

CIRR: a Rayleigh-Ritz type method with contour integral for generalized eigenvalue problems

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Abstract. We consider a Rayleigh-Ritz type eigensolver for finding a limited set of eigenvalues and their corresponding eigenvectors in a certain region of generalized eigenvalue problems. When the matrices are very large, iterative methods are used to generate an invariant subspace that contains the desired eigenvectors. Approximations are extracted from the subspace through a Rayleigh-Ritz projection. In this paper, we present a Rayleigh-Ritz type method with a contour integral (CIRR method). In this method, numerical integration along a circle that contains relatively small number of eigenvalues is used to construct a subspace. Since the process to derive the subspace can be performed in parallel, the presented method is suitable for master-worker programming models. Numerical experiments illustrate the property of the proposed method.

Key words: generalized eigenvalue problems, Rayleigh-Ritz procedure, Contour integral, master-worker type algorithm.

1. Introduction

In this paper, we consider a method for computing a limited set of eigenvalues and their corresponding eigenvectors in a certain region of the generalized eigenvalue problem

$$A\mathbf{x} = \lambda B\mathbf{x},$$

where $A, B \in \mathbb{R}^{n \times n}$ are symmetric and B is positive definite.

The generalized eigenvalue problems arise in many scientific and engineering applications. In such applications, the matrices are often very large, and iterative methods are used to generate a subspace that contains the desired eigenvectors. Approximations are extracted from the subspace through a Rayleigh-Ritz projection. Various methods can be derived from this scheme. Techniques based on the Krylov subspaces are powerful tools

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to building desired subspaces for large-scale eigenvalue problems [1, 2, 8, 9]. The relations among Krylov subspace methods, moment-matching approach and Padé approximation are shown in [2].

In [11], a moment-based method that finds eigenvalues in a given domain is presented, which is based on a root-finding method for an analytic function described in [4, 5, 10]. In this method, a small matrix pencil that has only the desired eigenvalues is derived by solving systems of linear equations constructed from A and B . These systems can be solved independently, thus we solve them on remote servers using asynchronous remote procedure calls. This approach is suitable for master-worker programming models. A parallel implementation of the method using a GridRPC system is presented in [12, 13].

Our purpose is to improve numerical stability of the method [11]. The computation of eigenvalues using explicit moments is sometimes numerically unstable. We show that a Rayleigh-Ritz procedure can be used to avoid the explicit use of moments. In the next section, we briefly describe the results about a moment-based eigensolver in [11]. In Section 3, we present a Rayleigh-Ritz type method with a contour integral. In this method, we can avoid the explicit use of the moments, and obtain a subspace which contains an invariant subspace spanned by the desired eigenvectors. In Section 4, some numerical experiments illustrate the property of our method.

2. A moment-based eigensolver

In this section, we review a moment-based method for generalized eigenvalue problems presented in [11]. This method, which is based on a moment-based root finding method [4], finds eigenvalues that are located inside a given circle.

Let $A, B \in \mathbb{R}^{n \times n}$ be symmetric, and let B be positive definite. Let $(\lambda_j, \mathbf{x}_j)$, $1 \leq j \leq n$ be eigenpairs of the matrix pencil (A, B) . The pencil (A, B) is called regular if $\det(\lambda B - A)$ is not identically zero for $\lambda \in \mathbb{R}$.

Suppose that m distinct eigenvalues $\lambda_1, \dots, \lambda_m$ are located inside a positively oriented closed Jordan curve Γ in \mathbb{C} . For a nonzero vector $\mathbf{v} \in \mathbb{R}^n$, we define the moments

$$\mu_k := \frac{1}{2\pi i} \int_{\Gamma} (z-\gamma)^k (B\mathbf{v})^T (zB-A)^{-1} B\mathbf{v} dz, \quad k = 0, 1, \dots, \quad (1)$$

where γ is located inside Γ . Let the $m \times m$ Hankel matrices H_m and $H_m^<$

