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GMRES implementations and residual smoothing techniques for solving ill-posed linear systems

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ABSTRACT

There are verities of useful Krylov subspace methods to solve nonsymmetric linear system of equations. GMRES is one of the best Krylov solvers with several different variants to solve large sparse linear systems. Any GMRES implementation has some advantages. As the solution of ill-posed problems are important. In this paper, some GMRES variants are discussed and applied to solve these kinds of problems. Residual smoothing techniques are efficient ways to accelerate the convergence speed of some iterative methods like CG variants. At the end of this paper, some residual smoothing techniques are applied for different GMRES methods to test the influence of these techniques on GMRES implementations.

1. Introduction

Iterativemethods for solving general, sparse linear systems of equations

$$Ax = b, \tag{1.1}$$

where $A \in R^{n\times n}$ and $x, b \in R^n$, have been gaining popularity in many areas of scientific computing. Many scientists have researched to solve (1.1) especially when the large sparse matrix A is severely ill-conditioned or is singular. Several different methods have been introduced to solve this problem. Most of the current researches on iterative methods focus on two sets of Krylov subspace methods and their variants [1]. Each set is based upon recursions which map the matrix A into a family of projection matrices which are then used to obtain approximations to a solution of (1.1). The first set is based upon the Arnoldi recursion and includes the Generalized Minimal Residual method (GMRES), the Full Orthogonalization method (FOM) and their variants while the second set of methods is based upon nonsymmetric Lanczos recursion and includes the Bi-Conjugate Gradient method (BiCG), the Quasi Minimal Residual method (QMR) and their variants [2–4]. The speed of convergence and stability of these methods are important. Then many implementations have also been introduced to improve these properties or create a simpler implementation for current iterative methods [5–10].

Some iterative methods like GMRES, LSQR and etc. are paying more attention to residual vector $r_k = b - Ax_k$ where x_k is the kth approximation solution of (1.1) by which the sequence of residual norms is decreased. GMRES is a popular method [3] which is widely used for solving linear system of equations. There are several implementations for this method that have been proposed for special goals with some advantages and disadvantages. Here, some GMRES implementations for solving ill-posed linear problems are applied to know which GMRES algorithm, with what extent, is more applicable to solve (nearly) singular problems and which one is not useful.

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This paper is organized as follows. In Section 2, some GMRES implementations and their properties are discussed. In Section 3, smoothing techniques that may modify the accuracy of some iterative methods like CG variants and the effects of residual smoothing on these methods are discussed. The solutions of ill-posed linear problems are applicable. But many iterative solvers are not able to compute meaningful solutions. To have a good comparison among different GMRES variants, in Section 4 they are applied to solve ill-posed problems. Moreover, some popular residual smoothing techniques are applied on GMRES implementations to test the influences of these techniques over convergence speed of GMRES solvers.

For simplicity, the square matrix A is assumed to be a real matrix and A^T means the transpose of A. Throughout this paper $\langle \cdot, \cdot \rangle$ is denoted for the inner product of two vectors and $\|\cdot\|$ is used for the associated norm.

2. Generalized minimal RESidual implementations

In 1986, Saad and Schultz proposed the well-known GMRES method for solving a nonsymmetric linear system of equations [11]. They gave a practical implementation based on the Arnoldi process [12], the so called "Standard GMRES". Next, many simple, stable or fast GMRES versions have been proposed and some of their implementations are discussed in this section, briefly.

Generally, there are two main steps for GMRES implementations. The first generates an orthogonal basis thanks to the Arnoldi process and the second solves a least squares problem to modify last approximation by generated orthogonal vectors. For solving (1.1), GMRES begins with an initial guess $x_0 \in R^n$ and characterizes the kth iterate as $x_k = x_0 + z_k$ where z_k is selected so the norm of corresponding residual r_k is minimized over $x_0 + K_k(r_0)$, then

$$\|r_k\| = \|r_0 - Az_k\| = \min_{z \in x_0 + K_k(r_0)} \|r_0 - Az\|, \tag{2.1}$$

where $r_0 = b - Ax_0$ and $K_k(v) = span\left\{v, Av, \ldots, A^{k-1}v\right\}$.

To generate a set of basis vectors for Krylov subspace $K_k(r_0)$, GMRES usually uses Arnoldi process at the first step which is as follows [11]:

Algorithm 1 (*Arnoldi (Modified Gram–Schmidt) Process*).

1. Given a vector v_1 with $\|v_1\| = 1$,
2. For $j = 1, \ldots, k$ do
   a. $v_{j+1} = Av_j$, For $i = 1, \ldots, j$ do $h_{i,j} = \langle v_{j+1}, v_i \rangle$, $v_{j+1} = v_{j+1} - h_{i,j}v_i$ End.
   b. $h_{j+1,j} = \| v_{j+1} \|$; $v_{j+1} = \frac{v_{j+1}}{h_{j+1,j}}$;
   End.

In brief, the steps 2a and 2b are shown with $v_{j+1} = \Pi_j^{\perp} Av_j / \|Av_j\|$. From this algorithm, the following important relation

$$AV_k = V_{k+1}\bar{H}_k, \tag{2.2}$$

which GMRES depends on, is obtained which the columns of V_k, i.e. $v_1, v_2, \ldots, v_k$, are a set of orthonormal basis vectors for $K_k(r_0)$ and upper Hessenberg matrix $\bar{H}_k = (h_{i,j}) \in R^{(k+1)\times k}$ is the matrix representation of A on $K_k(v_1)$ with respect to V_k. From (2.1) and (2.2) the basic formula of GMRES is obtained as

$$\begin{aligned} \min_{z \in x_0 + K_k(r_0)} \|r_0 - Az\| &= \min_{y \in R^k} \|r_0 - AV_k y\|, \\ &= \min_{y \in R^k} \|\beta e_1 - \bar{H}_k y\| \end{aligned} \tag{2.3}$$

with $\beta = \|r_0\|$ [11]. Note that the Arnoldi process breaks down at step k if and only if $h_{k+1,k} = 0$. In this case, matrix A is singular. Now if y_k minimizes the right hand side of least squares problem of (2.3), then $z_k = V_k\tilde{y}$ is the optimum solution of left hand side of (2.3) among the Krylov subspace $K_k(r_0)$. Generally, the algorithm of GMRES is written as follows.

Algorithm 2 (*Generalized Minimal RESidual Method*).

1. Given x_0, compute $r_0 = b - Ax_0$, $v_1 = \frac{r_0}{\|r_0\|}$.
2. Create $(k+1)$ orthogonal vectors $v_1, v_2, \ldots, v_{k+1}$ as a basis for $K_{k+1}(r_0)$.
3. Find $\tilde{y} \in R^k$ as solution of least squares problem (2.3).
4. Update $x_k = x_0 + V_k\tilde{y}$, if x_k does not satisfy, set $x_0 = x_k$ and go to 1.

According to this algorithm, GMRES is started with an initial guess x_0, after that orthogonalizing the vector v_{k+1} with $v_1, v_2, \ldots, v_k$ and finding the solution of a least squares problem, leads us to the next GMRES approximation so that the recursion of residual norms can be decreased.

Different GMRES methods have special properties, but they usually follow some regulations. For example two following questions are significant for GMRES implementations to be answered.