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CONTOUR INTEGRAL EIGENSOLVER FOR NON-HERMITIAN SYSTEMS: A RAYLEIGH-RITZ-TYPE APPROACH

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Abstract. The Rayleigh-Ritz-type approach of the contour integral (CIRR) eigensolver is extended to be generally applicable to non-Hermitian systems. The CIRR method can extract only the eigenvalues in a given domain, which was previously formulated for non-degenerated Hermitian systems. In this method, the Ritz space for the domain is constructed by numerical evaluation of a contour integral. The effect of the numerical approximation is analyzed from the viewpoint of a filter operator, which supports the use of moderate approximations. The numerical accuracy of the original moment-based approach is also assured. A block version of the CIRR method is proposed with a detailed algorithm, which allows us to resolve degenerated systems.

1. INTRODUCTION

The resolvent is one of the standard tools in linear algebra, providing a base to define analytic functions of matrices. Though the resolvent mostly appears in an analytic context, the direct evaluation of the resolvent is also possible with the powerful computers available nowadays, allowing novel numerical methods to be derived [1]. A contour integral eigensolver [2, 3, 4] is one example. With this eigensolver, a large-scale generalized eigenvalue problem is reduced to a handy one, from which only the eigen-components of interest are obtained. Originally, the contour integral method was formulated in a moment-based approach for diagonalizable and non-degenerated systems [2]. In this approach, the size-reduced eigen-problem is constructed from a set of contour integral calculations of a single-valued function, which is derived from the original problem. Though each evaluation of the function is costly, a series of these calculations can be processed in parallel independently, so

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that the method is suitable to modern computer architecture. To improve numerical stability, a Rayleigh-Ritz-type approach of the contour integral (CIRR) method was proposed for non-degenerated Hermitian systems [3]. In this approach, a set of Ritz vectors that spans the target eigen-subspace is constructed via contour integrals.

Recently, we have reformulated the moment-based approach, extending the applicability of the method to degenerated non-diagonalizable systems [4]. In this paper, we will similarly extend the Rayleigh-Ritz-type approach to degenerated non-Hermitian systems. A numerical aspect of the contour integral method, where the contour integral is approximated by some quadratures, is also discussed, based on the filter operator concept. In the next section, we will give a brief outline of the contour integral method, following the new formulation given in Ref. [4]. In Section 3, the new formulation for the Rayleigh-Ritz-type approach is given, and in Section 4, the numerical aspect of the contour integral method is discussed. A block version of the CIRR method is proposed in Section 5 with the detailed algorithm, and Section 6 concludes the paper.

2. Contour Integral Eigensolver

In this section, an outline of the contour integral method is surveyed, providing building blocks to be used in the later discussions. Let $A, B \in \mathbb{C}^{N\times N}$ and assume that the matrix pencil $zB - A$ is regular. The goal of the contour integral method is to solve a generalized eigenvalue problem,

$$(zB - A)x = 0, \tag{1}$$

for all z contained in a selected domain.

We will start from the Weierstrass canonical form for the regular matrix pencil [5].

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*

$$\begin{aligned} W &= \tilde{P}(zB - A)Q \\ &= \begin{pmatrix} z\mathbb{I}_{k_1} - \mathbb{J}_1 & & & & & & \\ & \ddots & & & & & \\ & & z\mathbb{I}_{k_d} - \mathbb{J}_d & & & & \\ & & & z\mathbb{N}_{d+1} - \mathbb{I}_{k_{d+1}} & & & \\ & & & & \ddots & & \\ & & & & & z\mathbb{N}_r - \mathbb{I}_{k_r} \end{pmatrix}, \end{aligned} \tag{2}$$

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.

