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A Filtered-Davidson Method for Large Symmetric Eigenvalue Problems

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Abstract. For symmetric eigenvalue problems, we constructed a three-term recurrence polynomial filter by means of Chebyshev polynomials. The new filtering technique does not need to solve linear systems and only needs matrix-vector products. It is a memory conserving filtering technique for its three-term recurrence relation. As an application, we use this filtering strategy to the Davidson method and propose the filtered-Davidson method. Through choosing suitable shifts, this method can gain cubic convergence rate locally. Theory and numerical experiments show the efficiency of the new filtering technique.

AMS subject classifications: 15A18, 65F15, 65F50, 34L15, 65N25.

Key words: Symmetric eigenproblem, filtering technique, Chebyshev polynomials, Krylov subspace, Davidson-type method.

1. Introduction

The Davidson method [1] is an efficient iterative procedure for computing a few eigenvalues and the corresponding eigenvectors of the standard eigenvalue problem

$$Ax = \lambda x, \quad \text{with} \quad \|x\| = 1, \tag{1.1}$$

where $A \in \mathbb{R}^{n\times n}$ is a large sparse symmetric matrix and $\|\cdot\|$ denotes the Euclidean norm. The Davidson method performs a so-called Rayleigh-Ritz procedure [12] on an increasing subspace which is extended by adding a preconditioned residual to the current subspace. For the unpreconditioned Davidson method, it is equivalent to the Lanczos method [12, 14, 15]. It has been known as a very successful method, especially, when dealing with certain diagonally dominant matrices for using diagonal preconditioner in its original paper. Subsequently, Morgan and Scott [7,8] generalized the Davidson method to a more general

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form. In the generalized Davidson method, they used a general preconditioner rather than a diagonal preconditioner.

In [17], Sleijpen and van der Vorst proposed a Jacobi-Davidson iteration method. In each step of the Jacobi-Davidson iteration method, a so-called correction equation needs to be solved. The Jacobi-Davidson iteration method is also a Davidson-type method, because the solution of the correction equation can be considered as a preconditioned residual vector. The coefficient matrix is a projection on the orthogonal complement of the current approximation which ensures the well-conditioned property of the correction equation when the approximate vector is near to the desired eigenvector. Furthermore, the Jacobi-Davidson iteration method can obtain cubic convergence rate locally. For more details of the Jacobi-Davidson iteration method and its convergence property, we refer to [16,17,19].

To obtain the preconditioned residual from the above discussions, we need to solve some linear systems which result in high computational costs, so as to the CPU time, especially for large problems. In [21], the authors proposed a new Chebyshev-Davidson method, in which the correction equation of the Davidson method is replaced by a Chebyshev polynomial filtering step which can amplify components of the desired eigenvector. This filtering technique can reduce the computational cost for just processing the matrix-vector products, although an indeterminate iteration step for the Chebyshev filter should be given in advance.

In this paper, we propose a new three-term recurrence polynomial filter by means of Chebyshev polynomials. This filter is located in the Krylov subspace spanned by a shifted matrix and the current approximate vector. Also, we give an estimate of the degree of the filtered polynomial. It can reduce the computational cost and conserve memory for its three-term recurrence relation. Furthermore, we give a stopping criterion resulted from the inverse iteration method [12,14] for the inner iteration step. For some suitable parameters, the new polynomial filter can reduce the iteration numbers for high convergence rate of the proposed filtered-Davidson method.

The remainder of this paper is organized as follows. In Section 2, some preliminaries for the filtering technique, Chebyshev polynomials and the Davidson method are given. In Section 3, the three-term recurrence polynomial is derived and we propose a stopping criterion which is easily verified. Furthermore, we propose the so-called filtered-Davidson method. Some details of the filtering technique are discussed in Section 4. We use some numerical experiments to demonstrate our results in Section 5 and, in the last section, we give some conclusions and remarks.

2. Preliminaries

In this paper, we use I to denote the identity matrix of suitable dimension. For a matrix $A \in \mathbb{R}^{n\times n}$, we use A^T to denote its transpose; this notation can be easily carried over to vectors. A Krylov subspace of order m associated with a matrix A and a vector $x \neq 0$ is defined by

$$K_m(A,x) = \mathrm{span}\{x, Ax, \cdots, A^{m-1}x\}.$$