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Recovering from accuracy deterioration in the contour integral-based eigensolver

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Abstract

We consider a contour integral-based eigensolver that finds eigenvalues in a given domain and the corresponding eigenvectors of the generalized eigenvalue problem. In the contour integral-based eigensolver, quadrature points are placed in the complex plane in order to approximate the contour integral. When eigenvalues exist near a quadrature point, the accuracy of other eigenvalues is deteriorated. We herein propose a method by which to recover the accuracy of the eigenpairs when eigenvalues exist near a quadrature point. A numerical experiment is conducted in order to verify that the proposed method is efficient.

Keywords generalized eigenvalue problem, contour integral, accuracy improvement

Research Activity Group Algorithms for Matrix / Eigenvalue Problems and their Applications

1. Introduction

The generalized eigenvalue problem involves finding eigenvalues $\lambda \in \mathbb{C}$ and the corresponding eigenvectors $\boldsymbol{x} \in \mathbb{C}^n \backslash \{\boldsymbol{0}\}$ that satisfy $A\boldsymbol{x} = \lambda B\boldsymbol{x}, A, B \in \mathbb{C}^{n\times n}$. We assume that the matrix pencil $zB - A$ is diagonalizable. In [1, 2], a contour integral-based eigensolver called the Sakurai-Sugiura method (SS method) was proposed for the generalized eigenvalue problem. The SS method can find eigenvalues located inside a given region and the corresponding eigenvectors by using a contour integral along a boundary of the given domain. The contour integral is approximated using some numerical integration rule. Then, quadrature points are on the boundary of the region. The quadrature points are usually set in the complex plane, e.g., along a circle or an ellipse. For the case that the matrices A, B are real and $zB - A$ has only real eigenvalues, an approach using real quadrature points was recently proposed [3].

When some eigenvalues exist near a quadrature point, the accuracy of other eigenpairs is deteriorated. Particularly, when using the real quadrature points for real eigenvalues, there is a higher probability that eigenvalues exist near a quadrature point than in the case of quadrature points in the complex plane. In the present paper, we propose a method to recover the accuracy of the target eigenpairs without moving the quadrature points.

The remainder of the paper is organized as follows. In the next section, we introduce the SS method. In Section 3, we discuss the reason for the accuracy deterioration. In Section 4, we present the proposed method. Its accuracy is discussed in Section 5. A numerical example of the proposed method is presented in Section 6. Finally, our conclusions are presented in Section 7.

2. Contour integral-based eigensolver

Let $\lambda_i, \boldsymbol{x}_i, i = 1, 2, \ldots, n$ be eigenvalues and the corresponding eigenvectors, and let m be the number of eigenvalues located in a certain open domain $\Omega \subset \mathbb{C}$. Moreover, let $L, K \in \mathbb{N}$ satisfy $LK \geq m$, and let $V \in \mathbb{C}^{n\times L}$ be an input matrix, e.g., a random matrix. We define matrices S and S_k as follows:

$$S := [S_0, S_1, \ldots, S_{K-1}],$$
$$S_k := \frac{1}{2\pi \mathrm{i}} \oint_\Gamma z^k (zB - A)^{-1} BV \mathrm{d}z, \tag{1}$$

where Γ is a Jordan curve surrounding the domain Ω. If the rank of the matrix S is m, then the range of S is spanned by the eigenvectors corresponding to the eigenvalues in Ω. In the numerical computation, the contour integral in (1) is approximated by the following N-point numerical integration:

$$S \approx \hat{S} := [\hat{S}_0, \hat{S}_1, \ldots, \hat{S}_{K-1}],$$
$$S_k \approx \hat{S}_k := \sum_{j=0}^{N-1} w_j z_j^k (z_j B - A)^{-1} BV, \tag{2}$$

where $w_j, j = 0, 1, \ldots, N-1$ are weights corresponding to the quadrature points. The approximate eigenvalues in Ω and the corresponding eigenvectors are extracted from $\hat{S}$ by the Rayleigh-Ritz procedure. The algorithm of the SS method is shown in Algorithm 1. In practice, for accurate computation scaled quadrature points are used instead of z_j^k.

