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A Multilevel Spectral Indicator Method for Eigenvalues of Large Non-Hermitian Matrices

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Abstract. Recently a novel family of eigensolvers, called spectral indicator methods (SIMs), was proposed. Given a region on the complex plane, SIMs first compute an indicator by the spectral projection. The indicator is used to test if the region contains eigenvalue(s). Then the region containing eigenvalues(s) is subdivided and tested. The procedure is repeated until the eigenvalues are identified within a specified precision. In this paper, using Cayley transformation and Krylov subspaces, a memory efficient multilevel eigensolver is proposed. The method uses less memory compared with the early versions of SIMs and is particularly suitable to compute many eigenvalues of large sparse (non-Hermitian) matrices. Several examples are presented for demonstration.

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Key words: Eigenvalue problems, spectral indicator method, non-Hermitian matrix.

1 Introduction

Consider the generalized eigenvalue problem

$$Ax = \lambda Bx, \tag{1.1}$$

where A,B are $n\times n$ large sparse non-Hermitian matrices. In particular, we are interested in the computation of all eigenvalues in a region $R\subset\mathbb{C}$, which contains p eigenvalues such that $1\ll p\ll n$ or $1\ll p\sim n$.

Many efficient eigensolvers are proposed in literature for large sparse Hermitian (or symmetric) matrices (see, e.g., [11]). In contrast, for non-Hermitian matrices, there exist

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much fewer methods including the Arnoldi method and Jacobi-Davidson method [2, 9]. Unfortunately, these methods are still far from satisfactory as pointed out in [12]:

"*In essence what differentiates the Hermitian from the non-Hermitian eigenvalue problem is that in the first case we can always manage to compute an approximation whereas there are non-symmetric problems that can be arbitrarily difficult to solve and can essentially make any algorithm fail.*"

Recently, a family of eigensolvers, called the spectral indicator methods (SIMs), was proposed [6, 7, 14]. The idea of SIMs is different from the classical eigensolvers. In brief, given a region $R \subset \mathbb{C}$ whose boundary ∂R is a simple closed curve, an indicator I_R is defined and then used to decide if R contains eigenvalue(s). When the answer is positive, R is divided into sub-regions and indicators for these sub-regions are computed. The procedure continues until the size of the sub-region(s) is smaller than the specified precision, e.g., 10^{-6}. The indicator I_R is defined using the spectral projection P, i.e., Cauchy contour integral of the resolvent of the matrix pencil (A,B) on ∂R [8]. In particular, one can construct I_R based on the spectral projection of a random vector $\boldsymbol{f}$. It is well-known that P projects $\boldsymbol{f}$ to the generalized eigenspace associated to the eigenvalues enclosed by ∂R [8]. $P\boldsymbol{f}$ is zero if there is no eigenvalue(s) inside R, and nonzero otherwise. Hence $P\boldsymbol{f}$ can be used to decide if R contains eigenvalues(s) or not. Evaluation of $P\boldsymbol{f}$ needs to solve linear systems at quadrature points on ∂R. In general, it is believed that computing eigenvalues is more difficult than solving linear systems of equations [5]. The proposed method converts the eigenvalue problem to solving a number of related linear systems.

Spectral projection is a classical tool in functional analysis to study, e.g., the spectrum of operators [8] and the finite element convergence theory for eigenvalue problems of partial differential equations [14]. It has been used to compute matrix eigenvalue problems in the method by Sakurai-Sugiura [13] and FEAST by Polizzi [10]. For example, FEAST uses spectral projection to build subspaces and thus can be viewed as a subspace method [15]. In contrast, SIMs use the spectral projection to define indicators and combines the idea of bisection to locate eigenvalues. Note that the use of other tools such as the condition number to define the indicator is possible.

In this paper, we propose a new SIM, called SIM-M. Firstly, by proposing a new indicator, the memory requirement is significantly reduced and thus the computation of many eigenvalues of large matrices becomes realistic. Secondly, a new strategy to speedup the computation of the indicators is presented. Thirdly, other than the recursive calls in the first two members of SIMs [6, 7], a multilevel technique is used to further improve the efficiency. Moreover, a subroutine is added to find the multiplicities of the eigenvalues. The rest of the paper is organized as follows. Section 2 presents the basic idea of SIMs and two early members of SIMs. In Section 3, we propose a new eigensolver SIM-M with the above features. The algorithm and the implementation details are discussed as well. The proposed method is tested by various matrices in Section 4. Finally, in Section 5, we draw some conclusions and discuss some future work.