



Global Range Restricted GMRES for Linear Systems with Multiple Right Hand Sides

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Abstract

This work concerns the solution of non-symmetric, sparse linear systems with multiple right hand sides by iterative methods. Herein a global version of the range restricted generalized minimal residual method (RRGMRES) is proposed for solving this sort of problems. Numerical results confirm that this new algorithm is applicable.

Keywords: Krylov subspace; GMRES; Range restricted GMRES; Multiple right hand sides

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1. Introduction

There are many applications for the solution of several sparse linear system of equations

$$Ax^{(i)} = b^{(i)}, \quad i = 1, \dots, s, \quad (1)$$

with the same $n \times n$ matrix A , but s different right hand sides $b^{(i)}$, $i = 1, \dots, s$. If all the right hand sides are available simultaneously, these s linear systems can be combined in a block form as:

$$AX = B, \quad (2)$$

where

$$X = [x^{(1)}, \dots, x^{(s)}] \text{ and } B = [b^{(1)}, \dots, b^{(s)}].$$

Several iterative methods have been proposed for finding the solution of such a problem. There are some block iterative methods like the block conjugate gradient (BI-CG) proposed by O'Leary (1980), and its variants Nikishin and Yeregin (1995), Saad (1987), to solve (2) when the matrix A is symmetric and positive definite. In last years, block Krylov subspace methods have been proposed for nonsymmetric problems. One of the most important methods for this aim is the block GMRES (BGMRES) Simoncini and Gallopoulos (1995, 1996). Similarly, several block iterative methods like block quasi minimal residual (BQMR) as well as block BiCGSTAB have been developed for nonsymmetric matrices Chan and Wang (1997), Cullum and Donath (1974), Freund and Malhotra (1997), Golub and Underwood (1977), Guennouni et al. (2003). The main goals of these methods are not only to reach the solution faster than solving s separate linear system of equations, but also to reduce the required computations. However, in BGMRES, block Arnoldi process is applied to generate an orthogonal basis that still requires higher computation and storage than the new methods.

In this context, Jbilou et al. (1999) proposed global GMRES (GI-GMRES) method with less arithmetic computation and storage requirement. Surprisingly, in this case, a real hessenberg least square problem with low dimension must be solved whilst in BGMRES, the corresponding least square matrix, which is used to reduce dimension A , is a block hessenberg matrix. Therefore, solving a least square problem with real elements is much easier than such problem with block matrices as its elements. After proposing GI-GMRES, some researchers have developed this method in different aspects Bellalij et al. (1991), Lin (2005). However, GMRES Saad and Schultz (1986), is a popular iterative method for solving nonsymmetric linear systems with variety of implementations such as simpler GMRES Walker (1994), GMRES with householder implementation Walker (1988), range restricted GMRES Calvetti et al. (2000, 2001) as well as generalization and modification GMRES methods Chen et al. (1999), that each implementation is practical for a set of problems. Among these variants, range restricted GMRES (RRGMRES) has been introduced for ill-posed linear system of equations. Here, this version of GMRES is considered for solving (2).

The outline of this paper is as follows: In Section 2, global GMRES is described briefly. In Section 3, a new global GMRES is explained with some explanations. Numerical experiment is in the next Section.

Throughout this paper, the following notations are used. Let $E = \mathbb{R}^{n \times s}$ to denote the vector space, on the field \mathbb{R} of matrices with dimension $n \times s$. For two vectors X and Y in E , and the inner product $\langle X, Y \rangle_F = tr(X^T Y)$, where $tr(Z)$ is the trace of square matrix Z and X^T is the transpose of the matrix X , are defined. The associated norm is the well-known Frobenius norm denoted by $\|\cdot\|_F$. For a matrix $V \in E$, the Krylov subspace $K_k(A, V)$ is defined by

$$K_k(A, V) = span \{V, AV, A^2V, \dots, A^{k-1}V\}.$$

A set of vectors is said to be F-orthonormal if it is orthonormal with respect to the scalar product $\langle \cdot, \cdot \rangle_F$.

1. GI-GMRES for solving matrix equations

GI-GMRES algorithm for multiple right hand side problems (2) was recently proposed by Jbilou et al. (1999). Here, let us recall a brief description of GI-GMRES. At first step, this method needs to generate a set of F-orthonormal vectors by the global Arnoldi orthogonalization procedure to project the square matrix A into an $(k + 1) \times k$ upper hessenberg matrix. So, the algorithm of global Arnoldi process, required for this aim, is written below:

Algorithm 2.1. Global Arnoldi process

1. Choose $V_1 \in E$ with $\|V_1\|_F = 1$.

2. For $j = 1, \dots, k$ do

$$V_{j+1} = AV_j,$$

For $i = 1, \dots, j$ do

$$h_{i,j} = \text{tr}(V_{j+1}^T V_i),$$

$$V_{j+1} = V_{j+1} - h_{i,j} V_i,$$

End

$$h_{j+1,j} = \|V_{j+1}\|_F,$$

$$V_{j+1} = V_{j+1} / h_{j+1,j},$$

End.

