International Journal of Engineering, Mathematical and Physical Sciences
ISSN: 2517-9934
Vol:8, No:9, 2014

Global GMRES with Deflated Restarting for Families of Shifted Linear Systems

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Abstract—Many problems in science and engineering field require the solution of shifted linear systems with multiple right hand sides and multiple shifts. To solve such systems efficiently, the implicitly restarted global GMRES algorithm is extended in this paper. However, the shift invariant property could no longer hold over the augmented global Krylov subspace due to adding the harmonic Ritz matrices. To remedy this situation, we enforce the collinearity condition on the shifted system and propose shift implicitly restarted global GMRES. The new method not only improves the convergence but also has a potential to simultaneously compute approximate solution for the shifted systems using only as many matrix vector multiplications as the solution of the seed system requires. In addition, some numerical experiments also confirm the effectiveness of our method.

Keywords—Shifted linear systems, global Krylov subspace, GLGMRESIR, GLGMRESIRsh, harmonic Ritz matrix, harmonic Ritz vector.

I. Introduction

We consider the solution of a sequence of families of linear systems:

$$(A - \sigma_i I)x_i^j = b^j, \tag{1}$$

with $j = 1, \ldots, p$ and $i = 1, \ldots, s$. Here $A \in \mathbb{C}^{n\times n}$ is a nonsingular matrix and all the $b^j \in \mathbb{C}^n$ are available simultaneously. Then (1) can be written as

$$(A - \sigma_i I)X_i = B, \tag{2}$$

where $B = [b^1, b^2, \ldots, b^p]$ and $X_i = [x_i^1, x_i^2, \ldots, x_i^p]$ are $N \times p$ rectangular matrices. We call the numbers $\{\sigma_i\}_{i=1}^s \in \mathbb{C}$ shifts.

Systems with multiple right hand sides and multiple shifts arise in many scientific and engineering applications. For example, control theory [4], time dependent differential equations [16] and lattice quantum chromodynamics (lattice QCD) [1].

For simplicity of discussion, we frequently will focus on one family of linear systems with only one shift and drop the index i, yielding two systems of the form

$$AX = B, \tag{3}$$

$$(A - \sigma I)X_\sigma = B, \tag{4}$$

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The first equation is referred as the seed systems while the second one is termed as the shifted systems. All of them are the systems with multiple right hand sides.

A number of recent articles have established the benefits of using the shift invariance when solving shift linear systems with a single right hand $(p = 1)$. Methods that are based on the nonsymmetric Lanczos process have been straightforwardly derived (1), such as CG [17], QMR, TFQMR [6], BiCGstab [7] and a recently proposed method IDR [15]. Restarted Krylov methods are not as straightforward. After a restart, all residual vectors formed at the end of a cycle of the Krylov method need to be parallel to each other. For FOM method, thid happens automatically [14]. However, this collinearity does not occur for restarted GMRES [8]. To handle this situation, Frommer and Glässner enforced the residuals to be collinear and proposed shifted GMRES [8]. This is an efficient method for solving families of shifted linear systems $(p = 1)$, but it inherits the properties of stagnation and unpredictable convergence exhibited by restarted GMRES, see, e.g. [13], [5]. Deflated version of restarted GMRES can improve this. One of these approaches is related to Morgan's GMRESDR [12], and in [3], this method has been extended to simultaneously solve a family of shift systems with a single right hand side.

Recently, Lin combine restarted global GMRES method with deflation technology and proposed the implicitly global GMRES (GLGMRESIR) approach [11] for solving the seed systems. It has been observed that significant improvements in convergence rates can be achieved from global Krylov subspace methods by adding these harmonic Ritz matrices. Therefore, we consider an extension of GLGMRESIR to solve shifted linear systems with multiple right hand sides and multiple shifts in this section. Thus, we will have an efficient method which not only improves the convergence but also has a potential to simultaneously compute approximate solution for the shifted systems as the expense of only p matrix vector multiplications per iteration.

The structure of the paper is as follows. In the next section, we recall some properties of global Krylov subspace. In Section III, we describe the implicitly global GMRES method aimed at accelerating convergence. We introduce our new method to address shifted linear systems in Section IV. The effectiveness of the proposed method is also demonstrated in Section V. Finally, some conclusions are summarized in Section VI.

