Accuracy analysis on the Rayleigh-Ritz type of the contour integral based eigensolver for solving generalized eigenvalue problems

Akira Imakura[1,*], Lei Du[2], and Tetsuya Sakurai[1,3]

[1]University of Tsukuba, Japan
[2]Dalian University of Technology, China.
[3]JST/CREST

[*]Email : imakura@cs.tsukuba.ac.jp

Abstract

We investigate the contour integral based eigensolvers for computing all eigenvalues located in a certain region and their corresponding eigenvectors. In this paper, we focus on the Rayleigh-Ritz type method and analyze its accuracy. From the results of our accuracy analysis, we conclude that the Rayleigh-Ritz type of the contour integral based eigensolver with enough subspace size can achieve high accuracy for target eigenpairs even if some eigenvalues exist outside, but near, the region.

1 Introduction

In this paper, we consider the contour integral based eigensolvers for computing all eigenvalues located in a certain region and their corresponding eigenvectors $(\lambda_i, \boldsymbol{x}_i)$ for the generalized eigenvalue problem of the form

$$A\boldsymbol{x}_i = \lambda_i B\boldsymbol{x}_i, \quad \boldsymbol{x}_i \in \mathbb{C}^n \setminus \{\boldsymbol{0}\}, \quad \lambda_i \in \Omega \subset \mathbb{C}, \tag{1}$$

where $A, B \in \mathbb{C}^{n\times n}$ and $A - zB$ is assumed to be nonsingular for any z on the boundary of Ω. Let m be the number of eigenvalues located in Ω, and is generally unknown. Such eigenvalue problems arise in many areas of computational science and engineering.

The contour integral based eigensolver for solving generalized eigenvalue problems (1) was first introduced by Sakurai and Sugiura in 2003 [10]. Since then, several authors have actively studied and proposed improvement techniques based on the concepts of Sakurai and Sugiura [4–6, 8, 11, 13]. The concepts of Sakurai and Sugiura have also been extended for solving nonlinear eigenvalue problems [1–3, 14].

In this paper, we specifically investigate the block and Rayleigh-Ritz type of the contour integral based eigensolver called the block SS-RR method [5] for solving (1). We analyze the accuracy of the eigenpairs obtained from the block SS-RR method with the numerical integration. We also analyze the accuracy when a certain computation in the numerical integration is contaminated; details will be described in Section 4. Here, we note that our analyses in this paper are not for roundoff errors, but only for errors from the numerical integration.

For our accuracy analyses, we also assume that the matrix pencil (A, B) is diagonalizable, i.e.,

$$\widetilde{P}^{\mathrm{H}}(zB - A)Q = z \begin{bmatrix} I_r & \\ & O_{n-r} \end{bmatrix} - \Lambda, \tag{2}$$

where $\Lambda := \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$ is a diagonal matrix and $\widetilde{P} := [\widetilde{\boldsymbol{p}}_1, \widetilde{\boldsymbol{p}}_2, \ldots, \widetilde{\boldsymbol{p}}_n]$, $Q := [\boldsymbol{q}_1, \boldsymbol{q}_2, \ldots, \boldsymbol{q}_n]$ are nonsingular matrices. I_r and O_{n-r} denote the r dimensional identity matrix and the $(n-r) \times (n-r)$ zero matrix with all their entries being zero, respectively. The generalized eigenvalue problem $A\boldsymbol{x}_i = \lambda_i B\boldsymbol{x}_i$ has $r := \mathrm{rank}(B)$ finite eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_r$ and $n-r$ infinite eigenvalues. The vectors $\widetilde{\boldsymbol{p}}_i$ and $\boldsymbol{q}_i$ are the corresponding left and right eigenvectors, respectively.

The remainder of this paper is organized as follows. In Section 2, we briefly describe the basic concepts of the contour integral based eigensolver, and the algorithm of the block SS-RR method with the continuous integration. In Section 3, we show the algorithm of the block SS-RR method with the numerical integration, and analyze its accuracy. In Section 4, we analyze the accuracy when a certain computation in the numerical integration is contaminated. Finally we draw some conclusions in Section 5.

Throughout, the following notations are used. Let $V = [\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_L] \in \mathbb{C}^{n \times L}$, then $\mathrm{span}\{V\} := \mathrm{span}\{\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_L\}$. Also, let $A \in \mathbb{C}^{n \times n}$, then $\mathcal{K}_k^{\square}(A, V)$ is the block Krylov subspace, and is defined by $\mathcal{K}_k^{\square}(A, V) := \mathrm{span}\{[V, AV, A^2V, \ldots, A^{k-1}V]\}$.

2 The contour integral based eigensolver

As a powerful algorithm for solving the generalized eigenvalue problem (1), the contour integral based eigensolver was first introduced by Sakurai and Sugiura in 2003 [10]; this is called the SS-Hankel method. For solving (1), they introduced the rational function

$$f(z) := \boldsymbol{u}^{\mathrm{H}}(zB - A)^{-1}B\boldsymbol{v}, \quad \boldsymbol{u}, \boldsymbol{v} \in \mathbb{C}^n \setminus \{\boldsymbol{0}\}, \tag{3}$$

whose poles are eigenvalues λ of the generalized eigenvalue problem; they then considered computing all poles located in Ω.

All poles located in a certain region of an analytic function can be computed by the algorithm in [7], which is based on the Cauchy's integral formula

$$f(a) = \frac{1}{2\pi \mathrm{i}} \oint_{\Gamma} \frac{f(z)}{z-a} \mathrm{d}z, \tag{4}$$

where Γ is the positively oriented Jordan curve (the boundary of Ω). Applying the algorithm in [7] to the rational function (3), the eigenpairs $(\lambda_i, \boldsymbol{x}_i)$ of the generalized eigenvalue problem (1) can be obtained from the generalized eigenvalue problem: $H_M^{<}\boldsymbol{u}_i = \theta_i H_M \boldsymbol{u}_i$, where H_M and $H_M^{<}$ are small $M \times M$ Hankel matrices whose entries consist of the moments

$$H_M(i,j) = \mu_{i+j-2}, \quad H_M^{<}(i,j) = \mu_{i+j-1}, \quad \mu_k := \frac{1}{2\pi \mathrm{i}} \oint_{\Gamma} z^k f(z) \mathrm{d}z.$$

For details, we refer to [10].

For more accurate eigenpairs, an improvement on the SS-Hankel method has been proposed [11] based on using the Rayleigh-Ritz procedure, and is called the SS-RR method. Block variants of the SS-Hankel method and the SS-RR method have also been proposed [4,5] for the higher stability of the algorithms, specifically when multiple eigenvalues exist in Ω. These are called the block SS-Hankel method and the block SS-RR method, respectively. Recently we have also introduced an Arnoldi-based interpretation of the contour integral based eigensolvers and proposed a new algorithm named as the block SS-Arnoldi method [6].

Algorithm 1 The block SS-RR method with the continuous integration

Input: $L, M \in \mathbb{N}, V \in \mathbb{C}^{n\times L}$
Output: Eigenpairs $(\lambda_i, \boldsymbol{x}_i)$ for $i = 1, 2, \ldots, LM$
1: Compute $S_k = \oint_\Gamma z^k (zB - A)^{-1} BV \mathrm{d}z$ for $k = 0, 1, \ldots, M-1$
2: Compute the orthogonalization of $S = [S_0, S_1, \ldots, S_{M-1}] : W = \mathrm{orth}(S)$
3: Compute eigenpairs $(\theta_i, \boldsymbol{u}_i)$ of the matrix pencil $(W^{\mathrm{H}}AW, W^{\mathrm{H}}BW)$, and $(\lambda_i, \boldsymbol{x}_i) = (\theta_i, W\boldsymbol{u}_i)$ for $i = 1, 2, \ldots, LM$

As another approach of the contour integral based eigensolver, Polizzi has proposed the FEAST eigensolver in 2009 [8] and developed it [13]. The FEAST eigensolver is the subspace iteration-type method based on the concepts of Sakurai and Sugiura, and one iteration of it can also be regarded as a special case of the block SS-Arnoldi method [6].

