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Nonlinear eigenvalue problems and contour integrals

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In this paper Beyn's algorithm for solving nonlinear eigenvalue problems is given a new interpretation and a variant is designed in which the required information is extracted via the canonical polyadic decomposition of a Hankel tensor. A numerical example shows that the choice of the filter function is very important, particularly with respect to where it is positioned in the complex plane.

1. Introduction

In this paper, we consider the following *nonlinear eigenvalue problem*. Given an integer $m \geq 1$, a domain $\Omega \subset \mathbb{C}$ and a matrix-valued function $T : \Omega \to \mathbb{C}^{m\times m}$ analytic in Ω, we want to determine the values $\lambda \in \Omega$ (eigenvalues) and $v \in \mathbb{C}^m$, $v \neq 0$ (eigenvectors) such that

$$T(\lambda)v = 0.$$

More specifically, given a closed contour $\Gamma \subset \Omega$ that has its interior in Ω, we consider the problem of approximating *all* eigenvalues (and corresponding eigenvectors) *inside* Γ. We observe that if the problem size m is equal to 1, then the problem reduces to that of computing all the zeros λ of the analytic scalar function T inside the closed contour Γ.

The approach discussed in this paper is based on (numerical approximations of) contour integrals of the resolvent operator $T(z)^{-1}$ applied to a rectangular matrix $\hat{V}$:

$$\frac{1}{2\pi i}\int_{\Gamma} f(z)T(z)^{-1}\hat{V}dz \quad \in \mathbb{C}^{m\times q}$$

where $f : \Omega \to \mathbb{C}$ is analytic in Ω and $\hat{V} \in \mathbb{C}^{m\times q}$ is a matrix chosen randomly or in another specified way, with $q \leq m$.

Using contour integrals to solve linear and nonlinear eigenvalue problems is a relatively recent development compared to the history of applying such methods to look for the zeros of a scalar analytic function, a problem that we investigated in [1]. Our approach was based on the pioneering work of Delves and Lyness [2] (see also [3] for a recent overview of numerical algorithms based on analytic function values at roots of unity). We reduced the problem to a generalized eigenvalue problem

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involving a Hankel matrix as well as a shifted Hankel matrix consisting of the moments of the analytic function T. For generalized linear eigenvalue problems corresponding to the pencil $A - zB$ Tetsuya Sakurai and his co-authors [4–7] (see also [8] for the specific case where $A, B \in \mathbb{R}^{m\times m}$ are symmetric and B is positive definite) use

$$\frac{1}{2\pi i}\int_{\Gamma}(z-\gamma)^p\hat{u}^H(zB-A)^{-1}\hat{v}\,dz, \quad p = 0, 1, 2, \ldots$$

where $\gamma \in \mathbb{C}$ belongs to the interior of Γ and the vectors $\hat{u}, \hat{v} \in \mathbb{C}^m$ have been chosen at random. Note that these contour integrals are scalar moments based on the resolvent $(zB - A)^{-1}$. Given an upper estimate q for the number of eigenvalues of $A - zB$ located inside Γ, these contour integrals are approximated via a quadrature formula (e.g., the trapezoidal rule if Γ is the unit circle) for $p = 0, 1, \ldots, 2q - 1$. The generalized eigenvalue problem (of size $q \times q$) involving the Hankel matrix and the shifted Hankel matrix based on the moments leads to approximations of the eigenvalues of $A - zB$ located inside Γ.

To approximate the eigenvectors, specific linear combinations are taken from the columns of the rectangular matrix given by

$$\frac{1}{2\pi i}\int_{\Gamma}(z-\gamma)^p(zB-A)^{-1}\hat{v}\,dz \quad \in \mathbb{C}^m$$

for $p = 0, 1, \ldots, q - 1$.

Eric Polizzi [9] studied the pencil $A - zB$ where $A, B \in \mathbb{C}^{m\times m}$ are Hermitian and B is positive definite. To compute all the eigenvalues located inside a compact interval on the real axis (enclosed by the contour Γ), he considered

$$S = \frac{1}{2\pi i}\int_{\Gamma}(zB-A)^{-1}B\hat{V}dz$$

for a rectangular matrix $\hat{V} \in \mathbb{C}^{m\times q}$ chosen at random, given an upper estimate q for the number of eigenvalues.

Polizzi's FEAST algorithm can be summarized as follows (see also Krämer et al. [10]; Tang and Polizzi [11]; Laux [12]; Güttel et al. [13]):

1. Choose $\hat{V} \in \mathbb{C}^{m\times q}$ of rank q.
2. Compute S by contour integration.
3. Orthogonalize S resulting in the matrix Q having orthonormal columns.
4. Form the Rayleigh quotients
$$A_Q = Q^HAQ \quad \text{and} \quad B_Q = Q^HBQ.$$
5. Solve the size-q generalized eigenvalue problem
$$A_Q\tilde{Y} = B_Q\tilde{Y}\tilde{\Lambda}.$$
6. Compute the approximate Ritz pairs $(\tilde{\Lambda}\ ,\ \tilde{X} = Q\tilde{Y})$.
7. If convergence is not reached, then go to Step 1, with $\hat{V} = \tilde{X}$.

To compute all the eigenvalues inside the contour Γ for a nonlinear analytic function T, Tetsuya Sakurai and his co-authors [14,15] (see also [16] for the specific case of polynomial eigenvalue problems) use the scalars

$$\frac{1}{2\pi i}\int_{\Gamma}z^p\hat{u}^HT(z)^{-1}\hat{v}\,dz, \quad p = 0, 1, 2, \ldots$$

where the vectors $\hat{u}, \hat{v} \in \mathbb{C}^m$ have been chosen at random. To approximate the eigenvectors, they consider the vectors

$$\frac{1}{2\pi i}\int_{\Gamma}z^pT(z)^{-1}\hat{v}\,dz, \quad p = 0, 1, 2, \ldots.$$

The eigenvectors are specific linear combinations of these vectors.

In this paper, we present a new interpretation of Beyn's algorithm [17]. Contrary to Beyn, who is not interested in the eigenvalues located outside the contour Γ, we will indicate that these eigenvalues, as well as the behaviour of the analytic function T outside but near Γ, play an important role to assess the accuracy of the computed eigenvalues. To simplify the technical details, we consider only simple eigenvalues. It is straightforward, however, to extend our approach to multiple eigenvalues by using the results that Beyn has described for this case.

Our paper is organized as follows. In Section 2, we start by summarizing Beyn's algorithm, which is based on Keldysh' theorem. For the sake of simplicity, we consider only simple eigenvalues. Section 3 describes the effect of approximating the contour integrals by numerical integration and introduces the corresponding filter function, which we use to reinterpret Beyn's algorithm in Section 4. In Section 5, we propose a variant of the most important substep of Beyn's algorithm: the extraction of the eigenvalue and eigenvector information from the computed moments. Our variant is based on the canonical polyadic decomposition of a Hankel tensor composed from the moments. Section 6 provides three strategies for solving a specific nonlinear eigenvalue problem. Finally, the conclusions are given in Section 7.