

A filter diagonalization for generalized eigenvalue problems based on the Sakurai-Sugiura projection method

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Abstract

The Sakurai-Sugiura projection method, which solves a generalized eigenvalue problem to find certain eigenvalues in a given domain, was reformulated by using the resolvent theory. A new interpretation based on the filter diagonalization was given, and the corresponding filter function was derived explicitly. The block version of the method was also proposed, which enabled to resolve degenerated eigenvalues. Two numerical examples were provided to illustrate the method.

Key words: Generalized eigenvalue problem, Spectral projection, Filter diagonalization

1 Introduction

There is a wide area of scientific and engineering applications that are reduced to the eigenvalue problem [3,11,2,6]. Generally speaking, the dimension of the system increases with the refinement of the corresponding physical model, which can reach few millions. Fortunately, it is often the case that not all of the eigenvalues are necessary, and those in the physically meaningful range may suffice. Iterative methods are typically used for those cases [1,10,5,14],

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which are suitable to extract eigenvalues with large absolute value. In some applications, however, it is required to extract eigenvalues embedded in the middle of the distribution.

In the last decade, a filter diagonalization [4,7] is developed to extract eigenvalues contained in a specified region G . It was first formulated based on time propagation of quantum wave packets [9], and soon was reformulated as a filter operator. Let H be a Hermitian matrix and v be an arbitrary vector. A filter function $f(x) = \sum_i c_i x^i$ is designed, such that $f(x) \simeq 0$ on outside of G . The filter operator is defined by replacing x with H as $f(H)$. When the operator is applied on v , eigen-elements of H whose eigenvalues are contained in G dominate in $f(H)v$. Starting from a set of initial vectors v_i , we can thus span an eigen-subspace localized on G by using a set of $f(H)v_i$. In typical applications, a gaussian function is chosen for $f(x)$, and Chebyshev series expansion is used instead of the Taylor series. Because the power series is employed in the expansion, however, it is inevitable for $f(x)$ to diverge as $x \rightarrow \pm\infty$. Therefore, we have to shift and scale H *a priori* such that all the eigenvalues of H are confined in the domain of $f(x)$.

The Sakurai-Sugiura (SS) method [12] also extract eigenvalues in the specified domain, though it takes a different approach. In the filter diagonalization, the domain G is determined numerically by the asymptotic behavior of $f(x)$. On the other hand, the SS method defines G mathematically by a Cauchy integral path that surrounds G . As a result, the SS method can deal with the non-Hermitian systems, where the eigenvalues may be located on the complex plane. The method is also applicable to the generalized eigenvalue problems, and is suitable to the modern distributed parallel computer.

In the present paper, we will reformulate the SS method in the context of the resolvent theory. The block version of the SS method is also proposed, in which the relation to the filter diagonalization is discussed. Next section is devoted to the derivation based on the resolvent theory. In Sec. 3, the SS method is investigated in the light of the filter diagonalization, and the algorithm of the block SS method is given. Two numerical examples are shown in Sec. 4, and Sec. 5 conclude.

2 Block Sakurai-Sugiura method

In this section, we reformulate the Sakurai-Sugiura (SS) projection method based on the resolvent of a matrix pencil, and propose a block version of the SS method. Let $A, B \in \mathbb{C}^{N \times N}$ form a regular matrix pencil $zB - A$. The regular pencil can be transformed into Weierstrass canonical form [15].

Theorem 1 (Weierstrass canonical form). *Let $zB - A$ be a regular pencil of order N . Then there exist nonsingular matrices $\tilde{P}, Q \in \mathbb{C}^{N \times N}$ such that*

$$\tilde{P}(zB - A)Q = \begin{pmatrix} z\mathbb{I}_{k_1} - \mathbb{J}_1 & & & & \\ & \ddots & & & \\ & & z\mathbb{I}_{k_d} - \mathbb{J}_d & & \\ & & & z\mathbb{N}_{d+1} - \mathbb{I}_{k_{d+1}} & \\ & & & & \ddots \\ & & & & & z\mathbb{N}_r - \mathbb{I}_{k_r} \end{pmatrix}, \quad (1)$$

where $\mathbb{J}_i, \mathbb{N}_i \in \mathbb{C}^{k_i \times k_i}$ are Jordan blocks, \mathbb{N}_i is nilpotent, and \mathbb{I}_k denotes the identity matrix of order k .