We let α_i be the eigenvalue of $\mathbb{J}_i$, and $\alpha_i = \infty$ for $i > d$. Because $\tilde{P}$ and Q are regular, there exist $P = \tilde{P}^{-1}$ and $\tilde{Q} = Q^{-1}$. According to the block structure of W, we partition the row vectors of $\tilde{P}$, $\tilde{Q}$ into $\tilde{P}_i, \tilde{Q}_i \in \mathbb{C}^{k_i \times N}$ for $i = 1, 2, \ldots, r$. Similarly, the column vectors of P, Q are partitioned into $P_i, Q_i \in \mathbb{C}^{N \times k_i}$. Under this partitioning, $zB - A = PW\tilde{Q}$ can be decomposed into

$$B = \sum_{i=1}^{d} P_i \tilde{Q}_i + \sum_{i=d+1}^{r} P_i \mathbb{N}_i \tilde{Q}_i, \tag{3}$$

$$A = \sum_{i=1}^{d} P_i \mathbb{J}_i \tilde{Q}_i + \sum_{i=d+1}^{r} P_i \tilde{Q}_i. \tag{4}$$

Note that the first vectors in $\tilde{P}_i$ and Q_i are the left and right eigenvectors of the matrix pencil $zB - A$, respectively, with eigenvalue α_i. (We employ an upper triangular form for the Jordan blocks.)

A moment matrix of the matrix pencil is defined based on the contour integral.

Definition 2. Let Γ be a positively oriented closed Jordan curve and G be 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

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

We pick up eigenvalues contained in G, and construct the following collective notations:

- The direct sum of $\mathbb{J}_i$ is taken over $i; \alpha_i \in G$ to form a Jordan matrix $\mathbb{J}_\Gamma \in \mathbb{C}^{k_\Gamma \times k_\Gamma}$, where $k_\Gamma = \sum_{i;\alpha_i \in G} k_i$.
- The corresponding P_i and Q_i are collected in the same order used to form the Jordan matrix above to form $P_\Gamma, Q_\Gamma \in \mathbb{C}^{N \times k_\Gamma}$. $\tilde{P}_\Gamma, \tilde{Q}_\Gamma \in \mathbb{C}^{k_\Gamma \times N}$ are defined similarly.

Under the collective notation, the moment matrix is written as [4]

$$M_n = Q_\Gamma \mathbb{J}_\Gamma^n \tilde{P}_\Gamma. \tag{6}$$

This expression leads to the basic theorem of the contour integral method [4]:

Theorem 3. *Let C and D be arbitrary $N \times m$ matrices, where $N > m \geq k_\Gamma$, and define a size-reduced moment matrix $\mathbb{M}_n = C^H M_n D (\in \mathbb{C}^{m \times m})$. If ranks of both $C^H Q_\Gamma$ and $\tilde{P}_\Gamma D$ are k_Γ, the non-singular part of a size-reduced matrix pencil $z\mathbb{M}_0 - \mathbb{M}_1$ is equivalent to $z\mathbb{I}_{k_\Gamma} - \mathbb{J}_\Gamma$.*

Note that the moment matrix was previously defined as M_nB [4]. The term B is dropped here for the convenience of the CIRR method, though the proof of the theorem is nearly identical.

The following addition theorem can also be derived from Eqs. (3), (4), and (6):

$$M_iBM_j = M_{i+j}, \tag{7}$$

$$M_iAM_j = M_{i+j+1}. \tag{8}$$

In the moment-based contour integral method, two $m \times m$ Hankel matrices $\mathbb{H}_m$ and $\mathbb{H}_m^<$ are prepared,

$$\mathbb{H}_m = \begin{pmatrix} \mu_0 & \mu_1 & \cdots & \mu_{m-1} \\ \mu_1 & \mu_2 & \cdots & \mu_m \\ \vdots & \vdots & & \vdots \\ \mu_{m-1} & \mu_m & \cdots & \mu_{2m-2} \end{pmatrix} \tag{9}$$

and

$$\mathbb{H}_m^< = \begin{pmatrix} \mu_1 & \mu_2 & \cdots & \mu_m \\ \mu_2 & \mu_3 & \cdots & \mu_{m+1} \\ \vdots & \vdots & & \vdots \\ \mu_m & \mu_{m+1} & \cdots & \mu_{2m-1} \end{pmatrix}, \tag{10}$$

where $\mu_n = u^H M_n v$ and $u, v \in \mathbb{C}^N$ are random vectors. By taking row vectors of C^H as $C_i^H = u^H M_i B$ and column vectors of D as $D_i = BM_i v$, and applying the addition theorem, the Hankel matrices become $\mathbb{H}_m = \mathbb{M}_0$ and $\mathbb{H}_m^< = \mathbb{M}_1$. Therefore, the non-singular part of the matrix pencil $z\mathbb{H}_m - \mathbb{H}_m^<$ is equivalent to $z\mathbb{I}_{k_\Gamma} - \mathbb{J}_\Gamma$, if u and v are random enough and the eigenvalues are not degenerated in G. A block version of the method was also proposed, in which the vectors u and v are replaced by random matrices $U, V \in \mathbb{C}^{N \times l}$. With the block version, up to the l-th order degeneracy can be resolved for the eigenvalues in G.