In this algorithm, the matrices $V_i \in E, i = 1, \dots, k, k + 1$ are F-orthonormal while the elements $h_{i,j}$ are real numbers. This algorithm will stagnate at step $j, (j < k)$, if $h_{j+1,j} < \varepsilon$ computationally. Here and throughout this paper W_k is denoted for the $n \times ks$ matrix $W_k = [V_1, \dots, V_k]$, \bar{H}_k is the $(k + 1) \times k$ upper Hessenberg matrix with nonzero entries $h_{i,j}$ and $\bar{H}_{\cdot,j}$ will show the j th column of \bar{H}_k . Notice that in block GMRES, the corresponding block hessenberg matrix \bar{H}_k is of dimension $(k + 1)s \times ks$ whilst in global GMRES this matrix is $(k + 1) \times k$. Then BGMRES needs much more storage and computation requirements than GI-GMRES for generating an orthonormal basis set of vectors for $K_k(A, V_1)$. To know better about global Arnoldi algorithm and its properties, the following definitions and propositions are useful.

Definition 2.2.

The grade of an $n \times s$ matrix $V \in E$ is the degree of the nonzero monic polynomial P with lowest degree that $P(A)V = 0$.

Definition 2.3.

Given $\alpha = [\alpha_1, \dots, \alpha_k]$ in R^k the symbol $*$ denotes the following

$$W_k * \alpha = \sum_{i=1}^k \alpha_i V_i, \quad (3)$$

and similarly

$$W_k * \bar{H}_k = [W_k * \bar{H}_{.,1}, W_k * \bar{H}_{.,2}, \dots, W_k * \bar{H}_{.,k}]. \quad (4)$$

From global Arnoldi process the following properties are also concluded.

Proposition 2.4.

If the global Arnoldi process does not breakdown until k th iterate, then the set $\{V_1, \dots, V_k\}$ is an F-orthonormal basis for the Krylov subspace $K_k(A, V_1)$.

Proposition 2.5.

The global Arnoldi process will stagnate at step k if the grade of V_1 is k .

The proofs of these two propositions are similar to those for the Arnoldi algorithm applied on a linear system with single right side Saad (1995, 1986).

Proposition 2.6.

For the matrix W_k and a real vector α , we have

$$\|W_k * \alpha\|_F = \|\alpha\|_2. \quad (5)$$

Proof:

From Definition 2.2, $W_k * \alpha = \sum_{i=1}^k \alpha_i V_i$, and the fact that the matrices $V_i, i = 1, \dots, k$ are F-orthonormal, i.e., $\langle V_i, V_j \rangle_F = \delta_{i,j}$, we have:

$$\|W_k * \alpha\|_F^2 = \left\langle \sum_{i=1}^k \alpha_i V_i, \sum_{i=1}^k \alpha_i V_i \right\rangle_F = \sum_{i=1}^k \alpha_i^2 = \|\alpha\|_2^2.$$

Proposition 2.7.

From the global Arnoldi algorithm, the following reduction relation is held

$$A W_k = W_{k+1} * \bar{H}_k, \tag{6}$$

where W_k and \bar{H}_k be as defined before and $W_{k+1} = [W_k \ V_{k+1}]$.

Proof:

Refer to Jbilou et al. (1999).

The global GMRES algorithm is summarized as follows.

Algorithm 2.8. Global GMRES

1. Choose X_0 , compute $R_0 = B - A X_0$, $\beta = \|R_0\|$ and set $V_1 = R_0 / \beta$.
2. For $j = 1, \dots, k$ run algorithm 1 with V_1 to build the F-orthonormal basis set $\{V_1, \dots, V_{k+1}\}$.
3. Compute $X_k = X_0 + W_k * \bar{y}$ where $\bar{y} = \arg \min_{y \in \mathbb{R}^k} \|\beta e_1 - \bar{H}_k \bar{y}\|$.

