A projection method for generalized eigenvalue problems

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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. The projection produces a small pencil with Hankel matrices.

1 Introduction

The generalized eigenvalue problem

$$Ax = \lambda Bx,$$

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 [14, 15, 16, 18, 19]. A comprehensive report on computational methods for eigenvalue problems was given by Golub and van der Vorst [6].

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 proposed approach is based on the root finding method for an analytic function proposed by Kravanja, Sakurai and Van Barel [11]. This method finds all of the zeros that lie in a circle by 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 [5, 10, 13].

In Section 2, we introduce a function that is derived via the resolvent of the matrix pencil. We show a projection method using numerical integration of this function. 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, 17]. In Section 4, a number of 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., Gantmacher [7]).

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*

$$P(zB - A)Q = \begin{pmatrix} zI_d - J_d & O \\ O & zJ_{n-d} - I_{n-d} \end{pmatrix}, \tag{1}$$

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 $J_d := \mathrm{diag}(\lambda_1, \ldots, \lambda_d)$. Let $p_1, \ldots, p_n \in \mathbb{C}^n$ be vectors such that

$$P^T = (p_1, \ldots, p_n),$$

and let $q_1, \ldots, q_n \in \mathbb{C}^n$ be

$$Q = (q_1, \ldots, q_n).$$

Let

$$\nu_j := u^H q_j p_j^H v, \quad 1 \le j \le d.$$

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*

$$f(z) = \sum_{j=1}^{d} \frac{\nu_j}{z - \lambda_j} + g(z), \tag{2}$$

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

$$\begin{aligned} f(z) &= u^H(zB - A)^{-1}v \\ &= u^H Q \begin{pmatrix} zI_d - J_d & O \\ O & zJ_{n-d} - I_{n-d} \end{pmatrix}^{-1} Pv \\ &= u^H Q_1(zI_d - J_d)^{-1}P_1 v + u^H Q_2(I_{n-d} - zJ_{n-d})^{-1}P_2 v. \end{aligned} \tag{3}$$

Since

$$(zI_d - J_d)^{-1} = \begin{pmatrix} (z-\lambda_1)^{-1} & & & \\ & (z-\lambda_2)^{-1} & & \\ & & \ddots & \\ & & & (z-\lambda_d)^{-1} \end{pmatrix},$$

it follows that

$$\begin{aligned} & u^H Q_1(zI_d - J_d)^{-1}P_1 v \\ &\quad = (u^H q_1, \ldots, u^H q_d)(zI_d - J_d)^{-1} \begin{pmatrix} p_1 v \\ \vdots \\ p_d v \end{pmatrix} \\ &\quad = \sum_{j=1}^{d} \frac{u^H q_j p_j^H v}{z - \lambda_j} \\ &\quad = \sum_{j=1}^{d} \frac{\nu_j}{z - \lambda_j}. \end{aligned}$$

Let

$$D = \begin{pmatrix} 0 & 1 & & \\ & 0 & \ddots & \\ & & \ddots & 1 \\ & & & 0 \end{pmatrix} \in \mathbb{R}^{k\times k}.$$

Then

$$(I - zD)^{-1} = (I + zD + (zD)^2 + \cdots + (zD)^{k-1}).$$

Therefore if the maximum size of Jordan blocks of $(I_{n-d} - zJ_{n-d})$ is K, then

$$g(z) := u^H Q_2 (I_{n-d} - zJ_{n-d})^{-1} P_2 v$$

is a polynomial of degree $K-1$. □

The resolvent form of a pencil has important roles in eigenvalue problems and matrix analysis (see e.g., [2] and [8]).