be

$$H_m := [\mu_{i+j-2}]_{i,j=1}^m = \begin{pmatrix} \mu_0 & \mu_1 & \cdots & \mu_{m-1} \\ \mu_1 & \mu_2 & \cdots & \mu_m \\ \vdots & \vdots & & \vdots \\ \mu_{m-1} & \mu_m & \cdots & \mu_{2m-2} \end{pmatrix}$$

and

$$H_m^< := [\mu_{i+j-1}]_{i,j=1}^m = \begin{pmatrix} \mu_1 & \mu_2 & \cdots & \mu_m \\ \mu_2 & \mu_3 & \cdots & \mu_{m+1} \\ \vdots & \vdots & & \vdots \\ \mu_m & \mu_{m+1} & \cdots & \mu_{2m-1} \end{pmatrix}.$$

Then we have the following theorem ([11]).

Theorem 1 *Let the matrix pencil (A, B) be regular. Then the eigenvalues of the pencil $(H_m^<, H_m)$ are given by $\lambda_1 - \gamma, \dots, \lambda_m - \gamma$.*

The corresponding eigenvectors $\mathbf{x}_1, \dots, \mathbf{x}_m$ are obtained using the contour integral

$$\mathbf{s}_k := \frac{1}{2\pi i} \int_{\Gamma} (z-\gamma)^k (zB-A)^{-1} B\mathbf{v} dz, \quad k = 0, 1, \dots, m-1. \quad (2)$$

Theorem 2 *Let \mathbf{u}_j ($1 \leq j \leq m$) be eigenvectors of the pencil $(H_m^<, H_m)$. Let $S = [\mathbf{s}_0, \dots, \mathbf{s}_{m-1}]$. Then the eigenvectors associated with $\lambda_1, \dots, \lambda_m$ are given by*

$$\mathbf{x}_j = S\mathbf{u}_j, \quad j = 1, 2, \dots, m.$$

Therefore, the original eigenvalue problem is reduced to the problem with the $m \times m$ Hankel matrices.

When Γ is a circle with the center γ and the radius ρ , we obtain the following approximations for μ_k by approximating the integral (1) via the N -point trapezoidal rule:

$$\mu_k \approx \hat{\mu}_k := \frac{1}{N} \sum_{j=0}^{N-1} (\omega_j - \gamma)^{k+1} (B\mathbf{v})^T (\omega_j B - A)^{-1} B\mathbf{v},$$

$$k = 0, 1, \dots,$$

where

$$\omega_j := \gamma + \rho e^{(2\pi i/N)(j+1/2)}, \quad j = 0, 1, \dots, N-1.$$

We also approximate \mathbf{s}_k by

$$\hat{\mathbf{s}}_k = \frac{1}{N} \sum_{j=0}^{N-1} (\omega_j - \gamma)^{k+1} (\omega_j B - A)^{-1} B \mathbf{v}, \quad k = 0, 1, \dots \quad (3)$$

In these computations, we need to solve the systems of linear equations

$$(\omega_j B - A) \mathbf{y}_j = B \mathbf{v}, \quad j = 0, 1, \dots, N-1. \quad (4)$$

When matrices A and B are large, the computational costs for solving the systems of linear equations (4) are dominant in the method. Since these linear systems are independent for each j , they can be solved in parallel. The implementation with GridRPC system is presented in [12, 13].

Defining the $m \times m$ Hankel matrices \hat{H}_m and $\hat{H}_m^<$ by

$$\hat{H}_m := [\hat{\mu}_{i+j-2}]_{i,j=1}^m \quad \text{and} \quad \hat{H}_m^< := [\hat{\mu}_{i+j-1}]_{i,j=1}^m,$$

we obtain the approximate eigenpairs by solving the eigenvalue problem with the matrix pencil $(\hat{H}_m^<, \hat{H}_m)$.