In global GMRES, the iterate $X_k = X_0 + \bar{Z} \in X_0 + K_k(A, R_0)$ is computed so that the vector \bar{Z} minimizes the residual Frobenius norm over $K_k(A, R_0)$, i.e.

$$\|R_k\|_F = \|R_0 - A\bar{Z}\|_F = \min_{Z \in K_k(A, R_0)} \|R_0 - AZ\|_F. \tag{7}$$

By multiplying W_{k+1} into $R_k = R_0 - A\bar{Z}$ with respect to product $*$, we have

$$\begin{aligned} W_{k+1} * R_k &= W_{k+1} * R_0 - W_{k+1} A\bar{Z} \\ &= \beta e_1 - \bar{H}_k W_k \bar{y}, \end{aligned}$$

because of $W_{k+1} * R_0 = \|R_0\|_F e_1$, and (6) where $e_1 = (1, 0, \dots, 0)^T \in \mathbb{R}^{k+1}$.

So, in global GMRES, this minimizing problem is transferred into an upper Hessenberg least square problem

$$\min_{y \in \mathbb{R}^k} \left\| \beta e_1 - \bar{H}_k y \right\|_2. \quad (8)$$

$$\|R_k\|_F = \min_{y \in \mathbb{R}^k} \left\| \beta e_1 - \bar{H}_k y \right\|_2. \quad (9)$$

For solving (8), Givens rotations are mainly used to transform (8) into an upper triangular linear system of equations of order k .

2. Global RRGMRES for multiple right hand side equations

The Range Restricted GMRES (RRGMRES) method proposed by Calvetti et al. (2000, 2001), is a variant of GMRES that has some advantages over standard GMRES. RRGMRES uses the Krylov subspace $K_k(A, AR_0) = AK_k(A, r_0)$ for the problem $Ax = b$ with one right side vector $b \in \mathbb{R}^n$. In this method, the Arnoldi decomposition algorithm is started with $v_1 = Ar_0 / \|Ar_0\|$ instead of $v_1 = r_0 / \|r_0\|$. Therefore the computed solution will be restricted to the range of A , i.e. $\mathfrak{R}(A)$, because $K_k(A, AR_0) \subseteq \mathfrak{R}(A)$ and this is the reason it is named as range restricted GMRES.

In this paper, the RRGMRES technique is applied for linear systems of equations with multiple right hand sides and this method will be the global RRGMRES (GI-RRGMRES). Let $X_0 \in E$ be the initial matrix guess and $R_0 = B - AX_0$ is the corresponding residual. Here, the global Arnoldi process is started with $V_1 = AR_0 / \|AR_0\|_F$ to generate the F-orthonormal basis set $\{V_1, \dots, V_k\}$ for the new Krylov subspace $K_k(A, AR_0)$. The iterates X_k , $k \geq 1$ computed by GI-RRGMRES satisfy

$$\|B - AX_k\| = \min_{X \in X_0 + K_k(A, AR_0)} \|B - AX\| = \min_{Z \in K_k(A, AR_0)} \|R_0 - AZ\|, \quad (10)$$

where

$$K_k(A, AR_0) = \text{span} \{AR_0, A^2R_0, \dots, A^kR_0\} \text{ and } X_k = X_0 + Z.$$

Global RRGMRES is relatively similar to global GMRES in many steps. Therefore, the Arnoldi reduction relation $AW_k = W_{k+1}\bar{H}_k$ is held for

$$W_k = [V_1, \dots, V_k], \quad W_{k+1} = [W_k \quad V_{k+1}],$$

and the $(k+1) \times k$ coefficients of the Hessenberg matrix $\bar{H}_k = (h_{i,j})$.

Now, for an arbitrary matrix $X = X_0 + Z$ where $Z \in K_k(A, AR_0)$, the matrix $Z \in K_k(A, AR_0)$ is determined by the following linear combination

$$Z = \sum_{i=1}^k y_i V_i = W_k * y, \tag{11}$$

for some vector $y \in \mathbb{R}^k$, because $\{V_1, \dots, V_k\}$ is a basis for $K_k(A, AR_0)$. Thus, by using (6), the following relation is obtained

$$R_0 - AZ = R_0 - (AW_k) * y = R_0 - W_{k+1} * (\bar{H}_k y). \tag{12}$$

To reach to RRGMRES condition for projecting goal, we multiply both sides of (12) by the $n \times (k + 1)$ s matrix $W_{k+1} = [V_1, \dots, V_k, V_{k+1}]$ using the product $*$.

