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Global FOM and GMRES algorithms for matrix equations

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Abstract

In the present paper, we present new methods for solving nonsymmetric linear systems of equations with multiple right-hand sides. These methods are based on global oblique and orthogonal projections of the initial matrix residual onto a matrix Krylov subspace. We first derive the global full orthogonalization method and give its properties. The second method which is a global orthogonal projection method is the global generalized minimum residual method. We then give some properties of this new algorithm. We also show how to apply these methods for solving the Lyapunov matrix equation. Finally, numerical examples will be given.

Keywords: Global Arnoldi; Matrix Krylov subspace; Block methods; Iterative methods; Nonsymmetric linear systems; Multiple right-hand sides

1. Introduction

Many applications require the solution of several sparse systems of linear equations

$$Ax^{(i)} = b^{(i)}, \quad i = 1, \ldots, s, \tag{1.1}$$

with the same coefficient matrix and different right-hand sides. When all the $b^{(i)}$s are available simultaneously, Eq. (1.1) can be written as

$$A\,X = B, \tag{1.2}$$

where A is an $N \times N$ real matrix, B and X are $N \times s$ rectangular matrices whose columns are $b^{(1)}, b^{(2)}, \ldots, b^{(s)}$ and $x^{(1)}, x^{(2)}, \ldots, x^{(s)}$, respectively. In practice, s is of moderate size $s \ll N$.

When A is symmetric and positive definite, the block conjugate gradient (Bl-BCG) algorithm of O'Leary [12] and its variants [11], are useful for solving the linear system (1.2). For nonsymmetric problems, some block Krylov subspace methods have been developed these last years. The most

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important ones, are the block biconjugate gradient (Bl-BCG) [12], the block generalized minimal residual (BGMRES) algorithm introduced by Vital [23] and studied by Simoncini and Gallopoulos [20] and the block quasi minimum residual (Bl-QMR) algorithm [4,9]; see also [3,5]. All these block Krylov subspace methods converge in at most $\lceil N/s \rceil$ iterations. The purpose of the block methods is to solve the problem (1.2) faster than solving each system separately.

Another alternative to those block solvers, is to use a single system called the seed system and generate by some method the corresponding Krylov subspace. Then, we project the residuals of the other systems onto this Krylov subspace. The process is repeated with an other seed system until all the systems are solved. This procedure has been used by Smith and al. [21] and Chan and Wang [2] for the conjugate gradient method. When the matrix A is nonsymmetric, Simoncini and Galopoulos [19] combined this technique with hybrid methods developed in [10], using the GMRES algorithm [17]. We note that this procedure is also attractive when the right-hand sides of (1.1) are not available at the same time; see [13,14,22].

In the present paper, we give a new alternative for solving the problem (1.2). Our iterative methods will be defined as global orthogonal and oblique projection methods onto a matrix Krylov subspace. The global full orthogonalization method (Gl-FOM) and the global generalized minimum residual method (Gl-GMRES) are obtained by projecting globally the initial matrix residual onto a matrix Krylov subspace. When solving one linear system of equations, these global methods reduce to the well known FOM and GMRES methods.

We also use these global methods for solving matrix equations such as the well known Lyapunov matrix equation $AX + XA^{\mathrm{T}} = -B$.

Throughout this paper, we use the following notations. Let $\mathbb{E} = \mathbb{M}_{N,s}$ denotes the vector space, on the field $\mathbb{R}$, of rectangular matrices of dimension $N \times s$. For X and Y two vectors in $\mathbb{E}$, we define the following inner product $\langle X, Y\rangle_F = \mathrm{tr}(X^{\mathrm{T}} Y)$, where $\mathrm{tr}(Z)$ denotes the trace of the square matrix Z and X^{T} the transpose of the matrix X. The associated norm is the well-known Frobenius norm denoted by $\|\cdot\|_F$. For a vector $V \in \mathbb{E}$, the matrix Krylov subspace $\mathcal{K}_m(A, V)$ is the subspace of $\mathbb{E}$ generated by the vectors (matrices) $V, AV, \ldots, A^{m-1}V$. Unless specified, the Frobenius norm will be used for matrices and vectors. A system of vectors of $\mathbb{E}$ is said to be F-orthogonal if it is orthogonal with respect to the scalar product $\langle\cdot,\cdot\rangle_F$.

The paper is organized as follows. In Section 2, we define the global Arnoldi algorithm and give some properties. Using this algorithm, we introduce in Section 3 the Gl-FOM methods. Section 4 describes the Gl-GMRES and some properties. This section ends with a theoretical comparison between the Gl-FOM and Gl-GMRES. In Section 5 we apply the global GMRES for solving the matrix Lyapunov equation. The last section reports on some numerical examples.

2. Global Arnoldi process

Let V be an $N \times s$ rectangular matrix and consider the matrix Krylov subspace $\mathcal{K}_k(A, V) = \mathrm{span}\{V, AV, \ldots, A^{k-1}V\}$. We note that $Z \in \mathcal{K}_k(A, V)$ means that

$$Z = \sum_{i=0}^{k-1} \alpha_i A^i V.$$

We recall that the minimal polynomial of $V \in \mathbb{E}$ is the nonzero monic polynomial of lowest degree such that $P(A)V = 0$. The degree of this polynomial is called the grade of V.

