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An Implicitly Restarted Block Arnoldi Method in a Vector-Wise Fashion†

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Abstract. In this paper, we develop an implicitly restarted block Arnoldi algorithm in a vector-wise fashion. The vector-wise construction greatly simplifies both the detection of necessary deflation and the actual deflation itself, so it is preferable to the block-wise construction. The numerical experiment shows that our algorithm is effective.

Key words: IRAM; Arnoldi-type algorithm; vector-wise block Arnoldi; implicit restart.

AMS subject classifications: 65F15

1 Introduction

Many scientific applications lead to large-scale eigenvalue problems, where typically only a few eigenvalues are of interest. For such problems Krylov methods are well suited.

In the first Krylov methods, the Krylov subspace, which is constructed by the Arnoldi factorization, is based on a single vector. By instead using a set of orthonormal vectors to generate the Krylov subspace, a block Arnoldi method is obtained.

As the iteration proceeds, the storage and computational requirements increase and the algorithm needs to be restarted. The earlier approaches considered explicit restarting, using information obtained from the Hessenberg matrix to construct an improved starting vector. Sorensen devised an approach for the single-vector Arnoldi, where instead the factorization is updated [7]. This is accomplished via an implicit shifted QR-iteration applied to the Arnoldi-factorization. Sorensen chose the shifts among the unwanted Ritz-values.

The implicit restarting technique was generalized to block Arnoldi by Lehoucq and Maschhoff [5]. In paper [4] which is about the model reduction problem, Freund introduces an algorithm which implements the block Arnoldi method in a vector-wise fashion, as opposed to the block-wise construction. The vector-wise construction is preferable to the block-wise construction because it greatly simplifies both the detection of necessary deflation and the actual deflation itself. And the choice of the initial block vector could be arbitrary, while in the block-wise case, an orthogonal one is needed.

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Since the deflation exists, it becomes necessary to exploit whether the structure of the matrices in the Arnoldi factorization after the truncation from $(k + p)$-order to k-order is right. In this paper, we first prove this point which means that the implicit restarting technique can be combined with the vector-wise block Arnoldi method, we then develop an implicitly restarted block Arnoldi algorithm in a vector-wise fashion to solve the large-scale eigenproblems.

In Section 2 we give some notations and the vector-wise block Arnoldi process which is introduced in [4]. In Section 3 we present our strategy for the computation of eigenvalues. In Section 4 we report our numerical experiments which demonstrate that the proposed algorithm is effective.

2 Arnoldi-type algorithm

2.1 Block Krylov subspaces

We first introduce our notion of block Krylov subspaces for multiple starting vectors. Let $A \in \mathbf{R}^{\mathrm{N}\times N}$ be a given $N \times N$ matrix and

$$R = [r_1 \;\; r_2 \;\; \cdots \;\; r_m] \in \mathbf{R}^{\mathrm{N}\times m} \tag{1}$$

be a given matrix of m right starting vectors $r_1, r_2, \cdots, r_m$. In contrast to the case $m = 1$, linear independence of the columns in the block Krylov sequence,

$$R, AR, A^2R, \cdots, A^{j-1}R, \cdots \tag{2}$$

is lost gradually in general. By scanning the columns of the matrices in (2) from left to right and deleting each column that is linearly dependent on earlier columns, we obtain the *deflated* block Krylov sequence

$$R_1, AR_2, A^2R_3, \cdots, A^{j_{max}-1}R_{j_{max}}. \tag{3}$$

This process of deleting linearly dependent vectors is referred to as *exact deflation* in the following. In (3), for each $j = 1, 2, \cdots, j_{max}$, R_j is a submatrix of R_{j-1}, with $R_j \neq R_{j-1}$ if, and only if, deflation occurred within the jth Krylov block $A^{j-1}R$ in (2). Here, for $j = 1$, we set $R_0 = R$. Denoting by m_j the number of columns of R_j, we thus have

$$m \geq m_1 \geq m_2 \geq \cdots \geq m_{j_{max}} \geq 1. \tag{4}$$

By construction, the columns of the matrices (3) are linearly independent, and for each n, the subspace spanned by the first n of these columns is called the *nth block Krylov subspace*(induced by A and R). In the following, we denote the nth Krylov subspace by $\mathcal{K}_n(A, R)$. For later use, we remark that for

$$n = m_1 + m_2 + \cdots + m_j \;, \tag{5}$$

where $1 \leq j \leq j_{max}$, the nth block Krylov subspace is given by

$$\mathcal{K}_n(A, R) = \text{Colspan}\{R_1, AR_2, A^2R_3, \cdots, A^{j-1}R_j\}. \tag{6}$$

2.2 Basis vectors

The columns of the deflated block Krylov sequence (3), which is used in the above definition of $\mathcal{K}_n(A, R)$, tend to be almost linearly dependent even for moderate values of n. Therefore,