A Convergent Restarted GMRES Method For Large Linear Systems

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Abstract The GMRES method is popular for solving nonsymmetric linear equations. It is generally used with restarting to reduce storage and orthogonalization costs. However, it is possible to show that the restarted GMRES method may not converge, i.e., it may be stationary. To remedy this difficulty, a new convergent restarted GMRES method is discussed in this paper.

Key words GMRES, Krylov subspace, iterative methods, nonsymmetric systems.

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1. Introduction

The restarted GMRES algorithm GMRES(m)[1] proposed by Saad and Schultz is one of the most popular iterative methods for solving large linear systems of equations

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

with a sparse, nonsymmetric, and nonsingular matrix A. It is known that when A is positive real, the restarted GMRES method will produce a sequence of approximates x_k that converge to the exact solution. However, when A is not positive real, this method often slows down convergence and stagnates. The analysis and implementation of the restarted GMRES algorithm continue to receive considerable attention [2,3,4,5,6,7,8]. For example, Y.Saad suggested a flexible inner-outer preconditioned GMRES method FGMRES(m)[2]. R.B.Morgan gave a restarted GMRES method augmented with eigenvectors [3] ,and Cao Zhihao et. al. presented a convergent restarted GMRES algorithm based on the algorithm FGMRES(m)[4]. We will now briefly review the algorithm GMRES in this section. A new restarted GMRES method and its analysis will be given in section 2, section 3 gives the examples and comparisons, and conclusions are given in section 4. The restarted GMRES can be briefly described as follows.

Algorithm 1: GMRES(m) for systems (1.1)

1. Start: Choose x_0 and compute $r_0 = b - Ax_0$ and $\beta = \|r_0\|$, $v_1 = r_0/\beta$.

2. Iterate: For $j = 1, 2, \cdots, m$ do:

$$h_{i,j} = (Av_j,\ v_i), \quad i = 1, 2, \cdots, j,$$
$$\bar{v}_{j+1} = Av_j - \sum_{i=1}^{j} h_{i,j} v_i,$$
$$h_{j+1,j} = \|\bar{v}_{j+1}\|,$$
$$v_{j+1} = \bar{v}_{j+1}/h_{j+1,j}.$$

3. Form the approximate solution:

   $x_m = x_0 + V_m y_m$, where y_m minimizes $\|\beta e_1 - H_m y\|$, $y \in R^m$. Here H_m is the $(m+1)$ by m matrix whose only nonzero entries are the elements $h_{i,j}$ defined in step 2. $V_m = [v_1, v_2, \cdots, v_m]$ and the vector e_1 is the first column of the $(m+1) \times (m+1)$ identity matrix.

4. Restart:

   Compute $r_m = b - Ax_m$, if satisfied then stop else compute $x_0 := x_m$, $r_0 := r_m$, $\beta := \|r_0\|$, $v_1 := r_0/\beta$ and go to 2.

If A is not positive real, then $r_0 \perp span\{Ar_0, A^2 r_0, \cdots, A^m r_0\}$ may happen. In this situation the restarted GMRES method is stationary. To avoid this disadvantage, we introduce and analyze a new convergent restarted GMRES method. Conveniently , we use the term CGMRES(m) to denote the method.

2. CGMRES(m)

The linear systems associated with (1.1) can be taken as the following form

$$\begin{bmatrix} I & A \\ -A^T & 0 \end{bmatrix} \begin{bmatrix} u^* \\ x \end{bmatrix} = \begin{bmatrix} f \\ g \end{bmatrix}, \tag{2.1}$$

where $I \in R^{n \times n}$ is the identity matrix , while $u^* \in R^n$ is a given vector and $f = u^* + b, g = -A^T u^* \in R^n$. Since A is nonsingular, thus the system (2.1) has an unique solution $z^* = \begin{bmatrix} u^* \\ x^* \end{bmatrix}$. Let z_0 is the initial approximate solution of (2.1), $B = \begin{bmatrix} I & A \\ -A^T & 0 \end{bmatrix}, \bar{r}_0 = \begin{bmatrix} f \\ g \end{bmatrix} - Bz_0$. Solving the systems (2.1) with GMRES(m),where $m \geq 2$, we have the following results:

Proposition 2.1 Denoting by $\beta_i, i = 1, 2, \cdots, n$, the eigenvalues of $A^T A$ and supposing

$$\beta_1 \geq \beta_2 \geq \cdots \geq \beta_n \geq 1/4, \tag{2.2}$$

then we have that the eigenvalues of matrix B have positive real part.

