Novel interpretation of
contour integral spectral projection methods for
solving generalized eigenvalue problems

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Abstract: For generalized eigenvalue problems, we consider computing all
eigenvalues located in a certain region and their corresponding eigenvectors.
Recently, contour integral spectral projection methods have been proposed for
such problems. In this study, from an analysis of the relationship between
the contour integral spectral projection and the Krylov subspace, we provide a
novel interpretation of these methods. We also propose a new algorithm based
on this interpretation.

1 Introduction

We consider computing all eigenvalues located in a certain region and their corresponding
eigenvectors \((\lambda_i, x_i), i = 1, 2, \ldots, m\) for the generalized eigenvalue problem in the form

\[ Ax_i = \lambda_i Bx_i, \quad x_i \in \mathbb{C}^n \setminus \{0\}, \quad \lambda_i \in \Omega \subset \mathbb{C}, \tag{1} \]

where \(A, B \in \mathbb{C}^{n \times n}\) and the matrix pencil \((A, B)\) is assumed to be regular, i.e., \(A - zB\)
is nonsingular for some \(z \in \mathbb{C}\). Such eigenvalue problems arise in many areas of
computational science and engineering.

A powerful algorithm for solving the generalized eigenvalue problem (1) is the contour
integral spectral projection method proposed by Sakurai and Sugiura in 2003 [5]. Since
then, several authors have actively studied and proposed improved techniques based on
the concepts of Sakurai and Sugiura [1, 2, 4, 6].

In this study, we analyze the relationship between the contour integral spectral pro-
jection and the Krylov subspace, and provide a novel interpretation of contour integral
spectral projection methods. We also propose a new algorithm based on this interpreta-
tion.

The remainder of this paper is organized as follows. In Section 2, we briefly describe
the basic concepts of contour integral spectral projection methods. In Section 3, we
provide a novel interpretation and propose a new algorithm based on this interpretation.
In Section 4, we show results from numerical experiments using our proposed algorithm,
and finally we draw some conclusions in Section 5.

Throughout this paper, the following notations are used. Let \(A = [a_1, a_2, \ldots, a_m] \in \mathbb{C}^{n \times m}\),
then \(\text{span}\{A\} := \text{span}\{a_1, a_2, \ldots, a_m\}\). Also, let \(\mathcal{V}, \mathcal{W}\) be subspaces,
then \(\mathcal{V} + \mathcal{W}\) denotes the sum of the subspaces of \(\mathcal{V}, \mathcal{W}\), i.e., \(\mathcal{V} + \mathcal{W} := \{v + w| v \in \mathcal{V}, w \in \mathcal{W}\}\).
Algorithm 1 The Rayleigh-Ritz procedure

**Input:** $m$ dimensional subspace $S_m$

**Output:** Eigenpairs $(\lambda_i, \mathbf{x}_i)$ for $i = 1, 2, \ldots, m$

1. Compute the orthonormal basis $W = [\mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_m]$ of the subspace $S_m$
2. Compute eigenpairs $(\lambda_i, \mathbf{u}_i)$ of the matrix pencil $(W^HAW, W^HBW)$, and $\mathbf{x}_i = W\mathbf{u}_i$ for $i = 1, 2, \ldots, m$

2 Contour integral spectral projection methods

For solving the generalized eigenvalue problem (1), a contour integral spectral projection method was first introduced by Sakurai and Sugiura in 2003 [5]. For solving (1), they introduced the rational function

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

whose poles are eigenvalues $\lambda$ of the generalized eigenvalue problem; they then considered computing all poles located in $\Omega$.

All poles located in a certain region of an analytic function can be computed by the algorithm in [3], which is based on the Cauchy’s integral formula. Applying the algorithm in [3] to the rational function (2), the eigenpairs $(\lambda_i, \mathbf{x}_i)$ of the generalized eigenvalue problem (1) can be obtained from the generalized eigenvalue problem with small Hankel matrices

$$H_M := \begin{pmatrix}
\mu_0 & \mu_1 & \cdots & \mu_{M-1} \\
\mu_1 & \mu_2 & \cdots & \mu_M \\
\vdots & \vdots & \ddots & \vdots \\
\mu_{M-1} & \mu_M & \cdots & \mu_{2M-2}
\end{pmatrix}, \quad H_M^\leq := \begin{pmatrix}
\mu_1 & \mu_2 & \cdots & \mu_M \\
\mu_2 & \mu_3 & \cdots & \mu_{M+1} \\
\vdots & \vdots & \ddots & \vdots \\
\mu_M & \mu_{M+1} & \cdots & \mu_{2M-1}
\end{pmatrix},$$

whose entries consist of the moments

$$\mu_k := \frac{1}{2\pi i} \oint_{\Gamma} (z - \gamma)^k f(z) \, dz, \quad k = 0, 1, \ldots,$$

where $\Gamma$ is the positively oriented Jordan curve (the boundary of $\Omega$), and $\gamma$ is located in $\Omega$. For details, we refer to [5].

