigma_i \in \Omega\} \approx \mathcal{R}(U_{S_1}^{(1)}) \). Therefore, the magnitude of the elements of \( q_i^{(1)} \) is expected to be much larger than that of \( q_i^{(2)} \).

Based on this concept, we detect spurious singular values using the following index:
\[
\tau_i := \frac{\|q_i\|_2^2}{\|q_i\|_{\Sigma_{S_1}^{-1}}^2} = \frac{q_i^T q_i}{q_i^T \Sigma_{S_1}^{-1} q_i}.
\]
If \( \tau_i \) is smaller than some constant \( \varepsilon \), we treat the eigenpair as a spurious singular values.
We set $(\log|f(\sigma)|, |f_g(\sigma)|)$.

Figure 1: The values of $|f(\sigma)|$ and $|f_g(\sigma)|$.

4 Numerical experiments

Here, we evaluate the performance of the proposed method (Algorithms 1 and 2). For Algorithm 2, we set $z = g(t) = \exp(t)$.

Let the quadrature points $z_j$ and $t_j$ be on an ellipse with center $\gamma$, major axis $\rho$ and aspect ratio $\alpha$, i.e.,

$$z_j = t_j = \gamma + \rho (\cos(\theta_j) + \alpha i \sin(\theta_j)), \quad \theta_j = \frac{2\pi}{N} \left( j - \frac{1}{2} \right), \quad j = 1, 2, \ldots, N.$$  

The corresponding weights are set as

$$\omega_j = \frac{\rho}{N} (\alpha \cos(\theta_j) + i \sin(\theta_j)), \quad \psi_j = \frac{\rho}{N} \exp(t_j) (\alpha \cos(\theta_j) + i \sin(\theta_j)).$$

We set $(\gamma, \rho, \alpha) = ((a^2 + b^2)/2, (b^2 - a^2)/2, 0.1)$ for Algorithm 1 and $(\gamma, \rho, \alpha) = (\log(a) + \log(b), \log(b) - \log(a), 0.1)$ for Algorithm 2.

In these numerical experiments, the algorithms were implemented in MATLAB R2019a. The input matrix $V_{in}$ was set as a random matrix generated by the Mersenne Twister in MATLAB and each linear system was solved using the MATLAB command “\".

4.1 Experiment I: filter function

Here, we compare the filter functions $f(\sigma)$ and $f_g(\sigma)$ for two cases. Figure 1 shows that the values of the filter functions $|f(\sigma)|$ and $|f_g(\sigma)|$ for $[a, b] = [0.8, 1.2]$ and $[10^{-3}, 10^{-1}]$.

As shown in Figure 1(a), in the case that the target region is around 1, there is no large difference between the filter functions $f(\sigma)$ and $f_g(\sigma)$. On the other hand, as shown in Figure 1(b), in the case that the target region is cross to 0, there is large difference. For the region of $\sigma > b$, both $|f(\sigma)|$ and $|f_g(\sigma)|$ decrease with increasing $\sigma$, specifically $|f(\sigma)|$ shows rapid decreasing. For the region of $0 < \sigma < a$, $|f(\sigma)|$ shows large value $|f(\sigma)| \approx 0.5$. Instead, $|f_g(\sigma)|$ drastically decrease. This result indicates that, a cluster of singular value in the region $[0, 10^{-4}]$ causes a negative effect on the accuracy of the SS-SVD based on $f(\sigma)$, but not the accuracy of the SS-SVD with nonlinear transform based on $f_g(\sigma)$.

4.2 Experiment II: model problem

In this subsection, we compare the accuracy of four methods:

- Naive: The block SS–CAA method [16] via the symmetric eigenvalue problem (2):

In these numerical experiments, the algorithms were implemented in MATLAB R2019a. The input matrix $V_{in}$ was set as a random matrix generated by the Mersenne Twister in MATLAB and each linear system was solved using the MATLAB command “\".
For the model problem 1, we compute 40 singular triplets such that singular values are uniformly distributed on the logarithmic scale. Then, the matrix $A$ is constructed as $A = U\Sigma V^T$ with orthogonal matrices $U$ and $V$ constructed from random matrices.