Because \tilde{P} and Q are the regular matrices, we can define $P = \tilde{P}^{-1}$ and $\tilde{Q} = Q^{-1}$. According to the Jordan block structures in Eq. (1), we will partition row vectors in \tilde{P} and \tilde{Q} into $\tilde{P}_i, \tilde{Q}_i \in \mathbb{C}^{k_i \times N}$, and column vectors in P and Q into $P_i, Q_i \in \mathbb{C}^{N \times k_i}$, respectively, for $i = 1, 2, \dots, r$.

Theorem 2. *Resolvent of the regular pencil $(zB - A)^{-1}$ is decomposed into*

$$(zB - A)^{-1} = \sum_{i=1}^d Q_i \left\{ \sum_{m=0}^{k_i-1} \frac{(\mathbb{J}_i - \alpha_i \mathbb{I}_{k_i})^m}{(z - \alpha_i)^{m+1}} \right\} \tilde{P}_i - \sum_{i=d+1}^r Q_i \left\{ \sum_{m=0}^{k_i-1} z^m \mathbb{N}_i^m \right\} \tilde{P}_i, \quad (2)$$

where α_i is an eigenvalue of Jordan block \mathbb{J}_i .

Proof. Let $W = \tilde{P}(zB - A)Q$. According to Theorem 1, we have

$$\begin{aligned} (zB - A)^{-1} &= QW^{-1}\tilde{P} \\ &= \sum_{i=1}^d Q_i (z\mathbb{I}_{k_i} - \mathbb{J}_i)^{-1} \tilde{P}_i + \sum_{i=d+1}^r Q_i (z\mathbb{N}_i - \mathbb{I}_{k_i})^{-1} \tilde{P}_i. \end{aligned} \quad (3)$$

Using the resolvent of the Jordan block,

$$R(z, \mathbb{J}_i) \equiv (z\mathbb{I}_{k_i} - \mathbb{J}_i)^{-1} = \sum_{m=0}^{k_i-1} \frac{(\mathbb{J}_i - \alpha_i \mathbb{I}_{k_i})^m}{(z - \alpha_i)^{m+1}}, \quad (4)$$

and $(z\mathbb{N}_i - \mathbb{I}_{k_i})^{-1} = -z^{-1}R(z^{-1}, \mathbb{N}_i)$, we get the result. \square

Definition 3. Let Γ be a positively oriented closed Jordan curve and G be the inside of Γ . For a non-negative integer n , the n -th order moment matrix

of the pencil $zB - A$, localized on G , is defined by

$$M_n = \frac{1}{2\pi i} \oint_{\Gamma} z^n (zB - A)^{-1} dz B. \quad (5)$$

Note that the moment matrix can be defined more generally, where a polynomial of z appears in place of z^n in Eq. (5). Such a matrix, however, can be represented by a linear combination of M_n .

Theorem 4. *The localized moment matrix is written as*

$$M_n = \sum_{i; \alpha_i \in G} Q_i \mathbb{J}_i^n \tilde{Q}_i. \quad (6)$$

Proof. Let Eq. (2) to Eq. (5),

$$M_n = \sum_{i=1}^d Q_i \left\{ \frac{1}{2\pi i} \oint_{\Gamma} j_i(z) dz \right\} \tilde{P}_i B - \sum_{i=d+1}^r Q_i \left\{ \frac{1}{2\pi i} \oint_{\Gamma} n_i(z) dz \right\} \tilde{P}_i B, \quad (7)$$

$$j_i(z) = z^n \sum_{m=0}^{k_i-1} \frac{(\mathbb{J}_i - \alpha_i \mathbb{I}_{k_i})^m}{(z - \alpha_i)^{m+1}}, \quad (8)$$

$$n_i(z) = z^n \sum_{m=0}^{k_i-1} z^m \mathbb{N}_i^m. \quad (9)$$

Using the relation

$$z^n = \sum_{j=0}^n \binom{n}{j} (z - \alpha)^{n-j} \alpha^j, \quad (10)$$

we have

$$\text{Res}_{z=\alpha} \left(\frac{z^n}{(z - \alpha)^{m+1}} \right) = \begin{cases} 0, & m > n, \\ \binom{n}{n-m} \alpha^{n-m}, & m \leq n, \end{cases} \quad (11)$$

where $\binom{n}{j}$ is a binomial coefficient and $\text{Res}_{z=\alpha}(g(z))$ gives a residue of $g(z)$ at a pole $z = \alpha$. Because $(\mathbb{J}_i - \alpha_i \mathbb{I}_{k_i})^m = 0$ for $m \geq k_i$, the residue of $j_i(z)$ is given by

$$\begin{aligned} \text{Res}_{z=\alpha_i}(j_i(z)) &= \sum_{m=0}^{\min(n, k_i-1)} \binom{n}{n-m} \alpha_i^{n-m} (\mathbb{J}_i - \alpha_i \mathbb{I}_{k_i})^m \\ &= \mathbb{J}_i^n. \end{aligned} \quad (12)$$

