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Inexact Iterative WYD Method for Eigenvalue Problems

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Abstract. In this paper, we propose a new inexact iterative subspace projection method for real symmetric positive definite generalized eigenvalue problems based on the WYD (an abbreviation of the initials of the proposers: Wilson, Yuan, and Dickens [1]) method. Firstly an analysis of the convergence condition of the approximate eigenvectors is given when $\mathbf{A}\mathbf{r}_{k+1}=\lambda\mathbf{B}\mathbf{r}_k$ is inexactly solved by the Krylov subspace methods. Then the inexact iterative WYD (IIWYD) method is constructed, which utilizes the approximate Ritz subspace generated by the WYD method with an inexact solver as the main search space. The IIWYD method improves the quality of the search space during the iterative process, significantly reduces the number of iteration steps, and improves the overall computational efficiency and stability. The results of numerical experiments show that the IIWYD method is more efficient and stable compared to the locally optimal block preconditioned conjugate gradient (LOBPCG) method and the Jacobi-Davidson (JD) method. In addition, we also discuss the effects of the refined strategy and the conjugate strategy in our method.

AMS subject classifications: 65F15, 65F10

Key words: Eigenvalue problems, iterative method, WYD, LOBPCG, Jacobi-Davidson.

1 Introduction

For a given real symmetric positive definite (SPD) matrix $\mathbf{A}$ and $\mathbf{B}$, there exists a set of real numbers λ with vectors $\mathbf{x}$ satisfying $\mathbf{A}\mathbf{x}=\lambda\mathbf{B}\mathbf{x}$, where λ and $\mathbf{x}$ are called the eigenvalues and the corresponding eigenvectors. For the SPD generalized eigenvalue problem, all eigenvalues are positive.

For small-scale eigenvalue problems, classical algorithms such as the Jacobi method and the QR decomposition method are wildly used. For larger-scale sparse problems,

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these algorithms are unsatisfactory in computational efficiency, because their time complexity is related to the cube of the dimension of matrices. Lanczos [2] and Arnoldi [3] gave efficient methods for large-scale symmetric and general eigenvalue problems, respectively. Since then many effective subspace projection methods have been developed [4–7]. Yuan proposed the WYD method [8] as an eigenvalue solver which is particularly effective for structural dynamic analysis problems, and showed the relationship between the WYD method and the Lanczos method.

The basic process of the subspace projection method is to form a search space firstly, then project the large-scale matrix to this subspace, and transform the original problem into a small-scale eigenvalue problem. Based on the eigenvalues and eigenvectors of this small-scale problem, a set of corresponding approximate eigenvalues and approximate eigenvectors of the original problem can be obtained in the search space [9], this process is often called the Rayleigh-Ritz process [10]. The subspace iterative method combines the Rayleigh-Ritz process with the vector simultaneous iterations to achieve much faster convergence for multiple eigenvalues and eigenvectors [11]. Earlier, methods for generating the search spaces were usually based on exact solvers. However, some more efficient eigenvalue solvers have since emerged, which use inexact linear solvers to generate the search spaces while still allowing the eigenvectors to converge. The most representative of such eigenvalue solvers include the Jacobi-Davidson method (JD) [12,13], the locally optimal block preconditioned conjugate gradient (LOBPCG) method [14], etc.

We introduce the inexact solver and iterative strategy into the WYD method and propose the inexact iterative WYD (IIWYD) method, which can efficiently solve large-scale SPD eigenvalue problems. In Section 2, the original WYD method is introduced. Then the complete IIWYD method is constructed and analyzed in Section 3. In Section 4, numerical experiments are conducted to demonstrate the convergence and computational efficiency of the IIWYD method. In Section 5, we give brief conclusions on the IIWYD method and discussions on the relationship between different acceleration strategies.

2 Original WYD method and optimization strategies

The WYD method [8] is based on the load-dependent Ritz vector (LDRV) method [1,15], which is proposed to be used for dynamic analysis originally. Yuan proposed that the Ritz vectors can be regarded as the approximation to the eigenvectors when the random vector is taken as the initial vector. When the number of Ritz vectors increases, the error in approximate eigenvectors will also decrease. Yuan also proved that, for the N-order eigenvalue problem, the projection matrix $\mathbf{A}^*$ of the WYD method and coefficient matrix $\mathbf{T}$ of the Lanczos method exactly satisfy $\mathbf{A}^*=\mathbf{T}^{-1}$ when both the WYD and Lanczos method perform N steps. Since the Lanczos vectors depend only on the previous two terms, and the Ritz vectors of the WYD method remain orthogonal, usually the Ritz vectors of the WYD method have better numerical stability and clearer physical meaning [8].

Chen [16] gives a more practical iterative form of the WYD method, which reduces the