Since then, an improvement on the Sakurai and Sugiura’s algorithm has been proposed for obtaining more accurate eigenpairs; this is called the CIRR method [6] and is based on using the Rayleigh-Ritz procedure (Algorithm 1). Block variants of the algorithms in [5] and in [6] have also been proposed [1, 2] for the higher stability of the algorithms, especially when many eigenvalues exist in $\Omega$.

Let $V \in \mathbb{C}^{n \times L} \setminus \{O\}$, e.g., a random matrix. Also, let $S = [S_0, S_1, \ldots, S_{M-1}] \in \mathbb{C}^{n \times ML}$, where

$$S_k = [s_k^{(1)}, \ldots, s_k^{(L)}] := \frac{1}{2\pi i} \oint_{\Gamma} (z - \gamma)^k (zB - A)^{-1}BV \, dz, \quad k = 0, 1, \ldots, M - 1.$$ 

Then, the block CIRR method [1] constructs the $ML$-dimensional subspace

$$S_M := \text{span}\{S\} = \text{span}\{s_0^{(1)}, \ldots, s_0^{(L)}, s_1^{(1)}, \ldots, s_1^{(L)}, \ldots, s_{M-1}^{(1)}, \ldots, s_{M-1}^{(L)}\}.$$
Algorithm 2 The block CIRR method

**Input:** $N, M, L \in \mathbb{N}, V \in \mathbb{C}^{n \times L}, \gamma, (z_j, \omega_j)$ for $j = 1, 2, \ldots, N$

**Output:** Eigenpairs $(\lambda_i, x_i)$ for $i = 1, 2, \ldots, ML$

1. Solve $Y_j = (z_jB - A)^{-1}V$ for $j = 1, 2, \ldots, N$
2. Compute $S_k = \frac{1}{N} \sum_{j=1}^{N} \omega_j(z_j - \gamma)^k Y_j$ for $k = 0, 1, \ldots, M - 1$
3. Compute the QR decomposition of $S = [S_0, S_1, \ldots, S_{M-1}] : S = WR$
4. Compute eigenpairs $(\theta_i, u_i)$ of the matrix pencil $(W^H AW, W^H BW)$, and $(\lambda_i, x_i) = (\theta_i, W u_i)$ for $i = 1, 2, \ldots, ML$

from the Rayleigh-Ritz procedure. The subspace $S_M$ contains all eigenvectors of (1): $S_M = \text{span}\{x_1, x_2, \ldots, x_m\}$ for $m \leq ML$. The block CIRR method with $L = 1$ reduces to the CIRR method.

In practice, the computation of the contour integral in (3) is approximated by some numerical integration rule such as the $N$-point trapezoidal rule

$$S_k \approx \tilde{S}_k = \frac{1}{N} \sum_{j=1}^{N} \omega_j(z_j - \gamma)^k(z_jB - A)^{-1}BV,$$

where $z_j$ are the quadrature points and $\omega_j$ are the corresponding weights. The simple formulation of the block CIRR method is shown in Algorithm 2; for details, we refer to [2,6].

3 A novel interpretation and a new algorithm

For a generalization of the Jordan canonical form to the matrix pencil, we have the following theorem.

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

$$\tilde{P}(zB - A)Q = \text{diag}(zI_{n_1} - J_1, \ldots, zI_{n_d} - J_d, zN_{d+1} - I_{nd+1}, \ldots, zN_r - I_{nr}),$$

where $J_i, N_i$ are Jordan blocks, $N_i$ is nilpotent, and $I_{n_i}$ denotes the identity matrix of order $n_i$.

Based on Theorem 1, in Section 3.1, we provide a novel interpretation of the contour integral spectral projection. In Section 3.2, we propose a new algorithm based on the block Arnoldi method.