Because $j_i(z)$ is regular for $z \neq \alpha_i$ and $n_i(z)$ is regular for $z \in \mathbb{C}$, we have, using the Cauchy's integral theorem,

$$M_n = \sum_{i; \alpha_i \in G} Q_i \mathbb{J}_i^n \tilde{P}_i B. \quad (13)$$

Meanwhile, by definition, the matrix B is expanded as

$$B = \sum_{i=1}^d P_i \tilde{Q}_i + \sum_{i=d+1}^r P_i \mathbb{N}_i \tilde{Q}_i. \quad (14)$$

Combining Eqs. (13) and (14), we get the result. \square

As shown below, we can use the localized moment matrix to extract Jordan blocks whose eigenvalues are contained in G . Here we employ the following collective notations: Those Jordan blocks $\mathbb{J}_i; \alpha_i \in G$ are collected to form $k_\Gamma \times k_\Gamma$ Jordan matrix \mathbb{J}_Γ , where $k_\Gamma = \sum_{i; \alpha_i \in G} k_i$. Similarly, the corresponding eigenvectors Q_i and \tilde{Q}_i are collected to form $Q_\Gamma \in \mathbb{C}^{N \times k_\Gamma}$ and $\tilde{Q}_\Gamma \in \mathbb{C}^{k_\Gamma \times N}$, respectively. Let C and D be arbitrary $N \times m$ matrices, where $N > m \geq k_\Gamma$. A size-reduced moment matrix is defined as

$$\mathbb{M}_n = C^H M_n D \in \mathbb{C}^{m \times m}. \quad (15)$$

Theorem 5. *If ranks of both $C^H Q_\Gamma$ and $\tilde{Q}_\Gamma D$ are k_Γ , non-singular part of a matrix pencil $z\mathbb{M}_0 - \mathbb{M}_1$ is equivalent to $z\mathbb{I}_{k_\Gamma} - \mathbb{J}_\Gamma$.*

Proof. Using the collective notations,

$$\mathbb{M}_n = C^H Q_\Gamma \mathbb{J}_\Gamma^n \tilde{Q}_\Gamma D. \quad (16)$$

Because ranks of $C^H Q_\Gamma$ and $\tilde{Q}_\Gamma D$ are k_Γ , there exist $m \times m$ regular matrices $\tilde{\mathbb{P}}_m$ and \mathbb{Q}_m , such that

$$\tilde{\mathbb{P}}_m C^H Q_\Gamma = \begin{pmatrix} \mathbb{I}_{k_\Gamma} \\ 0 \end{pmatrix}, \quad (17)$$

$$\tilde{Q}_\Gamma D \mathbb{Q}_m = (\mathbb{I}_{k_\Gamma}, 0). \quad (18)$$

Then, we have

$$\tilde{\mathbb{P}}_m (z\mathbb{M}_0 - \mathbb{M}_1) \mathbb{Q}_m = \begin{pmatrix} z\mathbb{I}_{k_\Gamma} - \mathbb{J}_\Gamma \\ 0 \end{pmatrix}, \quad (19)$$

which is the result of the theorem. \square

From Theorem 5, the interior eigenvalues of the original matrix pencil $zB - A$ are obtained by solving the size-reduced eigenvalue problem $z\mathbb{M}_0 - \mathbb{M}_1$. The corresponding eigenvectors are also obtained from the eigenvectors $\tilde{\mathbb{P}}_m$ and \mathbb{Q}_m of the size-reduced system. Let \mathbb{Q}_m be split into $(\mathbb{Q}_\Gamma, \mathbb{Q}_\emptyset)$, where $\mathbb{Q}_\Gamma \in \mathbb{C}^{m \times k_\Gamma}$

defines the non-singular components of the right-eigenvectors of $z\mathbf{M}_0 - \mathbf{M}_1$. Similarly, $\tilde{\mathbf{P}}_m$ is split into $(\tilde{\mathbf{P}}_\Gamma, \tilde{\mathbf{P}}_\emptyset)^T$, $\tilde{\mathbf{P}}_\Gamma \in \mathbb{C}^{k_\Gamma \times m}$. Note that $\tilde{\mathbf{P}}_\emptyset$ and \mathbf{Q}_\emptyset define right and left common null spaces of \mathbf{M}_n , respectively.