The global Arnoldi algorithm constructs an F-orthonormal basis $V_1, V_2, \ldots, V_k$, i.e., $\mathrm{tr}(V_i^{\mathrm{T}} V_j) = 0$ for $i \neq j$, $i, j = 1, \ldots, k$, and $\mathrm{tr}(V_i^{\mathrm{T}} V_i) = 1$, of the Krylov subspace $\mathcal{K}_k(A, V)$. The algorithm is described as follows:

Algorithm 2.1. Global Arnoldi algorithm

1. Choose an $N \times s$ matrix V_1 such that $\|V_1\|_F = 1$.
2. For $j = 1, \ldots, k$
   $h_{i,j} = \mathrm{tr}(V_i^{\mathrm{T}} A V_j)$, $i = 1, \ldots, j$,
   $\widetilde{V}_j = AV_j - \sum_{i=1}^{j} h_{i,j} V_i$,
   $h_{j+1,j} = \|\widetilde{V}_j\|_F$; if $h_{j+1,j} = 0$ stop,
   $V_{j+1} = \widetilde{V}_j / h_{j+1,j}$.

For the global Arnoldi algorithm, we have the following propositions:

Proposition 1. *If the global Arnoldi algorithm does not stop before the kth step, then the block system $\{V_1, V_2, \ldots, V_k\}$ is an F-orthonormal basis of the matrix Krylov subspace $\mathcal{K}_k(A, V_1)$.*

Proposition 2. *The global Arnoldi algorithm will stop at step m if and only if the grade of V_1 is m.*

The proofs of these propositions are similar to those given in [16] for the classical Arnoldi algorithm.

Let us now introduce some notations. $\mathcal{V}_k$ will denote the $N \times ks$ matrix: $\mathcal{V}_k = [V_1, V_2, \ldots, V_k]$. $\widetilde{H}_k$ denotes the $(k+1) \times k$ upper Hessenberg matrix whose nonzero entries $h_{i,j}$ are defined by Algorithm 2.1 and H_k is the $k \times k$ matrix obtained from $\widetilde{H}_k$ by deleting its last row. $H_{.,j}$ will denote the jth column of the matrix H_k. Note that the block matrix $\mathcal{V}_k$ is F-orthonormal which means that the blocks $V_1, \ldots, V_k$ are orthonormal with respect to the scalar product defined earlier.

Remark that the Hessenberg matrix H_k in the global Arnoldi algorithm is of dimension $k \times k$ while for the block Arnoldi algorithm [18], H_k is a block Hessenberg matrix of dimension $ks \times ks$. This is an important difference between the two procedures.

Next, we use the notation $*$ for the following product:

$$\mathcal{V}_k * \alpha = \sum_{i=1}^{k} \alpha_i V_i, \tag{2.1}$$

where $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_k)^{\mathrm{T}}$ is a vector of $\mathbb{R}^k$ and, by the same way, we set

$$\mathcal{V}_k * H_k = [\mathcal{V}_k * H_{.,1}, \mathcal{V}_k * H_{.,2}, \ldots, \mathcal{V}_k * H_{.,k}]. \tag{2.2}$$

It is easy to see that the following relations are satisfied:

$$\mathcal{V}_k * (\alpha + \beta) = (\mathcal{V}_k * \alpha) + (\mathcal{V}_k * \beta) \quad \text{and} \quad (\mathcal{V}_k * H_k) * \alpha = \mathcal{V}_k * (H_k \alpha), \tag{2.3}$$

where α and β are two vectors of $\mathbb{R}^k$. Using these notations, we have the following result which will be used later.

Proposition 3. *Let $\mathcal{V}_k$ be the matrix defined by $\mathcal{V}_k = [V_1, V_2, \ldots, V_k]$ where the $N \times s$ matrices V_i, $i = 1, \ldots, k$, are defined by the global Arnoldi algorithm. Then we have*

$$\|\mathcal{V}_k * \alpha\|_F = \|\alpha\|_2, \tag{2.4}$$

where α is a vector of $\mathbb{R}^k$.

Proof. From the definition of the product $*$, we have $\mathcal{V}_k * \alpha = \sum_{i=1}^{k} \alpha_i V_i$, and then

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

But, since the matrices V_i, $i = 1, \ldots, k$, are orthonormal with respect to the scalar product $\langle \cdot, \cdot \rangle_F$, it follows that

$$\|\mathcal{V}_k * \alpha\|_F^2 = \sum_{i=1}^{k} \alpha_i^2 = \|\alpha\|_2^2. \qquad \square$$

Theorem 1. *Let $\mathcal{V}_k$, H_k and $\widetilde{H}_k$ as defined before, then using the product $*$, the following relations hold:*

$$A\,\mathcal{V}_k = \mathcal{V}_k * H_k + Z_{k+1}, \tag{2.5}$$

where $Z_{k+1} = h_{k+1,k}\,[0_{N\times s}, \ldots, 0_{N\times s}, V_{k+1}]$, and

$$A\,\mathcal{V}_k = \mathcal{V}_{k+1} * \widetilde{H}_k. \tag{2.6}$$

Proof. From the global Arnoldi algorithm, we have

$$AV_j = \sum_{i=1}^{j+1} h_{i,j} V_i, \quad j = 1, \ldots, k,$$

where $h_{i,j} = \mathrm{tr}(V_i^{\mathrm{T}} A V_j)$. Using the block matrix $\mathcal{V}_k = [V_1, \ldots, V_k]$ and the product $*$ defined below, the preceding relation can be written as

$$A\,\mathcal{V}_k = \mathcal{V}_k * H_k + h_{k+1,k}\,[0_{N\times s}, \ldots, 0_{N\times s}, V_{k+1}].$$

To prove the relation (2.6), consider the product

$$\mathcal{V}_{k+1} * \widetilde{H}_k = [\mathcal{V}_k; V_{k+1}] * \begin{pmatrix} H_k \\ u_{k+1} \end{pmatrix}, \quad \text{with } u_{k+1} = (0, \ldots, 0, h_{k+1,k}).$$