Let:

$$W_{k+1} * R = u = \begin{pmatrix} u(1) \\ u(2) \\ \vdots \\ u(k+1) \end{pmatrix} = \begin{pmatrix} tr(V_1^T R) \\ tr(V_2^T R) \\ \vdots \\ tr(V_{k+1}^T R) \end{pmatrix} \in \mathbb{R}^{k+1}. \tag{13}$$

So, from (5), (12) and (13), the following relation is determined:

$$W_{k+1} * R = W_{k+1} * (R_0 - AZ) = u_0 - \bar{H}_k y. \tag{14}$$

$$\|R_k\|_F = \min_{y \in \mathbb{R}^k} \|u_0 - \bar{H}_k y\|. \tag{15}$$

To compute the iterate $X_k, k \geq 1$, by global RRGMRES, the residual norm has to be minimized over $K_k(A, AR_0)$. Thus, the corresponding residual F-norm is

$$\|R_k\|_F = \|B - AX_k\|_F = \min_{X \in X_0 + K_k(A, AR_0)} \|B - AX\|_F = \|u_0 - \bar{H}_k \bar{y}\|_2,$$

where

$$\bar{y} = \operatorname{argmin}_{y \in \mathbb{R}^k} \|u_0 - \bar{H}_k y\|.$$

From the above, the following theorem is concluded.

Theorem 3.1.

In GI-RRGMRES, the optimum iterative solution $X_k = X_0 + \bar{Z}$, for $k \geq 1$, satisfies $X_k = X_0 + K_k(A, AR_0)$, where:

$$\|R_k\|_F = \|R_0 - A\bar{Z}\|_F = \min_{y \in \mathbb{R}^k} \|u_0 - \bar{H}_k y\|_2,$$

and

$$X_k = X_0 + W_k * \bar{y}, \text{ where } \bar{y} = \operatorname{argmin}_{y \in \mathbb{R}^k} \|u_0 - \bar{H}_k y\|.$$

Now, the global RRGMRRES algorithm is as follows:

Algorithm 3.2. Global RRGMRRES

1. Choose X_0 , compute $R_0 = B - A X_0$, $\beta = \|AR_0\|$ and set $V_1 = AR_0 / \beta$.
2. For $j = 1, \dots, k$ run algorithm 1 with V_1 to build the basis set $\{V_1, V_2, \dots, V_{k+1}\}$.
3. Compute $X_k = X_0 + W_k * y_k$ where

$$y_k = \operatorname{argmin}_{y \in \mathbb{R}^k} \|u_0 - \bar{H}_k y\|, \text{ and } u_0 = W_{k+1} * R_0.$$

Suppose matrix A is (nearly) singular. The following theorem about GI-RRGMRES is derived.

Theorem 3.3.

Apply GI-RRGMRES on (2) until breakdown at step k . If $\operatorname{rank}(A) = k - 1$ and $\dim AK_{k-1}(A, AR_0) = k - 1$, then global RRGMRRES produces a least square solution of (2).

Proof:

By substituting $\|\cdot\|_F$ and $\langle \cdot, \cdot \rangle_F$ instead of ordinary vector product $\|\cdot\|_2$ and $\langle x, y \rangle = x^T y$ into the proof of theorem A2 in Cao and Wang (2002), it is proved.

3. Numerical experiments

The aim of this Section is to illustrate the convergence performance of global RRGMRRES for some linear system of equations with multiple right hand sides. All codes were written in Matlab and the experiments are done on 2.2 GHz personal computer with 1GB of RAM.

In all experiments, the right hand side matrix B is chosen so that the random matrix X of dimension $n \times s$ with values uniformly distributed in the interval $[-5,5]$, determined by the Matlab code $X = 5 * randn(n,s)$, is the solution of $AX = B$. The initial guess X_0 is taken to be $X_0 = zeros(n,s)$. The convergence tolerance $\varepsilon = 10^{-10}$ is considered with the stopping criterion $\|R_k\|_F < \varepsilon$. For each example, the figures show $\log_{10}(\|R_k\|_F)$ versus the number of iterations.

Example 4.1.

The matrix A is obtained by first discretizing the Poisson equation:

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) u(x, y) = f(x, y) \text{ for } (x, y) \in \Omega = [0,1] \times [0,1],$$

with Neumann boundary conditions:

$$\frac{\partial}{\partial x} u(x, y) = \phi(x, y) \text{ on } \partial\Omega,$$

on a uniform grid of mesh size $h = 1/M$ via central differences, and then by taking the unknowns in the red-black ordering. This matrix is explicitly written down in Saberi Najafi and Zareamoghaddam (2008), Sidi (2001) and it was considered therein for testing other GMRES implementations.

In our numerical experiments for this exam, we took $M = 39$ which the corresponding square matrix A is in order of 1600. The matrix $X = 5 * randn(1600,20)$ is chosen as the exact solution of (1) and the restart number is $k = 50$.