Theorem 6. *The right-eigenvectors of the original matrix pencil $zB - A$ is given by $\mathbf{Q}_\Gamma = \mathbf{M}_0 D \mathbf{Q}_\Gamma$, and its adjoint is given by $\tilde{\mathbf{Q}}_\Gamma = \tilde{\mathbf{P}}_\Gamma C^H \mathbf{M}_0$.*

Proof. Because $\mathbf{M}_0 = \mathbf{Q}_\Gamma \tilde{\mathbf{Q}}_\Gamma$, we have

$$\mathbf{M}_0 D \mathbf{Q}_\Gamma = \mathbf{Q}_\Gamma \tilde{\mathbf{Q}}_\Gamma D \mathbf{Q}_\Gamma = \mathbf{Q}_\Gamma \mathbf{I}_{k_\Gamma} = \mathbf{Q}_\Gamma. \quad (20)$$

Similarly, $\tilde{\mathbf{P}}_\Gamma C^H \mathbf{M}_0 = \tilde{\mathbf{Q}}_\Gamma$. \square

The left-eigenvectors are obtained by solving on the transposed system.

We can now derive the original SS method. Let $v \in \mathbb{C}^N$ be an arbitrary vector and $\mu_n = v^H \mathbf{M}_n v$. Two $m \times m$ Hankel matrices \mathbf{H}_m and $\mathbf{H}_m^<$ are defined as

$$\mathbf{H}_m = \begin{pmatrix} \mu_0 & \mu_1 & \cdots & \mu_{m-1} \\ \mu_1 & \mu_2 & \cdots & \mu_m \\ \vdots & \vdots & & \vdots \\ \mu_{m-1} & \mu_m & \cdots & \mu_{2m-2} \end{pmatrix} \quad (21)$$

and

$$\mathbf{H}_m^< = \begin{pmatrix} \mu_1 & \mu_2 & \cdots & \mu_m \\ \mu_2 & \mu_3 & \cdots & \mu_{m+1} \\ \vdots & \vdots & & \vdots \\ \mu_m & \mu_{m+1} & \cdots & \mu_{2m-1} \end{pmatrix}. \quad (22)$$

Theorem 7. *If all elements of $\tilde{\mathbf{Q}}_\Gamma v$ and $v^H \mathbf{Q}_\Gamma$ are non-zero, and there is no degeneracy in \mathbb{J}_Γ , then non-singular part of a matrix pencil $z\mathbf{H}_m - \mathbf{H}_m^<$ is equivalent to $z\mathbf{I}_{k_\Gamma} - \mathbb{J}_\Gamma$.*

Proof. By choosing row vectors of C^H and column vectors of D to be

$$(C^H)_{i,*} = v^H \mathbf{Q}_\Gamma \mathbb{J}_\Gamma^{i-1} \tilde{\mathbf{Q}}_\Gamma \quad (23)$$

and

$$D_{*,i} = \mathbf{Q}_\Gamma \mathbb{J}_\Gamma^{i-1} \tilde{\mathbf{Q}}_\Gamma v \quad (24)$$

for $i = 1, 2, \dots, m$, respectively, we have $\mathbf{H}_m = \mathbf{M}_0$ and $\mathbf{H}_m^< = \mathbf{M}_1$. As for the rank of $\tilde{\mathbf{Q}}_\Gamma D$, we consider that column vectors of $\tilde{\mathbf{Q}}_\Gamma D$ form the Krylov

series of \mathbb{J}_Γ starting from $\tilde{Q}_\Gamma v$. Because \mathbb{J}_Γ is not degenerated, and elements of $\tilde{Q}_\Gamma v$ are non-zero, these column vectors are linearly independent, and thus the rank of $\tilde{Q}_\Gamma D$ is k_Γ . Similarly, the rank of $C^H Q_\Gamma$ is k_Γ . From Theorem 5, we have the result of the theorem. \square

Rigorously, not all of the elements of $\tilde{Q}_\Gamma v$ need to be non-zero; the prerequisite non-zero elements are those corresponding to the last Jordan canonical vector for each Jordan blocks in \mathbb{J}_Γ .

A block version of the SS method is located between Theorems 5 and 7. Let V be an $N \times l$ matrix, whose column vectors are used as initial vectors. The block SS method is defined by replacing μ_n in Theorem 7 with matrices $V^H M_n V$. Apparently from the proof of the theorem, up to the l -th order degeneracy in \mathbb{J}_Γ can be separated in the block SS method.