The quadrature points are usually placed along a circle or an ellipse. If the matrices A, B are real and $zB-A$ has only real eigenvalues, using real quadrature points can reduce the memory requirements and the computational cost because only real arithmetic is required.

Algorithm 1 Sakurai-Sugiura method

Input: $L, K, N \in \mathbb{N}, V \in \mathbb{C}^{n\times L}, (z_j, w_j)$
Output: eigenpairs $(\lambda_i, \boldsymbol{x}_i), i = 1, 2, \ldots, LK$
1: Solve linear equations $(z_j B - A)Y_j = BV$ for $Y_j, j = 0, 1, \ldots, N-1$.
2: Compute $\hat{S}_k = \sum_{j=0}^{N-1} w_j z_j^k Y_j, k = 0, 1, \ldots, K-1$.
3: Construct an orthogonal basis Q from $\hat{S}$.
4: Compute the eigenpairs $(\theta_i, \boldsymbol{u}_i)$ of $Q^H AQ\boldsymbol{u} = \theta Q^H BQ\boldsymbol{u}$.
5: Set $(\lambda_i, \boldsymbol{x}_i) = (\theta_i, Q\boldsymbol{u}_i), i = 1, 2, \ldots, LK$.

One way to choose real quadrature points is to use the Chebyshev points [3].

3. Accuracy deterioration of the eigenpairs

When some eigenvalues are near a quadrature point, namely, $z_{j'}$, the matrix $z_{j'}B - A$ becomes ill-conditioned. Additionally, as will be shown in Section 6, the eigenpairs except for the eigenvalues that are near $z_{j'}$ are obtained with low accuracy, even if the linear equation $(z_{j'}B - A)Y_{j'} = V$ is solved with sufficiently high accuracy. In this section, we discuss the reason of the accuracy deterioration.

3.1 Filter function of the contour integral-based eigensolver

Let $\boldsymbol{y}_i, i = 1, 2, \ldots, n$ be left eigenvectors corresponding to the eigenvalues $\lambda_i, i = 1, 2, \ldots, n$, and let $\boldsymbol{v}_\ell$ be the ℓ-th column vector of the input matrix V. For $\hat{S}_k$ in (2), the following proposition holds [4].

Proposition 1 *The ℓ-th column vector of $\hat{S}_k$ denoted by $\hat{\boldsymbol{s}}_{k,\ell}$ is represented as follows:*

$$\hat{\boldsymbol{s}}_{k,\ell} = \sum_{i=1}^{n} \boldsymbol{y}_i^H B\boldsymbol{v}_\ell f_k(\lambda_i)\boldsymbol{x}_i, \quad f_k(\lambda_i) := \sum_{j=0}^{N-1} \frac{w_j z_j^k}{z_j - \lambda_i}. \tag{3}$$

We also have $f_k(\lambda) = \lambda^k f_0(\lambda), k = 1, 2, \ldots, K-1$ if the weights satisfy the following conditions:

$$\sum_{j=0}^{N-1} w_j z_j^k \begin{cases} \neq 0, & k = -1. \\ = 0, & k = 0, 1, \ldots, N-2. \end{cases} \tag{4}$$

We call $f_k(\lambda)$ defined in Proposition 1 the filter function. Proposition 1 shows that calculating $\hat{S}_k$ is equivalent to multiplying each eigen-component included in V by the filter function $f_k(\lambda_i)$.

The filter function $f_0(\lambda)$ for a circle centered at the origin with radius 1 and $N = 16$ is shown in Fig. 1. The absolute value of the filter function $f_0(\lambda)$ is approximately 1 inside the unit circle. However, since $z_j, j = 0, 1, \ldots, N-1$ are poles of the filter function, the filter function rises suddenly near the quadrature points. In the outer region of the unit circle, $|f_0(\lambda)|$ decreases gently. The absolute value of the filter function for the Chebyshev points on the interval $[-1, 1]$ with $N = 16$ is shown in Fig. 2. The filter function oscillates on the interval $[-1, 1]$ because the poles are on the interval $[-1, 1]$.

