A projection method for generalized eigenvalue problems using numerical integration

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Abstract

In this paper, we propose a method for finding certain eigenvalues of a generalized eigenvalue problem that lie in a given domain of the complex plane. The proposed method projects the matrix pencil onto a subspace associated with the eigenvalues that are located in the domain via numerical integration.

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1. Introduction

The generalized eigenvalue problem

\[ Ax = \lambda B x, \]

where \( A \) and \( B \) are \( n \times n \) real or complex matrices, arises in many applications of scientific computations. Often \( A \) and \( B \) are large and sparse, and only a few of the eigenvalues are desired. Due to the size of the problem, several methods for such eigenvalue problems are building sequences of subspaces that contain the desired eigenvectors, for example, see [4,5,15,16,18,20,21]. A comprehensive report on computational methods for eigenvalue problems was given by Golub and van der Vorst [8].

In this paper, we propose a method for determining certain eigenvalues that lie in a given domain of the complex plane. The proposed method projects the matrix pencil \( A - \lambda B \) onto a subspace
associated with the eigenvalues that are located in the domain. The approach is based on the root finding method for an analytic function proposed by Kravanja et al. [13]. This method finds all of the zeros that lie in a circle using numerical integration. Methods for the determination of zeros of analytic functions that are based on the numerical evaluation of integrals are called quadrature methods [3,11,14].

In Section 2, we introduce a function that is derived via the resolvent of the matrix pencil. This function can be regarded as a rational function, and we apply a method that finds poles of a function using numerical integrations. In Section 3, we present an algorithm for the case in which the domain is given by a circle and the numerical integration is evaluated via the trapezoidal rule. We present an error analysis of the method using the results described in [12,19]. In Section 4, several numerical examples are used to illustrate the properties of the proposed method.

2. A projection method

Let $A,B \in \mathbb{C}^{n \times n}$, and let $\lambda_1,\ldots,\lambda_d$ be finite eigenvalues of the matrix pencil $A - \lambda B$. The pencil $A - \lambda B$ is called regular if $\det(A - \lambda B)$ is not identically zero for $\lambda \in \mathbb{C}$.

For nonzero vectors $u,v \in \mathbb{C}^n$, we define

$$f(z) := u^H(zB - A)^{-1}v.$$ 

The function $f(z)$ is analytic when $zB - A$ is nonsingular.

We use the following result about Weierstrass’s canonical form (see e.g., [6]).

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

$$P(zB - A)Q = \begin{pmatrix} zI_d - J_d & O \\ O & zJ_{n-d} - I_{n-d} \end{pmatrix},$$

where $J_d$ and $J_{n-d}$ are in Jordan canonical form, $J_{n-d}$ is nilpotent, and $I_d$ denotes the identity matrix of order $d$.

We assume that $J_d$ is the diagonal matrix $J_d := \text{diag}(\lambda_1,\ldots,\lambda_d)$. Let $p_1,\ldots,p_n \in \mathbb{C}^n$ be vectors such that $P^H = (p_1,\ldots,p_n)$, and let $q_1,\ldots,q_n \in \mathbb{C}^n$ be $Q=(q_1,\ldots,q_n)$. Let $v_j := u^Hq_j p_j^Hv$, $1 \leq j \leq d$.

**Theorem 2.** Let $K$ be the maximum size of Jordan blocks of $J_{n-d}$. If $A - \lambda B$ is regular and $A$ is diagonalizable then

$$f(z) = \sum_{j=1}^d \frac{v_j}{z - \lambda_j} + g(z),$$

where $g(z)$ is a polynomial of degree $K - 1$. 