II. Preliminaries

A. Notations

Throughout this paper, $||.||_F$ denotes the Frobenius norm, ^{T} is referred to as the transpose conjugate operation of matrix, the identity matrix of order k is designated as I_k or I and $\mathbf{0}_{i\times j}$ is defined as the zero rectangular matrix with i rows and j columns. $\mathcal{R}(\cdot)$ and tol denote the range of the matrix and the convergence threshold, respectively. For two rectangular matrices X and Y, we define $< X, Y >_F = tr(X^TY)$, where tr$(\cdot)$ denotes the trace of the square matrix X^TY. If X is an $n \times p$ matrix, the $x = \text{vec}(X)$ is the ns vector obtained by stacking the p columns of the matrix X. The notations of MATLAB style are also used, for example, $U(1:i, 1:j)$ denotes the submatrix of the first i rows and the first j columns of U, $U(:, j)$ refers to its jth column and $U(i, j)$ corresponds to the $U_{i,j}$ entry of the matrix U.

B. Global Krylov Subspace

Let $X_0 \in \mathbb{C}^{n\times p}$ be the initial guess and $R_0 = B - AX_0$. Global Krylov subspace generated by A from R_0 is defined as follows

$$\mathcal{K}_m(A, R_0) := \text{ span}\{R_0, AR_0, A^2R_0, \ldots, A^{m-1}R_0\}.$$

Note that the definition of 'global span' means a linear combination of the $N \times p$ matrices, i.e., $\{\sum_{i=0}^{m-1} \gamma_i A^i R_0\}$, for some scalars $\gamma_i's \in \mathbb{C}$. We observe that the global Krylov subspace generated by A and R_0 is invariant under any shift, i.e.,

$$\mathcal{K}_m(A, R_0) = \mathcal{K}_m((A - \sigma I), R_0),$$

as long as the starting rectangular matrices are collinear.

Thus, any $Z \in \mathcal{K}_m(A, R_0)$ can be expressed as $Z = \Phi_{m-1}(A)R_0$ with Φ_{m-1} a polynomial of degree $\leq m-1$ or, equivalently, $Z = \Phi^{\sigma}_{m-1}(A - \sigma I)R_0$, where

$$\Phi^{\sigma}_{m-1}(t) = \Phi_{m-1}(t + \sigma).$$

Similar to the Krylov subspace, some properties of the global Krylov space were introduced in [10].

III. Implicitly global GMRES method

A. Global Arnoldi Process

We firstly review global Arnoldi Process that constructs an Frobenius orthonormal (Forthonormal) basis of the global Krylov subspace $\mathcal{K}_m(A, R_0)$, as described in [10].

The global Arnoldi algorithm constructs an Forthonormal basis $V_1, V_2, \ldots V_m$ satisfying

$$\begin{aligned} &\text{tr}(V_i^TV_j) = 0, \text{ for } i \neq j, i, j = 1, 2, \ldots, m, \\ &\text{tr}(V_i^TV_i) = 1, \text{ for } i = 1, 2, \ldots, m. \end{aligned} \tag{5}$$

Then we have a global Arnoldi relation

$$A\mathcal{V}_m = \mathcal{V}_{m+1}(H_m \otimes I_p) + h_{m+1,m}[0_{n\times p}, \ldots, 0_{n\times p}, V_{m+1}],$$

$$A\mathcal{V}_m = \mathcal{V}_{m+1}(\bar{H}_m \otimes I_p), \tag{6}$$

Algorithm 1 Global Arnoldi Process [10]

```
β = ||V||_F, V_1 = V/β;
for j = 1, ..., m, do
  U = AV_j;
  for i = 1, 2, ... j, do
    h_{i,j} =< U, V_i >_F;
    U = U − V_i h_{i,j};
  end for
  H_{j+1,j} = ||U||_F
  V_{j+1} = U/h_{j+1,j};
end for
```

where $\mathcal{V}_{m+1}$ denotes the $n \times (m+1)p$ rectangular matrix: $\mathcal{V}_{m+1} = [V_1, V_2, \ldots V_{m+1}]$, $\bar{H}_m$ denote the $(m+1)\times m$ upper Hessenberg matrix:

$$\begin{aligned} \bar{H}_m &= \begin{bmatrix} h_{1,1} & h_{1,2} & \ldots & h_{1,m} \\ h_{2,1} & h_{2,2} & \ldots & h_{2,m} \\ 0 & h_{3,2} & \ldots & h_{3,m} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & h_{m+1,m} \end{bmatrix} \\ &= \begin{bmatrix} H_m \\ h_{m+1,m}e_m^H \end{bmatrix} \in \mathbb{C}^{(m+1)\times m}, \end{aligned}$$

with $e_m = [0, \ldots, 0, 1]^T$ is the mth vector of the canonical basis of $\mathbb{R}^m$.