Proof We have

$$|\lambda I_1 - B| = \begin{vmatrix} (\lambda - 1)I & -A \\ A^T & \lambda I \end{vmatrix}, \tag{2.3}$$

where $I_1 \in R^{2n\times 2n}$ is a identity matrix.If $\lambda = 1$ is the eigenvalue of matrix B,by (2.3),we get

$$\begin{vmatrix} 0 & -A \\ A^T & I \end{vmatrix} = 0.$$

This is a contradiction with that matrix A is nonsingular.Hence,we have $\lambda \neq 1$. According to (2.3) and $\lambda \neq 1$,we have

$$\begin{aligned} |\lambda I_1 - B| &= \begin{vmatrix} (\lambda-1)I & -A \\ A^T & \lambda I \end{vmatrix} \\ &= \begin{vmatrix} (\lambda-1)I & -A \\ 0 & \lambda I + (\lambda-1)^{-1}A^T A \end{vmatrix} \\ &= |(\lambda-1)\lambda I + A^T A|. \end{aligned}$$

If $\{\lambda_{i,j} | i = 1, 2, \cdots, n; j = 1, 2\}$ denote the eigenvalues of B ,then $\lambda_{i,j}, j = 1, 2$, can be given by solving the following equation

$$(\lambda_{i,j} - 1)\lambda_{i,j} + \beta_i = 0, i = 1, 2, \cdots, n, j = 1, 2. \tag{2.4}$$

Solving (2.4) we obtain

$$\lambda_{i,1} = \frac{1 + \sqrt{1 - 4\beta_i}}{2} \tag{2.5}$$

and

$$\lambda_{i,2} = \frac{1 - \sqrt{1 - 4\beta_i}}{2}, \tag{2.6}$$

$i = 1, 2, \cdots, n$. Using (2.2) yields the desired result.

According to [1] and Proposition 2.1,we know that using the restarted GMRES method to solve (2.1) will produce a sequence of approximations which converges to the exact solution of (2.1) when $\beta_i \geq 1/4, i = 1, 2, \cdots, n$. If the conditions $\beta_i \geq 1/4, i = 1, 2, \cdots, n$ do not hold, we can use

Proposition 2.2 Assume that $y_k, k = 1, 2, \cdots, m$ minimizes $\|\beta e_1 - H_k y\|, y \in R^k$, H_k is the $(k+1) \times k$ matrix whose nonzero entries are the elements $h_{i,j}$ defined by GMRES(m) for (2.1),$z_k = z_0 + V_k y_k$ is the approximate solution of (2.1),where $V_k = [v_1, v_2, \cdots, v_k], v_i$ is the Arnoldi vector generated by GMRES(m) for (2.1),$i = 1, 2, \cdots, k,\ k = 1, 2, \cdots, m (m \geq 2)$. Suppose that $z_k = \begin{bmatrix} u_k \\ x_k \end{bmatrix} \in R^{2n}, u_k, x_k \in R^n$ and residual $\bar{r}_k = \begin{bmatrix} f \\ g \end{bmatrix} - Bz_k$,then the following results hold:

(1) $\|\bar{r}_m\|_2 < \|\bar{r}_0\|_2$ and z_k tents to the exact solution $z^* = \begin{bmatrix} u^* \\ x^* \end{bmatrix}$ of (2.1).

(2) x^* is the exact solution of (1.1).