Let Γ 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 Γ. We consider the problem to find all the poles of $f(z)$ inside Γ. Let

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

Let the $m \times m$ Hankel matrices H_m and $H_m^<$ be

$$H_m := [\mu_{i+j-2}]_{i,j=1}^m \quad \text{and} \quad H_m^< := [\mu_{i+j-1}]_{i,j=1}^m.$$

We have the following theorem:

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

Proof. Let V_m be the Vandermonde matrix

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

Let $D_m := \mathrm{diag}(\nu_1, \ldots, \nu_m)$ and $\Lambda_m := \mathrm{diag}(\lambda_1, \ldots, \lambda_m)$. The residue theorem implies that

$$\mu_k = \sum_{j=1}^m \nu_j \lambda_j^k, \quad k = 0, 1, \ldots. \tag{5}$$

Then, we can verify that

$$H_m = V_m D_m V_m^T$$

and

$$H_m^< = V_m D_m \Lambda_m V_m^T.$$

Therefore,

$$\begin{aligned} H_m^< - \lambda H_m &= V_m D_m \Lambda V_m^T - \lambda V_m D_m V_m^T \\ &= V_m D_m (\Lambda - \lambda I) V_m^T. \end{aligned}$$

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. □

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

3 The case in which Γ is given by a circle

In this section, we consider the case in which Γ is given by a circle and the integration is evaluated via a trapezoidal rule on the circle. Let γ and ρ be the center and the radius, respectively, of the given circle. Let N be a positive integer, and let

$$\omega_j := e^{\frac{2\pi \mathrm{i}}{N} j}, \quad j = 0, 1, \ldots, N-1.$$

If Γ is the unit circle, we obtain the following approximations for μ_k

$$\mu_k \approx \hat{\mu}_k := \frac{1}{N} \sum_{j=0}^{N-1} \omega_j^{k+1} f(\omega_j), \quad k = 0, 1, \ldots, \tag{6}$$

by approximating the integral of equation (4) via the N-point trapezoidal rule. Note that

$$f(\omega_j) = v^H (\omega_j B - A)^{-1} u,$$

and the equation (6) can be evaluated via the first Fourier transform.

When Γ is not the unit circle, we apply the shift and the scaling for $f(z)$, i.e., we use $f(\gamma + \rho\omega_j)$ instead of $f(\omega_j)$.

Let the $m \times m$ Hankel matrices $\hat{H}_m$ and $\hat{H}_m^<$ be

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

Let $\zeta_1, \ldots, \zeta_m$ be the eigenvalues of the pencil $\hat{H}_m^< - \lambda \hat{H}_m$. Then we regard $\hat{\lambda}_j = \gamma + \rho\zeta_j$, $1 \le j \le m$ as the approximations for $\lambda_1, \ldots, \lambda_m$.

Thus, we obtain the following:

Algorithm:

Input: $u, v \in \mathbb{C}^n$, N, m, γ, ρ

Output: $\hat{\lambda}_1, \ldots, \hat{\lambda}_m$

1. Set $\omega_j \leftarrow \exp(2\pi \mathrm{i} j/N), j = 0, \ldots, N-1$
2. Form $y_j = ((\gamma + \rho\omega_j)B - A)^{-1} u, j = 0, \ldots, N-1$
3. Set $f_j \leftarrow v^H y_j, j = 0, \ldots, N-1$
4. Compute $\hat{\mu}_k, k = 0, \ldots, 2m-1$

5. Compute the eigenvalues $\zeta_1, \ldots, \zeta_m$ of the pencil $\hat{H}_m^< - \lambda \hat{H}_m$.
6. Set $\hat{\lambda}_j \leftarrow \gamma + \rho\zeta_j$, $j = 1, \ldots, m$.

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 $H_m^< - \lambda H_m$ are presented in [12] and [17]. Let η be

$$\eta := \min_{j>m} \frac{|\lambda_j - \gamma|}{\rho}.$$

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 $N \geq 2m$.

4 Numerical examples

We provide various 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 Example 1, 2 and 3, the linear equations that appear in the calculation for $f(z)$ were solved via the Matlab command '\'. In Example 4, the linear equations were solved by the preconditioned Bi-CGSTAB method [20] in conjugation with the incomplete LU factorization. The stopping criterion for the residual was 10^{-12}.