Developing this product, we get

$$\mathcal{V}_{k+1} * \widetilde{H}_k = \mathcal{V}_k * H_k + h_{k+1,k}\,[0_{N\times s}, \ldots, 0_{N\times s}, V_{k+1}].$$

Hence from the relation (2.5), it follows that

$$A\,\mathcal{V}_k = \mathcal{V}_{k+1} * \widetilde{H}_k. \qquad \square$$

It is known that the Arnoldi algorithm which is based on the Gram–Schmidt process is not stable numerically. The modified version based on the modified Gram–Schmidt process for the global Arnoldi algorithm is given as follows:

Algorithm 2.2. Modified global Arnoldi algorithm

1. Choose an $N \times s$ matrix V_1 such that $\|V_1\|_F = 1$.
2. For $j = 1, \ldots, k$
   $\widetilde{V} = AV_j$,
   for $i = 1, 2, \ldots, j$,
   $h_{i,j} = \mathrm{tr}(V_i^{\mathrm{T}} \widetilde{V})$,
   $\widetilde{V} = \widetilde{V} - h_{i,j} V_i$,
   $h_{j+1,j} = \|\widetilde{V}\|_F$,
   $V_{j+1} = \widetilde{V} / h_{j+1,j}$.

The drawback with the Arnoldi algorithm is that firstly it becomes expensive as the dimension of the Krylov subspaces involved increase. The second drawback is the fact that we have to save all the previous vectors (blocks). A first possibility to overcome these drawbacks is to restart the algorithm and a second one is to use an incomplete orthogonalization of the blocks. These strategies have been used by Saad [16] to compute a few eigenpairs or for solving nonsymmetric linear systems. This was also applied for the block Arnoldi algorithm as described in [18] to obtain a banded block upper Hessenberg matrix.

3. The global full orthogonalization method

Consider the block linear system of equations (1.2) and let X_0 be an initial $N \times s$ matrix guess to the solution X and $R_0 = B - AX_0$ its associated residual. At the kth iterate, a correction Z_k is determined in the matrix Krylov subspace $\mathcal{K}_k = \mathcal{K}_k(A, R_0)$ such that the new residual is F-orthogonal to $\mathcal{K}_k$. This yields to

$$X_k - X_0 = Z_k \in \mathcal{K}_k \tag{3.1}$$

and

$$R_k = R_0 - AZ_k \perp_F \mathcal{K}_k. \tag{3.2}$$

Note that R_k is obtained by projecting R_0 onto $A\mathcal{K}_k$ along the F-orthogonal of the Krylov subspace $\mathcal{K}_k$. If $\mathcal{Q}_k$ denotes the projector onto $A\mathcal{K}_k$ along $\mathcal{K}_k^{\perp}$, then from the Galerkin relation (3.2), we have

$$R_k = R_0 - \mathcal{Q}_k R_0. \tag{3.3}$$

$Z_k \in \mathcal{K}_k$ can be written as $Z_k = \mathcal{V}_k * y_k$, where y_k is any vector in $\mathbb{R}^k$. Hence the residual R_k is given by

$$R_k = R_0 - A\mathcal{V}_k * y_k. \tag{3.4}$$

Now, since R_k is F-orthogonal to $\mathcal{K}_k$, we get

$$\langle V_i, R_0 \rangle_F = \langle V_i, A\mathcal{V}_k * y_k \rangle_F, \quad i = 1, \ldots, k, \tag{3.5}$$

where $\{V_1, V_2, \ldots, V_k\}$ is the global Arnoldi F-orthonormal basis of the matrix Krylov subspace $\mathcal{K}_k$. Using (2.3) and (2.5), the linear system (3.5) can be written as

$$H_k\, y_k = \|R_0\|_F\, e_1^{(k)}, \tag{3.6}$$

where $e_1^{(k)}$ is the first canonical basis vector in $\mathbb{R}^k$ and H_k is the $k \times k$ upper Hessenberg matrix defined as

$$H_k = \begin{pmatrix} \operatorname{tr}(V_1^{\mathrm{T}} A V_1) & \operatorname{tr}(V_1^{\mathrm{T}} A V_2) & & \ldots & \operatorname{tr}(V_1^{\mathrm{T}} A V_k) \\ \operatorname{tr}(V_2^{\mathrm{T}} A V_1) & \operatorname{tr}(V_2^{\mathrm{T}} A V_2) & & \ldots & \operatorname{tr}(V_2^{\mathrm{T}} A V_k) \\ 0 & \operatorname{tr}(V_3^{\mathrm{T}} A V_2) & & \ldots & \operatorname{tr}(V_3^{\mathrm{T}} A V_k) \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \ldots & 0 & \operatorname{tr}(V_k^{\mathrm{T}} A V_{k-1}) & \operatorname{tr}(V_k^{\mathrm{T}} A V_k) \end{pmatrix}.$$

From the relation (3.6), we see that at step k, we have to solve only one $k \times k$ linear system to get the k-dimensional vector y_k and then $X_k = X_0 + \mathcal{V}_k * y_k$. Using the global Arnoldi algorithm to determine an F-orthonormal basis of $\mathcal{K}_k$, the global full orthogonalization method (Gl-FOM) is summarized as follows:

Algorithm 3.1. Global full orthogonalization method

1. Choose X_0 and set $V_1 = R_0/\|R_0\|_F$.
2. At step k use the global Arnoldi algorithm to get an F-orthonormal basis of $\mathcal{K}_k$.
3. Form the approximation: $X_k = X_0 + \mathcal{V}_k * y_k$ with $H_k\, y_k = \|R_0\|_F\, e_1^{(k)}$.