3.1 A novel interpretation of the contour integral spectral projection

Since the matrices $P, Q$ are nonsingular, we define $P = \tilde{P}^{-1}, Q = \tilde{Q}^{-1}$. According to the Jordan block structure of (5), we partition row vectors in $P, Q$ into $\tilde{P}_i, \tilde{Q}_i \in \mathbb{C}^{n_i \times n}$ and column vectors in $P, Q$ into $P_i, Q_i \in \mathbb{C}^{n_i \times n}$, respectively, for $i = 1, 2, \ldots, r$. Then, we can derive the following lemma and theorem.
Lemma 2. Let $\psi_k(z)$ be a $k$-degree polynomial. Then, we have
\[
\frac{1}{2\pi i} \int_{\Gamma} \psi_k(z - \gamma)(zB - A)^{-1} dz = \psi_k(S_{\Gamma})P_{\Gamma},
\]
where
\[
S_{\Gamma} := \sum_{i: \lambda_i \in \Omega} Q_i(J_i - \gamma I)\tilde{Q}_i, \quad P_{\Gamma} := \sum_{i: \lambda_i \in \Omega} Q_i\tilde{P}_i.
\]

Proof. From [2, Theorem 4], we have the following relation
\[
\frac{1}{2\pi i} \int_{\Gamma} (z - \gamma)^k(zB - A)^{-1} dz = \sum_{i: \lambda_i \in \Omega} Q_i(J_i - \gamma I)^k\tilde{P}_i, \quad k = 0, 1, \ldots.
\]
Here, since $\tilde{Q}_iQ_i = I$ and $\tilde{Q}_iQ_j = 0$ for $i \neq j$,
\[
\sum_{i: \lambda_i \in \Omega} Q_i(J_i - \gamma I)^k\tilde{P}_i = \left( \sum_{i: \lambda_i \in \Omega} Q_i(J_i - \gamma I)\tilde{Q}_i \right)^k \left( \sum_{i: \lambda_i \in \Omega} Q_i\tilde{P}_i \right) = S_{\Gamma}^kP_{\Gamma}.
\]
Therefore, Lemma 2 is proved.

Definition. Let $A \in \mathbb{C}^{n \times n}$, $B = [b_1, b_2, \ldots, b_l] \in \mathbb{C}^{n \times l}$. Also, let $K_m(A, b_1)$ be the Krylov subspace defined by
\[
K_m(A, b_1) := \text{span}\{b_1, Ab_1, \ldots, A^{m-1}b_1\}
\]
Then, the subspace $K_m^\square(A, B)$ is defined by the sum of the Krylov subspaces, i.e.,
\[
K_m^\square(A, B) := K_m(A, b_1) + K_m(A, b_2) + \cdots + K_m(A, b_l) = \text{span}\{[B, AB, \ldots, A^{m-1}B]\}.
\]

Theorem 3. Let $S_M$ be the subspace of the block CIRR method defined by (4). Then, we have
\[
S_M = K_M^\square(S_{\Gamma}, P_{\Gamma}BV).
\]

Proof. From the definition of $S_k$ (3) and Lemma 2, we have $S_k = S_{\Gamma}^kP_{\Gamma}V$. Therefore,
\[
S_M = \text{span}\{[S_0, S_1, \ldots, S_k]\} = \text{span}\{[P_{\Gamma}BV, S_{\Gamma}P_{\Gamma}BV, \ldots, S_{\Gamma}^{M-1}P_{\Gamma}BV]\} = K_M^\square(S_{\Gamma}, P_{\Gamma}BV).
\]
Therefore, Theorem 4 is proved.

Remark. According to Theorem 4, the block CIRR method can be regarded as the Rayleigh-Ritz procedure based on the block Krylov subspace $K_M^\square(S_{\Gamma}, P_{\Gamma}BV)$. Here, we note that in the block CIRR method, the basis vectors of $K_M^\square(S_{\Gamma}, P_{\Gamma}BV)$ are explicitly computed by (3) and the QR decomposition of $S$ (Algorithm 2).
3.2 Proposal of a new algorithm based on the block Arnoldi method

In Section 3.1, we analyzed the relationship between the contour integral spectral projection and the block Krylov subspace. In this section, we consider applying the block Arnoldi procedure to the block Krylov subspace $K_{\square M}(S_\Gamma, P_\Gamma)$, and we propose a new algorithm based on the block Arnoldi method.

For the eigenpairs of the generalized eigenvalue problem (1) and matrix multiplications for $S_\Gamma$, we have the following two theorems.