Proof of (1) The residual vector of the approximate solution z_k can be written as

$$\bar{r}_k = \begin{bmatrix} f \\ g \end{bmatrix} - Bz_k = \begin{bmatrix} u^* + b - u_k - Ax_k \\ g + A^T u_k \end{bmatrix} = \begin{bmatrix} \bar{r}_{k1} \\ \bar{r}_{k2} \end{bmatrix}, k = 0, 1, \cdots, m.$$

Suppose further that $\bar{v}_1 = \bar{r}_0/\|\bar{r}_0\|_2 = \begin{bmatrix} \bar{v}_{1,1} \\ \bar{v}_{1,2} \end{bmatrix} \neq 0$. We find

$$\bar{v}_1^T B \bar{v}_1 = \bar{v}_{1,1}^T \bar{v}_{1,1} + \bar{v}_{1,1}^T A \bar{v}_{1,2} - \bar{v}_{1,2}^T A^T \bar{v}_{1,1} = \bar{v}_{1,1}^T \bar{v}_{1,1} \geq 0 \tag{2.7}$$

and if $\bar{v}_{1,1} = 0$,we have

$$\bar{v}_1^T B^2 \bar{v}_1 = \left[-\bar{v}_{1,2}^T A^T, 0\right] \begin{bmatrix} A\bar{v}_{1,2} \\ 0 \end{bmatrix} = -\bar{v}_{1,2}^T A^T A \bar{v}_{1,2} \leq 0 \tag{2.8}$$

Let $K_m = span\{\bar{r}_0, B\bar{r}_0, \cdots, B^{m-1}\bar{r}_0\}$. We have

$$\begin{aligned} \|\bar{r}_m\|_2 &= \min_{z \in K_m} \| \begin{bmatrix} f \\ g \end{bmatrix} - B[z_0 + z]\|_2 \\ &= \min_{z \in K_m} \|\bar{r}_0 - Bz\|_2 \\ &= \min_{y \in R^m} \|\beta \bar{v}_1 - BV_m y\|_2, \end{aligned} \tag{2.9}$$

where $z = V_m y$.
Using $BV_m = V_{m+1}H_m$, we get

$$\min_{y \in R^m} \|\beta \bar{v}_1 - BV_m y\|_2 = \min_{y \in R^m} \|\beta e_1 - H_m y\|_2, \tag{2.10}$$

where e_1 is the first column of the $(m+1) \times (m+1)$ identity matrix. By (2.9) and (2.10),we obtain

$$\|\bar{r}_m\|_2 = \min_{z \in K_m} \|\bar{r}_0 - Bz\|_2 \leq \|\bar{r}_0 - \frac{\beta \bar{v}_1^T B \bar{v}_1}{\|B\bar{v}_1\|_2^2} B\bar{v}_1\|_2. \tag{2.11}$$

Let

$$c_1 = \frac{\beta \bar{v}_1^T B \bar{v}_1}{\|B\bar{v}_1\|_2^2}, R_1 = \bar{r}_0 - c_1 B\bar{v}_1.$$

According to $\bar{v}_{1,1} \neq 0$ and (2.7),we have

$$c_1 > 0, R_1^T B \bar{v}_1 = 0$$

and

$$\begin{aligned} \|\bar{r}_0\|_2 &= \|\bar{r}_0 - c_1 B\bar{v}_1 + c_1 B\bar{v}_1\|_2 \\ &= \sqrt{\|R_1\|_2^2 + c_1^2 \|B\bar{v}_1\|_2^2} > \|R_1\|_2. \end{aligned} \tag{2.12}$$