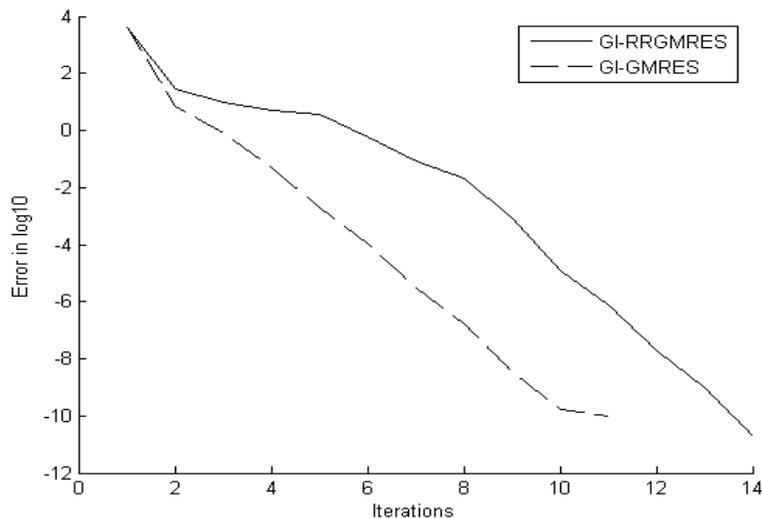


Figure 1. Graph of the residual for Example 4.1 with $A \in \mathbb{R}_{1600 \times 1600}$ and $X, B \in \mathbb{R}_{1600 \times 20}$

Figure 1, shows that both implementations perform well in the particular case of 20 different right hand sides. We know that for the problems with a single hand side the convergence speed of standard GMRES is a little faster than RRGMRES and this issue is repeated here too.

Example 4.2.

In this example, matrix A has the following structure:

$$A = \begin{pmatrix} 1 & 0 & 0.5 & & & \\ & 1 & 0 & \ddots & & \\ & & \ddots & \ddots & 0.5 & \\ & & & \ddots & 0 & \\ 1 & & & & & 1 \end{pmatrix} \in \mathbb{R}^{1000 \times 1000}.$$

This matrix is approximately upper triangular. The right hand side matrix B is chosen so that $X = 5 * \text{randn}(1000, 30)$ be the exact solution of (2). Figure 2, shows the behavior of residual norms of global GMRES implementations.

In this example, the restart number is $k = 30$. It can be seen from the graph that global RRGMRES reaches to the solution after 3 iterations similarly to the results of global GMRES. It is interesting that both of these methods solve a system of linear equations with 30 different right hand side vectors by the restart number $k = 30$ (e.g. GI-GMRES (30)) just after 3 outer iterates that shows these methods are powerful for solving such problems.

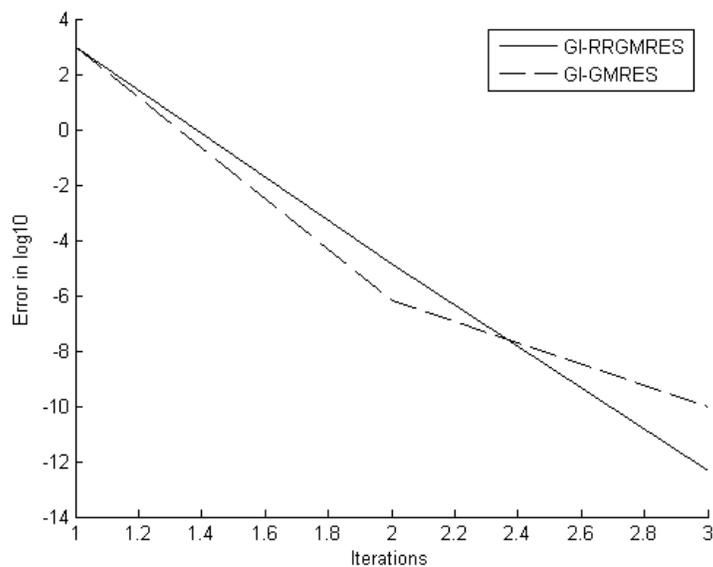


Figure 2. Graph of the residual for Example 4.2 with $A \in \mathbb{R}^{1000 \times 1000}$ and $X, B \in \mathbb{R}^{1000 \times 30}$

RRGMRES is a good iterative solver for ill-posed problems. The next problem, which has a singular square matrix A for even integers, is selected from Brown (1991).

4. Conclusion

RRGMRES is a variant of GMRES for solving linear equations with single right side which looks for the solution through the range of square matrix A . In this paper, a global RRGMRRES was proposed for solving linear system of equations with multiple right hand sides. GI-RRGMRES is not always as fast as GI-GMRES, however performs better when the square matrix is ill-posed or singular.

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