3 Filter diagonalization

From the viewpoint of the filter diagonalization, the localized moment matrix M_n is considered to be a filter operator. In the following, we focus on the case where the matrix pencil $zB - A$ is diagonalizable. In this case, \mathbb{J}_i is reduced to a scalar, α_i . Comparing Equations (5) and (6), a filter function corresponding to M_n is derived as

$$\begin{aligned} f_n(x) &= \frac{1}{2\pi i} \oint_\Gamma \frac{z^n}{z - x} dz \\ &= \begin{cases} x^n, & x \in G, \\ 0, & \text{otherwise.} \end{cases} \end{aligned} \quad (25)$$

When M_n is operated on the i -th right-eigenvector, its amplitude is modulated by $f_n(\alpha_i)$,

$$\tilde{Q}_i M_n Q_i = f_n(\alpha_i) \tilde{Q}_i Q_i. \quad (26)$$

In the conventional filter diagonalization, a single filter operator $f(H)$ is applied on a set of random vectors to construct a basis set that spans the filtered eigen-subspace. On the other hand, the SS method applies a set of modulated filter operators M_n on a single vector to build the basis set. From this point of view, the block SS method is considered naturally as a hybrid method between the filter diagonalization and the SS method.

In the actual calculations, the path integral in Eq. (5) is evaluated numerically by using an appropriate quadrature. Let z_j be the quadrature points on Γ and

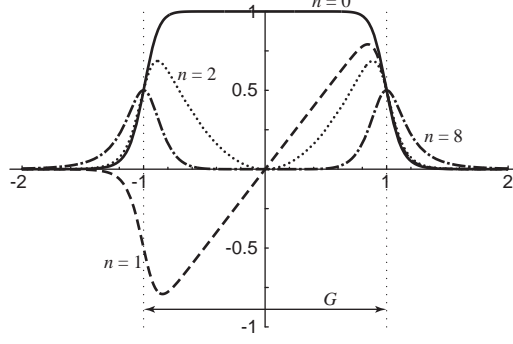


Fig. 1. Plots of filter functions $\tilde{f}_n(x)$ for $M = 16$, $\gamma = 0$, $\rho = 1$, $n = 0, 1, 2$, and 8 . w_j be the corresponding weights, where $j = 1, 2, \dots, M$. The localized moment matrix is then approximated by

$$\bar{M}_n = \sum_{j=1}^M w_j z_j^n (z_j B - A)^{-1} B. \quad (27)$$

Accordingly, the effective filter function $\bar{f}_n(x)$ is derived for the quadrature as

$$\bar{f}_n(x) = \sum_{j=1}^M w_j \frac{z_j^n}{z_j - x}. \quad (28)$$

Thanks to the explicit form of the filter function, several properties of the SS method can be analyzed quantitatively. As an example, let Γ be a circle of radius ρ centered at a point γ . Dividing the circle into M division and applying the trapezoidal rule, we have $z_j = \gamma + \rho \exp(\frac{2\pi i}{M}(j - \frac{1}{2}))$ and $w_j = (z_j - \gamma)/M$. From the numerical reason, the momental weight of z^n is also replaced by a shift-and-scaled one, $((z - \gamma)/\rho)^n$. Then, the filter function becomes

$$\tilde{f}_n(x) = \sum_{j=1}^M w_j \left(\frac{z_j - \gamma}{\rho} \right)^n \frac{1}{z_j - x} \quad (29)$$

$$= \frac{\tilde{x}^n}{1 + \tilde{x}^M} \quad (30)$$

where $\tilde{x} = (x - \gamma)/\rho$. In Fig. 1, $\tilde{f}_n(x)$ is plotted along the real axis for $M = 16$, $\gamma = 0$, $\rho = 1$, $n = 0, 1, 2$, and 8 . The shape of the effective filter functions deviates from the ideal rectangle, which exude outside of G . The value and the derivative at the boundary are $\tilde{f}_n(\gamma + \rho) = 1/2$ and $\tilde{f}'_n(\gamma + \rho) = (-M/4 + n/2)/\rho$ for $n = 0, 1, \dots, M-1$. From here, we notice that n should be kept well smaller than $M/2$.

The filtered subspace is spanned by the set of filtered vectors. If there exist multiple eigenvalues in G , we need as many vectors to span the subspace. Higher order moment matrices become necessary then, which may, in turn,

require large M . Instead, we can prepare multiple initial vectors and use the block SS method. The algorithm of the block SS method is shown below.

Algorithm 1 (Block SS method).

