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PRECONDITIONING BLOCK LANCZOS ALGORITHM FOR SOLVING SYMMETRIC EIGENVALUE PROBLEMS [*1)]

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Abstract

A preconditioned iterative method for computing a few eigenpairs of large sparse symmetric matrices is presented in this paper. The proposed method which combines the preconditioning techniques with the efficiency of block Lanczos algorithm is suitable for determination of the extreme eigenvalues as well as their multiplicities. The global convergence and the asymptotically quadratic convergence of the new method are also demonstrated.

Key words: eigenvalue, eigenvector, sparse matrices, Lanczos method, preconditioning

1. Introduction

The Lanczos process is an effective method [1, 2, 14, 21] for computing a few eigenvalues and corresponding eigenvectors of a large sparse symmetric matrix $A \in \mathbf{R}^{n\times n}$. If it is practical to factor the matrix $A-\rho I$ for one or more values of ρ near the desired eigenvalues, the Lanczos method can be used with the inverted operator and convergence will be very rapid[5,10,22]. In practical applications, however, the matrix A is usually large and sparse, so factoring A is either impossible or undesirable. The Lanczos algorithm can suffer from convergence problem if the desired eigenvalues are not well separated from the rest of the spectrum.

The conjugate gradient method [11] for solving linear equations has also convergence problem if the distribution of eigenvalues is unfavorable. Convergence of the conjugate gradient method can be improved by preconditioning techniques [3, 15, 16]. It would also be desirable to improve the convergence of the Lanczos algorithm with preconditioning techniques, but this is not straightforward. Preconditioning can be applied indirectly to eigenvalue problems by using the preconditioned conjugate gradient method or the preconditioned SOR method to solve equations for inverse iteration [6, 7, 20], the Rayleigh quotient iteration [23, 24] and shift-and-invert Lanczos method [5, 10, 22].

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The generalized Davidson method [17, 18] gives a more direct preconditioning approach to eigenvalue problems. The method generates a subspace with the operator $N(\rho) = (M - \rho I)^{-1}(A - \rho I)$, where ρ is the most recent approximation to the desired eigenvalue, M is any approximation to A. $M - \rho I$ can be viewed as a preconditioner to $A - \rho I$. Morgan and Scott[19] transformed $N(\rho)$ to a symmetric operator $L^{-1}(A - \rho I)L^{-T}$ so that the Lanczos algorithm can be applied, where LL^T is the Cholesky factorization of the preconditioner $M - \rho I$. Certainly, the preconditioner $M - \rho I$ is required to be symmetric positive definite. Then they gave a preconditioning Lanczos algorithm (called the PL algorithm). However it is difficult to determine the multiplicity of the computed eigenvalues by using the PL algorithm and there are some errors in the PL algorithm and the proof of its convergence.

The method we will describe, the preconditioning block Lanczos algorithm (called the PBL algorithm), is an extension of the PL algorithm. A double iteration scheme is also used. The Rayleigh-Ritz procedure and a certain preconditioned matrix are used in the outside loop; the block Lanczos algorithm[4,9] is applied in the inside loop. The PBL algorithm not only enables us to detect the multiplicity of the computed eigenvalues, but affords us improved rates of convergence. This algorithm can be very efficient if the matrix is fairly sparse and an approximation inverse is easily available.

In section 2 we formulate the PBL algorithm and discuss the various steps of the computations. In section 3 we analyze the global convergence of the algorithm and asymptotically quadratic convergence with respect to the outer loop. Section 4 looks at some implementation details and gives numerical experiments where a comparison with the block Lanczos algorithm is investigated.

2. Preconditioning Block Lanczos (PBL) Algorithm

Let the eigenvalues $\lambda_i (i = 1, 2, \cdots, n)$ of the symmetric matrix A be ordered as follows

$$\lambda_1 \le \lambda_2 \le \cdots \le \lambda_j \le \lambda_{j+1} \le \cdots \le \lambda_n \tag{1}$$

Suppose that we are interested in computing the j-th smallest eigenvalue and corresponding eigenvector of the matrix A. The preconditioning block Lanczos algorithm can be described as follows.

PBL Algorithm. Choose $m (m \ge j)$ linear independent vectors $x_i^{(0)} (i = 1, 2, \cdots, m)$, and let $X^{(0)} = [x_1^{(0)}, \cdots, x_m^{(0)}]$.

For $k = 0, 1, \cdots$, do 1) to 5)

1) Compute $A_k = X^{(k)^T} A X^{(k)}$, $B_k = X^{(k)^T} X^{(k)}$, and find the j smallest eigenvalues $\mu_1^{(k)}, \cdots, \mu_j^{(k)} (\mu_1^{(k)} \le \cdots \le \mu_j^{(k)})$ and corresponding eigenvectors $q_1^{(k)}, \cdots, q_j^{(k)}$ of the symmetric generalized eigenvalue problem

$$A_k q = \mu B_k q \tag{2}$$

and let $Q^{(k)} = [q_1^{(k)}, \cdots, q_j^{(k)}]$.

2) Choose M_k to be a symmetric positive definite matrix approximating $A - \mu_j^{(k)} I$, and compute the Cholesky factorization $M_k = L_k L_k^T$.