We describe the algorithm of the block SS-RR method. Let $V \in \mathbb{C}^{n\times L} \setminus \{O\}$ such that $V^{\mathrm{H}}[\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_m]$ is full rank, e.g., a random matrix. Then, the block SS-RR method [5] constructs the LM-dimensional subspace $\mathrm{span}\{S\}$ for the Rayleigh-Ritz procedure, where

$$S := [S_0, S_1, \ldots, S_{M-1}], \quad S_k := \frac{1}{2\pi \mathrm{i}} \oint_\Gamma z^k (zB - A)^{-1} BV \mathrm{d}z. \tag{5}$$

The algorithm of the block SS-RR method with the continuous integration (5) can be shown in Algorithm 1.

For the subspace constructed by the block SS-RR method with the continuous integration (Algorithm 1), we have the following theorem.

Theorem 1. *Let m be the number of eigenvalues of (1) and $m \le LM$. We also let $V \in \mathbb{C}^{n\times L}$ such that $V^{\mathrm{H}}[\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_m]$ is full rank. Then we have*

$$\mathrm{span}\{S\} = \mathrm{span}\{\boldsymbol{x}_i | \lambda_i \in \Omega, i = 1, \ldots, m\}.$$

Proof. From the diagonalization of the matrix pencil (2), we have

$$(zB - A)^{-1} = Q \left(z \begin{bmatrix} I_r & \\ & O_{n-r} \end{bmatrix} - \Lambda \right)^{-1} \widetilde{P}^{\mathrm{H}}, \quad B = P \begin{bmatrix} I_r & \\ & O_{n-r} \end{bmatrix} \widetilde{Q}^{\mathrm{H}},$$

where $P := \widetilde{P}^{-\mathrm{H}}, \widetilde{Q}^{\mathrm{H}} := Q^{-1}$. Here let $Q = [\boldsymbol{q}_1, \boldsymbol{q}_2, \ldots, \boldsymbol{q}_n], \widetilde{Q} = [\widetilde{\boldsymbol{q}}_1, \widetilde{\boldsymbol{q}}_2, \ldots, \widetilde{\boldsymbol{q}}_n]$ and $\Lambda = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$. Then, from the Cauchy's integral formula (4), the matrix S_k in (5) can be rewritten by

$$\begin{aligned} S_k &= \frac{1}{2\pi \mathrm{i}} \oint_\Gamma \sum_{i=1}^{r} \frac{z^k}{z - \lambda_i} \boldsymbol{q}_i \widetilde{\boldsymbol{q}}_i^{\mathrm{H}} V \mathrm{d}z \\ &= \sum_{i, \lambda_i \in \Omega} \lambda_i^k \boldsymbol{q}_i \widetilde{\boldsymbol{q}}_i^{\mathrm{H}} V \\ &= Q_\Gamma \Lambda_\Gamma^k \widetilde{Q}_\Gamma^{\mathrm{H}} V, \end{aligned}$$

where $\Lambda_\Gamma = \mathrm{diag}\{\lambda_i | \lambda_i \in \Omega\}, Q_\Gamma = [\boldsymbol{q}_i | \lambda_i \in \Omega], \widetilde{Q}_\Gamma = [\widetilde{\boldsymbol{q}}_i | \lambda_i \in \Omega]$. This leads to

$$S = [S_0, S_1, \ldots, S_{M-1}] = Q_\Gamma Y,$$

Algorithm 2 The block SS-RR method with the numerical integration

Input: $L, M, N \in \mathbb{N}, V \in \mathbb{C}^{n\times L}, (z_j, \omega_j), j = 1, 2, \ldots, N$
Output: Eigenpairs $(\lambda_i, \boldsymbol{x}_i)$ for $i = 1, 2, \ldots, LM$
1: Compute $\widehat{S}_k = \sum_{j=1}^{N} \omega_j z_j^k (z_j B - A)^{-1} BV$ for $k = 0, 1, \ldots, M-1$
2: Compute the orthogonalization of $\widehat{S} = [\widehat{S}_0, \widehat{S}_1, \ldots, \widehat{S}_{M-1}] : W = \mathrm{orth}(\widehat{S})$
3: Compute eigenpairs $(\theta_i, \boldsymbol{u}_i)$ of the matrix pencil $(W^{\mathrm{H}}AW, W^{\mathrm{H}}BW)$, and $(\lambda_i, \boldsymbol{x}_i) = (\theta_i, W\boldsymbol{u}_i)$ for $i = 1, 2, \ldots, LM$

where

$$Y := [\Lambda_\Gamma^0, \Lambda_\Gamma^1, \ldots, \Lambda_\Gamma^{M-1}] \begin{bmatrix} \widetilde{Q}_\Gamma^{\mathrm{H}} V & & & \\ & \widetilde{Q}_\Gamma^{\mathrm{H}} V & & \\ & & \ddots & \\ & & & \widetilde{Q}_\Gamma^{\mathrm{H}} V \end{bmatrix}.$$

Since $V^{\mathrm{H}}[\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_m]$ is full rank, $\widetilde{Q}_\Gamma^{\mathrm{H}} V$ and Y are also full rank matrices. Therefore $\mathrm{span}\{S\} = \mathrm{span}\{Q_\Gamma\} = \mathrm{span}\{\boldsymbol{x}_i | \lambda_i \in \Omega\}$ because of $\boldsymbol{q}_i = \boldsymbol{x}_i$. Thus Theorem 1 is proven. □

3 Accuracy analysis on the block SS-RR method

In this section, we introduce the algorithm of the block SS-RR method with the numerical integration, we then analyze its accuracy. We also experimentally evaluate the results of the accuracy analysis.

3.1 The block SS-RR method with the numerical integration

The continuous integration (5) is approximated by some numerical integration rule such as the N-point trapezoidal rule with $N \geq M - 1$

$$S \approx \widehat{S} := [\widehat{S}_0, \widehat{S}_1, \ldots, \widehat{S}_{M-1}], \quad \widehat{S}_k := \sum_{j=1}^{N} \omega_j z_j^k (z_j B - A)^{-1} BV, \tag{6}$$

where z_j are the quadrature points and ω_j are the corresponding weights. Here the weights ω_j are required to satisfy

$$\sum_{j=1}^{N} \omega_j z_j^k = 0, \quad k = 0, 1, \ldots, N-2, \tag{7}$$

as well as the Cauchy's integral theorem in the continuous integration. Using the numerical integration (6), the algorithm of the block SS-RR method with the numerical integration is shown in Algorithm 2.

Algorithm 2 can be modified in terms of the iteration technique. The basic concept is that the matrix $\widehat{S}_0^{(\ell-1)}$ is iteratively calculated, from the initial matrix $\widehat{S}_0^{(0)} = V$, as follows.

$$\widehat{S}_0^{(\ell_i)} := \sum_{j=1}^{N} \omega_j (z_j B - A)^{-1} B \widehat{S}_0^{(\ell_i - 1)}, \quad \ell_i = 1, 2, \ldots, \ell - 1. \tag{8}$$

Algorithm 3 The block SS-RR method with the iteration technique

Input: $L, M, N, \ell \in \mathbb{N}, \widehat{S}_0^{(0)} = V \in \mathbb{C}^{n\times L}, (z_j, \omega_j), j = 1, 2, \ldots, N$
Output: Eigenpairs $(\lambda_i, \boldsymbol{x}_i)$ for $i = 1, 2, \ldots, LM$
1: Compute $\widehat{S}_0^{(\ell_i)} = \sum_{j=1}^{N} \omega_j (z_j B - A)^{-1} B \widehat{S}_0^{(\ell_i - 1)}$ for $\ell_i = 1, 2, \ldots, \ell - 1$
2: Compute $\widehat{S}_k^{(\ell)} = \sum_{j=1}^{N} \omega_j z_j^k (z_j B - A)^{-1} B \widehat{S}_0^{(\ell-1)}$ for $k = 0, 1, \ldots, M - 1$
3: Compute the orthogonalization of $\widehat{S}^{(\ell)} = [\widehat{S}_0^{(\ell)}, \widehat{S}_1^{(\ell)}, \ldots, \widehat{S}_{M-1}^{(\ell)}] : W = \mathrm{orth}(\widehat{S}^{(\ell)})$
4: Compute eigenpairs $(\theta_i, \boldsymbol{u}_i)$ of the matrix pencil $(W^{\mathrm{H}} A W, W^{\mathrm{H}} B W)$, and $(\lambda_i, \boldsymbol{x}_i) = (\theta_i, W \boldsymbol{u}_i)$ for $i = 1, 2, \ldots, LM$