Input: $V \in \mathbb{C}^{N \times l}$, $\{z_j, w_j\}$ for $j = 1, 2, \dots, M$

Output: α_k for $k = 1, 2, \dots, K$

1. Solve $\tilde{V}_j = (z_j B - A)^{-1} B V$ and calculate $\mathbb{V}_j = V^H \tilde{V}_j \in \mathbb{C}^{l \times l}$
2. Compute $\bar{\mu}_n = \sum_{j=1}^M w_j z_j^n \mathbb{V}_j$
3. Construct Hankel matrices \mathbb{H}_m and $\mathbb{H}_m^{\leq} \in \mathbb{C}^{ml \times ml}$
4. Perform singular value decomposition, $\mathbb{H}_m = \mathbb{W} s \mathbb{U}$
5. Construct $\mathbb{H} = s^{-1/2} \mathbb{W}^H \mathbb{H}_m^{\leq} \mathbb{U}^H s^{-1/2} \in \mathbb{C}^{K \times K}$
6. Compute eigenvalues of \mathbb{H} to have α_k

If eigenvectors Q_k are also wanted, let q_k be eigenvectors of \mathbb{H} ,

7. Compute $\bar{S}_n = \sum_{j=1}^M w_j z_j^n \tilde{V}_j$
8. Compute $(Q_1, \dots, Q_K) = (\bar{S}_0, \dots, \bar{S}_{m-1}) \mathbb{U}^H s^{-1/2} (q_1, \dots, q_K)$

In the block SS method, the filtered subspace is implicitly spanned by the ml column vectors of \bar{S}_n . At steps 2 and 7, the momental weight z_j^n may as well be replaced by the shifted-and-scaled one. Note that the resulting eigenvalues are also shifted-and-scaled. At step 4, small singular value components are omitted, so that $s \in \mathbb{R}^{K \times K}$ where $K < ml$. If no ignorable singular values are found, there may be more eigenvalues than ml , and we should increase either m or l to span the subspace in higher dimensions. Because the effective filter function is not perfect, eigenvalues outside of G may be contaminated to be $K \geq k_\Gamma$.

4 Numerical examples

Two numerical examples are given in this section. The first one depicts how the localized moment matrix works as a filter operator. The other one demonstrates the improvement achieved by the block version of the SS method. The algorithm was implemented on Mathematica 5.2. The linear equation solver `LinearSolve[]` was used to evaluate $(z_j B - A)^{-1} B V$ numerically. The calculated eigenvalues are compared against those obtained by `Eigensystem[]`.

Example 8. Two random matrices, $A, B \in \mathbb{R}^{100 \times 100}$, were generated. The elements of A were taken randomly in $[-1, 1]$, while B was diagonal dominant, where random noises of $[-0.1, 0.1]$ were added to every entry of an identity matrix. The initial vector was setup artificially as a sum of all the right-eigenvectors, $v = \sum_i Q_i$. We define the i -th eigen-amplitude in v by $\tilde{Q}_i v$, so

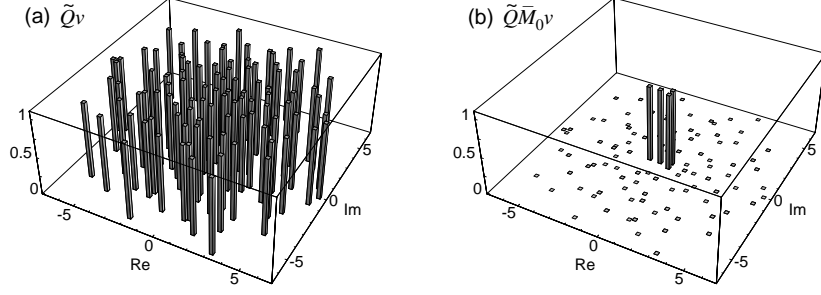


Fig. 2. Example 8: the eigen-amplitudes of a vector (a) before and (b) after the operation of the localized moment matrix.