**Theorem 4.** Let $H_M \in \mathbb{C}^{ML \times ML}$ be the banded Hessenberg matrix obtained from the matrix formula of the block Arnoldi procedure for the block Krylov subspace $K_{\square M}(S_\Gamma, P_\Gamma)$:

$$W^H S_\Gamma W = H_M,$$

where columns of $W$ are the orthonormal basis of $K_{\square M}(S_\Gamma, P_\Gamma)$. Also, let $(\theta_i, u_i)$ be the standard eigenpairs of $H_M$. Then, in the case of $m \leq ML$, the eigenpairs $(\lambda_i, x_i)$ of the generalized eigenvalue problem (1) are obtained by $(\lambda_i, x_i) = (\theta_i + \gamma, W u_i)$.

**Proof.** From the definitions of $S_\Gamma$ and $W$, Theorem 5 is proved.

**Theorem 5.** Let $U = [u_1, u_2, \ldots, u_L], u_i \in K_{\square M}(S_\Gamma, P_\Gamma)$, Then, there exist $(M - 1)$-degree polynomials $\psi_{M-1}(z)$ and $\Psi \in \mathbb{C}^{L \times L}$ such that

$$U = \psi_{M-1}(S_\Gamma)P_\Gamma V \Psi = \frac{1}{2\pi i} \int_{\Gamma} \psi_{M-1}(z)(zB - A)^{-1}BV \Psi dz.$$

We can also compute the matrix multiplications $S_\Gamma U$ based on the contour integral as follows:

$$S_\Gamma U = \frac{1}{2\pi i} \int_{\Gamma} (z - \gamma)\psi_{M-1}(z - \gamma)(zB - A)^{-1}BV \Psi dz. \quad (6)$$

**Proof.** From Lemma 2 and the definition of $K_{\square M}(S_\Gamma, P_\Gamma)$, Theorem 6 is proved.

**Remark.** According to Theorems 5 and 6, the generalized eigenvalue problem (1) can be solved by the block Arnoldi method for computing eigenpairs of $S_\Gamma$. Here, matrix multiplications for $S_\Gamma$ can be efficiently computed based on the contour integral (6).

Consequently, we propose a new algorithm based on the block Arnoldi method, as shown in Algorithm 3. Here, the computation of the contour integral is approximated by the $N$-point trapezoidal rule, just as in the block CIRR method (Algorithm 2).

When the contour integrals are computed without approximation (without numerical integration), the proposed method is mathematically equivalent to the block CIRR method and to the block variant of Hankel-based method proposed in [2]. The algorithm in [4] can also be regarded as a special case of the restarted version of the proposed algorithm with $M = 1$.

We show the contributions to the computational costs of the block CIRR method (Algorithm 2) and the proposed method (Algorithm 3) in Table 1. Here, we assume that $n \gg L, M, N$ and that the QR decomposition of an $n \times m$ matrix requires $2nm^2$ flops.
Algorithm 3 Proposed algorithm based on the block Arnoldi method

Input: $N, M, L \in \mathbb{N}, V \in \mathbb{C}^{n\times L}, \gamma, (z_j, \omega_j)$ for $j = 1, 2, \ldots, N$

Output: Eigenpairs $(\lambda_i, x_i)$ for $i = 1, 2, \ldots, ML$

1: Solve $Y_j = (z_j B - A)^{-1}BV$ for $i = 1, 2, \ldots, N$
2: $W_0 = (1/N) \sum_{j=1}^{N} \omega_j Y_j$
3: Compute the QR decomposition of $W_0$: $W_0 = W_1 R$
4: Set $\Psi_{1,j} = R^{-1}$ for $j = 1, 2, \ldots, N$
5: for $k = 1, 2, \ldots, M$ do:
6: $\widetilde{\Psi}_{k,j} = (z_j - \gamma) \Psi_{k,j}$ for $j = 1, 2, \ldots, N$
7: $W_k = (1/N) \sum_{j=1}^{N} \omega_j Y_j \widetilde{\Psi}_{k,j}$
8: for $i = 1, 2, \ldots, k$ do:
9: $H_{i,k} = W_i^{H} \widetilde{W}_k$
10: $\Psi_{k,j} = \Psi_{k,j} - \Psi_{i,j} H_{i,k}$ for $j = 1, 2, \ldots, N$
11: $\widetilde{W}_k = \widetilde{W}_k - W_i H_{i,k}$
12: end for
13: Compute the QR decomposition of $\widetilde{W}_k$: $\widetilde{W}_k = W_{k+1} H_{k+1,k}$
14: $\Psi_{k+1,j} = \Psi_{k+1,j} H_{k+1,k}^{-1}$ for $j = 1, 2, \ldots, N$
15: end for
16: Set $W = [W_1, W_2, \ldots, W_M]$ and $H_M = \{H_{i,j}\}_{1 \leq i,j \leq M}$
17: Compute eigenpairs $(\theta_i, u_i)$ of $H_M$, and $(\lambda_i, x_i) = (\theta_i + \gamma, W u_i)$ for $i = 1, 2, \ldots, ML$

