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ARNOLDI TYPE ALGORITHMS FOR LARGE UNSYMMETRIC MULTIPLE EIGENVALUE PROBLEMS[*1)]

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Abstract

As is well known, solving matrix multiple eigenvalue problems is a very difficult topic. In this paper, Arnoldi type algorithms are proposed for large unsymmetric multiple eigenvalue problems when the matrix A involved is diagonalizable. The theoretical background is established, in which lower and upper error bounds for eigenvectors are new for both Arnoldi's method and a general perturbation problem, and furthermore these bounds are shown to be optimal and they generalize a classical perturbation bound due to W. Kahan in 1967 for A symmetric. The algorithms can adaptively determine the multiplicity of an eigenvalue and a basis of the associated eigenspace. Numerical experiments show reliability of the algorithms.

Key words: Arnoldi's process, Large unsymmetric matrix, Multiple eigenvalue, Diagonalizable, Error bounds

1. Introduction

The Lanczos algorithm[20] is a very powerful tool for extracting a few extreme eigenvalues and associated eigenvectors of large symmetric matrices[4,5,22]. Since the 1980's, considerable attention has been paid to generalizing it to large unsymmetric problems. One of its generalizations is Arnoldi's method[1,25]. It can be used to compute outer part of the spectrum and corresponding eigenvectors[10,11,24,25,26,28]. In order to improve overall performance, Saad[27] suggested to use it in conjunction with the Chebyshev iteration. There are other variants available; see, e.g. [12, 13, 16, 17, 19, 24, 28].

To apply Arnoldi's algorithm and its variants to practical problems, one must account for the following difficulty[2,3,6,8]:

Difficulty* *Multiple eigenvalues are a common occurrence.*

In the symmetric case, Parlett and Scott[21] used the Lanczos algorithm with selective orthogonalization to solve Difficulty*. Their algorithm maintains the semi-orthogonality among the Lanczos vectors so as to avoid the occurrence of spurious

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eigenvalues and determines the multiplicities of the required eigenvalues and the associated eigenspaces by restarting. The key idea is that, before restarting, a new initial vector is orthogonalized with respect to all the converged eigenvectors until the eigenspace associated with a multiple eigenvalue is found.

In the unsymmetric case, the situation becomes much more complicated. The strategy of restarting[21] cannot solve Difficulty* since the eigenvectors of unsymmetric matrices are, in general, not mutually orthogonal just as those of symmetric matrices are. The mutual orthogonality of eigenvectors forms the basis of the algorithm in [12]. Theoretically speaking, a simple simulation of the idea used in [21] suggests that before restarting we use Arnoldi's method with a new initial vector orthogonal to all the left eigenvectors of the matrix A associated with all the converged right eigenvectors. Proceeding in such a way, we can find the multiplicities of the required eigenvalues and determine the associated eigenspaces. However, an easy analysis[23] shows that Arnoldi's method is inefficient for computing the left eigenvectors of A. Of course, one can apply Arnoldi's method to A^H, the conjugate transpose of A, to get the left eigenvectors of A, while this doubles the amount of computation.

In order to deal with Difficulty*, generalized block Lanczos methods are studied in [10, 14]. They can be used to compute outer part of the spectrum and corresponding eigenvectors, up to a multiplicity equal to block size when A is diagonalizable. However, if the multiplicities of the required eigenvalues are bigger than block size, the block algorithms themselves are not able to determine the multiplicity of an eigenvalue and the associated eigenspace. Therefore, to be able to detect the multiplicity, the block algorithms have to combine with other techniques in practice.

In this paper, we design Arnoldi type algorithms for solving Difficulty* when A is diagonalizable. As is seen from [10, 14], the proposed idea is important not only in its own right but also indispensable for the block Arnoldi method when block size is smaller than or equal to the multiplicities of the required eigenvalues.

In Section 2, we introduce the notation used and go through the underlying Arnoldi algorithm; in Section 3, assuming that A is diagonalizable, we present the theoretical background of the Arnoldi type algorithms to be proposed in Section 4. Some of the results, i.e. theoretical error bounds for eigenvectors, are new for both Arnoldi's method and a general perturbation problem; in Section 4 we present two Arnoldi type algorithms to solve Difficulty*; in Section 5, we discuss some implementations of the algorithms; in Section 6, we report three numerical examples to show reliability of the algorithms, followed by some concluding remarks in Section 7.

2. The Underlying Arnoldi Algorithm

2.1. Notation

Throughout the paper, assume that A is an $N \times N$ real diagonalizable matrix, $N \gg 1$ and it has M distinct eigenvalues λ_i, where the multiplicities of λ_i are d_i, $i = 1, 2, \cdots, M$. Under this assumption let $\mathcal{P}_i$ be the d_i-dimensional eigenspace associated with λ_i and the columns of $\Phi_{id_i} = (\varphi_{i1}, \varphi_{i2}, \cdots, \varphi_{id_i})$ form a basis of $\mathcal{P}_i$, where $\|\varphi_{ij}\| = 1$