Proof. Let $P$ be partitioned in the form
\[
P = \begin{pmatrix} P_1 \\ P_2 \end{pmatrix},
\]
where $P_1 \in \mathbb{C}^{d \times n}$ and $P_2 \in \mathbb{C}^{(n-d) \times n}$, and let $Q = (Q_1, Q_2)$, where $Q_1 \in \mathbb{C}^{n \times d}$ and $Q_2 \in \mathbb{C}^{n \times (n-d)}$. According to Theorem 1, we have
\[
f(z) = u^H(zB - A)^{-1}v = u^H\begin{pmatrix} zI_d - J_d & O \\ O & zJ_{n-d} - I_{n-d} \end{pmatrix}^{-1}Pv
\]
\[
= u^H Q_1(zI_d - J_d)^{-1}P_1 v - u^H Q_2(zJ_{n-d} - I_{n-d})^{-1} - P_2 v. \tag{3}
\]
Since
\[
(zI_d - J_d)^{-1} = \begin{pmatrix} (z - \lambda_1)^{-1} \\ (z - \lambda_2)^{-1} \\ \vdots \\ (z - \lambda_d)^{-1} \end{pmatrix},
\]
it follows that
\[
u^H Q_1(zI_d - J_d)^{-1}P_1 v = (u^H q_1, \ldots, u^H q_d)(zI_d - J_d)^{-1}
\begin{pmatrix} \begin{pmatrix} p_{11}^H \end{pmatrix} \\ \vdots \\ \begin{pmatrix} p_{1d}^H \end{pmatrix} \end{pmatrix} = \sum_{j=1}^{d} \frac{u^H q_j p_j^H v}{z - \lambda_j} = \sum_{j=1}^{d} \frac{v_j}{z - \lambda_j}.
\]
Let
\[
D = \begin{pmatrix} 0 & 1 \\ 0 & \ddots & \ddots \\ & \ddots & \ddots & 1 \\ 0 & & & 0 \end{pmatrix} \in \mathbb{R}^{k \times k}.
\]
Then
\[
(I - zD)^{-1} = I + zD + (zD)^2 + \cdots + (zD)^k.
\]
Therefore if the maximum size of Jordan blocks of $(I_{n-d} - zJ_{n-d})$ is $K$, then
\[
g(z) := -u^H Q_2(zJ_{n-d} - I_{n-d})^{-1}P_2 v
\]
is a polynomial of degree $K - 1$.  \qed
The resolvent form of a pencil has important roles in eigenvalue problems and matrix analysis (see e.g., [1,7,17]).

Let $\Gamma$ be a positively oriented closed Jordan curve in the complex plane. Let $\lambda_1, \ldots, \lambda_m$ be distinct eigenvalues that lie in the interior of $\Gamma$. We consider the problem to find all the poles of $f(z)$ inside $\Gamma$. Let

$$\mu_k := \frac{1}{2\pi i} \int_\Gamma (z - \gamma)^k f(z) \, dz, \quad k = 0, 1, \ldots, \quad (4)$$

where $\gamma$ is located inside $\Gamma$. Let the $m \times m$ Hankel matrices $H_m$ and $H_m^<$ be

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

and

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

We have the following theorem:

**Theorem 3.** If $v_j \neq 0$ for $1 \leq j \leq m$ then the eigenvalues of the pencil $H_m^< - \lambda H_m$ are given by $\lambda_1 - \gamma, \ldots, \lambda_m - \gamma$.

**Proof.** Let $V_m$ be the Vandermonde matrix

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

Let $D_m := \text{diag}(v_1, \ldots, v_m)$ and $A_m := \text{diag}(\lambda_1 - \gamma, \ldots, \lambda_m - \gamma)$. The residue theorem implies that

$$\mu_k = \sum_{j=1}^{m} v_j (\lambda_j - \gamma)^k, \quad k = 0, 1, \ldots, \quad (5)$$

Then, we can verify that

$$H_m = V_m D_m V_m^T$$

and

$$H_m^< = V_m D_m A_m V_m^T.$$
Therefore,
\[ H_m - \lambda H_m = V_mD_m A V_m^T - \lambda V_mD_m V_m^T = V_mD_m (A - \lambda I) V_m^T. \]
Since \( \lambda_1, \ldots, \lambda_m \) are distinct, \( V_m \) is nonsingular, and since \( D_m \) is also nonsingular, we have the result of the theorem. \( \square \)

Therefore, we can obtain the eigenvalues \( \lambda_1, \ldots, \lambda_m \) by solving the generalized eigenvalue problem \( H_m^L x = \lambda H_m x \). If we find an appropriate \( \Gamma \) that includes a small number of eigenvalues, then the size of the derived eigenproblem is small. Note that the elements of \( H_m \) and \( H_m^L \) are defined via the integration (4).