By (2.11) and (2.12), we can get

$$\|\bar{r}_m\|_2 \leq \|R_1\|_2 < \|\bar{r}_0\|_2. \tag{2.13}$$

In similar way, if $\bar{v}_{1,1} = 0$ then $\bar{v}_{1,2} \neq 0$ we have

$$\|\bar{r}_m\|_2 = \min_{z \in K_m} \|\bar{r}_0 - Bz\|_2 \leq \|\bar{r}_0 - \frac{\beta \bar{v}_1^T B^2 \bar{v}_1}{\|B^2 \bar{v}_1\|_2^2} B^2 \bar{v}_1\|_2, \tag{2.14}$$

where $m \geq 2$.
Let

$$c_2 = \frac{\beta \bar{v}_1^T B^2 \bar{v}_1}{\|B^2 \bar{v}_1\|_2^2}, R_2 = \bar{r}_0 - c_2 B^2 \bar{v}_1.$$

According to $\bar{v}_{1,2} \neq 0$ and (2.8),we have

$$c_2 < 0, R_2^T B^2 \bar{v}_1 = 0$$

and

$$\begin{aligned} \|\bar{r}_0\|_2 &= \|\bar{r}_0 - c_2 B^2 \bar{v}_1 + c_2 B^2 \bar{v}_1\|_2 \\ &= \sqrt{\|R_2\|_2^2 + c_2^2 \|B^2 \bar{v}_1\|_2^2} > \|R_2\|_2. \end{aligned} \tag{2.15}$$

Thus, we can get

$$\|\bar{r}_m\|_2 \leq \|R_2\|_2 < \|\bar{r}_0\|_2. \tag{2.16}$$

Applying (2.13) and (2.16),we know if $\bar{r}_0 \neq 0$ then $\|\bar{r}_m\|_2 < \|\bar{r}_0\|_2$, the result (1) holds.

Proof of (2) Since $z^* = \begin{bmatrix} u^* \\ x^* \end{bmatrix}$ satisfies (2.1),we can find

$$-A^T u^* = g \tag{2.11}$$

and

$$Ax^* = (f - u^*) = b \tag{2.12}$$

By (2.12) we have thus obtained the result (2) .

According to Propositions 2.1 and 2.2, using algorithm GMRES(m) to solve system (2.1), we can obtain and approximate solution of (1.1). Now the CGMRES(m) algorithm can be briefly described as follows:

Algorithm 2: CGMRES(m) for systems (1.1)

1. Start: Choose z_0 and compute $r_0 = \begin{bmatrix} f \\ g \end{bmatrix} - Bz_0$ and $\beta = \|r_0\|$, $v_1 = r_0/\beta$.

2. Iterate: For $j = 1, 2, \cdots, m$ do:

$$h_{i,j} = (Bv_j,\ v_i), \quad i = 1, 2, \cdots, j,$$

$$\bar{v}_{j+1} = Bv_j - \sum_{i=1}^{j} h_{i,j} v_i,$$

$$h_{j+1,j} = \|\bar{v}_{j+1}\|,$$

$$v_{j+1} = \bar{v}_{j+1}/h_{j+1,j}.$$

3. Form the approximate solution of (2.1):

   $z_m = z_0 + V_m y_m$, where $V_m = [v_1, v_2, \cdots, v_m]$ and y_m minimizes $\|\beta e_1 - H_m y\|$, $y \in R^m$. Here H_m is the $(m+1)$ by m matrix whose only nonzero entries are the elements $h_{i,j}$ defined in step 2, and e_1 is the first column of the $(m+1) \times (m+1)$ identity matrix.

4. Form the approximate solution of (1.1):

$$x_m = \left[z^{(n+1)}, z^{(n+2)}, \cdots, z^{(2n)}\right]^T, \text{where } z_m = \left[z^{(1)}, z^{(2)}, \cdots, z^{(2n)}\right]^T$$

5. Restart:

Compute $r_m = b - Ax_m$, if satisfied, then stop , else compute $r_m = \begin{bmatrix} f \\ g \end{bmatrix} - Bz_m$, set $z_0 := z_m, r_0 := r_m$, $\beta := \|r_0\|$, $v_1 := r_0/\beta$, and go to 2.