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

$$\widehat{S}^{(\ell)} := [\widehat{S}_0^{(\ell)}, \widehat{S}_1^{(\ell)}, \ldots, \widehat{S}_{M-1}^{(\ell)}], \quad \widehat{S}_k^{(\ell)} := \sum_{j=1}^{N} \omega_j z_j^k (z_j B - A)^{-1} B \widehat{S}_0^{(\ell-1)}, \tag{9}$$

and $\mathrm{span}\{\widehat{S}^{(\ell)}\}$ is used for the Rayleigh-Ritz procedure instead of $\mathrm{span}\{\widehat{S}\}$.

Based on the iteration technique (8) and (9), the algorithm of the block SS-RR method with the iteration technique is shown in Algorithm 3. Algorithm 3 with $\ell = 1$ is equivalent to Algorithm 2. It has been experimentally shown that Algorithm 3 can achieve higher accuracy even with small N.

In practice for Algorithms 2 and 3, z^k are scaled for accurate calculation and the matrix $\widehat{S}^{(\ell)}$ is also approximated by a low rank matrix for reducing the cost of the Rayleigh-Ritz procedure.

In the next subsection, we analyze the accuracy of the block SS-RR method with the iteration technique (Algorithm 3).

3.2 Accuracy analysis on the block SS-RR method with numerical integration

Here, we analyse the accuracy of the block SS-RR method using the filter function that was used for analyses on some eigensolvers [4, 12]. As with Theorem 1 for the continuous integration, Eq. (8) for the numerical integration can be decomposed into each eigenpairs

$$\widehat{S}_0^{(\ell_i)} = \sum_{j=1}^{N} \sum_{i=1}^{r} \frac{\omega_j}{z_j - \lambda_i} \boldsymbol{q}_i \widetilde{\boldsymbol{q}}_i^{\mathrm{H}} \widehat{S}_0^{(\ell_i - 1)}, \quad \ell_i = 1, 2, \ldots, \ell - 1.$$

Here, let $f(\lambda_i)$ be the filter function defined by

$$f(\lambda_i) := \sum_{j=1}^{N} \frac{\omega_j}{z_j - \lambda_i}.$$

Then, $\widehat{S}_0^{(\ell-1)}$ can be written by

$$\widehat{S}_0^{(\ell-1)} = \sum_{i=1}^{r} f^{\ell-1}(\lambda_i) \boldsymbol{q}_i \widetilde{\boldsymbol{q}}_i^{\mathrm{H}} V,$$

and this leads to

$$\widehat{S}_k^{(\ell)} = \sum_{j=1}^{N}\sum_{i=1}^{r} \frac{\omega_j z_j^k}{z_j - \lambda_i} f^{\ell-1}(\lambda_i)\boldsymbol{q}_i\widetilde{\boldsymbol{q}}_i^{\mathrm{H}} V. \tag{10}$$

Here we have the following proposition.

Proposition 1. *Let (z_j, ω_j) be quadrature points and the corresponding weights satisfying (7). Then we have*

$$\sum_{j=1}^{N} \frac{\omega_j z_j^k}{z_j - \lambda} = \lambda^k \sum_{j=1}^{N} \frac{\omega_j}{z_j - \lambda}, \quad k = 0, 1, \ldots, N-1, \tag{11}$$

where we define that $0^0 = 1$.

Proof. In the case of $\lambda = 0$, Eq. (11) is naturally satisfied from (7) such that

$$\sum_{j=1}^{N} \frac{\omega_j z_j^k}{z_j - \lambda} = \lambda^k \sum_{j=1}^{N} \frac{\omega_j}{z_j - \lambda} = \begin{cases} \sum_{j=1}^{N} \omega_j / z_j & (k = 0) \\ 0 & (k = 1, 2, \ldots, N-1) \end{cases}.$$

Therefore we prove when $\lambda \neq 0$. We have

$$\frac{\omega_j z_j^k}{z_j - \lambda} = \frac{\omega_j}{z_j - \lambda}\lambda^k \left(\frac{z_j}{\lambda}\right)^k = \frac{\omega_j}{z_j - \lambda}\lambda^k \left(1 + \frac{z_j - \lambda}{\lambda}\right)^k.$$

Here, from the binomial theorem $(a+b)^k = \sum_{p=0}^{k} \binom{k}{p} a^{k-p} b^p$, this is rewritten by

$$\frac{\omega_j z_j^k}{z_j - \lambda} = \frac{\omega_j}{z_j - \lambda}\lambda^k \sum_{p=0}^{k} \binom{k}{p} \left(\frac{z_j - \lambda}{\lambda}\right)^p.$$

Therefore, the left term of Eq. (11) is

$$\begin{aligned} \sum_{j=1}^{N} \frac{\omega_j z_j^k}{z_j - \lambda} &= \sum_{j=1}^{N} \frac{\omega_j}{z_j - \lambda}\lambda^k \sum_{p=0}^{k} \binom{k}{p} \left(\frac{z_j - \lambda}{\lambda}\right)^p \\ &= \lambda^k \sum_{p=0}^{k} \binom{k}{p} \lambda^{-p} \sum_{j=1}^{N} \omega_j (z_j - \lambda)^{p-1}. \end{aligned}$$

Here from (7), we have

$$\sum_{j=1}^{N} \omega_j (z_j - \lambda)^{p-1} = 0, \quad p = 1, 2, \ldots, N-1.$$

Therefore, for $k = 0, 1, \ldots, N-1$,

$$\sum_{j=1}^{N} \frac{\omega_j z_j^k}{z_j - \lambda} = \lambda^k \binom{k}{0} \lambda^{-0} \sum_{j=1}^{N} \omega_j (z_j - \lambda)^{-1} = \lambda^k \sum_{j=1}^{N} \frac{\omega_j}{z_j - \lambda}.$$

Therefore Proposition 1 is proven. □

Proposition 1 means that Eq. (10) can be rewritten by

$$\begin{aligned}\widehat{S}_k^{(\ell)} &= \sum_{i=1}^{r} \lambda_i^k \left(\sum_{j=1}^{N} \frac{\omega_j}{z_j - \lambda_i} \right) f^{\ell-1}(\lambda_i) \boldsymbol{q}_i \widetilde{\boldsymbol{q}}_i^{\mathrm{H}} V \\ &= \sum_{i=1}^{n} \lambda_i^k f^{\ell}(\lambda_i) \boldsymbol{q}_i \widetilde{\boldsymbol{q}}_i^{\mathrm{H}} V \\ &= Q_r \Lambda_r^k f^{\ell}(\Lambda_r) \widetilde{Q}_r^{\mathrm{H}} V, \end{aligned} \tag{12}$$

where $\Lambda_r := \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_r)$, $f(\Lambda_r) := \mathrm{diag}(f(\lambda_1), f(\lambda_2), \ldots, f(\lambda_r))$, $Q_r := [\boldsymbol{q}_1, \boldsymbol{q}_2, \ldots, \boldsymbol{q}_r]$ and $\widetilde{Q}_r := [\widetilde{\boldsymbol{q}}_1, \widetilde{\boldsymbol{q}}_2, \ldots, \widetilde{\boldsymbol{q}}_r]$. From Eqs. (9) and (12), $S^{(\ell)}$ can be shown by

$$\widehat{S}^{(\ell)} = F^{\ell} U, \tag{13}$$

where

$$\begin{aligned} F &:= Q_r f(\Lambda_r) \widetilde{Q}_r^{\mathrm{H}}, \\ U &:= [V, C_r V, C_r^2 V, \ldots, C_r^{M-1} V], \\ C_r &:= Q_r \Lambda_r \widetilde{Q}_r^{\mathrm{H}}. \end{aligned}$$

Here $F \in \mathbb{C}^{n \times n}$ is the diagonalizable matrix whose eigenpairs are $(f(\lambda_i), \boldsymbol{q}_i) = (f(\lambda_i), \boldsymbol{x}_i)$, and $U \in \mathbb{C}^{n \times LM}$ such that $\mathrm{span}\{U\} = \mathcal{K}_M^{\square}(C_r, V)$. Eq. (13) means that $\mathrm{span}\{\widehat{S}^{(\ell)}\}$ is constructed by the subspace iteration method of F with the input matrix U.