3. Rayleigh-ritz-type Approach

In this section, we will give a new proof for the Rayleigh-Ritz-type contour integral method, which allows us to use it for non-Hermitian systems. In general, the Rayleigh-Ritz-type approach constructs the left and right Ritz vectors L_i and R_i, which are collectively noted as $L, R \in \mathbb{C}^{N \times m}$, respectively. The original matrix pencil $zB - A$ is projected onto the Ritz space to form a size-reduced pencil, $z\mathbb{B} - \mathbb{A} \in \mathbb{C}^{m \times m}$, where $\mathbb{B} = L^H BR$ and $\mathbb{A} = L^H AR$. In the context of the contour integral method, the Ritz space is constructed by using the moment matrix.

Taking $L^H = C^H M_0$ and $R = M_0 D$, the addition theorem leads to $\mathbb{B} = \mathbb{M}_0$ and $\mathbb{A} = \mathbb{M}_1$. According to Theorem 3, the non-singular part of the matrix pencil $z\mathbb{B} - \mathbb{A}$ is equivalent to $z\mathbb{I}_{k_\Gamma} - \mathbb{J}_\Gamma$, if ranks of $C^H Q_\Gamma$ and $\tilde{P}_\Gamma D$ are k_Γ.

In this crude approach, both the left and right Ritz spaces need be constructed, and thus the approach is more costly than the moment-based one; the evaluation of $\mu_n = u^H M_n v$ requires only the right Ritz space. As shown in the next theorem, however, only one of the Ritz spaces is actually necessary to solve the problem.

Theorem 4. *Let $L, D \in \mathbb{C}^{N\times m}$ be arbitrary matrices, and $R = M_0 D$. A projected matrix pencil $z\mathbb{B} - \mathbb{A}$ is defined by $\mathbb{B} = L^H B R$ and $\mathbb{A} = L^H A R$. If ranks of both $L^H P_\Gamma$ and $\tilde{P}_\Gamma D$ are k_Γ, the non-singular part of the projected matrix pencil is equivalent to $z\mathbb{I}_{k_\Gamma} - \mathbb{J}_\Gamma$.*

Proof. Let $C^H = L^H P \tilde{Q}$. Because P and $\tilde{Q}$ are regular, $L^H = C^H Q \tilde{P}$. From Eqs. (3), (4), and (6), we have

$$Q\tilde{P}BM_n = M_n, \tag{11}$$

$$Q\tilde{P}AM_n = M_{n+1}, \tag{12}$$

so that $\mathbb{B} = C^H M_0 D = \mathbb{M}_0$ and $\mathbb{A} = C^H M_1 D = \mathbb{M}_1$. Because $C^H Q_\Gamma = L^H P_\Gamma$, the rank of $C^H Q_\Gamma$ is k_Γ. From Theorem 3, we get the result. ■

Similar to the moment-based method, the Ritz space can be constructed from a single initial vector. Starting from a random initial vector $v \in \mathbb{C}^N$, the right Ritz vectors are constructed as $R_i = M_i v$, while the left Ritz vectors are arbitrary. If there is no degeneracy in G, we can apply Theorem 4 by taking $D_i = BM_i v$.

When the left Ritz vectors are constructed as $L_i^H = u^H M_i$ in addition to $R_i = M_i v$, we have $\mathbb{B} = \mathbb{H}_m$ and $\mathbb{A} = \mathbb{H}_m^<$, and the CIRR method becomes identical to the moment-based method. This observation is especially important for Hermitian systems, where A and B are self-adjoint and B is positive definite. In this case, the moment matrix M_n also becomes self-adjoint, and the the left Ritz space is obtained at no additional cost as $L_i = R_i$ by taking $u = v$. This is the Rayleigh-Ritz-type method originally discussed in Ref. [3]. As shown in the next section, the generation of both Ritz spaces improves the numerical accuracy of the method.

