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Weighted and flexible versions of block CMRH method for solving nonsymmetric linear systems with multiple right-hand sides

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ABSTRACT

Block Krylov subspace methods are the most popular algorithms for solving large nonsymmetric linear systems with multiple right-hand sides. One of them is the block CMRH method. This method generates a (non orthogonal) basis of the Krylov subspace through the block Hessenberg process. To accelerate the convergence of the block CMRH method, we will introduce two new methods. First, we present the block CMRH method with weighting strategy. In this method, the block CMRH method uses a different product at each restart. Second, we introduce a flexible version of the block CMRH algorithm that allows varying preconditioning at every step of the algorithm. Numerical experiments illustrate the benefits of the presented methods.

1. Introduction

Block iterative methods are used for large systems with multiple right-hand sides of the form

$$AX = B, \tag{1}$$

where $A \in \mathbb{R}^{n\times n}$ is a large nonsymmetric real matrix and X and B are rectangular matrices of dimension $n \times s$, and s is of moderate size (i.e., $s \ll n$). This problem arises in many areas of science and engineering, such as computational biology, electromagnetic structure computation, control theory, and so on [1–4].

When A is a large sparse matrix, block iterative methods, e.g., block CG method [5], block GMRES method [6], block Lanczos method [7], block QMR method [1], block BiCGSTAB method [8], block LSQR method [9], the block OSGCR(s)/OSOmin(s,k) methods [10,11], or block CMRH method [12,13] are natural candidates for solving (1). The purpose of these block methods is to provide the solutions of a multiple right-hand sides system faster than their single right-hand side counterparts. They are generally more efficient when the matrix of the linear system is relatively dense or when preconditioners are used.

The global methods form another family that can be applied to the solution of multiple linear systems. These methods are based on the use of a global projection process onto a matrix Krylov subspace and they are particularly suitable for sparse multiple linear systems. References on this class include global FOM and GMRES methods [14,15], global BCG and BiCGSTAB methods [16,17], global CGS algorithm [18,19], Gl-LSQR algorithm [20], Gl-BCR and Gl-CRS algorithms [21], global Hessenberg and CMRH methods [22], and global SCD algorithm [23]. In order to improve the convergence property of the Krylov subspace methods the weighted and flexible versions of these methods have been proposed. The weighting strategy has been successfully developed for solving linear systems [24] and matrix equations [24–28]. Several flexible versions of

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Krylov Subspace Methods have been implemented successfully. These include the flexible GMRES method [29], GMRESR [30], flexible CG [31–33], flexible QMR [34], flexible BiCG and flexible BiCGSTAB [35]. See also [36] for a general theory where the preconditioner itself is a Krylov subspace method.

For nonsymmetric problems, the block CMRH [12,13] is one such method, but it may need restarting. Here we give two new versions of the restarted block CMRH method to improve convergence. First to accelerate the convergence of the block CMRH method we apply a weighting technique. We introduce a weighted block Hessenberg process for constructing a basis of the block Krylov subspace by using the weighting matrix D. Second we propose a flexible version of the block CMRH.

Throughout the paper, all vectors and matrices are assumed to be real. For a matrix X, $\|X\|_F$ denotes the Frobenius norm $\|X\|_F = \sqrt{\mathrm{tr}(X^TX)}$. For a matrix $V \in \mathbb{R}^{n\times s}$, the block Krylov subspace $\mathcal{K}_k(A, V)$ is the subspace generated by the columns of the matrices $V, AV, A^2V, \ldots, A^{k-1}V$. Some MATLAB notation is used; for instance, $H_k(i+1 : m+1, 1 : m)$ denotes the portion of H_k with rows from $i+1$ to $m+1$ and columns from 1 to m. Finally, $0_{m\times n}$ and I_s will denote the zero and the identity matrices in $\mathbb{R}^{m\times n}$ and $\mathbb{R}^{s\times s}$, respectively.