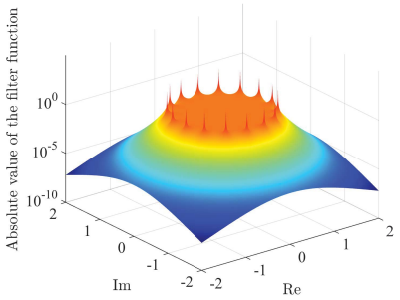

Fig. 1. Absolute value of the filter function $f_0(\lambda)$ on the complex plane. The quadrature points are placed along a circle centered at the origin with radius 1 for $N = 16$.

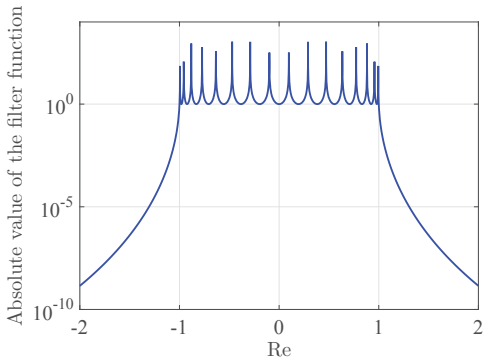

Fig. 2. Absolute value of the filter function $f_0(\lambda)$ on the real axis. The quadrature points are the Chebyshev points in the interval $[-1, 1]$ for $N = 16$.

3.2 Reason for the accuracy deterioration

We consider the case that the eigenvalue $\lambda_{i'}$ is near $z_{j'}$ such that $|f_k(\lambda_{i'})| \gg |f_k(\lambda_i)|, i \neq i'$. We assume that $||\boldsymbol{x}_i||_2 = 1$ and $|\boldsymbol{y}_{i'}^H B\boldsymbol{v}_\ell| \approx |\boldsymbol{y}_i^H B\boldsymbol{v}_\ell|, i \neq i'$. This assumption holds when the input matrix is set as a random matrix. We define $\alpha_{i,k,\ell} := f_k(\lambda_i)\boldsymbol{y}_i^H B\boldsymbol{v}_\ell$. Then, $|\alpha_{i',k,\ell}| \gg |\alpha_{i,k,\ell}|, i \neq i'$. From Proposition 1, we have

$$\frac{1}{\alpha_{i',k,\ell}}\hat{\boldsymbol{s}}_{k,\ell} = \boldsymbol{x}_{i'} + \sum_{i=1, i\neq i'}^{n} \frac{\alpha_{i,k,\ell}}{\alpha_{i',k,\ell}}\boldsymbol{x}_i, \quad \left|\frac{\alpha_{i,k,\ell}}{\alpha_{i',k,\ell}}\right| \ll 1.$$

From the above discussion, the Rayleigh-Ritz procedure with the subspace spanned by $\hat{\boldsymbol{s}}_{k,\ell}$ provides high accuracy eigenpair for $(\lambda_{i'}, \boldsymbol{x}_{i'})$. In contrast, other eigenpairs are obtained with low accuracy due to rounding error.

4. Proposed method for recovering the accuracy

In Section 3, we observed that the accuracy deterioration is caused by the oscillation of the filter function. Here, we propose a method to recover the accuracy by suppressing the oscillation. We assume that there are one or more eigenvalues near just one quadrature point and the linear equations are solved with sufficiently high accuracy.

Since a large absolute value of the filter function of the eigenvalues near a quadrature point adversely affects the accuracy of the eigenpairs, we need to prevent this influence. The following approach is a simple

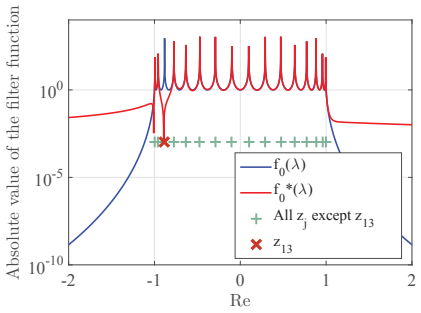

Fig. 3. Absolute value of the filter function $f_0^*(\lambda)$ for $j' = 13$ and $f_0(\lambda)$ on the real axis. The quadrature points ('+' and '×') are the Chebyshev points on the interval $[-1, 1]$ for $N = 16$.