As for the classical full orthogonalization method (FOM) the norm of the residual at the kth iteration can be determined without actually having to compute the correction. In fact, using the relations (2.3) and (2.5), the norm of the residual R_k can be expressed as

$$\|R_k\|_F = \big\|R_0 - \mathcal{V}_k * H_k y_k - h_{k+1,k}[0_{N\times s}, \ldots, 0_{N\times s}, V_{k+1}] * y_k\big\|_F,$$

but since $H_k\, y_k = \|R_0\|_F\, e_1^{(k)}$ and $R_0 = \|R_0\|_F \mathcal{V}_k * e_1^{(k)}$, it follows that

$$\|R_k\|_F = h_{k+1,k}\big\|[0_{N\times s}, \ldots, 0_{N\times s}, V_{k+1}] * y_k\big\|_F = h_{k+1,k}\big|y_k^{(k)}\big|,$$

where $y_k^{(k)}$ is the last component of the vector y_k.

One of the drawbacks of the algorithm is the fact that it could break down. Another drawback as explained earlier is that it becomes expensive in time of cost and memory as k increases. One possibility is to restart the algorithm every m iterations for a chosen integer m and the second one is to truncate the global Arnoldi process.

In the next section, we give a global version of the GMRES algorithm for solving linear systems of equations with multiple right-hand sides.

4. The global generalized minimal residual method

As we have seen, the norm of the residual obtained by the Gl-FOM is not minimized at each step and hence it may oscillate. The global GMRES method overcomes this drawback and is defined as follows.

Starting from an initial guess X_0 and the corresponding residual R_0 we construct, at step k, the new approximation X_k of the solution of the block linear system (1.2) such that

$$X_k - X_0 = Z_k \in \mathcal{K}_k, \tag{4.1}$$

with the F-orthogonality relation

$$R_k \perp_F \mathcal{W}_k = A\mathcal{K}_k. \tag{4.2}$$

If $\mathcal{P}_k$ denotes the F-orthogonal projector onto the matrix Krylov subspace $\mathcal{W}_k$, then the residual R_k can be expressed as

$$R_k = R_0 - \mathcal{P}_k R_0. \tag{4.3}$$

As we are dealing with an orthogonal projection method onto the Krylov subspace $\mathcal{W}_k$, we have a minimization property and the relation (4.3) implies

$$\|R_k\|_F = \min_{Z\in\mathcal{K}_k} \|R_0 - AZ\|_F. \tag{4.4}$$

Consider now the F-orthonormal basis $\{V_1, \ldots, V_k\}$, of the subspace $\mathcal{K}_k$, obtained from the global Arnoldi process with $V_1 = R_0/\|R_0\|_F$. Then the following result will allow us to transform the minimization problem (4.4) with the Frobenius norm to a minimization problem with the l_2-norm and this will be very useful for the practical implementation of the global GMRES.

Theorem 2. *Let $\mathcal{V}_k$ denotes the block matrix $\mathcal{V}_k = [V_1, \ldots, V_k]$, where $\{V_1, V_2, \ldots, V_k\}$ form the F-orthonormal basis of $\mathcal{K}_k$ obtained from Algorithm* 2.1. *Let $\widetilde{H}_k$ be the $(k+1)\times k$ upper Hessenberg matrix whose entries are $h_{i,j} = \mathrm{tr}(V_i^{\mathrm{T}} A V_j)$, then*

$$\|R_k\|_F = \min_{y\in\mathbb{R}^k} \big\|\|R_0\|_F e_1^{(k+1)} - \widetilde{H}_k\, y\big\|_2,$$

where $e_1^{(k+1)}$ is the first canonical basis vector in $\mathbb{R}^{k+1}$ and y is a vector of $\mathbb{R}^k$.

Proof. From (4.4), the norm of the residual R_k is given as

$$\|R_k\|_F = \min_{y\in\mathbb{R}^k} \|R_0 - A\mathcal{V}_k * y\|_F. \tag{4.5}$$

From the relation (2.6), we have $A\mathcal{V}_k = \mathcal{V}_{k+1} * \widetilde{H}_k$. On the other hand, since $R_0 = \|R_0\|_F V_1$ and since $V_1 = \mathcal{V}_{k+1} * e_1^{(k+1)}$, we get

$$R_0 = \|R_0\|_F\, \mathcal{V}_{k+1} * e_1^{(k+1)}. \tag{4.6}$$

Replacing (4.6) in (4.5), we obtain

$$\|R_k\|_F = \min_{y\in\mathbb{R}^k} \big\|\|R_0\|_F \mathcal{V}_{k+1} * e_1^{(k+1)} - \big(\mathcal{V}_{k+1} * \widetilde{H}_k\big) * y\big\|_F. \tag{4.7}$$

Now, using the properties (2.3) of the product $*$, the relation (4.7) becomes

$$\|R_k\|_F = \min_{y\in\mathbb{R}^k} \big\|\mathcal{V}_{k+1} * \big(\|R_0\|_F e_1^{(k+1)} - \widetilde{H}_k y\big)\big\|_F. \tag{4.8}$$

Finally, applying Theorem 1, it follows that

$$\|R_k\|_F = \min_{y\in\mathbb{R}^k} \big\|\|R_0\|_F e_1^{(k+1)} - \widetilde{H}_k y\big\|_2. \qquad \square$$

The global generalized minimal residual Gl-GMRES algorithm is summarized as follows:

Algorithm 4.1. Global generalized minimal residual algorithm

1. Choose X_0, compute $R_0 = B - AX_0$ and $V_1 = R_0/\|R_0\|_F$.
2. For $j = 1, 2, \ldots, k$ construct the F-orthonormal basis $V_1, V_2, \ldots$ by Algorithm 2.1.
3. Solve the problem

$$\min_{y\in\mathbb{R}^k} \left\| \|R_0\|_F e_1^{(k+1)} - \widetilde{H}_k y \right\|_2$$

and compute $X_k = X_0 + \mathcal{V}_k * y_k$, where y_k is the solution of the preceding least squares problem.