Table 1: Main contributions to the computational costs of the block CIRR method and the proposed algorithm. Here, GEP and SEP denote the generalized and standard eigenvalue problems, respectively.

<table>
<thead>
<tr>
<th>Operation type</th>
<th>Block CIRR</th>
<th>Proposed algorithm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solve $(z_j B - A) Y_j = BV$</td>
<td>$N$ [times]</td>
<td>$N$ [times]</td>
</tr>
<tr>
<td>Mat-Vec for $A$ and $B$</td>
<td>$ML$ (for $A$) + $ML$ (for $B$) [time]</td>
<td>$0$ [times]</td>
</tr>
<tr>
<td>Solve small eigenvalue problem</td>
<td>GEP: 1 [time] SEP: 1 [time]</td>
<td></td>
</tr>
<tr>
<td>Construct the orthonormal basis</td>
<td>$2nLMN + 2n(LM)^2$ [flops]</td>
<td>$2nLM^2 N + 2n(LM)^2$ [flops]</td>
</tr>
<tr>
<td>Set small eigenvalue problem</td>
<td>$4n(LM)^2$ [flops]</td>
<td>$0$ [flops]</td>
</tr>
<tr>
<td>Compute eigenvectors</td>
<td>$2nML \times m$ [flops]</td>
<td>$2nML \times m$ [flops]</td>
</tr>
</tbody>
</table>

Table 1 shows that the proposed algorithm is more efficient than the block CIRR method. Note that the proposed algorithm has approximately the same storage requirements as the block CIRR method.

As another advantage of the proposed algorithm, which is based on the block Arnoldi method, it is expected that some improvement techniques used for the (block) Arnoldi method can be applied to the proposed algorithm (Algorithm 3), such as some type of restart techniques, the (block) Lanczos method.
Figure 1: Relative residuals of eigenpairs: $\|Ax_i - \lambda_i Bx_i\|_2/ (\|Ax_i\|_2 + |\lambda_i|\|Bx_i\|_2)$ from computational results for the two test problems.

4 Numerical examples and results

To confirm that the proposed algorithm (Algorithm 3) can solve generalized eigenvalue problems (1) just as well as the block CIRR method, we provide two numerical examples. The algorithms were implemented in MATLAB R2013a, and the computation of the contour integral was approximated by the $N$-point trapezoidal rule. The input matrix $V$ was set as a random matrix generated by the MATLAB command “rand”, and each linear system was solved by the MATLAB command “\”.

The first test problem was taken from a model analysis of dissipative magnetohydrodynamics (MHD). The obtained matrices $A$ and $B$ were real nonsymmetric and $n = 416$. We set $\Gamma$ to be the circle with center $\gamma = -0.2 + 0.6i$ and radius $\rho = 0.05$, and consider finding five eigenvalues located within the circle. We also set $L = 1, M = 5$, and $N = 64$.

The second test problem was taken from an electronic structure calculation (ESC) for a system of silicon. The obtained matrices $A$ and $B$ were Hermitian, and $B$ was positive definite, where $n = 1726$. The eigenvalues are located on the real axis. To find sixteen eigenvalues in the interval $[-0.17, 0.17]$, we set $\Gamma$ to be the circle with center $\gamma = 0$ and radius $\rho = 0.17$. We also set $L = 4, M = 4$, and $N = 64$.

The relative residuals of eigenpairs for the first and second test problems are shown in Figures 1(a) and 1(b), respectively. Figure 1 shows that the proposed method (Algorithm 3) can compute eigenpairs with approximately the same accuracy as the block CIRR method (Algorithm 2).

5 Conclusions

In this paper, we have provided a novel interpretation of contour integral spectral projection methods for solving the generalized eigenvalue problem (1). We have also proposed a new algorithm based on the block Arnoldi method.

In future, we will propose and analyze efficient improvements in the proposed algorithm based on some techniques that are applied to the block Arnoldi method.
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References