Now we consider a method to evaluate eigenvectors. Let
\[ s_k := \frac{1}{2\pi i} \int_{\Gamma} (z - \gamma)^k (zB - A)^{-1} v \, dz, \quad k = 0, 1, \ldots. \]
Then we have the following theorem.

**Theorem 4.** Let
\[ \sigma_j := p_j^H v, \quad j = 1, 2, \ldots, m. \]
Then
\[ [s_0, \ldots, s_{m-1}] = [\sigma_1 q_1, \ldots, \sigma_m q_m] V_m^T. \]  

**Proof.** Since \( \mu_k = u^H s_k \), it follows from Eqs. (5) and (6) that
\[ s_k = \sum_{j=1}^{m} q_j p_j^H v (\lambda_j - \gamma)^k = \sum_{j=1}^{m} \sigma_j q_j (\lambda_j - \gamma)^k, \]
for \( k = 0, 1, \ldots, m - 1 \). Thus we have the result of the theorem. \( \square \)

From Eq. (7), we can evaluate eigenvectors \( q_1, \ldots, q_m \) when the eigenvalues \( \lambda_1, \ldots, \lambda_m \) are given. Note that \( s_k, 0 \leq k \leq m - 1 \), can be obtained in a process to calculate \( f(z) \).

**3. The case in which \( \Gamma \) is given by a circle**

In this section, we consider the case in which \( \Gamma \) is given by a circle and the integration is evaluated via a trapezoidal rule on the circle. Let \( \gamma \) and \( \rho \) be the center and the radius, respectively, of the given circle. Let \( N \) be a positive integer, and let
\[ \omega_j := \gamma + \rho e^{(2\pi i/N)j}, \quad j = 0, 1, \ldots, N - 1. \]
By approximating the integral of Eq. (4) via the \( N \)-point trapezoidal rule, we obtain the following approximations for \( \mu_k \):
\[ \mu_k \approx \hat{\mu}_k := \frac{1}{N} \sum_{j=0}^{N-1} (\omega_j - \gamma)^{k+1} f(\omega_j), \quad k = 0, 1, \ldots \]
Let the $m \times m$ Hankel matrices $\hat{H}_m$ and $\hat{H}_m^\leq$ be $\hat{H}_m := [\hat{\mu}_{i+j-2}]_{i,j=1}^m$ and $\hat{H}_m^\leq := [\hat{\mu}_{i+j-1}]_{i,j=1}^m$. Let $\zeta_1, \ldots, \zeta_m$ be the eigenvalues of the pencil $\hat{H}_m^\leq - \hat{\lambda} \hat{H}_m$. We regard $\hat{\lambda}_j = \gamma + \zeta_j$, $1 \leq j \leq m$ as the approximations for $\lambda_1, \ldots, \lambda_m$.

Let
\[ y_j := (\omega_j B - A)^{-1}v, \quad j = 0, 1, \ldots, N - 1, \]
and let
\[ \hat{s}_k := \frac{1}{N} \sum_{j=0}^{N-1} (\omega_j - \gamma)^{k+1} y_j, \quad k = 0, 1, \ldots. \]
(9)

Note that
\[ f(\omega_j) = u^H (\omega_j B - A)^{-1}v = u^H y_j. \]

Let $\hat{V}_m$ be the Vandermonde matrix with respect to $\zeta_1, \ldots, \zeta_m$. Then the approximations for the eigenvectors are obtained by
\[ [\hat{q}_1, \ldots, \hat{q}_m] = [\hat{s}_0, \ldots, \hat{s}_{m-1}] \hat{V}_m^{-T}. \]
(10)

Since $\hat{V}_m$ is a Vandermonde matrix, the elements of $\hat{V}_m^{-T}$ can be obtained by evaluating the coefficients of the Lagrange polynomials
\[ \phi_j(z) := \prod_{l=1, l \neq j}^{m} \frac{z - \zeta_l}{\zeta_j - \zeta_l}, \]
for $j = 1, 2, \ldots, m$ [9].

Thus, we obtain the following algorithm.