We see from Algorithm 4.1, that we have to solve only one k-dimensional l_2-least-squares problem to get the k-dimensional vector y_k. This leads to considerable savings compared to the block GMRES algorithm where the Hessenberg matrix H_k is of dimension $ks \times ks$ or to the simple GMRES algorithm where s least-squares problems have to be solved at each iteration.

As for the Gl-FOM, the storage and the number of operations increase at each iteration. To remedy these difficulties, one can restart the algorithm every m iterations.

For the practical implementation, we have to solve the k-dimensional l_2 minimization problem

$$\min_{y\in\mathbb{R}^k} \left\| \|R_0\|_F\, e_1^{(k+1)} - \widetilde{H}_k y \right\|_2.$$

As described in [17], $\widetilde{H}_k$ is maintained in a factored form and the factors are updated with each increment k. Typically, the matrix $\widetilde{H}_k$ is factored as $\widetilde{Q}_k \widetilde{H}_k = \widetilde{R}_k$, where $\widetilde{Q}_k$ is a product of Givens rotations and $\widetilde{R}_k$ is upper triangular. In practice, the QR-factorization is implemented, at each step, by performing this factorization on the new column of $\widetilde{H}_k$; the details of this implementation are given in [17].

When solving one linear system of equations by the GMRES algorithm, we can obtain the norm of the residual without explicitly computing the new approximation. This important property is also valid for the Gl-GMRES. In fact using the QR-factorization of $\widetilde{H}_k$, we have

$$\|R_k\|_F = \min_{y\in\mathbb{R}^k} \left\| \|R_0\|_F\, e_1^{(k+1)} - \widetilde{H}_k y \right\|_2 = \min_{y\in\mathbb{R}^k} \left\| \widetilde{Q}_k \left(\|R_0\|_F\, e_1^{(k+1)} - \widetilde{H}_k y \right) \right\|_2.$$

Since the last row of $\widetilde{R}_k$ is zero, the Frobenius norm of the residual R_k is the last component of the vector $\|R_0\|_F\, \widetilde{Q}_k\, e_1^{(k+1)}$.

Let m be the grade of R_0 hence $h_{m+1,m} = 0$ and as we have seen in Section 2 (Proposition 2), V_{m+1} cannot be computed and the matrix Krylov subspace $\mathcal{K}_m$ is invariant. In this case the relation (2.5) becomes $A\mathcal{V}_m = \mathcal{V}_m * H_m$. The Frobenius norm of the mth residual is given as

$$\|R_m\|_F = \min_{y\in\mathbb{R}^m} \left\| \mathcal{V}_m * \left(\|R_0\|_F\, e_1^{(m)} - H_m y \right) \right\|_F.$$

Using Theorem 1, the last relation becomes

$$\|R_m\|_F = \min_{y\in\mathbb{R}^m} \left\| \|R_0\|_F\, e_1^{(m)} - H_m y \right\|_2.$$

Now as H_m is nonsingular, the minimum is zero and the approximation X_m is the exact solution of (2.1). This shows that the Gl-GMRES algorithm converges in at most m iterations.

We will give now some convergence results on the Gl-GMRES algorithm.

Proposition 4. *Assume that* $A = U\Lambda U^{-1}$ *is diagonalizable, where* $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_N)$. *Then, at step* k, *the residual norms produced by the Gl-GMRES satisfy*

$$\|R_k\|_F \leqslant \kappa_F(U)\,\|R_0\|_F\,\sqrt{N}\,\min_{p\in\mathcal{P}_k,\ p(0)=1}\Big(\max_{i=1,\ldots,N}|p(\lambda_i)|\Big),$$

where $\kappa_F(U) = \|U\|_F\,\|U^{-1}\|_F$ *and* $\mathcal{P}_k$ *is the set of polynomials of degree less or equal than* k.

Proof. At step k, the residual R_k produced by the Gl-GMRES can be written as $R_k = p_k(A)R_0$, where the polynomial p_k is of degree $\leqslant k$ and $p_k(0) = 1$. Then the minimization property (4.4) can be expressed as

$$\|R_k\|_F = \min_{p\in\mathcal{P}_k,\ p(0)=1}\big\|p(A)R_0\big\|_F.$$

On the other hand, since $A = U\Lambda U^{-1}$, we have

$$\|R_k\|_F = \min_{p\in\mathcal{P}_k,\ p(0)=1}\big\|U\,p(\Lambda)\,U^{-1}R_0\big\|_F. \tag{4.9}$$

Then

$$\|R_k\|_F \leqslant \kappa_F(U)\,\|R_0\|_F\,\min_{p\in\mathcal{P}_k,\ p(0)=1}\big\|p(\Lambda)\big\|_F. \tag{4.10}$$

As Λ is a diagonal matrix, it follows that

$$\big\|p(\Lambda)\big\|_F \leqslant \sqrt{N}\,\max_{i=1,\ldots,N}|p(\lambda_i)|.$$