method for improving the accuracy of the eigenpairs. After obtaining the approximate eigenpairs by the SS method, we apply the SS method again with quadrature points set away from the approximate eigenvalues. As a result, improved approximate eigenpairs are obtained. However, this approach requires linear equations again. In the SS method, the computation time for solving the linear equations accounts for most of the total computation time [5]. Therefore, we propose a method that avoids solving linear equations again.

We introduce a filter function $f_k^*(\lambda)$ defined as follows:

$$f_k^*(\lambda) := \sum_{j=0, j\neq j'}^{N-1} \frac{w_j z_j^k}{z_j - \lambda}.$$

This filter function is equivalent to $f_k(\lambda)$ with $w_{j'} = 0$ and is shown in Fig. 3. By using the filter function $f_k^*(\lambda)$, the oscillation of the filter function $f_k(\lambda)$ around $\lambda = z_{j'}$ is suppressed because $f_k^*(\lambda)$ does not have the pole $z_{j'}$. To avoid the accuracy deterioration due to the oscillation of $f_k(\lambda)$, we propose a method based on $f_k^*(\lambda)$.

After obtaining the approximate eigenpairs by the SS method, we compute the value of the filter function at each approximate eigenvalue and find the nearest quadrature point $z_{j'}$ from the eigenvalue for which the absolute value of the filter function is the largest. Then, we compute the matrix $\hat{S}^*$ by

$$S^* := [\hat{S}_0^*, \hat{S}_1^*, \ldots, \hat{S}_{K-1}^*], \quad \hat{S}_k^* := \sum_{j=0, j\neq j'}^{N-1} w_j z_j^k Y_j. \quad (5)$$

We extract the approximate eigenpairs from $\hat{S}^*$ by the Rayleigh-Ritz procedure. Finally, we compare the accuracy of the eigenpairs extracted from $\hat{S}^*$ and the accuracy of the eigenpairs obtained by the SS method. The eigenpairs with higher accuracy are adopted as solutions. The algorithm of the proposed method is shown in Algorithm 2. Since the proposed method can obtain improved eigenpairs without solving linear equations again, the computational cost is low.

5. Accuracy of the proposed method

First, we present a theory regarding the accuracy of the eigenpairs obtained by the SS method [4]. In this section, we assume that the weights satisfy (4) and true

Algorithm 2 Proposed method

Input: $L, K, N \in \mathbb{N}, V \in \mathbb{C}^{n\times L}, (z_j, w_j)$
Output: eigenpairs $(\lambda_i^*, \boldsymbol{x}_i^*), i = 1, 2, \ldots, LK$

1: Apply the SS method and compute approximate eigenpairs $(\lambda_i, \boldsymbol{x}_i), i = 1, 2, \ldots, LK$.
2: Compute the values of the filter function $f_0(\lambda_i), i = 1, 2, \ldots, LK$.
3: Set $i' = \arg\max_i(|f_0(\lambda_i)|), j' = \arg\min_j(|\lambda_{i'} - z_j|)$.
4: Compute $\hat{S}_k^*, k = 0, 1, \ldots, K-1$ by (5).
5: Construct an orthogonal basis Q^* from $\hat{S}^*$.
6: Compute the eigenpairs $(\theta_i^*, \boldsymbol{u}_i^*)$ of $Q^{*H}AQ^*\boldsymbol{u}^* = \theta^* Q^{*H}BQ^*\boldsymbol{u}^*$.
7: Set $(\lambda_i^*, \boldsymbol{x}_i^*) = (\theta_i^*, Q^*\boldsymbol{u}_i^*), i = 1, 2, \ldots, LK$.
8: Set $(\lambda_i^*, \boldsymbol{x}_i^*) = (\lambda_i, \boldsymbol{x}_i)$ if the accuracy of $(\lambda_i, \boldsymbol{x}_i)$ is better than $(\lambda_i^*, \boldsymbol{x}_i^*)$.

eigenpairs $(\lambda_i, \boldsymbol{x}_i), i = 1, 2, \ldots, n$, are ordered in decreasing order of $|f_0(\lambda_i)|$.