Since $h_{i,j} =< U, V_i >_F = \text{tr}(V_i^TU) = \text{vec}(V_i)^T\text{vec}(U)$, $h_{j+1,j} = ||U||_F = ||\text{vec}(U)||_2$, the global Arnoldi process over the matrix A with starting rectangle matrix V is equivalent with the classical Arnoldi process over the matrix $(I_p \otimes A)$ with starting vector vec(V). Then we have the following relation:

$$\begin{aligned} &(I_p \otimes A)[\text{vec}(V_1), \text{vec}(V_2), \ldots, \text{vec}(V_m)] \\ &\quad = [\text{vec}(V_1), \text{vec}(V_2), \ldots, \text{vec}(V_m)]H_m \\ &\quad + h_{m+1,m}\text{vec}(V_{m+1})e_m^T, \\ &\quad = [\text{vec}(V_1), \text{vec}(V_2), \ldots, \text{vec}(V_m), \text{vec}(V_{m+1})]\bar{H}_m. \end{aligned} \tag{7}$$

B. Implicitly Restarted Global GMRES

Let us assume that a global Arnoldi relation of type $A\mathcal{V}_m = \mathcal{V}_{m+1}(\bar{H}_m \otimes I_s)$ holds. In the GLGMRESIR method, harmonic Ritz matrices corresponding to the small eigenvalues $\theta_i's$ are kept in the restarting scheme. We denote these harmonic Ritz matrices $Y_k = \mathcal{V}_m(g_k \otimes I_p)$, where the k vectors g_i's corresponding to the smallest eigenvalues are obtained as solutions of the following generalized eigenvalue problem

$$< A\mathcal{V}_m, A\mathcal{V}_m(g_i \otimes I_p) - \mathcal{V}_m(\theta_i g_i \otimes I_p) >_F = 0. \tag{8}$$

Using (6), this becomes

$$(H_m + h_{m+1,m}^2 H_m^{-T} e_m e_m^{-T})g_i = \theta_i g_i, \ 1 \leq i \leq k. \tag{9}$$

Let R_0 be the initial residual for the linear equations at the start of the new cycle. Together with harmonic Ritz matrices, these matrices $([Y_1, \ldots, Y_k, R_0])$ are used to construct a new

Forthogonal basis of dimension $k+1$. It allows us to compute new matrices $\mathcal{V}_{k+1}^{new}$ and H_k^{new} such that

$$A\mathcal{V}_k^{new} = \mathcal{V}_{k+1}^{new}(H_k^{new} \otimes I_p),$$
$$< \mathcal{V}_k^{new}, \mathcal{V}_k^{new} >_F = I_{k+1},$$

where $\mathcal{V}_k^{new}$ is the Forthogonal basis of $[Y_1, \ldots, Y_k, R_0]$ and H_k^{new} is a $(k+1) \times k$ rectangular matrix. Then we run $m-k-1$ steps of the global Arnoldi process with starting matrices $\mathcal{V}_{k+1}^{new}(:, kp+1 : (k+1)p)$ to eventually build $\mathcal{V}_{m+1}$ and $\bar{H}_m$. At the end of each cycle of GLGMRESDR, a global Arnldi relation is generated,

$$A\mathcal{V}_m = \mathcal{V}_{m+1}(\bar{H}_m \otimes I_s),$$
$$< \mathcal{V}_{m+1}, \mathcal{V}_{m+1} >_F = I_{m+1},$$

where $V_i = \mathcal{V}_{k+1}^{new}(:, (i-1)p+1 : ip), 1 \le i \le k+1$ and $\bar{H}_m$ now is an upper Hessenberg matrix, except for a full leading $k+1$ by $k+1$ portion. Remarkably, $\mathcal{V}_m$ is the Forthonormal basis of a global Krylov subspace of dimension m,

$$\mathcal{S} = \text{span}\{Y_1, Y_2, \ldots, Y_k, R_0, AR_0, A^2R_0, \ldots, A^{m-k-1}R_0\}.$$

An approximate solution $X_m \in \mathbb{C}^{n\times p}$ is then found by minimizing the residual norm $||R_0 - A\mathcal{V}_m Y||$ over the space $X_0 + \mathcal{S}$. Details of the GLGMRESIR method are given in Algorithm 2.