So using this in (4.10) we obtain the desired result. □

We consider now the case where the matrix A is not diagonalizable. We first recall the definition of the ε-pseudospectrum of A [10]:

$$\Lambda_\varepsilon = \big\{z\in\mathbb{C}:\ \big\|(zI - A)^{-1}\big\| \geqslant \varepsilon^{-1}\big\},\quad \text{where } \varepsilon > 0.$$

$\Lambda_\varepsilon(A)$ is the set of the eigenvalues of $A + E$ with $\|E\| < \varepsilon$. Let $\partial\Lambda_\varepsilon(A)$ be the boundary of $\Lambda_\varepsilon(A)$ and let L_ε be the arc length of the boundary of $\Lambda_\varepsilon(A)$. We have the following result:

Proposition 5. *The norm of the residual produced by the Gl-GMRES at step* k, $k = 1, 2, \ldots$, *satisfy the following inequality*:

$$\|R_k\|_F \leqslant \frac{L_\varepsilon}{2\pi\varepsilon}\|R_0\|_F\,\min_{p\in\mathcal{P}_k,\ p(0)=1}\Big(\sup_{\lambda\in\Lambda_\varepsilon}|p(\lambda)|\Big).$$

Proof. Let Γ be the contour or the union of contours enclosing the ε-pseudospectrum $\Lambda_\varepsilon(A)$ and consider the integral representation

$$p(A) = \frac{1}{2\pi\,\mathrm{i}}\int_\Gamma p(z)(zI - A)^{-1}\,\mathrm{d}z.$$

It follows that

$$\big\|p(A)\big\|_F \leqslant \frac{1}{2\pi\,\varepsilon}\,\sup_{\lambda\in\Lambda_\varepsilon}|p(\lambda)|\int_\Gamma |\mathrm{d}z|.$$

Hence,

$$\|p(A)\|_F \leqslant \frac{L_\varepsilon}{2\pi\varepsilon} \sup_{\lambda\in\Lambda_\varepsilon} |p(\lambda)|. \tag{4.11}$$

Now, as the norm of the Gl-GMRES residuals verifies

$$\|R_k\|_F = \min_{p\in\mathcal{P}_k,\ p(0)=1} \|p(A)\,R_0\|_F,$$

it follows that

$$\|R_k\|_F \leqslant \|R_0\|_F \min_{p\in\mathcal{P}_k,\ p(0)=1} \|p(A)\|_F.$$

Then, using (4.11), we get

$$\|R_k\|_F \leqslant \frac{L_\varepsilon}{2\pi\varepsilon}\|R_0\|_F \min_{p\in\mathcal{P}_k,\ p(0)=1} \Big(\sup_{\lambda\in\Lambda_\varepsilon} |p(\lambda)|\Big). \qquad \square$$

Next, we will give a connection between the Frobenius norm of the residuals obtained from the Gl-FOM and Gl-GMRES methods. This comparison will be easy understood by using angles between vectors and subspaces.

We define the acute angle between two matrices X and Y in the space $\mathbb{E}$ as follows:

$$\cos(X,Y) = \frac{\langle X,Y\rangle_F}{\|X\|_F\|Y\|_F}.$$

Let $\mathcal{S}$ be any subspace of $\mathbb{E}$, then the acute angle between X and $\mathcal{S}$ is defined by

$$\cos(X,\mathcal{S}) = \max_{Y\in\mathcal{S}-\{0\}} \cos(X,Y).$$

Denote by R_k^{gg} the kth residual of the Gl-GMRES and let θ_k be the acute angle between R_0 and the matrix Krylov subspace $\mathcal{W}_k = A\mathcal{K}_k$. Then as $\mathcal{P}_k$ is an F-orthogonal projector onto $\mathcal{W}_k$, it follows that

$$\|R_k^{\mathrm{gg}}\|_F^2 = (1-\cos^2\theta_k)\|R_0\|_F^2. \tag{4.12}$$

Consider now the kth residual R_k^{gf} of the Gl-FOM starting from the same initial guess X_0 as for the Gl-GMRES. Let ϕ_k be the acute angle between R_0 and $\mathcal{Q}_k R_0$, where $\mathcal{Q}_k R_0$ is the oblique projection onto $\mathcal{W}_k$ along the F-orthogonal of $\mathcal{K}_k$. Then using the relation (3.3), it easily follows that

$$\|R_k^{\mathrm{gf}}\|_F^2 = \tan^2\phi_k \|R_0\|_F^2. \tag{4.13}$$

The relations (4.12) and (4.13) allow us to compare the norms of the residuals of the Gl-FOM and the Gl-GMRES methods, starting from the same initial guess. In fact, using these last two relations, we obtain

$$\|R_k^{\mathrm{gg}}\|_F^2 = \frac{1-\cos^2\theta_k}{\tan^2\phi_k}\|R_k^{\mathrm{gf}}\|_F^2. \tag{4.14}$$

Now from the definitions of the acute angles θ_k and ϕ_k, Eq. (4.14) implies

$$\|R_k^{\mathrm{gg}}\|_F \leqslant \cos\phi_k \|R_k^{\mathrm{gf}}\|_F.$$

When solving one linear system of equations, these relations reduce to those given in [8]. Note also that the comparison between FOM and GMRES obtained by Brown [1] is still valid for the global methods.