Theorem 2 *We define $\hat{\mathcal{P}}$, the orthogonal projector onto the subspace* range$(\hat{S})$. *Moreover, we define P_{LK}, the spectral projector associated with the invariant subspace associated with $\lambda_1, \lambda_2, \ldots, \lambda_{LK}$. We assume* rank$(P_{LK}V) = L$. *Then, the following relation holds:*

$$||(I - \hat{\mathcal{P}})\boldsymbol{x}_i||_2 \leq \alpha\beta_i \left|\frac{f_0(\lambda_{LK+1})}{f_0(\lambda_i)}\right|,$$

where $\alpha = ||X||_2||X^{-1}||_2$, $X = [\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n]$, and β_i depends on the input matrix.

The above theorem indicates that if the subspace size LK is sufficiently large so that $|f_0(\lambda_{LK+1})|$ is sufficiently small, the obtained eigenpairs have high accuracy.

In [4], the following case is also considered. The solution $Y_{j'}$ of the linear equation at the j'-th quadrature point is contaminated, namely, $Y_{j'}$ is replaced by $Y_{j'} + E$, where a matrix $E \in \mathbb{C}^{n\times L}$ satisfies rank$(E) = L$. Here, we define $\hat{S}'$ and $\hat{S}'_k$ as follows:

$$\hat{S}' := [\hat{S}'_0, \hat{S}'_1, \ldots, \hat{S}'_{K-1}], \quad \hat{S}'_k := \sum_{j=0}^{N-1} w_j z_j^k (Y_j + \delta_{j,j'}E),$$

where $\delta_{i,j}$ is the Kronecker delta. We assume that the input matrix V satisfies a similar condition as Theorem 2. (For details, refer to [4, Theorem 3].) Then, as in Theorem 2, a theorem regarding the accuracy of the eigenpairs holds.

Theorem 3 *We define $\hat{\mathcal{P}}'$, the orthogonal projector onto the subspace* range$(\hat{S}')$. *Then, the following relation holds:*

$$||(I - \hat{\mathcal{P}}')\boldsymbol{x}_i||_2 \leq \alpha\beta'_i \left|\frac{f_0(\lambda_{LK-L+1})}{f_0(\lambda_i)}\right|,$$

where β'_i depends on the input matrix.

The accuracy of the eigenpairs extracted from $\hat{S}$ depends on the $(LK+1)$-st largest absolute value of the filter function, whereas Theorem 3 indicates that the accuracy of the eigenpairs extracted from $\hat{S}'$ depends on the $(LK - L + 1)$-st largest absolute value of the filter function.

In the proposed method, the filter function $f_k^*(\lambda)$ is used. However, the accuracy of the eigenpairs can be analyzed by using $f_0(\lambda)$, not $f_0^*(\lambda)$.

Theorem 4 *We define $\hat{\mathcal{P}}^*$, the orthogonal projector onto the subspace* range$(\hat{S}^*)$. *We assume* rank$(Y_{j'}) = L$. *Then, the following relation holds:*

$$||(I - \hat{\mathcal{P}}^*)\boldsymbol{x}_i||_2 \leq \alpha\beta_i^* \left| \frac{f_0(\lambda_{LK-L+1})}{f_0(\lambda_i)} \right|, \qquad (6)$$

where β_i^* depends on the input matrix.

Proof The matrix $\hat{S}^*$ is equal to $\hat{S}'$ with $E = -Y_{j'}$. Since the rank of $Y_{j'}$ is L, from Theorem 3, we have (6). **(QED)**

This indicates that, if the subspace size $LK - L$ is sufficiently large so that $|f_0(\lambda_{LK-L+1})|$ is sufficiently small, then the obtained eigenpairs have high accuracy, even if the filter function $f_k^*(\lambda)$ is used.