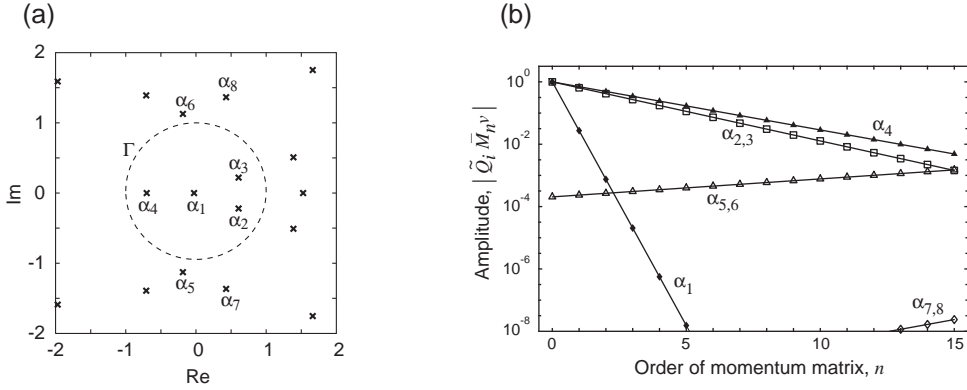


Fig. 3. Example 8: (a) distribution of the eigenvalues around the origin, and (b) eigen-amplitudes of $\bar{M}_n v$ for $\alpha_{1\sim 8}$.

that all the amplitudes in the initial vector were unity. The integral path Γ was taken to be a unit circle centered at origin. The M -point trapezoidal rule was employed for the quadrature, where $M = 64$, $\gamma = 0.0$, and $\rho = 1.0$.

The eigen-amplitudes of v and $\bar{M}_0 v$ are plotted in Fig. 2. Each box is located at the eigenvalue point on the complex plane, and the real part of the amplitude is plotted as its height; the imaginary part was negligibly small. As can be seen from the figure, four primary eigen-elements remained in $\bar{M}_0 v$, which are located inside of Γ . Detailed location of these eigenvalues, $\alpha_{1\sim 4}$, are plotted in Fig. 3(a), along with four more eigenvalues, $\alpha_{5\sim 8}$, located on the periphery of Γ . The eigen-amplitudes are modulated as we change the order of the moment matrix n . In Fig. 3(b), absolute values of the amplitudes are plotted as a function of n . The amplitudes of other eigen-elements than $\alpha_{1\sim 8}$ were lower than the plotted area. For the primary eigen-elements, $\alpha_{1\sim 4}$, the amplitude became smaller as n increases, which is roughly proportional to $|\alpha_i|^n$. On the other hand, the amplitude of the contaminant eigen-elements, $\alpha_{5\sim 8}$, increased with n . It is because the tail of the filter function $\tilde{f}_n(x)$ extends more outward for larger n . In the present example, $\tilde{f}_{15}(x)$ becomes lower than the threshold of 10^{-14} at $x > 1.9$ along the real axis.

To obtain the eigenvalues, $\mathbb{H}_m, \mathbb{H}_m^< \in \mathbb{C}^{16 \times 16}$ were calculated. The singular value decomposition was performed on \mathbb{H}_m to extract the non-singular part from the size-reduced matrix pencil. The singular values were compared with the largest one, and those components relatively smaller than 1.1×10^{-14} were removed. Two component were rejected at this step, and the approximated eigenvalues were calculated with the rest of 14 components. The accuracy of thus obtained eigenvalues are not uniform. The maximum error in the primary eigenvalues $\alpha_{1 \sim 4}$ was 1.7×10^{-14} . The corresponding eigenvectors are mainly spanned by the large singular value components, which are calculated in high accuracy. The smaller components also participate, though the contributions are so small that their inferior accuracy doesn't affect. Next two eigenvalues, α_5 and α_6 , are located near the periphery of G , the error of which was 2.4×10^{-12} . The errors in the following 7 eigenvalues were $3.2 \times 10^{-8} \sim 1.5 \times 10^{-6}$. These eigenvectors are spanned by the smaller singular value components. The rest eigenvalue could not be assigned to any exact correspondents, the eigenvector of which is spanned by the trace singular value components.

The original SS method has a difficulty to resolve nearly degenerated eigenvalues congested around the center of Γ . It is because the filter functions of large n are flat at the center, which makes the filtered vectors linearly dependent. The next example shows that the difficulty can be removed by the block SS method.

Example 9. A real symmetric matrix $A \in \mathbb{R}^{400 \times 400}$ was prepared, which has five primary eigenvalues, -10.03, -10.02, -10.01, -10.00, and -9.99, in the range of $[-10.5, -9.5]$. Other eigenvalues were taken randomly in the range $[-40, 40]$, and a random unitary matrix was prepared to construct A . An identity matrix was used for B . The circular integral path and the trapezoidal rule was employed, with the center and radius as $\gamma = -10$ and $\rho = 0.5$, respectively. The shifted-and-scaled momental weight was employed as described in Sec. 3.