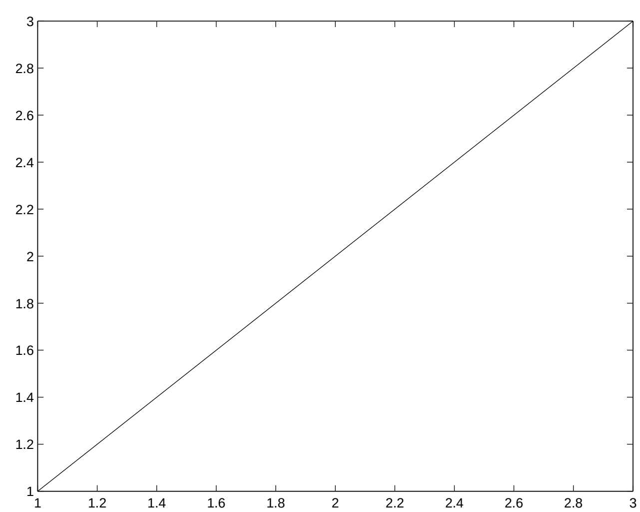
In comparing algorithm CGMRES(m) with GMRES(m) , where $m \geq 2$,it is clear that CGMRES(m) has the all advantages of algorithm GMRES(m) and is a convergent algorithm ,but it needs more storage than is required by GMRES(m) ,and costs nearly as much as by GMRES(m) in each inner loop.

3.Numerical experiments

In this section we report a few numerical experiments comparing the performances of CGMRES(m) with GMRES(m).

Example 1 . Consider $A = Toeplitz([1, -\underline{3.5}, 1, 1, 1]) \in R^{200\times 200}$, where the diagonal element of the matrix underlined .The matrix A has extreme singular value $\sigma_{200} = 4.1375 \times 10^{-11}$ and $\sigma_1 = 5.4955$. Let $b = A[2, 2, \cdots, 2]^T$,$x_0 = [0, 0, \cdots, 0]^T \in R^{200}$, $m = 10$, and $z_0 = [0, 0, \cdots, 0]^T \in R^{400}$. The logarithm of the norm of relative residual is given by $\log_{10}(\|b - Ax_m\|/\|b\|)$. Figure 1 exhibits the convergence histories of GMRES(m) and CGMRES(m) against the number of matrix-vector products.

Example 2 . Consider $A = Toeplitz([1, \underline{0.0}, 1, 1, 1]) \in R^{200\times 200}$, and $b = A[2, 2, \cdots, 2]^T \in R^{200}$,x_0, m, and z_0 as in Example 1. Figure 2 exhibits the convergence histories of GMRES(m) and CGMRES(m) against the number of matrix-vector products.



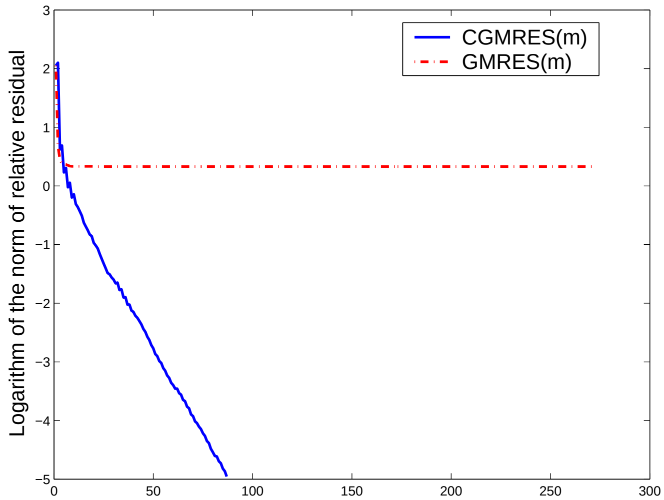


Figure 2: Number of matrix−vector products

4. Conclusion

Algorithm CGMRES(m) is useful especially when GMRES(m) is stationary . It can avoid stagnation arising from algorithm GMRES(m).However, we can't draw the conclusion that the convergence rate of CGMRES(m) is faster than GMRES(m) when GMRES(m) is convergent.

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