Algorithm 2 GLGMRESIR [11]

Input: $A \in \mathbb{C}^{n\times n}$ nonsingular, $B \in \mathbb{C}^{n\times p}$. $X_0 = \mathbf{0}_{n\times p}$, tol
Output: $X_m \in \mathbb{C}^{n\times p}$ with $X_m \approx A^{-1}B$.

1: Choose an initial guess matrix X_0 and compute the residual matrix $R_0 = B - AX_0$. $\beta_0 = ||R_0||_F$, $V_1 = R_0/\beta_0$. Generate $\mathcal{V}_{m+1}$ and $\bar{H}_m$ with the global Arnoldi process. Set $c = [\beta^T, 0, \ldots, 0]^T$.
2: Solve $\min ||c - \bar{H}_m y||_2$ for Y_m. Set $X_m = X_0 + \mathcal{V}_m(y_m \otimes I_p)$, $R_m = B - AX_m$. Check residual norms for convergence, and process if not satisfied.
3: Compute the k smallest eigenpairs (θ_j, g_j) of $(H_m + h_{m+1,m}^2 H_m^{-T} e_m e_m^{-T})$.
4: Orthonormalize the vectors g_i's by the first separating into real and imaginary parts if complex, to form the columns of $G_k \in \mathbb{R}^{m\times k}$. (It may be necessary to adjust k to include both the real and imaginary part of complex eigenvectors.)
5: Extend with zero entries the vectors $p_1, \ldots, p_k$ to length $m+1$, then orthonormalize the columns of $z = c - \bar{H}_m y_m$ against the columns of $\begin{bmatrix} G_k \\ 0 \end{bmatrix}$ to form g_{k+1}. Set $G_{k+1} = \begin{bmatrix} G_k & \\ 0 & g_{k+1} \end{bmatrix}$
6: Set $\mathcal{V}_{k+p}^{new} = \mathcal{V}_{m+1}(G_{k+1} \otimes I_p)$, $H_k^{new} = G_{k+1}^T \bar{H}_m G_k$. Apply the global Arnoldi algorithm to extend H_k^{new} and V_{k+p}^{new} to $\bar{H}_m$ and $\mathcal{V}_{m+1}$.
7: Let $c_i =< V_i, R_m >_F, i = 1, \ldots, m+1$ and $X_0 = X_m$. Go to step 2.

Let $\bar{\mathcal{V}}_m = [\text{vec}(V_1), \text{vec}(V_2), \ldots, \text{vec}(V_m)]$. Note that (8) is equivalent with

$$(I_p \otimes A)\bar{\mathcal{V}}_m \perp [(I_p \otimes A)\bar{\mathcal{V}}_m g_i - \theta_i \bar{\mathcal{V}}_m g_i]. \qquad (10)$$

The residual vector $\text{vec}(R_m)$ is orthogonal to the subspace spanned by the columns of $(I_p \otimes A)\bar{\mathcal{V}}_m$. From (9), we observe that harmonic residual vectors $\text{vec}(\tilde{R}_j) = (I_p \otimes A)\text{vec}(Y_j) - \theta_j \text{vec}(Y_j)$ is also is orthogonal to the subspace $\mathcal{R}((I_p \otimes A)\bar{\mathcal{V}}_m)$. The harmonic residual vectors and the residual vector $\text{vec}(R_m)$ all reside in the Krylov subspace of dimension $m+1$ and are orthogonal to the same subspace of dimension m, so they must be multiples of each other, i.e., $\text{vec}(\tilde{R}_j) = \zeta_j \text{vec}(R_m), j = 1, \ldots, k$. Then we have

$$\tilde{R}_j = AY_j - \theta_j Y_j = \zeta_j R_m, j = 1, \ldots, k.$$

IV. GLGMRESIR for shifted linear systems

As mentioned above, GLGMRESIR generates the matrix subspace of dimension m, i.e., $\mathcal{S}$. Any vector $X_k \in X_0 + \mathcal{S}$ can be represented as

$$X_m = X_0 + P_{m-k-1}(A)R_0 + \sum_{i=1}^{k} \alpha_i Y_i, \qquad (11)$$

where P_{m-k-1} is a polynomial of degree $\le m-k-1$ with $P_{m-k-1}(0) = 1$. Then, the corresponding residual $R_m = B - AX_m$ satisfies

$$R_m = R_0 - AP_{m-k-1}(A)R_0 - \sum_{i=1}^{k} \alpha_i AY_i$$
$$= \Phi_{m-k}(A)R_0 - \sum_{i=1}^{k} \alpha_i AY_i$$

where $\Phi_{m-k}(t) = 1 - tP_{m-k-1}(t)$ is a polynomial of degree $\le m-k$ with $\Phi_{m-k}(0) = 1$.