The influence of the quadrature error for the eigenvalues of the pencil $(\hat{H}_m^<, \hat{H}_m)$ are discussed in [5] and [10]. The accuracy of the results is sometimes improved by using the $M \times M$ Hankel matrices with $M (> m)$ instead of m .

For the moment-based method with the contour integral, we need the estimation of the circles that include appropriate number of eigenvalues. The method using the substructuring of the matrices can be used to estimate such circles ([14]).

If some of the eigenvalues in Γ are very close, the derived Hankel matrices become ill-conditioned and we can not separate these close eigenvalues. In the next section, we show a Rayleigh-Ritz type method with the contour integral. By this approach, we can avoid the explicit use of moments, and improves numerical accuracy for close eigenvalues.

3. A Rayleigh-Ritz type method with a contour integral

3.1. A Rayleigh-Ritz procedure

Many methods for finding eigenvalues and eigenvectors of a large-scale matrix pencil proceed by generating a sequence of subspace containing approximations to the desired eigenvectors. A Rayleigh-Ritz procedure is widely used to accomplish this end.

We apply a Rayleigh-Ritz procedure with an orthonormal basis $Q \in \mathbb{R}^{n \times m}$. The projected matrices are given by $\tilde{A} = Q^T A Q$ and $\tilde{B} = Q^T B Q$. The Ritz values of the projected pencil (\tilde{A}, \tilde{B}) are taken as approximate eigenvalues for the original pencil (A, B) with corresponding Ritz vectors. The algorithm is as follows.

Rayleigh-Ritz Procedure

1. Construct an orthonormal basis Q .
2. Form $\tilde{A} = Q^T A Q$ and $\tilde{B} = Q^T B Q$.
3. Compute the eigenpairs (θ_j, \mathbf{w}_j) ($1 \leq j \leq m$) of (\tilde{A}, \tilde{B}) .
4. Set $\mathbf{p}_j = Q \mathbf{w}_j$, $j = 1, \dots, m$.

The Galerkin approximation to the matrix pencil (A, B) on the subspace spanned by $[\mathbf{x}_1, \dots, \mathbf{x}_m]$ provides the exact eigenpairs $(\lambda_j, \mathbf{x}_j)$ ($1 \leq j \leq m$) by this procedure ([7, 9]).

3.2. The CIRR method

Now we present a method using the Rayleigh-Ritz procedure with an orthonormal basis Q which is derived by the integration.

Concerning the contour integral (2), we have the following lemma.

Lemma 1 *Let \mathbf{s}_k be defined by (2). Suppose that \mathbf{v} is expanded by the eigenvectors $\{\mathbf{x}_1, \dots, \mathbf{x}_n\}$ as*

$$\mathbf{v} = \sum_{j=1}^n \alpha_j \mathbf{x}_j. \quad (5)$$

Then

$$\mathbf{s}_k = \sum_{j=1}^m \alpha_j (\lambda_j - \gamma)^k \mathbf{x}_j, \quad k = 0, 1, \dots, m-1. \quad (6)$$

Proof. It follows from (2) and (5) that

$$\mathbf{s}_k = \frac{1}{2\pi i} \int_{\Gamma} \sum_{j=1}^n \alpha_j (z-\gamma)^k (zB-A)^{-1} B \mathbf{x}_j dz. \quad (7)$$

Since $(\lambda_j, \mathbf{x}_j)$ is an eigenpair of the matrix pencil (A, B) , we have

$$(zB - A)\mathbf{x}_j = (z - \lambda_j)B\mathbf{x}_j,$$

and thus

$$(zB - A)^{-1} B \mathbf{x}_j = (z - \lambda_j)^{-1} \mathbf{x}_j.$$

Therefore, from (7), we have

$$\mathbf{s}_k = \sum_{j=1}^n \frac{1}{2\pi i} \int_{\Gamma} \frac{\alpha_j (z-\gamma)^k}{z - \lambda_j} \mathbf{x}_j dz, \quad k = 0, 1, \dots, m-1. \quad (8)$$