The CIRR method can also be viewed from a filter operator standpoint [6, 7]. Obviously, from (6), the right Ritz space constructed by $M_0 D$ is contained in the subspace spanned by Q_Γ. In other words, the eigen-components outside of G are filtered out from D by the operation of M_0. More precisely, the operation of M_n can be interpreted as a manipulation of an eigen-spectrum. Assume that the matrix pencil $zB - A$ is diagonalizable, and define the i-th P- and Q-amplitude of a vector

v as $\tilde{P}_i v$ and $\tilde{Q}_i v$, respectively. The P-amplitude of v is related to the Q-amplitude of $M_n v$ as

$$\tilde{Q}_i M_n v = f_n(\alpha_i)\tilde{P}_i v, \tag{13}$$

where the filter function $f_n(x)$ is given by

$$\begin{aligned} f_n(x) &= \frac{1}{2\pi i}\oint_\Gamma \frac{z^n}{z-x}dz \\ &= \begin{cases} x^n, & x \in G, \\ 0, & \text{otherwise.} \end{cases} \end{aligned} \tag{14}$$

The filter function $f_n(x)$ is a localized function, which is zero outside of G. The moment matrix M_n correspondingly works as a filter operator, which diminishes eigen-components outside of G.

4. Numerical Approximation

In practical applications, the integral in Eq. (5) is approximated numerically by an appropriate quadrature. In this section, we will discuss on the numerical aspect of the contour integral method. First, a numerical example is shown, demonstrating inconsistent numerical accuracies in the moment-based method. The inconsistency is solved in the subsection 4.2, by attributing the numerically-approximated moment-based method to the CIRR method. The numerical accuracy of the CIRR method is further discussed quantitatively in the subsection 4.3, and the superior accuracy of the CIRR method for Hermitian systems is explained in the last subsection. To make the discussions simple, we assume hereafter that the matrix pencil $zB - A$ is diagonalizable.

4.1. Numerical example

One of the mysteries in the moment-based method is that eigenpairs are calculated accurately, even though the numerical accuracy of μ_n is far less comparable. To start with, we will show a numerical demonstration.

Example 5. A real symmetric matrix $A \in \mathbb{R}^{400\times 400}$ was setup by preparing a random unitary matrix and random eigenvalues in the range $[-80, 80]$. An identity matrix was used for B. A unit circle placed at the origin was taken as Γ, inside of which we found 4 eigenvalues. A random initial vector $v \in \mathbb{R}^{400}$ was prepared to calculate

$$\mu_n = \frac{1}{2\pi i}\oint_\Gamma z^n v^H (z\mathbb{I} - A)^{-1} v dz, \tag{15}$$

which was used to construct Hankel matrices $\mathbb{H}_m$ and $\mathbb{H}_m^<$ with $m = 16$. The integral in Eq. (15) was approximated by the M-point trapezoidal rule, where

M was varied to tune the numerical accuracy. We will refer to the approximated matrices as $\bar{\mathbb{H}}_m$ and $\bar{\mathbb{H}}_m^<$. We assume $M = 256$ calculations to be exact, and any numerical errors of the matrices at any other M are examined against them. The relative root mean square deviations (RMSD) of the matrix elements, $\|\bar{\mathbb{H}}_m - \mathbb{H}_m\|_{\mathrm{F}}/\|\mathbb{H}_m\|_{\mathrm{F}}$ and $\|\bar{\mathbb{H}}_m^< - \mathbb{H}_m^<\|_{\mathrm{F}}/\|\mathbb{H}_m^<\|_{\mathrm{F}}$, are plotted in Fig. 1 for various M. The four interior eigenpairs (e_i, Q_i) of $z\mathbb{I} - A$ were derived from solutions of a generalized eigenvalue problem $z\bar{\mathbb{H}}_m - \bar{\mathbb{H}}_m^<$. The eigenvectors were normalized and the residual norms of the eigenpairs were calculated by $\|(\alpha_i\mathbb{I} - A)Q_i\|_2$, which are also plotted in Fig. 1. The Hankel matrices become accurate as M increases, though they are far from the numerical limit. Nevertheless, the eigenpairs are obtained at 10^{-10} accuracy, even though the matrices are erroneous by a factor of $10^{-2} \sim 1$.

