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Designing rational filter functions for solving eigenvalue problems by contour integration



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ABSTRACT

Solving (nonlinear) eigenvalue problems by contour integration, requires an effective discretization for the corresponding contour integrals. In this paper it is shown that good rational filter functions can be computed using (nonlinear least squares) optimization techniques as opposed to designing those functions based on a thorough understanding of complex analysis. The conditions that such an effective filter function should satisfy, are derived and translated in a nonlinear least squares optimization problem solved by optimization algorithms from Tensorlab. Numerical experiments illustrate the validity of this approach.

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1. Introduction

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

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

Note that this formulation reduces to the linear eigenvalue problem in case $T(z) = A - zB$, and to the polynomial eigenvalue problem when $T(z)$ is a polynomial matrix. 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 in the domain Ω .

The number of eigenvalues could be large, e.g., when m is large, or in case of a polynomial eigenvalue problem when the degree of the polynomial matrix is large. In several applications, one is not interested in *all* eigenvalues but only in those lying in a certain region(s) of the complex plane. Therefore, we can reduce the original problem of finding *all* eigenvalues into one where we are only interested in those eigenvalues (and corresponding eigenvectors) lying within (or in the neighborhood) of a given closed contour $\Gamma \subset \Omega$. The relevant information to approximate these eigenvalues (and corresponding eigenvectors) can be extracted from the function $T(z)$ by using (approximate) contour integrals to the resolvent operator $T(z)^{-1}$ applied to a rectangular matrix \hat{V} :

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

for different choices of the function $f(z)$, e.g., $f(z) = z^0, z^1, z^2, \dots$. Here, $f : \Omega \rightarrow \mathbb{C}$ is analytic in Ω and $\hat{V} \in \mathbb{C}^{m \times q}$ is a matrix chosen randomly or in another specified way, with $q \leq m$.

For a detailed overview of the history and current research on solving eigenvalue problems by contour integration, we refer the interested reader to the introduction section of [25]. Here, only some key references are mentioned without having the intention of being complete. Based on the pioneering work of Delves and Lyness [6], the author of this paper together with Peter Kravanja developed several methods to compute the zeros of a scalar analytic function $t(z)$ (for a synthesis of these results, see [14]) reducing the problem to a generalized eigenvalue problem involving a Hankel matrix as well as a shifted Hankel matrix consisting of the moments of the analytic function $t(z)$. Later on Tetsuya Sakurai joined us in our study and co-authored some papers [13,19,12]. To solve eigenvalue problems, Sakurai and his co-authors applied the idea of the generalized eigenvalue problem involving the Hankel and shifted Hankel matrix using moments based on the resolvent function [20,10,15,9,21,27,1,2]. Eric Polizzi and co-authors also used contour integrals based on the resolvent function resulting in the FEAST algorithm [18, 24,7].

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