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A PROCESS FOR SOLVING A FEW EXTREME EIGENPAIRS OF LARGE SPARSE POSITIVE DEFINITE GENERALIZED EIGENVALUE PROBLEM *

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Abstract

In this paper, an algorithm for computing some of the largest (smallest) generalized eigenvalues with corresponding eigenvectors of a sparse symmetric positive definite matrix pencil is presented. The algorithm uses an iteration function and inverse power iteration process to get the largest one first, then executes $m-1$ Lanczos-like steps to get initial approximations of the next $m-1$ ones, without computing any Ritz pair, for which a procedure combining Rayleigh quotient iteration with shifted inverse power iteration is used to obtain more accurate eigenvalues and eigenvectors. This algorithm keeps the advantages of preserving sparsity of the original matrices as in Lanczos method and RQI and converges with a higher rate than the method described in [12] and provides a simple technique to compute initial approximate pairs which are guaranteed to converge to the wanted m largest eigenpairs using RQI. In addition, it avoids some of the disadvantages of Lanczos and RQI, for solving extreme eigenproblems. When symmetric positive definite linear systems must be solved in the process, an algebraic multilevel iteration method (AMLI) is applied. The algorithm is fully parallelizable.

Key words: Eigenvalue, sparse problem

1. Introduction

We are concerned in this work with finding a few extreme eigenvalues and their corresponding eigenvectors of a generalized large scale eigenvalue problem in which the matrices are sparse and symmetric positive definite.

Although finding a few extreme eigenpairs is of interest both in theory and practice, there are only few usable and efficient methods up to now. Reinsch and Bauer ([12]), suggested a QR algorithm with Newton shift for the standard eigenproblem which included an ingenious method to evaluate the shift. Their algorithm has a lower asymptotic convergence rate than a normal QL process with Wilkinson's shift or Rayleigh quotient iteration with inverse power iteration (RQI) and their strategy to calculate the shift can not be extended to the situation where any other shift which is different from the Newton shift and with a higher convergence rate is used. There are some works for selecting different shifts and acceleration techniques, see [11], [16], [17], [18].

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There is lack of efficient methods of computing extreme eigenvalues, in particular for the generalized problem. Although in theory it can be transformed into a standard problem as long as one of the two matrices A and B is positive definite, such a transformation will destroy the sparse structure of the initial matrices and is therefore inapplicable in practice.

Lanczos-like method and shifted inverse power iteration combined with Rayleigh quotient shift (or other evaluable shift) are expected to have a good efficiency for sparse eigenvalue problem either a standard one or a generalized one because it will not destroy the sparsity of matrices and the RQI method has a higher convergence rate, see [7], [3], [9]. But there exist several difficulties when using such a method to an extreme eigenvalue problem. First, it seems to be impossible to decide how many steps must be executed in the Lanczos process for getting the m largest eigenvalues. This means one must perform many more Lanczos steps than m and it still does not guarantee obtaining enough extreme eigenpairs as required. Another problem is that it is not certain whether it will converge to those expected m largest eigenpairs during the RQI process in which such Ritz pairs are taken as initial values.

We suggest an algorithm in Section 2 which avoids the above two weak points, i.e., it produces just m original pairs, without solving the Ritz pairs of the matrix pencil, and which will be guaranteed to tend to the m largest needed eigenpairs and even with a higher rate. Furthermore it also preserves the sparse structure of the original matrices and is fully parallelizable.

A sequence of shifts $\{\sigma_k\}$, which converges to the largest generalized eigenvalue of matrix pencil is computed first, by using an iteration function and then the largest eigenpair is computed by an inverse power iteration process. Subsequently, $m-1$ steps of a Lanczos-like procedure from this pair are performed to compute $m-1$ values and vectors which are good approximate extreme generalized eigenpairs, as will be proved in Section 3. More precisely, instead of solving the Ritz pairs of the original matrices, we could take them as initial pairs immediately and get the required m largest eigenpairs by Rayleigh quotient iteration and inverse power iteration which, furthermore, will converge with a cubic rate asymptotically since each original pair is very close to the corresponding final pair.

We present some further theoretical analysis in Section 3. In Section 4, we discuss some practical computational aspects, such as how to construct the iteration function, how to calculate function values and derivative values of the eigenpolynomial, how to solve the corresponding linear system and parallelization aspects, etc. Some numerical examples and concluding remarks are found in the two final sections.

2. Algorithm

Consider the generalized eigenvalue problem

$$A\mathbf{z} = \lambda B\mathbf{z} \tag{1}$$

where both A and B are $n \times n$ sparse real symmetric matrices and in addition B is positive definite. Let the n eigenpairs be $(\lambda_1, \mathbf{z}_1)$, $(\lambda_2, \mathbf{z}_2)$,...,$(\lambda_n, \mathbf{z}_n)$. We assume

$$(B\mathbf{z}_i, \mathbf{z}_j) = \delta_{ij}$$

i.e., $\{\mathbf{z}_i\}$ is a B-orthogonal basis and $\|\mathbf{z}_i\|_B = 1$, where the norm $\|\cdot\|_B = \sqrt{(B\cdot,\cdot)}$ and

$$\lambda_1 > \lambda_2 > \ldots > \lambda_n \tag{2}$$