Here, we describe a general result of the subspace iteration method. With respect to the subspace constructed by the subspace iteration method

$$V_\ell = A^\ell V_0, \quad V_0 \in \mathbb{C}^{n \times m} \tag{14}$$

for a diagonalizable matrix A, we have the following lemma, see e.g., [9, Theorem 5.2]

Lemma 1. *Let V_ℓ be the matrix obtained from the subspace iteration method (14) for a diagonalizable matrix $A \in \mathbb{C}^{n \times n}$, where $A = X^{\mathrm{H}} \Lambda X$, $X = [\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n]$, $\Lambda = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$. Assume that the eigenvalues are ordered in decreasing order of magnitude $|\lambda_i| \geq |\lambda_{i+1}|$. Defining $\mathcal{P}^{(\ell)}$ and $\mathcal{P}_m$ to be the orthogonal projectors onto the subspaces $\mathrm{span}\{V_\ell\}$ and $\mathrm{span}\{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_m\}$, respectively.*

Assume that V_0 such that $\mathcal{P}_m V_0$ is full rank. Then for each eigenvector $\boldsymbol{x}_i, i = 1, 2, \ldots, m$, there exists a unique vector $\boldsymbol{s}_i$ in the subspace $\mathrm{span}\{V_0\}$ such that $\mathcal{P}_L \boldsymbol{s}_i = \boldsymbol{x}_i$. Moreover, the following inequality is satisfied

$$\|(I - \mathcal{P}^{(\ell)}) \boldsymbol{x}_i\|_2 \leq \alpha\beta \left| \frac{\lambda_{m+1}}{\lambda_i} \right|^{\ell},$$

where α is some constant independent on ℓ, and $\beta = \|\boldsymbol{x}_i - \boldsymbol{s}_i\|_2$.

Proof. See e.g., [9, Theorem 5.2]. □

In [9, Theorem 4.6], a result of an accuracy analysis of the Rayleigh-Ritz procedure for solving standard eigenvalue problems is given. We can extend it for solving generalized eigenvalue problems as follows:

Lemma 2. *Let $(\lambda_i, \boldsymbol{x}_i)$ be the exact eigenpairs of the matrix pencil (A, B). Defining $\mathcal{P}_{\mathcal{V}}$ to be the orthogonal projector onto the subspace $\mathcal{V}$. Then, the residual norm of the pairs of $(\lambda_i, \boldsymbol{x}_i)$ for the linear operators $A_{\mathcal{V}} := \mathcal{P}_{\mathcal{V}} A \mathcal{P}_{\mathcal{V}}, B_{\mathcal{V}} := \mathcal{P}_{\mathcal{V}} B \mathcal{P}_{\mathcal{V}}$ satisfy*

$$\|(A_{\mathcal{V}} - \lambda_i B_{\mathcal{V}})\boldsymbol{x}_i\|_2 \leq \gamma \|(I - \mathcal{P}_{\mathcal{V}})\boldsymbol{x}_i\|_2,$$

where $\gamma = \|\mathcal{P}_{\mathcal{V}}(A - \lambda_i B)(I - \mathcal{P}_{\mathcal{V}})\|_2$.

Proof. From the definition of $A_{\mathcal{V}}, B_{\mathcal{V}}$, we have

$$\begin{aligned} \|(A_{\mathcal{V}} - \lambda_i B_{\mathcal{V}})\boldsymbol{x}_i\|_2 &= \|\mathcal{P}_{\mathcal{V}}(A - \lambda_i B)(\boldsymbol{x}_i - (I - \mathcal{P}_{\mathcal{V}})\boldsymbol{x}_i)\|_2 \\ &= \|\mathcal{P}_{\mathcal{V}}(A - \lambda_i B)(I - \mathcal{P}_{\mathcal{V}})\boldsymbol{x}_i\|_2 \\ &= \|\mathcal{P}_{\mathcal{V}}(A - \lambda_i B)(I - \mathcal{P}_{\mathcal{V}})(I - \mathcal{P}_{\mathcal{V}})\boldsymbol{x}_i\|_2 \\ &\leq \gamma \|(I - \mathcal{P}_{\mathcal{V}})\boldsymbol{x}_i\|_2. \end{aligned}$$

Therefore Lemma 2 is proven. □

Recall that the block SS-RR method with the numerical integration and the iteration technique (Algorithm 3) is based on the Rayleigh-Ritz procedure with $\mathrm{span}\{\widehat{S}^{(\ell)}\}$ constructed by Eq. (13). Therefore, applying Lemmas 1 and 2 to Eq. (13), we provide the following theorem with respect to the accuracy of the block SS-RR method (Algorithm 3).

Theorem 2. *Assume that $f(\lambda_i)$ are ordered in decreasing order of magnitude $|f(\lambda_i)| \geq |f(\lambda_{i+1})|$. Defining $\mathcal{P}^{(\ell)}$ and $\mathcal{P}_{LM}$ to be the orthogonal projectors onto the subspaces $\mathrm{span}\{\widehat{S}^{(\ell)}\}$ and $\mathrm{span}\{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_{LM}\}$, respectively.*

Assume that U such that $\mathcal{P}_{LM} U$ is full rank. Then for each eigenvector $\boldsymbol{x}_i, i = 1, 2, \ldots, LM$, there exists a unique vector $\boldsymbol{s}_i$ in the subspace $\mathcal{K}_M^{\square}(C_r, V)$ such that $\mathcal{P}_{LM}\boldsymbol{s}_i = \boldsymbol{x}_i$. Then, the residual norm of the pairs of $(\lambda_i, \boldsymbol{x}_i)$ for the linear operators $A^{(\ell)} := \mathcal{P}^{(\ell)} A \mathcal{P}^{(\ell)}, B^{(\ell)} := \mathcal{P}^{(\ell)} B \mathcal{P}^{(\ell)}$ satisfy

$$\|(A^{(\ell)} - \lambda_i B^{(\ell)})\boldsymbol{x}_i\|_2 \leq \alpha\beta\gamma \left| \frac{f(\lambda_{LM+1})}{f(\lambda_i)} \right|^{\ell},$$

where α is some constant independent on ℓ, $\beta = \|\boldsymbol{x}_i - \boldsymbol{s}_i\|_2$, and $\gamma = \|\mathcal{P}^{(\ell)}(A - \lambda_i B)(I - \mathcal{P}^{(\ell)})\|_2$.

Proof. From Lemmas 1 and 2, we have

$$\|(A^{(\ell)} - \lambda_i B^{(\ell)})\boldsymbol{x}_i\|_2 \leq \gamma \|(I - \mathcal{P}^{(\ell)})\boldsymbol{x}_i\|_2 \leq \alpha\beta\gamma \left| \frac{f(\lambda_{LM+1})}{f(\lambda_i)} \right|^{\ell}.$$

Therefore Theorem 2 is proven. □

Here we note that γ is bounded from above by the norms of the matrices such that $\gamma \leq \|A\|_2 + |\lambda_i| \|B\|_2$, and β strongly depends on the input subspace $\mathrm{span}\{U\}$. Because of $\mathrm{span}\{U\} = \mathcal{K}_M^{\square}(C_r, V)$, if $V \in \mathbb{C}^{n \times L}$ such that $\mathrm{span}\{V\}$ equally contains the components of the eigenvectors corresponding to $\lambda_i \in \Omega$, e.g., the random matrix, and the region Ω is not so large, then it is expected that all β have almost the same value for $\lambda_i \in \Omega$.