Table 1
Costs for Gl-GMRES(m) and BGMRES(m)

Cost	BGMRES(m)	Gl-GMRES(m)
$M \times v$	$s(m+1)$	$s(m+1)$
Solve triangular system	s (dim $ms \times ms$)	1 (dim $m \times m$)
Mult. of blocks of dim $N \times s$ and $s \times s$	$m(m+1)/2$	
N-vector DOT	$m(m+1)s^2/2$	$m(m+1)s/2$
MGS on $N \times s$ block	$m-1$	
Leading scalar costs	$O(m^2s^3 + m^3s^2)$	$O(m^2)$

In the Gl-GMRES and Gl-FOM, the work and storage increase with the iteration step. This may cause difficulties for large steps. As we said earlier, a first way is to restart these algorithms every m iterations many times as necessary for convergence. In practice, this is usually done for the GMRES algorithm.

A second way to overcome these problems, is to truncate the global Arnoldi process by performing an incomplete global Gram–Schmidt orthogonalization which could be obtained by F-orthogonalizing, at each step, the current block against the m previous ones. In this case, the relations (2.5) and (2.6) are still valid but the matrix H_k is a banded Hessenberg matrix with bandwidth of $m+1$.

For operation requirements, the main difference between the three algorithms is: if we apply the GMRES to each right-hand side, then we have to solve, at each iteration k, s least-squares problems with Hessenberg matrices of dimension $(k+1) \times k$. For the BGMRES the corresponding Hessenberg matrix is of dimension $(k+1)s \times ks$ and for the Gl-GMRES we have to solve one least-squares problem with a Hessenberg matrix of dimension $(k+1) \times k$. As pointed out in [19], although the BGMRES algorithm converges in at most $\lceil N/s \rceil$ iterations, the algorithm becomes very expensive as s increases. Table 1 lists the computational costs for Gl-GMRES(m) and BGMRES(m).

5. Application to the Lyapunov matrix equation

In the following section, we will show how to apply the Gl-GMRES for solving a Lyapunov matrix equation. We will not give any theoretical results.

We consider the following Lyapunov matrix equation:

$$AX + XA^{\mathrm{T}} + B = 0, \tag{5.1}$$

where A, B and X are $N \times N$ matrices. Such a matrix equation play an important role in control theory. This equation has a unique solution if and only if A and $-A$ have disjoint spectra.

The problem (5.1) can be solved by iterative methods such as the GMRES algorithm applied to the equivalent problem

$$\widetilde{\mathcal{A}}x = \widetilde{b} \tag{5.2}$$

with $\widetilde{\mathcal{A}} = I \otimes A + A \otimes I \in \mathbb{R}^{N^2 \times N^2}$, where $\otimes$ denotes the Kronecker product and

$$\widetilde{b} = -(B_{1,1}, \ldots, B_{N,1}, \ldots, B_{N,N})^{\mathrm{T}} \in \mathbb{R}^{N^2}.$$

As in [6], we define the operator $\mathcal{A}$ as

$$\mathcal{A}: X \to AX + XA^{\mathrm{T}}.$$

Hence the problem (5.1) can be expressed as

$$\mathcal{A}X = -B. \tag{5.3}$$

The matrix equation (5.3) can be solved by the Gl-GMRES by replacing in Algorithm 4.1 the matrix product AX by the new one $\mathcal{A}X = AX + XA^{\mathrm{T}}$. At step k, the residual $R_k = -AX_k - X_kA^{\mathrm{T}} - B$ is obtained by projecting orthogonally the initial residual $R_0 = -AX_0 - X_0A^{\mathrm{T}} - B$ onto the matrix Krylov subspace $\mathcal{A}\mathcal{K}_k(\mathcal{A}, R_0)$. Note that as $\widetilde{\mathcal{A}}$ is an $N^2 \times N^2$ matrix, the system (5.2) could be very large.

The Gl-GMRES algorithm for solving the Lyapunov matrix equation (5.1) is as follows:

Algorithm 5.1.

1. Choose a matrix X_0, compute $R_0 = -B - AX_0 - X_0A^{\mathrm{T}}$ and $V_1 = R_0/\|R_0\|_F$.
2. For $j = 1, 2, \ldots, k$ construct the F-orthonormal basis $V_1, V_2, \ldots$, by Algorithm 2.1 with the operator $\mathcal{A}$, of the Krylov subspace

$$\mathcal{K}_k(\mathcal{A}, R_0) = \operatorname{span}\{R_0, \mathcal{A}R_0, \ldots, \mathcal{A}^{k-1}R_0\}.$$

3. Solve the problem

$$\min_{y \in \mathbb{R}^k} \left\| \|R_0\|_F e_1^{(k+1)} - \widetilde{H}_k y \right\|_2$$

and compute $X_k = X_0 + \mathcal{V}_k * y_k$, where y_k is the solution of the preceding least squares problem.

We note that $\mathcal{A}^k R_0$ is defined recursively as $\mathcal{A}(\mathcal{A}^{k-1}R_0)$. Other iterative methods for solving (5.1) have been derived in [6,7,15].

In the case where B is a symmetric matrix, we have the following result:

Proposition 6. *If the $N \times N$ matrices B and X_0 are symmetric, then the iterates X_k, $k = 1, 2, \ldots$, produced by Algorithm* 5.1 *are all symmetric.*

Proof. As B and X_0 are symmetric, the residual $R_0 = -B - AX_0 - X_0A^{\mathrm{T}}$ and $V_1 = R_0/\|R_0\|_F$ are also symmetric. Then it is easily verified by induction that $V_1, V_2, \ldots, V_k$, constructed by Algorithm 2.1 with the operator $\mathcal{A}$, are all symmetric. Hence, as $X_k = X_0 + \mathcal{V}_k * y_k$, it follows that the iterates X_k, $k = 1, 2, \ldots$, are symmetric. □

Other theoretical results and preconditioning techniques for the matrix Lyapunov equation and more generally for the Sylvester equation are under investigation.