By the residue theorem, we obtain the result of this lemma. \square

Define the $m \times m$ Vandermonde matrix with $\lambda_1 - \gamma, \dots, \lambda_m - \gamma$ by

$$V = \begin{pmatrix} 1 & (\lambda_1 - \gamma) & \cdots & (\lambda_1 - \gamma)^{m-1} \\ 1 & (\lambda_2 - \gamma) & \cdots & (\lambda_2 - \gamma)^{m-1} \\ \vdots & \vdots & \cdots & \vdots \\ 1 & (\lambda_m - \gamma) & \cdots & (\lambda_m - \gamma)^{m-1} \end{pmatrix}.$$

From the equation (6) we have

$$S = XDV, \quad (9)$$

where $S = [\mathbf{s}_0, \mathbf{s}_1, \dots, \mathbf{s}_{m-1}]$, $X = [\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_m]$, and $D = \text{diag}(\alpha_1, \dots, \alpha_m)$.

With the orthonormal basis $\{\mathbf{q}_1, \dots, \mathbf{q}_m\}$ of the subspace spanned by $\{\mathbf{s}_0, \dots, \mathbf{s}_{m-1}\}$, we have the following theorem.

Theorem 3 *If $\lambda_1, \dots, \lambda_m$ are distinct and $\alpha_j \neq 0$ for $1 \leq j \leq m$ then*

$$\text{span}\{\mathbf{q}_1, \dots, \mathbf{q}_m\} = \text{span}\{\mathbf{x}_1, \dots, \mathbf{x}_m\} \quad (10)$$

Proof. Since $\lambda_1, \dots, \lambda_m$ are mutually distinct and $\alpha_j \neq 0$ for $1 \leq j \leq m$, V and D are nonsingular. Therefore, it follows from (9) that

$$\text{span}\{\mathbf{s}_0, \dots, \mathbf{s}_{m-1}\} = \text{span}\{\mathbf{x}_1, \dots, \mathbf{x}_m\}.$$

Since the column vectors $\{\mathbf{q}_1, \dots, \mathbf{q}_m\}$ are orthonormal basis of $\text{span}\{\mathbf{s}_0, \dots, \mathbf{s}_{m-1}\}$, the equation (10) holds. \square

This theorem implies that the eigenpairs $(\lambda_j, \mathbf{x}_j)$ ($1 \leq j \leq m$) are extracted by using

$$Q = [\mathbf{q}_1, \dots, \mathbf{q}_m]$$

for the projection in the Rayleigh-Ritz procedure ([7, 9]).

To obtain the orthonormal basis Q , we need to evaluate the contour integral (2). We use the N -point trapezoidal rule defined in (3) to approximate the integration. In the explicit moment method, it is efficient to set the size of Hankel matrices larger than the exact number of eigenvalues in the circle to decrease the influence of the quadrature error suffered from eigenvalues located outside Γ . For the presented method in this section, it is also efficient to set the larger size of subspace. Thus we construct M ($\geq m$) orthonormal basis $\{\mathbf{q}_1, \dots, \mathbf{q}_M\}$ from $\{\mathbf{s}_0, \dots, \mathbf{s}_{M-1}\}$. When M is larger than the number of eigenvalues inside Γ , some Ritz values are located outside Γ , or their corresponding residuals are not small. In this case we shall remove them as a ghost. We show the algorithm in Table 1.

