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Mathematics and Computers in Simulation 82 (2012) 2238–2252

MATHEMATICS AND COMPUTERS IN SIMULATION

www.elsevier.com/locate/matcom

Original Article

Simpler GMRES with deflated restarting

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Received 28 September 2010; received in revised form 29 February 2012; accepted 11 May 2012
Available online 28 June 2012

Abstract

In this paper we consider the simpler GMRES method augmented by approximate eigenvectors for solving nonsymmetric linear systems. We modify the augmented restarted simpler GMRES proposed by Boojhawon and Bhuruth to obtain a simpler GMRES with deflated restarting. Moreover, we also propose a residual-based simpler GMRES with deflated restarting, which is numerically more stable. The main advantage over the augmented version is that the simpler GMRES with deflated restarting requires less matrix-vector products per restart cycle. Some details of implementation are also considered. Numerical experiments show that the residual-based simpler GMRES with deflated restarting is effective.

MSC: 65F10; 65F30

Keywords: Linear system; Eigenvector; Harmonic Ritz vector; GMRES; Simpler GMRES; Restarting

1. Introduction

In this paper we consider iterative methods for solving the large sparse nonsymmetric system of linear equations

$$Ax = b, \tag{1}$$

where $A \in \mathbb{R}^{n\times n}$ is nonsingular, $b \in \mathbb{R}^n$ is a right-hand side vector, and $x \in \mathbb{R}^n$ is the sought-after solution.

One of the most popular iterative methods for solving such a system is the generalized minimal residual (GMRES) method developed by Saad and Schultz [12]. Let $x_0 \in \mathbb{R}^n$ be the initial guess, and $r_0 = b - Ax_0$ the initial residual vector. At the iteration step m, GMRES finds, in the affine subspace $x_0 + \mathcal{K}_m(A, r_0)$, the approximate solution x_m, which minimizes the Euclidean norm of the residual, i.e.,

$$\|r_m\| = \|b - Ax_m\| = \|b - A(x_0 + z_m)\| = \min_{z\in\mathcal{K}_m(A,r_0)} \|b - A(x_0 + z)\| = \min_{z\in\mathcal{K}_m(A,r_0)} \|r_0 - Az\|. \tag{2}$$

Here and in the following,

$$\mathcal{K}_m(A, r_0) = \text{span}\{r_0, Ar_0, \ldots, A^{m-1}r_0\}$$

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http://dx.doi.org/10.1016/j.matcom.2012.05.019

is the mth Krylov subspace generated by the matrix A and the initial residual vector r_0. It is easy to see that (2) is equivalent to the orthogonality condition

$$r_m \perp A\mathcal{K}_m(A, r_0), \tag{3}$$

where the orthogonality relation is based on the Euclidean inner product.

The classical implementation of GMRES is based on the Arnoldi process; see, for example [11]. Application of m steps of the Arnoldi process to the matrix A with the nonzero residual vector r_0 yields the Arnoldi factorization

$$AV_m = V_{m+1}\widehat{H}_m,$$

where the columns of the matrix V_m form the orthonormal basis of the Krylov subspace $\mathcal{K}_m(A, r_0)$ and $\widehat{H}_m \in \mathbb{R}^{(m+1)\times m}$ is an upper Hessenberg matrix. The least-squares problem can be reformulated as the reduced minimization problem

$$\|b - Ax_m\| = \|b - A(x_0 + V_m y_m)\| = \min_{y\in\mathbb{R}^m} \|\beta e_1 - \widehat{H}_m y\|,$$

where $\beta = \| r_0 \|$ and e_1 is the first column of an identity matrix of order $m+1$. The reduced minimization problem can be solved by the QR factorization of $\widehat{H}_m$ with Givens rotations.

A cheaper implementation of GMRES is called simpler GMRES. This method is proposed by Walker and Zhou [13] and further analyzed by Jiránek et al. [5]. Instead of building an orthonormal basis of $\mathcal{K}_m(A, r_0)$, it establishes an orthonormal basis V_m of $A\mathcal{K}_m(A, r_0)$ and then carries out the orthogonality relation (3). Specifically, let $Z_m = [z_1, z_2, \ldots, z_m]$ be a basis of $\mathcal{K}_m(A, r_0)$. Then, the orthonormal basis V_m of $A\mathcal{K}_m(A, r_0)$ can be obtained from the QR factorization of AZ_m, i.e.,

$$AZ_m = V_m R_m,$$

where $V_m = [v_1, v_2, \ldots, v_m]$ has orthonormal columns and R_m is an $m \times m$ nonsingular and upper triangular matrix. By carrying out the orthogonality relation (3), we can compute the mth residual vector r_m recursively as

$$r_m = r_0 - V_m(V_m^T r_0) = r_{m-1} - \alpha_m v_m, \quad m \geq 1,$$

where $\alpha_m = v_m^T r_0$. The corresponding approximate solution is

$$x_m = x_0 + Z_m t_m,$$

where t_m is the solution of the upper triangular system

$$R_m t_m = [\alpha_1, \alpha_2, \ldots, \alpha_m]^T.$$

As the iteration proceeds, the amount of storage and computational work required for GMRES or simpler GMRES increases significantly. It makes standard GMRES or simpler GMRES impractical. To overcome this disadvantage, the restarted version of these algorithms is used, that is, in restarted GMRES (GMRES(m)) or restarted simpler GMRES (SGMRES(m)), GMRES or simpler GMRES is restarted once the Krylov subspace reaches dimension m, and the current approximate solution becomes the new initial guess for the next m iterations. We present some details of SGMRES(m) in Algorithm 1.

Algorithm 1 *(SGMRES(m)).*

Input: A : *the coefficient matrix;* b : *the right-hand side;* x_0 : *an initial approximation;* m : *the maximal dimension of the Krylov subspace;* ε : *a tolerance.*
Output: *An approximate solution* x.

1. *Compute* $r_0 = b - Ax_0$, $z_1 = r_0/\| r_0 \|$, $\widehat{z}_1 = Az_1$, $r_{11} = \|\widehat{z}_1\|$, $v_1 = \widehat{z}_1/r_{11}$.
2. *Compute* $\alpha_1 = v_1^T r_0$, $r_1 = r_0 - \alpha_1 v_1$.
3. *For* $j = 2, 3, \ldots, m$
   3.1. $z_j = v_{j-1}$.
   3.2. $\widehat{z}_j = Az_j$.
   3.3. *For* $i = 1, 2, \ldots, j-1$