6. Numerical examples

The tests reported in this section were run on SUN Microsystems workstations using Matlab.

We compared the Gl-GMRES algorithm for solving the problem (1.2) with the standard GMRES algorithm applied to one right-hand side. As reported in [19] for similar matrices, the BGMRES algorithm is more expensive than the GMRES algorithm, so in our tests we did no comparison with BGMRES.

Table 2
Effectiveness of Gl-GMRES(10) measured by $t(s)/t(1)$. $N = 3600$, $\delta = 0.5$

s	10	20	30	40
B_1	3.62(15)	6.07(14)	8.04(14)	9.95(13)
B_2	3.6(15)	4.86(15)	7.60(15)	8.99(15)
B_3	3.47(17)	4.32(16)	5.68(16)	6.99(15)

Table 3
Effectiveness of Gl-GMRES(20) for Harwell–Boeing collection; $s = 10$

	B_1	B_2	B_3
PDE900 ($N = 900$)	6.40	6.09	6.04
SHERMAN4 ($N = 1140$)	4.5	6.24	6.35
SHERMAN5 ($N = 3312$)	5.01	6.30	6.45

For all the experiments, the initial guess was taken to be zero. The tests were stopped as soon as $\max_{1\leqslant j\leqslant s}(\|R_k^{(j)}\|/\|R_0^{(j)}\|) \leqslant 10^{-7}$.

For the first set of experiments, the matrix A represents the 5-point discretization of the operator

$$L(u) = -u_{xx} - u_{yy} + \delta u_x$$

on the unit square [0,1] $\times$ [0,1] with homogeneous Dirichlet boundary conditions. The discretization was performed using a grid size of $h = \frac{1}{61}$ which yields a matrix of dimension $N = 3600$; we chose $\delta = 0.5$. We considered three matrices for the right-hand sides: $B = B_1 = I_{N,s}$, $B = B_2 = \text{rand}(N, s)$, where function rand creates an $N \times s$ random matrix with coefficients uniformly distributed in [0, 1], and $B = B_3$, where B_3 is the $N \times s$ matrix whose ith column has all components equal to one except the ith component which is zero.

In Table 2, we give the ratio $t(s)/t(1)$, where $t(s)$ is the CPU time for Gl-GMRES(10), and $t(1)$ is the CPU time obtained when applying GMRES(10) for one right-hand side linear system. Note that the time obtained by GMRES(10) for one right-hand side depends on which right-hand side was used. So, in our experiments, $t(1)$ was obtained by dividing by s the time needed for the s right-hand sides using repeated GMRES(10). We note that Gl-GMRES(10) is effective if the indicator $t(s)/t(1)$ is less than s.

In Table 2, we listed $t(s)/t(1)$ for $s = 10$, 20, 30 and 40. In parentheses, we give the number of restarts for Gl-GMRES(10) to converge. The results obtained in Table 2 show the effectiveness of Gl-GMRES(10).

For the second set of experiments, we used matrices from the Harwell–Boeing collection: $A_1 =$ PDE900, $A_2 =$ SHERMAN4 and $A_3 =$ SHERMAN5. In Table 3, we listed the ratio $t(s)/t(1)$ obtained with Gl-GMRES(20) and GMRES(20). In these experiments, we set $s = 10$. As shown in Tables 2 and 3,

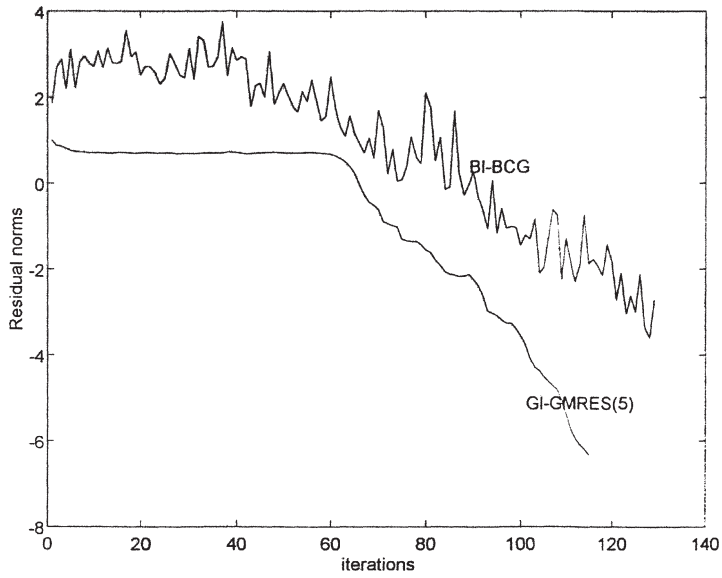

Fig. 1. Gl-GMRES(5); Bl-BCG.

the Gl-GMRES(20) algorithm is less expensive than the GMRES(20) algorithm applied to each right-hand side.

For the third experiment, the matrix A is the one considered in the first set of experiments with $N = 2500$ and $\delta = 1$. The matrix B of right-hand sides was $B = \text{rand}(N, s)$ with $s = 8$. Fig. 1 shows the behaviour of the Frobenius residual norms, in a logarithmic scale, versus the number of iteration for Gl-GMRES(5) and Bl-BCG.

7. Conclusion

In this paper, we have proposed and analyzed a global GMRES algorithm for solving the matrix equation $AX = B$. Experimental results show that the proposed method is effective and less expensive than the GMRES algorithm applied to each right-hand side. We have also noted how this algorithm could be applied to other matrix equations such as the matrix Lyapunov equation. Theoretical results for this problem and numerical experiments with preconditioning techniques are under investigation and will be given in the future.

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