Algorithm: CIRR method

Input: $\mathbf{v} \in \mathbb{R}^n$, N , M , γ , ρ

Output: $\hat{\lambda}_1, \dots, \hat{\lambda}_m, \hat{\mathbf{x}}_1, \dots, \hat{\mathbf{x}}_m$

1. Set $\omega_j \leftarrow \gamma + \rho \exp(2\pi i(j + 1/2)/N)$, $j = 0, \dots, N - 1$
2. Solve $(\omega_j B - A)\mathbf{y}_j = B\mathbf{v}$ for \mathbf{y}_j , $j = 0, \dots, N - 1$
3. Compute $\hat{\mathbf{s}}_k$, $k = 0, \dots, M - 1$ by (3)
4. Construct an orthonormal basis Q from $\{\hat{\mathbf{s}}_0, \dots, \hat{\mathbf{s}}_{M-1}\}$.
5. Form $\tilde{A} = Q^T A Q$ and $\tilde{B} = Q^T B Q$.
6. Compute the eigenpairs (θ_j, \mathbf{w}_j) ($1 \leq j \leq M$) of (\tilde{A}, \tilde{B}) .
7. Set $\mathbf{p}_j = Q\mathbf{w}_j$, $j = 1, \dots, M$.
8. Select the approximate eigenpairs $(\hat{\lambda}_1, \hat{\mathbf{x}}_1), \dots, (\hat{\lambda}_m, \hat{\mathbf{x}}_m)$ from (θ_j, \mathbf{p}_j) ($1 \leq j \leq M$).

Table 1. Algorithm of the CIRR method

In the CIRR method, the invariant subspace associated with the eigenvalues in a given domain is obtained by a projection with the orthonormal matrix Q constructed from S . Therefore the projected pencil (\tilde{A}, \tilde{B}) preserves the numerical stability of the original pencil (A, B) . This implies

In Fig. 1, we show the relative error of the approximate eigenvalues obtained by the explicit moment method and the CIRR method with various size of subspaces M according to the number of nodes N . The parameter were $\gamma = 4.0$ and $\rho = 0.0001$. We found six eigenvalues in the circle, i.e., $m = 6$. From the figure, we can see that the relative errors of approximate eigenvalues were improved by using the Rayleigh-Ritz procedure when $M > m$.

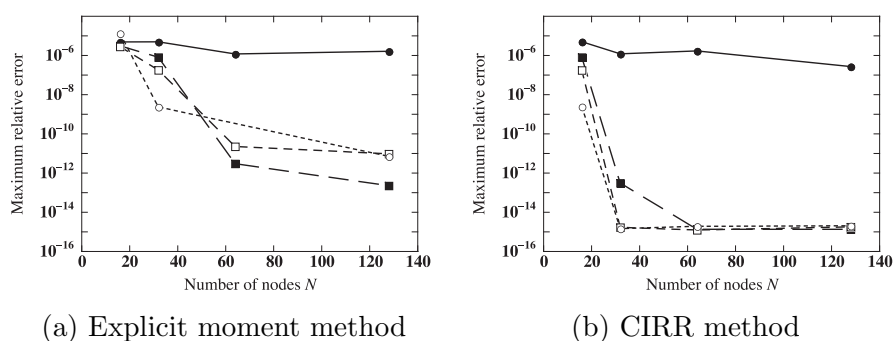


Fig. 1. Comparison of the relative errors in Example 1 with $\gamma = 4.0$ and $\rho = 0.0001$ (\bullet : $M = 6$, \blacksquare : $M = 9$, \square : $M = 12$, \circ : $M = 15$).

In Table 2, we show the maximum relative error

$$\max_{1 \leq j \leq m} \frac{|\hat{\lambda}_j - \lambda_j|}{|\lambda_j|}$$

with $\rho = 0.000125$. Seven eigenvalues were included in the circle. We also show the results with $\rho = 0.00015$ in Table 3. Nine eigenvalues were included in the circle.

Example 2 The test matrices were derived from computation of the molecular orbitals of lysozyme (129 amino-acid residues, 1,961 atoms) with 20,758 basis functions [3]. The structure of the lysozyme molecule has been determined experimentally, and we added counter-ions and water molecules around the lysozyme molecule in order to simulate in vivo conditions. The size of A and B was $n = 20,758$, and the number of nonzero elements was $\text{NZ} = 10,010,416$.