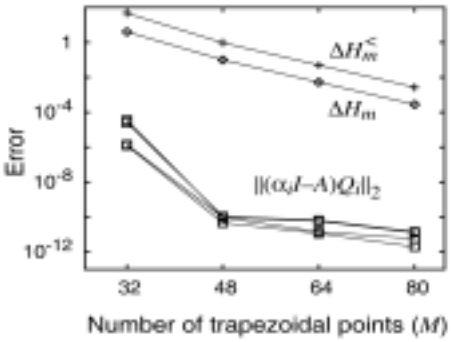

Fig. 1. Numerical errors of the Hankel matrices $\mathbb{H}_m$ and $\mathbb{H}_m^<$, and residual norms of four eigenpairs located inside of Γ.

4.2. Quadrature approximated moment-based method

The discrepancy between the precision of the matrix pencil and its eigenpairs is explained by the equivalence of the moment-based method to the CIRR method. Let z_j be quadrature points on Γ and w_j be the corresponding weights, where $j = 1, 2, \ldots, M$. The moment matrix M_n is approximated by the quadrature as

$$\bar{M}_n = \sum_{j=1}^{M} w_j z_j^n (z_j B - A)^{-1}. \tag{16}$$

We will first show that the approximated moment matrix $\bar{M}_n$ also works as a filter operator.

Theorem 6. *Let $zB - A$ be a diagonalizable regular matrix pencil, and $v \in \mathbb{C}^N$ be arbitrary. The i-th P-amplitude of v is related to the Q-amplitude of $\bar{M}_n v$ as*

$$\tilde{Q}_i \bar{M}_n v = \bar{f}_n(\alpha_i)\tilde{P}_i v, \tag{17}$$

where

$$\bar{f}_n(x) = \sum_{j=1}^{M} w_j \frac{z_j^n}{z_j - x}, \tag{18}$$

$$\bar{f}_n(\infty) = -\sum_{j=1}^{M} w_j z_j^n. \tag{19}$$

Proof. When the matrix pencil $zB - A$ is diagonalizable, its resolvent is written as [4]

$$(zB - A)^{-1} = \sum_{i=1}^{d} \frac{Q_i \tilde{P}_i}{z - \alpha_i} - \sum_{i=d+1}^{r} Q_i \tilde{P}_i. \tag{20}$$

Inserting Eq. (20) into Eq. (16), we have

$$\bar{M}_n = \sum_{i=1}^{r} \bar{f}_n(\alpha_i) Q_i \tilde{P}_i. \tag{21}$$

Operating $\tilde{Q}_i$ from the left side, we obtain the result of the theorem. ∎

Typically, $\bar{f}_n(x)$ becomes a fairly localized function around G, though the boundary is not as sharp as that of Eq. (14). For example, let Γ be a unit circle centered at the origin, and apply the M-point trapezoidal rule. The quadrature points and weights are given by $z_j = \exp(\frac{2\pi i}{M}(j - \frac{1}{2}))$ and $w_j = z_j/M$, respectively. This quadrature gives the filter function of

$$\bar{f}_n(x) = \frac{x^n}{1 + x^M}, \tag{22}$$

for $0 \leq n < M$. Note that, under the trapezoidal rule with the circular path, we have $\bar{f}_n(\infty) = 0$, so that the eigen-amplitude of the infinite eigenvalues is exactly nullified. When the filter operator was defined by $\bar{M}_n B$ [4], the operation of B effectively collapses the subspace with infinite eigenvalues, so that the eigencomponents $i > d$ could be ignored. In the CIRR method, however, we have to pay attention, so that such components do not contaminate the filtered subspace.

