

A New Subspace Iteration Algorithm for Solving Generalized Eigenvalue Problems

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Abstract

It is needed to solve generalized eigenvalue problems (GEP) in many applications, such as the numerical simulation of vibration analysis, quantum mechanics, electronic structure, etc. The subspace iteration is a kind of widely used algorithm to solve eigenvalue problems. To solve the generalized eigenvalue problem, one kind of subspace iteration method, Chebyshev-Davidson algorithm, is proposed recently. In Chebyshev-Davidson algorithm, the Chebyshev polynomial filter technique is incorporated in the subspace iteration [15]. In this paper, based on Chebyshev-Davidson algorithm, a new subspace iteration algorithm is constructed. In the new algorithm, the Chebyshev filter and inexact Rayleigh quotient iteration techniques are combined together to enlarge the subspace in the iteration. Numerical results of a vibration analysis problem show that the number of iteration and computing time of the proposed algorithm is much less than that of the Chebyshev-Davidson algorithm and some typical GEP solution algorithms. Furthermore, the new algorithm is more stable and reliable than the Chebyshev-Davidson algorithm in the numerical results.

Keywords: Generalized eigenvalue problem, Davidson algorithm, Chebyshev filter, Rayleigh quotient iteration, Acceleration

Mathematics Subject Classification (2010): 65F15, 65N25, 65H17

1 Introduction

Consider the following symmetric generalized eigenvalue problem (GEP)

$$\mathbf{A}\mathbf{x} = \lambda\mathbf{B}\mathbf{x}, \quad \text{with} \quad \|\mathbf{x}\|_{\mathbf{B}} = 1, \quad (1)$$

where $\mathbf{A} \in \mathbb{R}^{N \times N}$ and $\mathbf{B} \in \mathbb{R}^{N \times N}$ are large, sparse and symmetric matrices with $\mathbf{B}$ being positive definite, $\|\mathbf{x}\|_{\mathbf{B}}$ is the $\mathbf{B}$ -norm of the vector $\mathbf{x}$ which will be defined later. In many applications, it is needed to solve GEP (1), such as the vibration analysis, quantum mechanics, electronic structure calculations, etc. In (1), the matrix $\mathbf{A}$ is the stiffness matrix, and $\mathbf{B}$ represents the mass matrix. λ is an eigenvalue of the matrix pencil $(\mathbf{A}, \mathbf{B})$, and the nonzero vector $\mathbf{x}$ is the corresponding eigenvector. $(\lambda, \mathbf{x})$ is called an eigenpair of GEP. If $\mathbf{B}$ is a diagonal matrix, then the generalized eigenvalue problem reduces to the standard eigenvalue problem (SEP). Usually, the smallest eigenvalues and the corresponding eigenvectors play more important role in real applications than the largest ones. We are interested in the computation for the smallest eigenvalues and corresponding eigenvectors of a large sparse eigenvalue problem in this paper.

By now, many algorithms have been developed for solving eigenvalue problems [6, 25, 29]. These algorithms can be divided roughly into two classes: the direct methods and iterative methods. For large

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