Theorem 2 means that the accuracy of the block SS-RR method in terms of the residual 2-norm $\|(A^{(\ell)} - \lambda_i B^{(\ell)})\boldsymbol{x}_i\|_2$ is evaluated by the ratio of the magnitude of the filter function $|f(\lambda_i)|$ to the $(LM + 1)$-th largest one $|f(\lambda_{LM+1})|$. The magnitude of the filter function

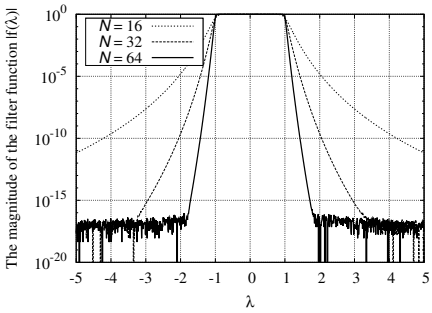


Fig. 1: The magnitude of the filter function $|f(\lambda)|$ of the N-point trapezoidal rule with $N = 16, 32, 64$ for the circle region Ω with the center $\rho = 0$ and radius $\gamma = 1$.

$|f(\lambda_i)|$ of the N-point trapezoidal rule with $N = 16, 32, 64$ for the circle region Ω with the center $\rho = 0$ and radius $\gamma = 1$ can be shown in Fig. 1. The filter function has $|f(\lambda)| \approx 1$ inside the region Ω, $|f(\lambda))| \approx 0$ far from the region and $0 < |f(\lambda)| < 1$ outside but near the region.

Therefore we observe from Theorem 2 that, using enough subspace size LM such that $|f(\lambda_{LM+1})|^\ell \approx 0$, the block SS-RR method achieves high accuracy for the target eigenpairs (the eigenvalue is inside Ω) even if some eigenvalues exist outside, but near, the region.

3.3 Experimental evaluation of the accuracy analysis

In this subsection, we experimentally evaluate the results of Theorem 2. We apply the block SS-RR method (Algorithm 3) to the model problem

$$\begin{gathered} A\boldsymbol{x}_i = \lambda B\boldsymbol{x}_i, \\ A = \mathrm{diag}(0.01, 0.11, 0.21, \ldots, 9.91) \in \mathbb{R}^{100\times 100}, \quad B = I_{100}, \\ \lambda_i \in \Omega : \mathrm{circle\ with\ center}\ \ \rho = 0, \mathrm{radius}\ \ \gamma = 1, \end{gathered} \tag{15}$$

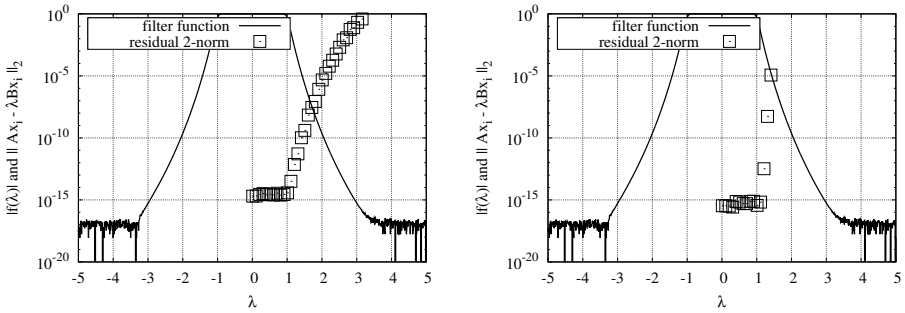
and evaluate its accuracy. Here, for the model problem, the number of eigenvalues located in Ω is $m = 10$ and outside nearest eigenvalue is 1.01.

We evaluate the relation of the accuracy with the number of subspace size LM and the number of iteration ℓ. For the first example to evaluate the relation with LM, we fixed the parameters as $L = 10, N = 32, \ell = 1$, and tested four cases $M = 1, 2, 3, 4$ ($LM = 10, 20, 30, 40$). For the second example to evaluate the relation with ℓ, we fixed the parameters as $L = 5, M = 3, N = 32$, and tested four cases $\ell = 1, 2, 3, 4$. For these examples we set the quadrature points as follows:

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

The algorithm was implemented in MATLAB R2014a. The input matrix V was set as a random matrix generated by the Mersenne Twister in MATLAB, and each linear system was solved by the MATLAB command "\".

The numerical results are presented in Fig. 2 and Table 1. We show the residual 2-norm $\|\boldsymbol{r}_i\|_2 := \|A\boldsymbol{x}_i - \lambda_i B\boldsymbol{x}_i\|_2$ with $L = 10, M = 4, N = 32, \ell = 1$ in Fig. 2(a), and with $L = 5, M = 3, N = 32, \ell = 4$ in Fig. 2(b), respectively. We also show the relationship of the



(a) $L = 10, M = 4, N = 32, \ell = 1$ (b) $L = 5, M = 3, N = 32, \ell = 4$

Fig. 2: The accuracy of the block SS-RR method and the filter function.

Table 1: Relationship of the accuracy of the block SS-RR method with LM and ℓ.

(a) Relationship with LM ($\ell = 1$)

M (LM)	$\lvert f(\lambda_{LM+1})\rvert$	$\min_{\lambda_i \in \Omega} \lVert \boldsymbol{r}_i \rVert_2$	$\max_{\lambda_i \in \Omega} \lVert \boldsymbol{r}_i \rVert_2$
1 (10)	4.21×10^{-1}	1.76×10^{-2}	1.34×10^{-1}
2 (20)	1.98×10^{-10}	2.29×10^{-10}	2.11×10^{-9}
3 (30)	5.03×10^{-16}	1.44×10^{-15}	1.20×10^{-14}
4 (40)	5.20×10^{-18}	2.03×10^{-15}	3.46×10^{-15}

(b) Relationship with ℓ ($LM = 15$)

ℓ	$\lvert f(\lambda_{LM+1})\rvert^{\ell}$	$\min_{\lambda_i \in \Omega} \lVert \boldsymbol{r}_i \rVert_2$	$\max_{\lambda_i \in \Omega} \lVert \boldsymbol{r}_i \rVert_2$
1	2.41×10^{-7}	1.68×10^{-7}	7.07×10^{-6}
2	5.80×10^{-14}	2.36×10^{-13}	1.32×10^{-11}
3	1.40×10^{-20}	1.67×10^{-16}	1.37×10^{-15}
4	3.36×10^{-27}	2.66×10^{-16}	7.78×10^{-16}

minimum and the maximum values of $\|\boldsymbol{r}_i\|_2$ in $\lambda_i \in \Omega$ with LM in Table 1(a) and with ℓ in Table 1(b), respectively.

Fig. 2(a) and Table 1(a) show that $\min_{\lambda_i \in \Omega} \|\boldsymbol{r}_i\|_2$ has approximately the same order with $|f(\lambda_{LM+1})|$, and the difference between $\min_{\lambda_i \in \Omega} \|\boldsymbol{r}_i\|_2$ and $\max_{\lambda_i \in \Omega} \|\boldsymbol{r}_i\|_2$ are not so large. We can also observe from Fig. 2(b) and Table 1(b) that $\|\boldsymbol{r}_i\|_2$ for $\lambda_i \in \Omega$ decrease exponentially with increasing ℓ, although they are bounded by the machine epsilon $\approx 10^{-16}$. As a result, the block SS-RR method with enough subspace size LM such that $|f(\lambda_{LM+1})|^{\ell} \approx 0$ shows high accuracy independent on the eigenvalues outside but near the region. This means that Theorem 2 is experimentally supported by these results.