Next, we will connect the moment-based and CIRR methods under the approximated moment matrix $\bar{M}_n$. Let $u, v \in \mathbb{C}^N$ be random vectors and $\bar{\mu}_n = u^H \bar{M}_n v$, which is used to build the approximated Hankel matrices. Let the right Ritz vectors be $R_i = \bar{M}_i v$ for $i = 0, 1, \ldots, m-1$. Based on Theorem 4, the moment-based method becomes identical to the CIRR method, if we can choose left Ritz vectors that satisfy

$$L_i^H B R_j = \bar{\mu}_{i+j} \quad \text{and} \quad L_i^H A R_j = \bar{\mu}_{i+j+1}. \tag{23}$$

In general, such a set of L_i exists if $N \geq 2m$. Especially, if the quadrature satisfies $\bar{f}_n(\infty) = 0$, we have, from Eq. (18), $\bar{f}_{n+1}(x) = x\bar{f}_n(x)$. In this case, we can take the left Ritz vectors explicitly as $L_i^H = u^H(Q\tilde{P}A)^i Q\tilde{P}$. From these observations, the numerically-approximated moment-based method can be considered as a special case of the CIRR method, which separates the the numerical accuracy of $\bar{\mu}_n$ from the accuracy of eigenvalues. In the next subsection, we will discuss on the accuracy of the numerically-approximated CIRR method.

4.3. Quadrature approximated CIRR method

We have shown that the moment-based method is identical to the CIRR method with the right Ritz vectors defined by $R_i = \bar{M}_i v, i = 0, 1, \ldots, m-1$. In this subsection, we will discuss on the numerical properties of the Ritz vectors. The moment operator $\bar{M}_n$ modulates the eigen-spectrum of v, filtering out the eigen-components far from G. Due to the numerical approximation, the eigen-components near G are not exterminated completely. The filter performance of $\bar{M}_n$ is determined by the filter function $\bar{f}_n(x)$, which is dependent on the quadrature. In Fig. 2, the asymptotic behavior of the filter function is depicted for some of $\bar{f}_n(x)$ used in Example 5. In that example, we were trying to extract eigen-components in the domain $[-1, 1]$ along the real axis. The ideal filter function $f_0(x)$ is a window

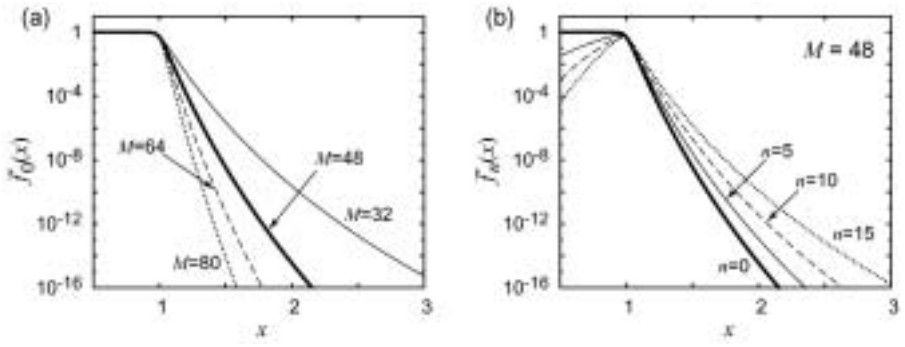

Fig. 2. The filter function $\bar{f}_n(x)$ of the M-point trapezoidal rule on the unit circle centered at the origin. (a) $\bar{f}_0(x)$ for various M. (b) $\bar{f}_n(x)$ of $M = 48$ for various n.

function with sharp edges at $x = -1$ and 1. Because of the numerical approximation, however, the actual filter functions $\bar{f}_0(x)$ have dull edges as shown in Fig. 2(a). Still, they are well localized functions, and reflecting the functional form of Eq. (18), they are guaranteed to approach zero asymptotically. The extent of the asymptotic tail depends on the quality of the quadrature. In the present case, the larger the number of trapezoidal points M, the sharper the edge becomes. In the moment-based method, the higher order moment matrices $\bar{M}_n, n > 0$ are also used.