For the shifted systems, we have

$$X_m^\sigma = X_0^\sigma + P_{m-k-1}^\sigma(A - \sigma I)R_0^\sigma + \sum_{i=1}^{k} \alpha_i^\sigma Y_i,$$

$$R_m^\sigma = R_0^\sigma - (A - \sigma I)P_{m-k-1}^\sigma(A - \sigma I)R_0^\sigma - \sum_{i=1}^{k} \alpha_i^\sigma (A - \sigma I)Y_i$$
$$= \Phi_{m-k}^\sigma(A - \sigma I)R_0^\sigma - \sum_{i=1}^{k} \alpha_i^\sigma (A - \sigma I)Y_i$$

where $\Phi_{m-k}(t) = 1 - tP_{m-k-1}(t)$ is a polynomial of degree $\le m-k$ with $\Phi_{m-k}(0) = 1$.

A. Collinear Residuals

Following the similar steps as in [9], we provide a simple analysis which justifies the residual R_m^σ is unique if the approximate collinearity condition exist.

Suppose that the initial residuals for the base and shifted systems are collinear, $R_0^\sigma = \beta_0 R_0,\ \beta_0 \in \mathbb{C}$. We enforce the condition that the residual R_m^σ is parallel to the minimized residual R_m, i.e.,

$$R_m^\sigma = \beta_m R_m,\ \beta_m \in \mathbb{C},$$

which amounts to

$$\beta_0\Phi^{\sigma}_{m-k}(A-\sigma I)R^{\sigma}_0 - \sum_{i=1}^{k}\alpha_i^{\sigma}(A-\sigma I)Y_i = \beta_s\Phi_{m-k}(A)R_0 - \sum_{i=1}^{k}\alpha_i AY_i.$$

Combining the conditions $AY_i - \theta_i Y_i = \tilde{R}_i$, $(A-\sigma I)Y_i = (\theta_i-\sigma)Y_i + \tilde{R}_i$ and $\tilde{R}_i = \zeta_i R_m$ yield

$$\begin{aligned}\beta_0\Phi^{\sigma}_{m-k}(A-\sigma I)R_0 - \sum_{i=1}^{k}(&\alpha_i^{\sigma}\zeta_i \\ &- \beta_s\alpha_i\zeta_i)R_0 - \beta_s\Phi_{m-k}(A)R_0 \\ &= \sum_{i=1}^{k}(\alpha_i^{\sigma}(\theta_i-\sigma) - \beta_s\alpha_i\theta_i)Y_i.\end{aligned}$$

Since the vectors $Y_1,\ldots,Y_k,R_0,AR_0,\ldots,A^{m-k-1}R_0$ are Forthogonal, it holds that

$$\beta_0\Phi^{\sigma}_{m-k}(t-\sigma) - \sum_{i=1}^{k}(\alpha_i^{\sigma}\zeta_i - \beta_s\alpha_i\zeta_i) - \beta_s\Phi_{m-k}(t) = 0$$

$$\alpha_i^{\sigma}(\theta_i-\sigma) - \beta_s\alpha_i\theta_i = 0,\ i=1,\ldots,k.$$

Using the relation $\Phi^{\sigma}_{m-k}(0)=1$, we have

$$\begin{pmatrix} \Phi_{m-k}(\sigma) - \sum_{i=1}^{k}\alpha_i\zeta_i & \zeta_1 & \ldots & \zeta_k \\ \alpha_1\zeta_1 & \sigma-\theta_1 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \alpha_k\zeta_k & 0 & \ldots & \sigma-\theta_k \end{pmatrix}\begin{pmatrix}\beta_s\\ \alpha_1^{\sigma}\\ \vdots\\ \alpha_k^{\sigma}\end{pmatrix} = \begin{pmatrix}\beta_0\\0\\\vdots\\0\end{pmatrix}. \tag{12}$$

Observe that when $\theta_j \neq \sigma, i=1,\ldots,k$ and $\Phi_{m-k}(\sigma) \neq \sum_{i=1}^{k}\alpha_i\zeta_i\sigma/(\sigma-\theta_i)$, the above system has a unique solution. It is shown that the colinearity condition cannot be satisfied, but if it can, the residual R^{σ}_m is unique.

