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An Efficient Variant of the GMRES(m) Method Based on the Error Equations

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Abstract. The GMRES(m) method proposed by Saad and Schultz is one of the most successful Krylov subspace methods for solving nonsymmetric linear systems. In this paper, we investigate how to update the initial guess to make it converge faster, and in particular propose an efficient variant of the method that exploits an *unfixed update*. The mathematical background of the unfixed update variant is based on the error equations, and its potential for efficient convergence is explored in some numerical experiments.

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1. Introduction

In recent years, there has been extensive research on Krylov subspace methods for solving large and sparse linear systems of the form

$$A\boldsymbol{x} = \boldsymbol{b}, \quad A \in \mathbb{R}^{n\times n}, \quad \boldsymbol{x}, \boldsymbol{b} \in \mathbb{R}^n , \tag{1.1}$$

where the coefficient matrix A is assumed to be nonsymmetric and nonsingular. These linear systems often arise from the discretization of partial differential equations in computational science and engineering. The CG method [10] and the MINRES method [16] are two well known Krylov subspace methods for solving symmetric linear systems, but for general nonsymmetric linear systems the GMRES method [17] and the Bi-CGSTAB method [25] (and its variants [9, 20, 28]) are the most widely used. The IDR(s) method [22] proposed by Sonneveld and van Gijzen has recently also attracted considerable attention [21, 24]. Further details may be found in several surveys [8, 18, 19].

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In this paper, we focus on further developments in the GMRES method context. Let us first note that the original GMRES method [17] has shown good convergence, but it has considerable computational cost and storage requirements due to long-term recurrence. This is avoided in the GMRES(m) method [17] now widely used in practice, which involves a so-called *restart* that can be described as follows. In the first restart cycle, the restart frequency m is chosen and an initial guess $\boldsymbol{x}_0^{(1)}$ is made. For any lth restart cycle, the GMRES method using the initial guess $\boldsymbol{x}_0^{(l)}$ is applied with m iterations to the linear system (1.1), to produce the approximate solution $\boldsymbol{x}_m^{(l)}$ that may then be used to update the initial guess (i.e. $\boldsymbol{x}_0^{(l+1)} := \boldsymbol{x}_m^{(l)}$) in the $(l+1)$th restart cycle. This process is repeated until there is satisfactory convergence.

However, although the restart procedure avoids the computational cost and storage drawbacks of the GMRES method, it usually slows down the convergence. To improve the convergence of the GMRES(m) method, several techniques have recently been proposed for the "inside part" of m iterations [1–5, 7, 12–15, 23, 27]. When the initial guess of each restart cycle is updated via $\boldsymbol{x}_0^{(l+1)} := \boldsymbol{x}_m^{(l)}$ as outlined above, we call this the *fixed update* procedure. To further improve the convergence, in this paper we propose *variants of the GMRES(m) method* with *unfixed update*, mathematically based on the error equations and iterative refinement scheme.

The paper is organized as follows. In Section 2, we briefly discuss the GMRES(m) method. The proposed GMRES(m) method with unfixed update, and its mathematical background based on the error equations and iterative refinement scheme, is then presented in Section 3. An example variant of the GMRES(m) method with unfixed update is considered in Section 4, and in particular its convergence is explored in some numerical experiments in Section 5. Our conclusions are summarized in Section 6.

2. The GMRES(m) Method

Let $\boldsymbol{x}_0$ denote an initial guess for the solution of system (1.1), and $\boldsymbol{r}_0 := \boldsymbol{b} - A\boldsymbol{x}_0$ the corresponding initial residual. The Krylov subspace methods form a family of projection methods that extract an approximate solution $\boldsymbol{x}_k$ from an affine space spanned by the initial guess $\boldsymbol{x}_0$ and the Krylov subspace $\mathscr{K}_k(A, \boldsymbol{r}_0) \equiv \mathrm{span}\{\boldsymbol{r}_0, A\boldsymbol{r}_0, \cdots, A^{k-1}\boldsymbol{r}_0\}$ such that

$$\boldsymbol{x}_k = \boldsymbol{x}_0 + \boldsymbol{z}_k, \qquad \boldsymbol{z}_k \in \mathscr{K}_k(A, \boldsymbol{r}_0).$$

The GMRES method [17] constructs the approximate solution $\boldsymbol{x}_k$ by the minimum residual condition as follows:

$$\boldsymbol{x}_k = \boldsymbol{x}_0 + V_k\boldsymbol{s}_k, \qquad \boldsymbol{s}_k = \arg\min_{\boldsymbol{s}\in\mathbb{R}^k} \|\boldsymbol{r}_0 - AV_k\boldsymbol{s}\|_2, \tag{2.1}$$

where V_k is the $n \times k$ matrix with columns the orthogonal basis of the Krylov subspace $\mathscr{K}_k(A, \boldsymbol{r}_0)$ often obtained by the Arnoldi procedure. Thus in the GMRES algorithm, the minimization problem (2.1) is transformed by using the matrix formula of the Arnoldi procedure, and solved by QR factorization based on the Givens rotation. However, the computational cost of the GMRES method grows by at least $\mathrm{O}(k^2 n)$ and storage requirements