4 Accuracy analysis when a solution of a linear system is contaminated

In this section, we analyze the accuracy of the block SS-RR method with the numerical integration (Algorithm 2) when the solution of the linear system in Algorithm 2 step 1 is contaminated, and experimentally evaluate the results of the accuracy analysis.

Here we consider the case that the solution of the linear system at j'-th quadrature point is contaminated as follows:

$$(z_{j'}B - A)^{-1}BV + E, \tag{16}$$

where $E \in \mathbb{C}^{n\times L}$ is an error matrix of $\mathrm{rank}(E) = L'$. Note that here we have no assumption on the norm of the error matrix E.

4.1 Accuracy analysis on the block SS-RR method with a contaminated solution of the linear system

By the contamination of the solution of the linear system (16), the matrix $\widehat{S}_k$ can be replaced as

$$\begin{aligned}\widehat{S}'_k &:= \sum_{j=1}^{N}\omega_j z_j^k\left\{(z_jB - A)^{-1}BV + \delta_{jj'}E\right\},\\ &= \widehat{S}_k + \omega_{j'}z_{j'}^k E,\end{aligned}$$

where $\delta_{jj'}$ denotes the Kronecker delta. Therefore, the matrix $\widehat{S}$ of (6) is also replaced by

$$\widehat{S}' = \widehat{S} + E', \quad E' := [\omega_{j'}E, \omega_{j'}z_{j'}E, \ldots, \omega_{j'}z_{j'}^{M-1}E], \tag{17}$$

where $E' \in \mathbb{C}^{n\times LM}$ and $\mathrm{rank}(E') = L'$. Then, the subspace $\mathrm{span}\{\widehat{S}'\}$ is used for the Rayleigh-Ritz procedure of the block SS-RR method with the contaminated solution (16).

Here, we provide a general result of the accuracy analysis of the Rayleigh-Ritz procedure using the contaminated subspace $\mathrm{span}\{V'\} := \mathrm{span}\{V + E\}$ with a low rank error matrix E, where $V, E \in \mathbb{C}^{n\times m}$ and $\mathrm{rank}(E) = m' < m$. Let $E_V \in \mathbb{C}^{n\times m'}$ be a matrix whose columns are basis vectors of $\mathrm{span}\{E\}$. Then, there exists a permutation matrix $P \in \mathbb{R}^{m\times m}$ such that

$$EP = E_V[E_{Y_1}E_{Y_2}], \tag{18}$$

where $E_{Y_1} \in \mathbb{C}^{m'\times m'}$ is a nonsingular matrix and $E_{Y_2} \in \mathbb{C}^{m'\times(m-m')}$. We also let

$$VP = [V_1, V_2], \quad \widetilde{V} := V_2 - V_1E_{Y_1}^{-1}E_{Y_2}, \tag{19}$$

where $V_1 \in \mathbb{C}^{n\times m'}$, $V_2, \widetilde{V} \in \mathbb{C}^{n\times(m-m')}$. Then we have the following lemma.

Lemma 3. *Let $(\lambda_i, \boldsymbol{x}_i)$ be the exact eigenpairs of the matrix pencil (A, B). Defining $\mathcal{P}'$ and $\widetilde{\mathcal{P}}$ to be the orthogonal projectors onto the subspaces $\mathrm{span}\{V'\}$ and $\mathrm{span}\{\widetilde{V}\} \subseteq \mathrm{span}\{V\}$, respectively. Then, the residual norm of the pairs of $(\lambda_i, \boldsymbol{x}_i)$ for the linear operators $A_{\mathcal{P}'} := \mathcal{P}'A\mathcal{P}'$, $B_{\mathcal{P}'} := \mathcal{P}'B\mathcal{P}'$ satisfy*

$$\|(A_{\mathcal{P}'} - \lambda_i B_{\mathcal{P}'})\boldsymbol{x}_i\|_2 \le \gamma'\|(I - \widetilde{\mathcal{P}})\boldsymbol{x}_i\|_2,$$

where $\gamma' = \|\mathcal{P}'(A - \lambda_i B)(I - \mathcal{P}')\|_2$.

Proof. From the Eq. (18) and (19), we have

$$\begin{aligned}\mathrm{span}\{V'\} &= \mathrm{span}\{(V+E)P\}\\ &= \mathrm{span}\{[V_1+E_VE_{Y_1}, V_2+E_VE_{Y_2}]\}\\ &= \mathrm{span}\{[V_1+E_VE_{Y_1}, V_2-V_1E_{Y_1}^{-1}E_{Y_2}]\}\\ &\supseteq \mathrm{span}\{V_2-V_1E_{Y_1}^{-1}E_{Y_2}\}\\ &= \mathrm{span}\{\widetilde{V}\}. \end{aligned} \tag{20}$$

From Lemma 2 and (20),

$$\|(A_{\mathcal{P}'}-\lambda_i B_{\mathcal{P}'})\boldsymbol{x}_i\|_2 \le \gamma'\|(I-\mathcal{P}')\boldsymbol{x}_i\|_2 \le \gamma'\|(I-\widetilde{\mathcal{P}})\boldsymbol{x}_i\|_2$$

is satisfied. Therefore Lemma 3 is proven. □

Recall that the block SS-RR method (Algorithm 2) with the contaminated solution (16) is based on the Rayleigh-Ritz procedure with $\mathrm{span}\{\widehat{S}'\} = \mathrm{span}\{\widehat{S}+E'\}$ defined by Eq. (17). Let $E_V \in \mathbb{C}^{n\times L'}$ be a matrix whose columns are the basis vectors of $\mathrm{span}\{E\}$. Then, since $\mathrm{rank}(E) = L'$, there exists a permutation matrix $P \in \mathbb{R}^{L\times L}$ such that

$$EP = E_V[E_{Y_1}, E_{Y_2}],$$

where $E_{Y_1} \in \mathbb{C}^{L'\times L'}$ is a nonsingular matrix and $E_{Y_2} \in \mathbb{C}^{L'\times(L-L')}$. Defining $P' := \mathrm{diag}(P, P, \ldots, P) \in \mathbb{R}^{LM\times LM}$, then we have

$$E'P' = E_V[E'_{Y_1}, E'_{Y_2}],$$

where $E'_{Y_1} \in \mathbb{C}^{L'\times L'}$ and $E'_{Y_2} \in \mathbb{C}^{L'\times(LM-L')}$ can be written by

$$\begin{aligned} E'_{Y_1} &:= \omega_{j'}E_{Y_1},\\ E'_{Y_2} &:= [\omega_{j'}E_{Y_2}, \omega_{j'}z_{j'}E_{Y_1}, \omega_{j'}z_{j'}E_{Y_2}, \ldots, \omega_{j'}z_{j'}^{M-1}E_{Y_1}, \omega_{j'}z_{j'}^{M-1}E_{Y_2}], \end{aligned}$$

because of the definition of E' (17). We also let

$$\begin{aligned} \widehat{S}'P' &= [\widehat{S}'_1, \widehat{S}'_2], & \widetilde{S} &:= \widehat{S}'_2 - \widehat{S}'_1E_{Y_1}'^{-1}E'_{Y_2},\\ UP' &= [U_1, U_2], & \widetilde{U} &:= U_2 - U_1E_{Y_1}'^{-1}E'_{Y_2}, \end{aligned}$$

where $\widehat{S}'_1, U_1 \in \mathbb{C}^{n\times L'}$, $\widehat{S}'_2, \widetilde{S}, U_2, \widetilde{U} \in \mathbb{C}^{n\times(LM-L')}$.

Here, from the relationship: $\widehat{S}' = \widehat{S}+E' = FU+E'$, we have

$$\widetilde{S} = F\widetilde{U}, \quad F := Q_r f(\Lambda_r)\widetilde{Q}_r^{\mathrm{H}}. \tag{21}$$

Therefore, from Lemmas 1 and 3, we provide the following theorem with respect to the accuracy of the block SS-RR method with the contaminated solution (16).