For the model problem 1, we compute 40 singular triplets such that $\sigma_i \in [0.8, 1.2]$ and for the model problem 2, we compute 40 singular triplets such that $\sigma_i \in [10^{-3}, 10^{-1}]$. We set the parameters as $(L, M, N, \ell, \delta) = (20, 4, 32, 1, 10^{-20})$.

| $\sigma^*/\sigma^*$ | $|\sigma^* - \sigma^*|/\sigma^*$ | $f(\sigma)$ | $fg(\sigma)$ | Naive | Naive with NT | SS–SVD | SS–SVD with NT | Approx. (17) | Approx. (15) |
|---------------------|----------------------------------|-------------|-------------|-------|--------------|--------|--------------|-------------|-------------|
| $10^{-18}$           |                                  | 0.05        | 0.05        | 0.8   | 0.8          | 0.8    | 0.8          | 0.8         | 0.8         |
| $10^{-16}$           |                                  | 0.1         | 0.1         | 1.0   | 1.0          | 1.0    | 1.0          | 1.0         | 1.0         |
| $10^{-14}$           |                                  | 0.2         | 0.2         | 1.2   | 1.2          | 1.2    | 1.2          | 1.2         | 1.2         |
| $10^{-12}$           |                                  | 0.3         | 0.3         | 1.4   | 1.4          | 1.4    | 1.4          | 1.4         | 1.4         |
| $10^{-10}$           |                                  | 0.4         | 0.4         | 1.6   | 1.6          | 1.6    | 1.6          | 1.6         | 1.6         |
| $10^{-8}$            |                                  | 0.5         | 0.5         | 1.8   | 1.8          | 1.8    | 1.8          | 1.8         | 1.8         |
| $10^{-6}$            |                                  | 0.6         | 0.6         | 2.0   | 2.0          | 2.0    | 2.0          | 2.0         | 2.0         |
| $10^{-4}$            |                                  | 0.7         | 0.7         | 2.2   | 2.2          | 2.2    | 2.2          | 2.2         | 2.2         |
| $10^{-2}$            |                                  | 0.8         | 0.8         | 2.4   | 2.4          | 2.4    | 2.4          | 2.4         | 2.4         |
| $10^0$               |                                  | 0.9         | 0.9         | 2.6   | 2.6          | 2.6    | 2.6          | 2.6         | 2.6         |
| $10^2$               |                                  | 1.0         | 1.0         | 2.8   | 2.8          | 2.8    | 2.8          | 2.8         | 2.8         |

Figure 2: Relative error $|\sigma^*_i - \sigma_i|/\sigma^*_i$ of singular values and residual 2-norm $|r_i|$.

Figure 3: Residual norm and its approximation.
Table 1: The target region $[a, b]$, the number $t$ of the target singular triplets and parameter setting for the proposed method.

|        | $[a, b]$ | $t$ | $L$ | $M$ |
|--------|----------|-----|-----|-----|
| Exterior | [0.120, 1.01] | 21  | 15  | 4   |
|         | [0.080, 1.01] | 40  | 30  | 4   |
|         | [0.045, 1.01] | 79  | 60  | 4   |
|         | [0.025, 1.01] | 153 | 120 | 4   |
| Interior| [0.060, 0.08] | 17  | 15  | 4   |
|         | [0.045, 0.08] | 39  | 30  | 4   |
|         | [0.030, 0.08] | 85  | 60  | 4   |
|         | [0.020, 0.08] | 158 | 120 | 4   |

Figure 4: The computation time v.s. the number of the target singular triplets.

In Figure 2, we show relative error of singular value $|\sigma_i^* - \tilde{\sigma}_i|/\sigma_i^*$, where $\sigma_i^*$ is the exact singular value, and residual 2-norm $\|r_i\|_2 = \|A^T \tilde{u}_i - \tilde{\sigma}_i \tilde{v}_i\|_2$. In the case of the model problem 1 \((18)\) whose singular values are uniformly distributed, as shown in Figure 2(a), all methods show almost the same accuracy both for the relative error and residual 2-norm. On the other hand, in the case of the model problem 2 \((19)\) whose singular values are uniformly distributed on the logarithmic scale, as shown in Figure 2(b), the nonlinear transformation shows drastically improves the accuracy. Specifically, the SS-SVD with the nonlinear transformation shows the best results both for relative error and residual 2-norm.