Since the matrix $\omega_j B - A$ with complex ω_j is complex symmetric, the COCG method [15] with incomplete Cholesky factorization with a complex

Table 2. Comparison of the relative errors in Example 1 with $\gamma = 4.0$ and $\rho = 0.000125$ ($m = 7$).

M	Explicit moment method	CIRR method
4	7.61×10^{-6}	7.59×10^{-6}
8	2.58×10^{-10}	7.40×10^{-16}
12	6.15×10^{-13}	8.88×10^{-16}
16	1.18×10^{-12}	8.88×10^{-16}
20	1.07×10^{-12}	7.40×10^{-16}
24	2.52×10^{-10}	1.18×10^{-15}

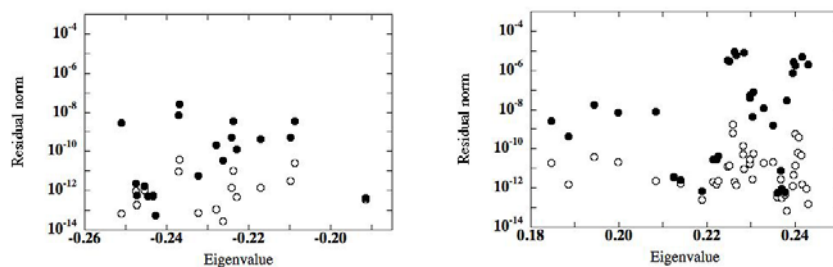
Table 3. Comparison of the relative errors in Example 1 with $\gamma = 4.0$ and $\rho = 0.00015$ ($m = 9$).

M	Explicit moment method	CIRR method
4	4.69×10^{-6}	3.55×10^{-6}
8	3.62×10^{-6}	6.16×10^{-6}
12	7.33×10^{-6}	4.52×10^{-8}
16	4.44×10^{-6}	8.07×10^{-14}
20	7.84×10^{-6}	1.78×10^{-15}
24	7.52×10^{-6}	1.62×10^{-15}

shift [6] was used. In this case, a complex shift was effective to decrease the number of iterations. The stopping criterion for the relative residual was 10^{-12} . Computation was performed in double-precision arithmetic.

The parameter of circles were estimated by the method in [14]. These circles include the energy levels of the highest occupied molecular orbitals (HOMO) and the lowest unoccupied molecular orbitals (LUMO), which are key factors in the amount of energy needed to add or remove electrons in a molecule. The parameters are chosen as $N = 32$ and $M = 24$, and $\mathbf{v} = (1, 1, \dots, 1)^T$.

In Fig. 2, we show the residuals $\|A\hat{\mathbf{x}}_j - \hat{\lambda}_j B\hat{\mathbf{x}}_j\|_2$ for each approximate eigenpairs. In the figure, the mark \bullet shows the residuals by the explicit moment method, and the mark \circ shows those of the CIRR method. We can see that the CIRR method gives smaller residuals. In case that we



(a) Residuals around HOMO (b) Residuals around LUMO

Fig. 2. Comparison of residuals $\|A\hat{x}_j - \hat{\lambda}_j B\hat{x}_j\|_2$ in Example 2 (\bullet : Explicit moment method, \circ : CIRR method)

choose larger N , the residuals were decreased. However, from a view point of computational costs, it is preferable to choose smaller N . It depends on a requirement of applications.

5. Conclusions

In this paper we present a Rayleigh-Ritz type method with numerical integration for generalized eigenvalue problems. In this method, a contour integral is used to construct a subspace for the Rayleigh-Ritz projection.

For the computation of the contour integral, we solve a certain number of systems of linear equations derived from matrices A and B . When A and B are large, the computational costs for solving systems of linear equations are dominant in the method. Since these linear systems can be solved independently, the process to derive the subspace is performed in parallel. Therefore the presented method is suitable for master-worker programming models.

Through the numerical experiments, we can see that the presented method gives good numerical results. More precise error analysis of the CIRR method is a part of our future work.

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