Example 1 Let us illustrate the results in the previous sections using a simple example [18]. Let

$$A = \begin{pmatrix} \frac{99}{100} & \frac{1}{100} & 0 & \cdots & 0 \\ 0 & \frac{98}{100} & \ddots & & 0 \\ \vdots & \ddots & \ddots & & \vdots \\ 0 & \cdots & 0 & \frac{1}{100} & \frac{1}{100} \\ 0 & \cdots & 0 & 0 & \frac{0}{100} \end{pmatrix}, \tag{7}$$

and let $B = I$. The eigenvalues of the pencil $A - \lambda B$ are $\lambda_j = (j-1)/100$ for $j = 1, \ldots, 100$.

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

$$\begin{aligned} \hat{\lambda}_1 &= -0.0000000220414688, \\ \hat{\lambda}_2 &= 0.0099996628360414, \\ \hat{\lambda}_3 &= 0.0199994536835002, \\ \hat{\lambda}_4 &= 0.0299998807651666. \end{aligned}$$

The maximum error of $\{\hat{\lambda}_j\}$ was 5.5×10^{-7}. 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

$$\begin{aligned}
\hat{\lambda}_1 &= -0.000000000000082, \\
\hat{\lambda}_2 &= 0.009999999999377, \\
\hat{\lambda}_3 &= 0.019999999999253, \\
\hat{\lambda}_4 &= 0.029999999999877.
\end{aligned}$$

The maximum error of $\{\hat{\lambda}_j\}$ was 7.5×10^{-13}, and $\eta^{2m-N} = \eta^{-120} \approx 2.3 \times 10^{-12}$.

Example 2 A is given by (7). B is an $n \times n$ matrix

$$B = \begin{pmatrix} 0 & 0 \\ 0 & I_4 \end{pmatrix}$$

where I_4 is an identity matrix of size four. n this case, B is nonsingular, and the the pencil has only four eigenvalues at $0, 0.01, 0.02$ and 0.03. All of the eigenvalues are located inside the circle.

The computational results obtained using $N = 16$ and $m = 4$ are given by

$$\begin{aligned}
\hat{\lambda}_1 &= 0.0000000000000000, \\
\hat{\lambda}_2 &= 0.0099999999999999, \\
\hat{\lambda}_3 &= 0.0200000000000001, \\
\hat{\lambda}_4 &= 0.0300000000000000.
\end{aligned}$$

The maximum error of $\{\hat{\lambda}_j\}$ was 3.2×10^{-16}.

Example 3 A problem that arises in the modal analysis of dissipative magnetohydrodynamics (MHD) [3]. Both A and B are nonsymmetric, and $n = 416$.

In Figure 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 Γ, 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 8.5×10^{-7}.

Example 4 A problem that is derived from the finite element method for a molecular electronic state [9]. 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, λ_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.

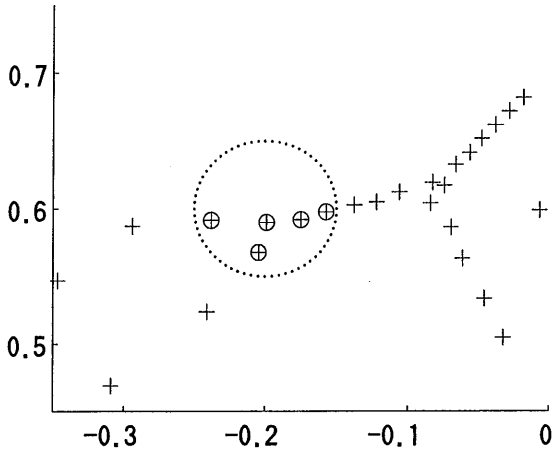

Figure 1: Approximate eigenvalues for Example 3

Table 1: Example 4: $\gamma = -9$, $\rho = 1$, $N = 32$, $m = 4$

j	$\hat{\lambda}_j$	$\lvert\hat{\lambda}_j - \lambda_j^*\rvert$
1	$-9.01565065746990 - 0.00000000921016i$	1.6×10^{-6}
2	$-8.98265731343177 - 0.00000003453753i$	6.6×10^{-6}
3	$-8.91765400027911 - 0.00000000888371i$	2.0×10^{-6}
4	$-8.57926086161660 - 0.00000000000034i$	1.4×10^{-11}