In Figure 3, we show the residual 2-norm and its estimations \((15)\) and \((17)\) for the proposed methods. We observe that the both approximations well estimated the exact residual 2-norms for both problems.

### 4.3 Experiment III: real-world problem

We evaluate the computation time of the proposed method compared with that of MATLAB functions $\text{svd}$ for computing all the singular triplets and $\text{svds}$ for computing partial singular triplets. We used a $60000 \times 784$ sparse matrix obtained from a 10-class classification of handwritten digits (MNIST) [21]. The average nonzero elements per row is 149.9. We normalized the matrix as the largest singular value is 1. For $\text{svds}$, we computed the largest $10, 20, \ldots, 160$ singular triplets. For the proposed method, the target interval, the number $t$ of the target singular triplets and parameters $L, M$ are shown in Table 1. Here, we fix $M = 4$ and set $L$ as $LM \approx 3t$. We also set $(N, \ell, \delta) = (32, 1, 10^{-20})$.

The computation time of all methods are shown in Figure 4. The breakdown of the computation time and accuracy of the proposed method are also shown in Table 2. As shown in
Table 2: Breakdown of the computation time and accuracy of the proposed method.

| region          | Computation time [sec.] | accuracy |                |                |
|-----------------|-------------------------|----------|----------------|----------------|
|                 | Steps 1–2 | 3 | 4 | 5 | Total | error | residual |
| [a, b]          |                |            |              |              |        |        |
| [0.120, 1.01]   | 0.809 | 0.002 | 0.144 | 0.006 | 0.962 | 1.67E-15 | 1.57E-13 |
| [0.080, 1.01]   | 0.842 | 0.005 | 0.299 | 0.017 | 1.146 | 1.70E-15 | 1.90E-14 |
| [0.045, 1.01]   | 0.886 | 0.015 | 0.792 | 0.049 | 1.693 | 2.94E-15 | 1.03E-14 |
| [0.025, 1.01]   | 0.997 | 0.054 | 1.847 | 0.178 | 2.898 | 2.48E-15 | 3.90E-15 |

| region          | Computation time [sec.] | accuracy |                |                |
|-----------------|-------------------------|----------|----------------|----------------|
|                 | Steps 1–2 | 3 | 4 | 5 | Total | error | residual |
| [a, b]          |                |            |              |              |        |        |
| [0.060, 0.08]   | 0.830 | 0.002 | 0.150 | 0.006 | 0.983 | 1.09E-15 | 8.26E-14 |
| [0.045, 0.08]   | 0.858 | 0.005 | 0.286 | 0.017 | 1.148 | 2.62E-15 | 8.99E-14 |
| [0.030, 0.08]   | 0.886 | 0.015 | 0.795 | 0.047 | 1.695 | 2.18E-15 | 5.02E-13 |
| [0.020, 0.08]   | 1.024 | 0.056 | 1.762 | 0.184 | 2.842 | 2.48E-15 | 3.99E-16 |

Figure 4: The computation time of \texttt{svds} increases with increasing the number $t$ of the target singular values. Then, in this experiment, \texttt{svd} is faster than \texttt{svds} when $t > 30$. Instead, the proposed method is much faster than \texttt{svds} and \texttt{svd} for both exterior and interior cases, although the computation time, specifically Step 4, of the proposed method increases with increasing $t$ and $L$.

5 Conclusions

Based on the concept of the complex moment-based eigensolvers, in this paper, we proposed a novel complex moment-based method to compute interior singular triplets (\texttt{I}). We also analysed error bounds of the proposed method and proposed an improvement technique using a nonlinear transformation to improve accuracy of the proposed method. The proposed method has high parallel efficiency as the complex moment-based parallel eigensolvers. From the numerical experiments, the proposed complex moment-based method with the nonlinear transformation can compute accurate singular triplets for both exterior and interior problems. The computation time of the proposed method is much faster than \texttt{svds} and \texttt{svd}.

In the future, we will evaluate the parallel performance of the proposed method for more large real-world problems.

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