6. Numerical example

In this section, we confirm the validity of the proposed method. We compare the relative residual of the eigenpairs obtained by the SS method and the eigenpairs obtained by the proposed method. A matrix A is generated as $A = Q^T DQ$, where

$$D = \mathrm{diag}(0.09, 0.18, \ldots, 45) \in \mathbb{R}^{500\times 500},$$

and $Q \in \mathbb{R}^{500\times 500}$ is an orthogonal matrix. The matrix B is the identity matrix. We replace the $(5,5)$ entry of the matrix D by 0.637462, which is an eigenvalue near a quadrature point. The absolute value of the filter function of the eigenvalue 0.637462 is approximately 5.7×10^4. The algorithm is implemented in MATLAB R2013b. In order to satisfy the assumption that the linear equations are solved with high accuracy, we use multiple-precision arithmetic (25 digits) when solving the linear equations. After solving the linear equations, double-precision arithmetic is used. The linear equations are solved via the MATLAB command "\". The input matrix V is a random matrix generated by a uniform distribution. The parameters of the SS method are $N = 16, L = 7$, and $K = 8$. We compute eleven eigenvalues in the interval $[-1, 1]$ and the corresponding eigenvectors. We use the Chebyshev points as the quadrature points. The quadrature points z_j and the corresponding weights w_j are set as $z_j = \cos(\theta_j), w_j = (-1)^j/N \cdot \sin(\theta_j)$, where $\theta_j = (2j+1)\pi/(2N), j = 0, 1, \ldots, N-1$. The computational results are shown in Table 1.

Among the eigenpairs obtained by the SS method, only the eigenvalue (0.637462) near a quadrature point has high accuracy. The approximate eigenvalues whose absolute values of the filter function are smaller than that of the eigenvalue 0.637472 have lower accuracy. In the proposed method, the accuracy of the eigenpairs are improved.

The relative residual of the eigenvalue 0.637462 extracted from $\hat{S}^*$ is approximately 1.6×10^{-11}. The eigencomponents corresponding to eigenvalues near the extracted quadrature point $z_{j'}$ included in $\hat{S}^*$ are smaller than its eigen-components included in $\hat{S}$, and the accuracy of the eigenpairs becomes lower [4]. Thus, the accuracy of the eigenvalue 0.637462 extracted from $\hat{S}^*$ deteriorates. According to the algorithm of the proposed method, the approximate eigenpair obtained by the SS method is adopted.

Table 1. Relative residuals for each eigenpair in [-1,1].

		relative residual	
Eigenvalue	Filter value	SS method	Proposed method
0.09	7.3	6.7×10^{-11}	4.0×10^{-13}
0.18	1.0	5.8×10^{-10}	2.9×10^{-12}
0.27	2.8	6.1×10^{-10}	9.3×10^{-13}
0.36	1.1	2.1×10^{-9}	5.4×10^{-12}
0.45	2.4	1.6×10^{-9}	3.3×10^{-12}
0.54	1.1	2.8×10^{-9}	2.6×10^{-11}
0.637462	5.7×10^4	3.2×10^{-14}	3.2×10^{-14}
0.72	1.0	1.7×10^{-9}	1.5×10^{-11}
0.81	1.3	1.5×10^{-9}	5.4×10^{-12}
0.90	2.1	5.8×10^{-10}	1.4×10^{-12}
0.99	1.1	7.8×10^{-10}	5.2×10^{-12}

7. Conclusion

In the present paper, we stated the reason why the eigenpairs obtained by the SS method may have a low accuracy when eigenvalues are near a quadrature point. We proposed a method to recover the accuracy of the eigenpairs. If the subspace size $LK - L$ is sufficiently large, the approximate eigenpairs obtained via the proposed method have high accuracy. Moreover, the proposed method has low computational cost because resolving the linear equations is not necessary. We demonstrated the validity of the proposed method.

The proposed method is effective when eigenvalues are near only one quadrature point. However, if eigenvalues are near several quadrature points, the proposed method may not be valid due to insufficiency of the subspace size. Methods for improving the accuracy of the eigenpairs remain a subject for future research.

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