The block SS method was examined on this system with varying the number of initial vectors l . Those initial vectors of \mathbb{R}^{400} were generated randomly and ortho-normalized. The result is summarized in Table 1. To maintain the computational amount nearly the same, the number of trapezoidal points M was reduced as l increased. The order of the Hankel matrix m was taken to be large enough for the size-reduced matrix pencil $\frac{z-\gamma}{\rho}\mathbb{H}_m - \mathbb{H}_m^<$ to have a singular part. This process certifies the over-completeness of the basis set that spans the filtered subspace. The linear dependence of the basis set was removed by the singular value decomposition on \mathbb{H}_m , where the threshold of the singularity was taken to be 1.1×10^{-14} . For $l = 1 \sim 3$, a total of 12 vectors were (implicitly) generated, while 16 vectors were necessary for $l = 4$, due to the duller filter function with $M = 32$.

Starting from a single initial vector, only four dimensions out of five could

Table 1

Example 9: errors of eigenvalues calculated by the block SS method. The columns, from left to right, are the number of initial vectors, the number of trapezoidal points, the order of the Hankel matrix, the number of obtained eigenvalues, errors of the eigenvalues in G , and errors of the contaminant eigenvalues, respectively.

l	M	m	N_α	$ \Delta\alpha_{\in G} $	$ \Delta\alpha_{\notin G} $
1	128	12	6	$1.3 \times 10^{-6} \sim 4.1 \times 10^{-3\#}$	$8.0 \times 10^{-11} \sim 6.9 \times 10^{-9}$
2	64	6	8	$7.7 \times 10^{-12} \sim 9.5 \times 10^{-8}$	$3.0 \times 10^{-12} \sim 6.5 \times 10^{-5}$
3	42	4	10	$4.5 \times 10^{-13} \sim 1.1 \times 10^{-10}$	$8.1 \times 10^{-13} \sim 2.3 \times 10^{-2}$
4	32	4	14	$1.8 \times 10^{-15} \sim 1.5 \times 10^{-12}$	$4.8 \times 10^{-14} \sim 8.1 \times 10^{-2}$

only four eigenvalues out of five were obtained.

be extracted for the primary subspace. Because the primary eigenvalues are located near the origin, the corresponding eigen-elements diminished quickly in $M_n v$, as $n \geq 1$ increased. As a result, peripheral eigen-elements overwhelmed in $M_n v$, leaving the basis set incomplete in the primary subspace. The situation is the same for $l > 1$, but in these cases the column vectors of $M_0 V$ already span l -dimensions with moderate linear independency. The eigenvalues became more accurate as l increases, reflecting the improved linear independency in the primary subspace. With the large l , the order of the moment m can also be kept smaller, where the practical filter functions are expected to behave better (see Fig. 1).

In this example, the number of linear equations to be solved were kept nearly constant to average the computation cost among different l . It is often the case, however, that the cost to solve a linear equation $A(x_1, x_2) = (v_1, v_2)$ is much smaller than twice the cost of $Ax = v$. This observation makes the block version of the SS method preferable, especially when the size of the matrix is large and preconditioning is necessary. The block SS method also inherits the adaptability to the parallel computing in the original, which makes the method attractive from a computational point of view.

5 Conclusion

The SS method was reformulated based on the resolvent theory, and its block version was proposed. The numerical example indicated that the block version has a potential not only to resolve degeneracies, but also to achieve higher accuracy under the same computational cost. The method was also interpreted in the context of the filter diagonalization. The explicit form of the filter function was derived for the SS method, which helps to investigate several properties of the method quantitatively.

In the Rayleigh-Ritz approach of the SS method [13], we don't use the Hankel matrices, but construct a size-reduced matrix pencil directly in the filtered subspace. In this approach, the quadrature for the path integral needs not be accurate enough, as far as the corresponding filter function $\bar{f}_n(x)$ is well localized. More specifically, $\bar{f}_0(x)$ need not be flat in $x \in G$, as far as $\bar{f}_0(x) \simeq 0$ for $x \notin G$. Indeed, Murakami proposed a novel filter operator similar to Eq. (27) [8], where the momental weight is replaced by constants and $\{z_j, w_j\}$ are chosen specifically. The corresponding filter function does oscillate in G , and falls off quickly outside of G . Liberation from the accuracy allows us to choose the integral path and quadrature points more freely, and to tweak the quadrature weight to make the filter function tail off faster. For example, if the quadrature points can be arranged on an even grid, the survey of the eigenvalue distribution becomes much easier, because we can reuse most of the quadrature points for different integral paths. Designing such an optimized quadrature is a part of our future work.

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