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

j	$\hat{\lambda}_j$	$\lvert\hat{\lambda}_j - \lambda_j^*\rvert$
1	$-9.01565230691512 - 0.00000000000001i$	2.7×10^{-13}
2	$-8.98266396293680 - 0.00000000000003i$	3.0×10^{-13}
3	$-8.91765596597219 - 0.00000000000000i$	2.3×10^{-13}

References

[1] W. E. Arnoldi, The principle of minimized iteration in the solution of the matrix eigenproblem, Quarterly of Appl. Math. 9 (1951) 17–29.

[2] F. Chatelin, Eigenvalues of Matrices, John Wiley & Sons, Chichester, 1993.

[3] J. Cullum, W. Kerner and R. Willoughby, A generalized nonsymmetric Lanczos procedure, Computer Phys. Communications 59 (1989) 19–48.

[4] E. R. Davidson, The iterative calculation of a few of the lowest eigenvalues and corresponding eigenvectors of large real symmetric matrices, J. Comput. Phys. 17 (1975) 87–94.

[5] L. M. Delves and J. N. Lyness, A numerical method for locating the zeros of an analytic functions, Math. Comput. 21 (1967) 543–560.

[6] G. H. Golub and H. A. van der Vorst, Eigenvalue computation in the 20th century, J. Comput. Appl. Math. 123 (2000) 35–65.

[7] F. R. Gantmacher, The theory of Matrices, Chelsea, New York, 1959.

[8] I. Gohberg, P. Lancaster and I. Rodman, Matrix Polynomials, Academic Press, New York, 1982.

[9] S. Hyodo, Meso-scale fusion: A method for molecular electronic state calculation in inhomogeneous materials, Proc. the 21st Century, Mikkabi, 2001, in T. Mitsui (Ed.), Special issue of J. Comput. Appl. Math. (to be published).

[10] N. I. Ioakimidis, Quadrature methods for the determination of zeros of transcendental functions–a review, in P. Keast and G. Fairweather (Eds.), Numerical Integration: Recent Developments, Software and Applications, Reidel, Dordrecht, 1987, 61–82.

[11] P. Kravanja, T. Sakurai and M. Van Barel, On locating clusters of zeros of analytic functions, BIT 39 (1999) 646–682.

[12] P. Kravanja, T. Sakurai, H. Sugiura and M. Van Barel, An error analysis of two related quadrature methods for computing zeros of analytic functions, Part II, Tech. Report Leuven TW-338 (2002).

[13] P. Kravanja and M. Van Barel, Computing the Zeros of Analytic Functions, Lecture Notes in Mathematics 1727, Springer, Berlin, 2000.

[14] C. C. Paige, Computational variants of the Lanczos method for the eigenproblems, J. Inst. Math. Appl. 10 (1972), 373–381.

[15] B. N. Parlett, The Symmetric Eigenvalue Problem, Prentice-Hall, Englewood Cliffs, NJ, 1980.

[16] A. Ruhe, Rational Krylov sequence methods for eigenvalue computation, Linear Algebra Appl. 58 (1984) 391–405.

[17] T. Sakurai, P. Kravanja, H. Sugiura and M. Van Barel, An error analysis of two related quadrature methods for computing zeros of analytic functions, J. Comput. Appl. Math. (to appear).

[18] G. De Samblanx and A. Bultheel, Using implicitly filtered RKS for generalized eigenvalue problems, J. Comput. Appl. Math. 107 (1999) 195–218.

[19] G. L. G. Sleipen and H. A. Van Der Vorst, A Jacobi-Davidson iteration method for linear eigenvalue problem, SIAM J. Matrix Anal. Appl. 17 (1996) 401–425.

[20] H. A. van der Vorst, Bi-CGSTAB: A fast and smoothly converging variant of Bi-CG for the solution of nonsymmetric linear systems, SIAM J. Sci. Statist. Comput. 13 (1992) 631–644.