**Algorithm.**

Input: $u, v \in \mathbb{C}^n$, $N$, $m$, $\gamma$, $\rho$
Output: $\hat{\lambda}_1, \ldots, \hat{\lambda}_m$, $\hat{q}_1, \ldots, \hat{q}_m$
1. Set $\omega_j := \gamma + \rho \exp(2\pi i j/N)$, $j = 0, \ldots, N - 1$
2. Form $y_j := (\omega_j B - A)^{-1}v$, $j = 0, \ldots, N - 1$
3. Set $f_j := u^H y_j$, $j = 0, \ldots, N - 1$
4. Compute $\hat{\mu}_k$, $k = 0, \ldots, 2m - 1$ by (8)
5. Compute the eigenvalues $\zeta_1, \ldots, \zeta_m$ of the pencil $\hat{H}_m^\leq - \hat{\lambda} \hat{H}_m$
6. Compute $\hat{q}_1, \ldots, \hat{q}_m$ by (10)
7. Set $\hat{\lambda}_j^\gamma + \zeta_j$, $j = 1, \ldots, m$

Let us now investigate the influence of the quadrature error of $\hat{\mu}_k$ in the algorithm. Error analyses for the eigenvalues of the pencil $\hat{H}_m^\leq - \hat{\lambda} \hat{H}_m$ are presented in [12] and [19]. Let $\eta$ be
\[ \eta := \min_{j>m} \frac{|\hat{\lambda}_j - \gamma|}{\rho}. \]

Then, we have the following error estimation for the computational results:
\[ |\hat{\lambda}_j - \lambda_j| = O(\eta^{2m-N}), \quad 1 \leq j \leq m, \]
if $N \geq 2m + K$. The term $K$ comes from the fact that the coefficients of $g(z)$ have an influence to $\hat{\mu}_{N-K-1}, \ldots, \hat{\mu}_{N-1}$. Note that $\eta$ does not depend on the eigenvalues that are located inside $\Gamma$. 
4. Numerical examples

We provide several numerical examples of the proposed method. The algorithm was implemented in Matlab Ver. 6.0 for a Linux operating system. Computation was done with double precision arithmetic. The vectors $u$ and $v$ were chosen randomly using the Matlab function ‘rand’. In Examples 5 and 6, the linear equations that appear in the calculation for $f(z)$ were solved via the Matlab command ‘\’. In Example 7, the linear equations were solved by the Bi-CGSTAB method [22]. The stopping criterion for the residual was $10^{-12}$.

Example 5. Let us illustrate the results in the previous sections using a simple example. Let

$$A = \begin{pmatrix}
99/100 & 1/100 & 0 & \cdots & 0 \\
0 & 98/100 & \ddots & \ddots & 0 \\
\vdots & \ddots & \ddots & \ddots & \vdots \\
0 & \cdots & 0 & 1/100 & 1/100 \\
0 & \cdots & 0 & 0 & 0
\end{pmatrix}, \quad B = \begin{pmatrix}
0 & \cdots & \cdots & \cdots & 0 \\
\cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots \\
0 & \cdots & \cdots & \cdots & 0 \\
0 & \cdots & \cdots & \cdots & I_{20}
\end{pmatrix} \in \mathbb{R}^{100 \times 100}, \quad (11)$$

where $I_{20}$ is the identity matrix of order 20. The eigenvalues of the pencil $A - \lambda B$ are $\lambda_j = (j - 1)/100$ for $j = 1, \ldots, 20$.

The eigenvalues in the circle with center $\gamma = 0.015$ and radius $\rho = 0.02$ are $\hat{\lambda} = 0.0, 0.01, 0.02$ and 0.03. The computational results obtained using the parameters $m = 4$ and $N = 64$ are given by

$$\hat{\lambda}_1 = 0.000000015646111, \quad \hat{\lambda}_2 = 0.0099953916913,$$
$$\hat{\lambda}_3 = 0.01999794844274, \quad \hat{\lambda}_4 = 0.03000075760470.$$

The maximum error of $\{\hat{\lambda}_j\}$ was $2.1 \times 10^{-6}$. In this case, $\eta = 1.25$, and $\eta^{2m-N} = \eta^{-56} \approx 3.7 \times 10^{-6}$. The computational results for $N = 128$ are given by

$$\hat{\lambda}_1 = 0.0000000000000100, \quad \hat{\lambda}_2 = 0.09999999999706,$$
$$\hat{\lambda}_3 = 0.019999999998694, \quad \hat{\lambda}_4 = 0.03000000000479.$$

The maximum error of $\{\hat{\lambda}_j\}$ was $1.3 \times 10^{-12}$, and $\eta^{2m-N} = \eta^{-120} \approx 2.3 \times 10^{-12}$.