Theorem 3. *Assume that $f(\lambda_i)$ are ordered in decreasing order of magnitude $|f(\lambda_i)| \ge |f(\lambda_{i+1})|$. Defining $\mathcal{P}', \widetilde{\mathcal{P}}$ and $\mathcal{P}_{LM-L'}$ to be the orthogonal projectors onto the subspaces $\mathrm{span}\{\widehat{S}'\}, \mathrm{span}\{\widetilde{S}\}$ and $\mathrm{span}\{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_{LM-L'}\}$, respectively.*

Assume that $\widetilde{U}$ such that $\mathcal{P}_{LM-L'}\widetilde{U}$ is full rank. Then for each eigenvector $\boldsymbol{x}_i, i = 1, 2, \ldots, LM-L'$, there exists a unique vector $\boldsymbol{s}_i$ in the subspace $\mathrm{span}\{\widetilde{U}\} \subseteq \mathrm{span}\{U\}$

such that $\mathcal{P}_{LM-L'}\boldsymbol{s}_i = \boldsymbol{x}_i$*. Then, the residual norm of the pairs of* $(\lambda_i, \boldsymbol{x}_i)$ *for the linear operators* $A_{\mathcal{P}'} := \mathcal{P}'A\mathcal{P}'$, $B_{\mathcal{P}'} := \mathcal{P}'B\mathcal{P}'$ *satisfy*

$$\|(A_{\mathcal{P}'} - \lambda_i B_{\mathcal{P}'})\boldsymbol{x}_i\|_2 \leq \alpha'\beta'\gamma' \left| \frac{f(\lambda_{LM-L'+1})}{f(\lambda_i)} \right|,$$

where α' *is some constant,* $\beta' = \|\boldsymbol{x}_i - \boldsymbol{s}_i\|_2$*, and* $\gamma' = \|\mathcal{P}'(A - \lambda_i B)(I - \mathcal{P}')\|_2$.

Proof. Applying Lemma 1 to Eq. (21) and also applying Lemma 3 to Eq. (17), we have

$$\|(A_{\mathcal{P}'} - \lambda_i B_{\mathcal{P}'})\boldsymbol{x}_i\|_2 \leq \gamma'\|(I - \widetilde{\mathcal{P}})\boldsymbol{x}_i\|_2 \leq \alpha'\beta'\gamma' \left| \frac{f(\lambda_{LM-L'+1})}{f(\lambda_i)} \right|.$$

Therefore Theorem 3 is proven. □

Theorem 3 means that the accuracy of the block SS-RR method with the contaminated solution, in terms of the residual 2-norm $\|(A_{\mathcal{P}'} - \lambda_i B_{\mathcal{P}'})\boldsymbol{x}_i\|_2$, is evaluated by the ratio of the magnitude of the filter function $|f(\lambda_i)|$ to the $(LM - L' + 1)$-th largest one $|f(\lambda_{LM-L'+1})|$. Therefore we observe that, using the enough subspace size LM such that $|f(\lambda_{LM-L'+1})| \approx 0$, the block SS-RR method achieves high accuracy for the target eigenpairs (the eigenvalue is inside Ω) even if the solution of the linear system is contaminated by a low rank error matrix (16).

We note that Theorem 3 can be naturally extended in the case when some solutions of the linear systems in different quadrature points are contaminated.

4.2 Further analysis on the results of Theorem 3

In Theorem 3, γ' is bounded above such that $\gamma' \leq \|A\|_2 + |\lambda_i|\|B\|_2$ just as γ in Theorem 2. In this subsection, we consider the magnitude of β' in Theorem 3 for each $\lambda_i \in \Omega$, which strongly depends on the input subspace $\mathrm{span}\{\widetilde{U}\}$. Let $VP = [V_1, V_2]$, where $V_1 \in \mathbb{C}^{n\times L'}$ and $V_2 \in \mathbb{C}^{n\times(L-L')}$, then U_1, U_2 can be rewritten by

$$\begin{aligned} U_1 &= V_1, \\ U_2 &= [V_2, C_r V_1, C_r V_2, \ldots, C_r^{M-1}V_1, C_r^{M-1}V_2]. \end{aligned}$$

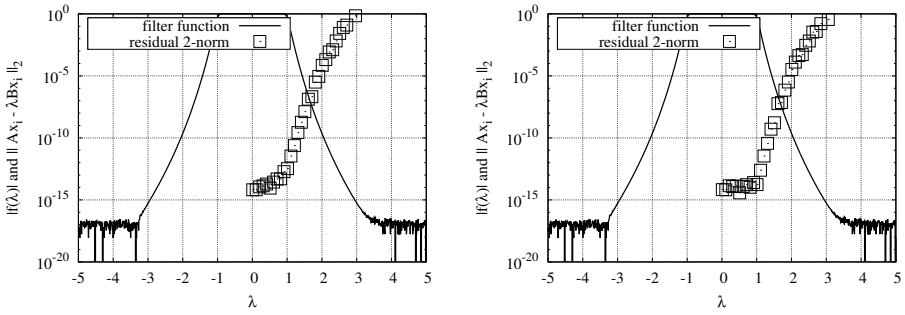
From the definition of $\widetilde{U}$ we have

$$\begin{aligned} \mathrm{span}\{\widetilde{U}\} &= \mathrm{span}\{U_2 - U_1 E_{Y_1}'^{-1} E_{Y_2}'\} \\ &= \mathrm{span}\{U_2 - U_1(\omega_{j'}E_{Y_1})^{-1}[\omega_{j'}E_{Y_2}, \ldots, \omega_{j'}z_{j'}^{M-1}E_{Y_1}, \omega_{j'}z_{j'}^{M-1}E_{Y_2}]\} \\ &= \mathrm{span}\{[V_2, C_r V_1, C_r V_2, \ldots, C_r^{M-1}V_1, C_r^{M-1}V_2] \\ &\qquad - V_1[E_{Y_1}^{-1}E_{Y_2}, z_{j'}I, z_{j'}E_{Y_1}^{-1}E_{Y_2}, \ldots, z_{j'}^{M-1}I, z_{j'}^{M-1}E_{Y_1}^{-1}E_{Y_2}]\} \\ &= \mathrm{span}\{[W_1, W_2]\}, \end{aligned} \tag{22}$$

where $W_1 \in \mathbb{C}^{n\times L'(M-1)}$ and $W_2 \in \mathbb{C}^{n\times(L-L')M}$ are defined by

$$\begin{aligned} W_1 &:= [(C_r - z_{j'}I)V_1, (C_r^2 - z_{j'}^2 I)V_1, \ldots, (C_r^{M-1} - z_{j'}^{M-1}I)V_1], \\ W_2 &:= [V_2 - V_1 E_{Y_1}^{-1}E_{Y_2}, C_r V_2 - z_{j'}V_1 E_{Y_1}^{-1}E_{Y_2}, \ldots, C_r^{M-1}V_2 - z_{j'}^{M-1}V_1 E_{Y_1}^{-1}E_{Y_2}]. \end{aligned}$$

We can observe from Eq. (22) and the definition of $C_r := Q_r \Lambda_r \widetilde{Q}_r^{\mathrm{H}}$ that, subspaces $\mathrm{span}\{W_1\}$ and also $\mathrm{span}\{\widetilde{U}\}$ weakly contain the components of the eigenvectors corresponding to the eigenvalues λ_i near the contaminated quadrature point $z_{j'}$. Therefore β' may become larger for λ_i near $z_{j'}$ than others, specifically for the case of $L' = L$.



(a) $z_{j'} = z_1$ (b) $z_{j'} = z_{16}$

Fig. 3: The accuracy of the block SS-RR method when the solution of the linear system is contaminated for $L = 10, L' = 10, M = 4, N = 32$.

4.3 Experimental evaluation of the accuracy analysis

In this subsection, we experimentally evaluate the results of Theorem 3 and of the analysis in Section 4.2. We apply the block SS-RR method (Algorithm 2) with the contaminated solution (16) to the model problem (15), and evaluate its accuracy.