As in [37], we need the definition of the left inverse of a rectangular matrix. Let Z_k be the $n \times k$ matrix. We partition this matrix as follows:

$$Z_k = \begin{bmatrix} Z1_k \\ Z2_k \end{bmatrix},$$

where $Z1_k$ is a $k \times k$ square matrix. If the matrix $Z1_k$ is nonsingular, we define Z_k^L a left inverse of Z_k by

$$Z_k^L = \left[Z1_k^{-1}, 0_{k\times(n-k)}\right].$$

The structure of the paper is as follows. In Section 2, we briefly describe the block CMRH method for solving nonsymmetric linear systems with multiple right-hand sides. A weighted version of the block CMRH algorithm is presented in Section 3. In Section 4, we propose the fixed and flexible preconditioned block CMRH algorithm. In Section 5, we demonstrate the effectiveness of the proposed methods. Finally, conclusions are summarized in Section 6.

2. Block CMRH method

The block CMRH method [12,13] is a generalization of the well-known CMRH method [37]. The essential component of the block CMRH method is the block Hessenberg process. Let $X_0 \in \mathbb{R}^{n\times s}$ be an initial matrix for the solution of system (1) and $R_0 = B - AX_0$ its residual. The block Hessenberg process computes a unit trapezoidal matrix $\mathcal{L}_m = [L_1, L_2, \ldots, L_m]$, whose matrices $L_i \in \mathbb{R}^{n\times s}$, for $i = 1, 2, \ldots, m$, form a basis of the Krylov subspace $\mathcal{K}_m(A, R_0) = \mathrm{span}\{R_0, AR_0, \ldots, A^{m-1}R_0\}$, by using the following formulas:

$$\begin{cases} R_0 = L_1U_1, \\ L_{k+1}H_{k+1,k} = AL_k - \displaystyle\sum_{j=1}^{k} L_jH_{j,k}, \qquad \text{for } k = 1, \ldots, m, \end{cases} \tag{2}$$

where the unit trapezoidal matrix L_{k+1} and the upper triangular matrix $H_{k+1,k} \in \mathbb{R}^{s\times s}$ are determined by the LU factorization of $W = AL_k - \sum_{j=1}^{k} L_jH_{j,k}$, and the matrices $H_{j,k} \in \mathbb{R}^{s\times s}$ are determined such that

$$L_{k+1} \perp E_1, E_2, \ldots, E_k, \tag{3}$$

where E_i, for $i = 1, 2, \ldots, k$, is the $n \times s$ matrix which is zero except for the ith s rows, which are the $s \times s$ identity matrix. Let $\overline{\mathcal{H}}_m \equiv (H_{i,j})_{1\le i\le m+1, 1\le j\le m}$ be an $(m+1)s \times ms$ block upper Hessenberg matrix. From the block Hessenberg process, we can deduce the relation

$$A\mathcal{L}_m = \mathcal{L}_{m+1}\overline{\mathcal{H}}_m = \mathcal{L}_m\mathcal{H}_m + L_{m+1}H_{m+1,m}E_m^T, \tag{4}$$

where $\mathcal{H}_m$ is the $ms\times ms$ matrix obtained from $\overline{\mathcal{H}}_m$ by deleting the last s rows and E_m is the $ms\times s$ matrix which is zero except for the mth s rows, which are the $s \times s$ identity matrix.

The block Hessenberg process can breakdown if the LU factorization of R_0 or W does not exist [13]. For avoiding such a breakdown, we use pivoting strategy.

The block CMRH method constructs an approximate solution of the form $X_m^{BC} = X_0 + \mathcal{L}_mY_m^{BC}$, where Y_m^{BC} is the solution of the minimizing problem

$$\min_{Y\in\mathbb{R}^{ms\times s}} \|E_1U_1 - \overline{\mathcal{H}}_mY\|_F, \tag{5}$$

where $E_1 \in \mathbb{R}^{(m+1)s\times s}$ is the first s columns of the identity matrix.

In Algorithm 1, we summarize the restarted block CMRH method with pivoting strategy (denoted by BCMRH(m)). More detail can be found in [13]. We mention that the block CMRH algorithm given in [12] is similar to the Algorithm 1. The main difference between these algorithms is the generation of the matrices H_m and W in the block Hessenberg processes.

We end this section by giving a relation between the residual norms of the block CMRH method and the block GMRES method denoted by $\|R_m^{BC}\|_F$ and $\|R_m^{BG}\|_F$, respectively, which is stated in the following lemma [13].