As shown in Fig. 2(b), the tail of the corresponding filter functions $\bar{f}_n(x)$ extends as n increases. In Example 5, the dimension of the Hankel matrices was $m = 16$, so that the right Ritz space was spanned by $\bar{M}_i v, i = 0, 1, \ldots 15$. Therefore, in the case of $M = 48$ and with a machine epsilon of 10^{-16}, those eigen-components with eigenvalues $1 < \alpha_i < 3$ may be contaminated in the result. Indeed, the non-singular part of the matrix pencil $z\mathbb{H}_m - \mathbb{H}_m^<$ is enlarged as M decreases. It must be noted that only a trace amount of the peripheral eigen-components is contained in the constructed Ritz vectors, so that those peripheral eigenpairs are obtained with fewer significant digits than the interior ones. In other words, the accuracy of the obtained eigenpairs is not uniform. Besides calculating the residual norms, the reliability of the eigenpairs may be assessed by a singular value analysis on a set of the constructed Ritz vectors.

4.4. Accuracy gain by the left Ritz space

As shown in Theorem 4, the left Ritz space can be arbitrary, if an exact moment matrix M_n is used to construct the right Ritz space. When the moment matrix is approximated numerically, however, the situation is not the same. Besides the right Ritz vectors $R_i = \bar{M}_i v$, let the left Ritz vectors be constructed as $L_i^H = u^H \bar{M}_i$. We also assume that the filter function satisfies $\bar{f}_n(\infty) = 0$, and thus $\bar{f}_{n+1}(x) = x\bar{f}_n(x)$. From Eq. (21), these Ritz vectors give the projected matrices $\mathbb{A}$ and $\mathbb{B}$ as

$$\mathbb{B}_{ij} = L_i^H B R_j = u^H \left(\sum_{k=1}^{r} \alpha_k^{i+j} \bar{f}_0(\alpha_k)^2 Q_k \tilde{P}_k \right) v, \tag{24}$$

$$\mathbb{A}_{ij} = L_i^H A R_j = u^H \left(\sum_{k=1}^{r} \alpha_k^{i+j+1} \bar{f}_0(\alpha_k)^2 Q_k \tilde{P}_k \right) v. \tag{25}$$

In fact, the identical projection can be obtained with another set of Ritz vectors given by

$$L_i^H = u^H (Q\tilde{P}A)^i Q\tilde{P}, \tag{26}$$

$$R_i = \left(\sum_{k=1}^{r} \bar{f}_0(\alpha_k) \bar{f}_i(\alpha_k) Q_k \tilde{P}_k \right) v. \tag{27}$$

Equation (27) indicates that the right Ritz vectors are constructed by a set of filter operators characterized by filter function $\bar{g}_i(x) = \bar{f}_0(x)\bar{f}_i(x)$. In general, the filter function $\bar{g}_i(x)$ is sharper than $\bar{f}_i(x)$ used in the moment-based method. Therefore, the construction of the left Ritz space will make the filter performance better, which narrows the non-singular space of the projected matrix pencil $z\mathbb{B} - \mathbb{A}$.

Usually, the construction of the left Ritz space is costly, so that it is less favorable than using better quadratures. In the case of Hermitian systems, however, the left

Ritz space is constructed implicitly at no additional cost, as described in Section 3. The observed improvement of the CIRR method over the moment-based method [3] may originate from the better filter performance achieved by the implicit construction of the left Ritz space.

5. Block CIRR

Similar to the moment-based method, a block version of the CIRR method can be derived by preparing multiple initial vectors. Let $V \in \mathbb{C}^{N\times l}$ be a random matrix and $S_n = M_n V$ where $n = 0, 1, \ldots, m-1$. In the block CIRR method, the right Ritz space is spanned by the column vectors of S_n.

The advantage of the block version is three-fold. First, degenerated eigen-components in G can be resolved. If the Ritz space is constructed from a single vector, degenerated eigen-components cannot be separated, because eigen-amplitudes of those components are modulated in the same way (see Eq. (13)). By preparing l independent initial vectors, up to the l-th order degeneracy can be resolved. Second, we can keep the order of the moment matrix small. In the CIRR method, the dimension of the Ritz space must be much larger than k_Γ, because the filter performance of $\bar{M}_n$ is not sharp enough. If the Ritz space is constructed from a single vector, we have to choose $m > k_\Gamma$, and the use of higher order moment matrices is inevitable. As shown in Fig. 2(b), however, the filter performance is worse for the higher moment matrix, and the contamination from the peripheral eigen-components becomes more severe. Because the dimension of the Ritz space is multiplexed to ml in the block version, we can keep the order of the moment matrix small, which allows us to use moderate quadratures. Finally, accidental oversights of eigen-components can be avoided. From Eq. (13), if there is no P-amplitude in the initial vector, the corresponding eigen-component is missing in the constructed Ritz space, even if it is located inside of Γ. Such an accidental situation is less probable in the block version, where many independent vectors are prepared initially.