We evaluate the relation of the accuracy with the number of subspace size LM and the contaminated quadrature point. To evaluate the relation of the accuracy, we fixed the parameters as $L = 10, L' = 10, N = 32$, and tested four cases $M = 1, 2, 3, 4$ ($LM = 10, 20, 30, 40$). The contaminated quadrature point is also tested two cases:

$$z_{j'} = \begin{cases} z_1 & = \cos\left(\frac{\pi}{32}\right) + \mathrm{i}\sin\left(\frac{\pi}{32}\right) \quad \approx 0.9956 + 0.0980\mathrm{i}, \\ z_{16} & = \cos\left(\frac{31\pi}{32}\right) + \mathrm{i}\sin\left(\frac{31\pi}{32}\right) \quad \approx -0.9956 + 0.0980\mathrm{i}, \end{cases}$$

where z_1 is near some eigenvalues in Ω, e.g., $\lambda_9 = 0.91$, on the other hand, z_{16} is far from all eigenvalues in Ω. The error matrix E was set as a different random matrix from V, and also was generated by the Mersenne Twister in MATLAB. Other conditions are the same as the experiment in Section 3.3.

The numerical results are presented in Fig. 3 and Table 2. We show the residual 2-norm $\|\boldsymbol{r}_i\|_2 := \|A\boldsymbol{x}_i - \lambda_i B\boldsymbol{x}_i\|_2$ with $L = 10, L' = 10, M = 4, N = 32, z_{j'} = z_1$ in Fig. 3(a), and with $L = 10, L' = 10, M = 4, N = 32, z_{j'} = z_{16}$ in Fig. 3(b), respectively. We also show the relationship of the minimum and the maximum values of $\|\boldsymbol{r}_i\|_2$ in $\lambda_i \in \Omega$ with LM for $z_{j'} = z_1$ in Table 2(a) and for $z_{j'} = z_1$ in Table 2(b), respectively.

Fig. 3 and Table 2 show that $\min \|\boldsymbol{r}_i\|_2$ have approximately the same order with $|f(\lambda_{LM-L'+1})|$. In this regard, however, for $z_{j'} = z_1$, the difference between $\min_{\lambda_i \in \Omega} \|\boldsymbol{r}_i\|_2$ and $\max_{\lambda_i \in \Omega} \|\boldsymbol{r}_i\|_2$ are larger than for $z_{j'} = z_{16}$; see Table 2. This is based on the fact that $\|\boldsymbol{r}_i\|_2$ corresponding to λ_i near the contaminated quadrature point $z_{j'}$ are larger than others; see Fig. 3(a). As a result, for the case that $z_{j'}$ is far from all $\lambda_i \in \Omega$, the block SS-RR method with enough subspace size LM shows high accuracy even if the solution of the linear system is contaminated. This means that Theorem 3 and the analysis in Section 4.2 are experimentally supported by this results.

Table 2: Relationship of the accuracy of the block SS-RR method with LM when the solution of the linear system is contaminated.

(a) z_1 is contaminated

M (LM)	$\lvert f(\lambda_{LM-L'+1})\rvert$	$\min_{\lambda_i\in\Omega}\lVert\boldsymbol{r}_i\rVert_2$	$\max_{\lambda_i\in\Omega}\lVert\boldsymbol{r}_i\rVert_2$
1 (10)	1.00×10^{0}	5.32×10^{-1}	2.84×10^{0}
2 (20)	4.21×10^{-1}	1.84×10^{-2}	2.63×10^{-1}
3 (30)	1.98×10^{-10}	2.43×10^{-10}	1.63×10^{-8}
4 (40)	5.03×10^{-16}	6.57×10^{-15}	1.91×10^{-13}

(b) z_{16} is contaminated

M (LM)	$\lvert f(\lambda_{LM-L'+1})\rvert$	$\min_{\lambda_i\in\Omega}\lVert\boldsymbol{r}_i\rVert_2$	$\max_{\lambda_i\in\Omega}\lVert\boldsymbol{r}_i\rVert_2$
1 (10)	1.00×10^{0}	5.54×10^{-1}	2.89×10^{0}
2 (20)	4.21×10^{-1}	4.11×10^{-2}	4.84×10^{-1}
3 (30)	1.98×10^{-10}	7.05×10^{-10}	4.96×10^{-9}
4 (40)	5.03×10^{-16}	3.71×10^{-15}	2.51×10^{-14}

5 Conclusions

In this paper, we investigated the accuracy of the block SS-RR method with the numerical integration. Then we provided two theorems for the accuracy analysis with the iteration technique (Theorem 2) and for the accuracy analysis with the contaminated solution of the linear system (Theorem 3). From the results of our accuracy analyses, we concluded that the block SS-RR method with enough subspace size can achieve high accuracy for target eigenpairs even if some eigenvalues exist outside but near the region, and also even if the solution of the linear system is contaminated. This also means that the block SS-RR method has error resilience property, and will lead to an algorithm-based fault tolerance technique different from checkpoint restart techniques and redundant computations.

In future work, we will analyze for the case of non-diagonalizable matrix pencils. We will also analyze the accuracy of the Hankel type of the contour integral based eigensolver.

Acknowledgements

This work was supported in part by MEXT SPIRE Field 5, JICFuS, JST/CREST and KEKENHI (Grant No. 25286097, 25870099).

References

[1] Asakura, J., Sakurai, T., Tadano, H., Ikegami, T., Kimura, K.: A numerical method for nonlinear eigenvalue problems using contour integrals. JSIAM Letters, **1**(2009), 52–55.

[2] Asakura, J., Sakurai, T., Tadano, H., Ikegami, T., Kimura, K.: A numerical method for polynomial eigenvalue problems using contour integral. Japan J. Indust. Appl. Math, **27**(2010), 73–90.

[3] Beyn, W.-J.: An integral method for solving nonlinear eigenvalue problems. Lin. Alg. Appl., **436**(2012), 3839–3863.

[4] Ikegami, T., Sakurai, T., Nagashima, U.: A filter diagonalization for generalized eigenvalue problems based on the Sakurai-Sugiura projection method. J. Comput. Appl. Math., **233**(2010), 1927–1936.

[5] Ikegami, T., Sakurai, T.: Contour integral eigensolver for non-Hermitian systems: a Rayleigh-Ritz-type approach. Taiwan. J. Math., **14** (2010), 825–837.

[6] Imakura, A., Du, L. Sakurai, T.: A block Arnoldi-type contour integral spectral projection method for solving generalized eigenvalue problems, Applied Mathematics Letters, **32** (2014), 22–27.

[7] Kravanja, P., Sakurai, T., van Barel, M.: On locating clusters of zeros of analytic functions. BIT, **39** (1999), 646–682.

[8] Polizzi, E.: A density matrix-based algorithm for solving eigenvalue problems. Phys. Rev. B, **79** (2009), 115112.

[9] Saad, Y.: Numerical Methods for Large Eigenvalue Problems, 2nd edition. SIAM, Philadelphia, PA, (2011).

[10] Sakurai, T., Sugiura, H.: A projection method for generalized eigenvalue problems using numerical integration. J. Comput. Appl. Math., **159** (2003), 119–128.

[11] Sakurai, T. Tadano, H.: CIRR: a Rayleigh-Ritz type method with counter integral for generalized eigenvalue problems. Hokkaido Math. J., **36** (2007), 745–757.

[12] Schofield, G., Chelikowsky, J. R., Saad, Y.: A spectrum slicing method for the Kohn-Sham problem. Comput. Phys. Commun., **183**(2012), 497–505.

[13] Tang, P. T. P., Polizzi, E.: FEAST as a subspace iteration eigensolver accelerated by approximate spectral projection. arXiv:1302.0432 [math.NA].

[14] Yokota, S., Sakurai, T.: A projection method for nonlinear eigenvalue problems using contour integrals. JSIAM Letters, **5**(2013), 41–44.