Example 6. A problem that arises in the modal analysis of dissipative magnetohydrodynamics (MHD) [2]. Both $A$ and $B$ are nonsymmetric, and $n = 416$.

In Fig. 1, we show the results obtained using parameters $\gamma = -0.2 + 0.6i$, $\rho = 0.05$, $m = 5$ and $N = 64$. The $+$ symbol denotes $\{\lambda_j^*\}$ that are evaluated via the Matlab command ‘eig’. The circle formed by the dotted line shows $\Gamma$, and the $\circ$ symbol denotes $\{\hat{\lambda}_j\}$. The presented method found five eigenvalues inside the circle. The maximum error of $\{\hat{\lambda}_j\}$ was $8.5 \times 10^{-7}$.
In Fig. 2, we show the results obtained using parameters $\gamma = 0.0$, $\rho = 0.002$, $m = 3$, and $N = 64$. In this case, more than 90 eigenvalues are located in the small area that is covered with a circle of radius $10^{-4}$ around the origin. Our algorithm located one approximate eigenvalue at this cluster. Thus one cluster of eigenvalues and two other eigenvalues in the circle of radius 0.002 at the origin were found with the parameter $m = 3$.

**Example 7.** A problem that is derived from the finite element method for a molecular electronic state [10]. Both $A$ and $B$ are real symmetric, and $n = 9264$. The number of nonzero elements is 240968 in both $A$ and $B$.

We computed four eigenvalues in the interval $[-10, -8]$. The results obtained using $\gamma = -9$, $\rho = 1$, $N = 32$ and $m = 4$ are given in Table 1. In the table, $\hat{\lambda}_j$ was evaluated via the Matlab command ‘eigs’ with the starting value $\hat{\lambda}_j$.

The results obtained using $\gamma = -9$, $\rho = 0.1$, $N = 32$ and $m = 3$ are given in Table 2.

In these examples, the evaluation of $f(\omega_j)$, $j = 0, \ldots, N - 1$ at Steps 2 and 3 in the algorithm occupies a large percent of the computational costs. Since $f(\omega_j)$ can be evaluated independently at
Table 1
Example 4: \( \gamma = -9, \rho = 1, N = 32, m = 4 \)

| \( j \) | \( \hat{\lambda}_j \) | \( |\hat{\lambda}_j - \hat{\lambda}_j^*| \) |
|---|---|---|
| 1 | \(-9.01565065746990 - 0.0000000921016i\) | \(1.6 \times 10^{-6}\) |
| 2 | \(-8.98265731343177 - 0.0000003453753i\) | \(6.6 \times 10^{-6}\) |
| 3 | \(-8.91765400027911 - 0.000000088371i\) | \(2.0 \times 10^{-5}\) |
| 4 | \(-8.57926086161660 - 0.000000000034i\) | \(1.4 \times 10^{-11}\) |

Table 2
Example 4: \( \gamma = -9, \rho = 0.1, N = 32, m = 3 \)

| \( j \) | \( \hat{\lambda}_j \) | \( |\hat{\lambda}_j - \hat{\lambda}_j^*| \) |
|---|---|---|
| 1 | \(-9.01565230691512 - 0.0000000000001i\) | \(2.7 \times 10^{-13}\) |
| 2 | \(-8.98266396293680 - 0.0000000000003i\) | \(3.0 \times 10^{-13}\) |
| 3 | \(-8.91765596597219 - 0.0000000000000i\) | \(2.3 \times 10^{-13}\) |

each \( \omega_j \), the presented algorithm provides a good performance in parallel computation. When \( A \) and \( B \) are symmetric, \( \omega_jB - A \) is symmetric with complex elements. In this case an iterative method for a symmetric complex matrix [23] is efficient.

Our algorithm requires a region that includes several eigenvalues and the number of eigenvalues or clusters in the region. Some numerical properties of a quadrature method for the determination of the number of clusters in a given region were discussed in [13]. The estimation of suitable \( m \) is remaining for our future work.

References