A detailed algorithm of the block CIRR method is given below.

Algorithm 1. (Block CIRR)
Input: $V \in \mathbb{C}^{N\times l}$, $\{z_j, w_j\}$ for $j = 1, 2, \ldots, M$
Output: (α_i, Q_i) for $i = 1, 2, \ldots, K$

1. Solve $\tilde{V}_j = (z_j B - A)^{-1} V$ at each quadrature point.
2. Compute $\bar{S}_n = \sum_{j=1}^{M} w_j z_j^n \tilde{V}_j$ for $n = 0, 1, \ldots, m-1$.
3. Perform singular value decomposition on the collection of $\bar{S}_n$:
   $S = (S_0, S_1, \ldots, S_{m-1}) \in \mathbb{C}^{N\times ml}$,
   $S = U s W^H$ where $U \in \mathbb{C}^{N\times K}$, $s \in \mathbb{C}^{K\times K}$, and $W \in \mathbb{C}^{ml\times K}$,

$K \leq ml$, $U^H U = W^H W = \mathbb{I}_K$, and s is diagonal and positive definite.

4. Compute $\mathbb{B} = U^H B U$ and $\mathbb{A} = U^H A U$, and obtain eigenpairs (α_i, q_i) of the projected matrix pencil $z\mathbb{B} - \mathbb{A} \in \mathbb{C}^{K \times K}$.
5. Compute $Q_i = U q_i$.

Some notes on the algorithm follow:

- Though Step 1 is the most time-consuming part, the linear equations can be solved independently parallel for each quadrature point z_j. This makes the algorithm efficient on modern parallel computer architecture.
- In Step 2, the momental weight of z_j^n can be replaced by the shifted-and-scaled one, $((z_j - \gamma)/\rho)^n$. For the numerical reason, γ and ρ should be chosen such that a circle with a center γ and radius ρ mostly covers the region G. Different from the moment-based method, the obtained eigenvalues are not shifted-and-scaled.
- At Step 3, the column vectors of S should span the right eigen-subspace around G in an overcomplete manner. Otherwise, the dimension of the subspace is larger than ml, so that we have to increase either m or l. The orthonormal set to span the subspace is extracted as U, omitting components with trace singular values.
- In Step 3, the column vectors of $U = (U_1, U_2, \ldots, U_K)$ span the right Ritz space. Though they form an orthonormal set, the reliability of the U_k direction is not uniform: the smaller the singular value s_{kk}, the less reliable U_k is. The reliability of U_k propagates to the eigenvectors Q_i, which can be assessed by an index $\sum_{k=1}^{K} s_{kk} |q_{ik}|^2$.
- In Step 4, U is also used for the left Ritz space. Though the left space can be taken arbitrarily, the present choice is better, at least for Hermitian systems.

6. Conclusion

The CIRR method is reformulated to be applicable to non-Hermitian systems. The generalization is achieved by the basic theorem on the contour integral method, which is based on the generalized resolvent [4]. In practical applications, the contour integral is numerically approximated by an appropriate quadrature. The effect of the numerical approximation is analyzed from the viewpoint of the filter operator, where the moment matrix is considered as an operator that modifies an eigen-spectrum of the operand. The performance of the filter operator is quantitatively related to the employed quadrature, which may serve to show what happens when sloppy quadratures are employed, encouraging more careful use of them in the future. The numerical version of the moment-based method is successfully attributed to

the special case of the CIRR method, supporting the numerical soundness of the moment-based method. We have also proposed a block version of the CIRR method, which not only can resolve degenerated eigen-components, but also is numerically beneficial.

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