In practice, the corresponding polynomials Φ_{m-k} are not calculated. We now work out how the shifted systems can be practically computed when the GLGMRESIR iteration is performed on the seed systems.

Our basic assumption is that $R^{\sigma}_0 = \beta_0 R_0$. As mentioned above, at the end of each cycle of GLGMRESIR, a global Arnoldi relation is generated

$$A\mathcal{V}_m = \mathcal{V}_{m+1}(\bar{H}_m \otimes I_p),$$

with a shifted Arnoldi relation

$$(A-\sigma I)\mathcal{V}_m = \mathcal{V}_{m+1}((\bar{H}_m - \sigma I_m)\otimes I_p),$$

We enforce the condition that the residual for the shifted system is parallel to the minimized residual of the base system, i.e.,

$$R^{\sigma}_m = \beta_m R_m. \tag{13}$$

So

$$\begin{aligned} B - (A-\sigma I)(X^{\sigma}_0 + \mathcal{V}_m(y^{\sigma}_m\otimes I_p)) &= \beta_m\mathcal{V}_{m+1}(z\otimes I_p)\\ \beta_0R^{\sigma}_0 - \mathcal{V}_{m+1}((\bar{H}_m-\sigma I_m)y^{\sigma}_m\otimes I_p) &= \mathcal{V}_{m+1}(\beta_m z\otimes I_p)\\ \mathcal{V}_{m+1}((\beta_0 c - (\bar{H}_m-\sigma I_m)y^{\sigma}_m)\otimes I_p) &= \mathcal{V}_{m+1}(\beta_m z\otimes I_p)\end{aligned} \tag{14}$$

By straightforward computations, it is shown that if $z = c - \bar{H}_m y_m$ then for (13) to hold, we must have

$$(\bar{H}_m - \sigma I_m)y^{\sigma}_m + z\beta_m = \beta_0 c$$

Thus, we can compute both y^{σ}_m and β_m by solving the augmented linear system,

$$\begin{bmatrix} \bar{H}_m - \sigma I_m, & z \end{bmatrix}\begin{bmatrix} y^{\sigma}_m \\ \beta_m\end{bmatrix} = \beta_0 c \tag{15}$$

Note that we only compute the minimum residual solution using a Petrov Galerkin condition for the base systems. We enforce collinearity of the residuals to compute the approximation for the shifted systems. It is shown that a solution to (13) is exist if and only is the residual polynomial satisfies $\theta_j \neq \sigma, i=1,\ldots,l$ and $\Phi_{m-k}(\sigma) \neq \sum_{i=0}^{k}\alpha_i\zeta_j\sigma/(\sigma-\theta_j)$, otherwise, the system is singular. We can compute the QR factorization of $[\bar{H}_m - \sigma I_m, z] = QR$ to detect numerical singularity by examining the last diagonal entry of R. In the case that the solution does not exist, we simply perform one more iteration and check condition again.

To make this idea more concrete, we present outline of the shifted GLGMRESIR (GLGMRESIRsh) for solving the systems (1) in Algorithm 3.

Algorithm 3 GLGMRESIRsh algorithm.

1: At the beginning of a cycle of GLGMRESIRSh, assume the current problem is $(A-\sigma_i I)(X_i - X_{0,i}) = \beta_i R_0$, with $\beta_1 = 1$, and where $X_{0,i}$ is the current approximate solution to the ith shifted system.
2: Apply GLGMRESIR to A and generate equation $A\mathcal{V}_m = \mathcal{V}_{m+1}(\bar{H}_m \otimes I_p)$.
3: For the base system, solve the minimum residual reduced problem $\min||c-\bar{H}_m y||$ for y_1, where $c_i =< V_i^T R_m >_F$, $i=1,\ldots,m+1$. The new approximate solution is $X_1 = X_{0,1} + \mathcal{V}_m(y_1\otimes I_p)$; The new residual vector is $R_1 = R_{0,1} - A\mathcal{V}_m y_1 = R_{0,1} - \mathcal{V}_{m+1}(\bar{H}_m y_1\otimes I_p)$
4: For the other shifted systems $i,\ldots,s$, form $z = c - \bar{H}_m y_1$. Apply a QR factorization : $[\bar{H}_m - \sigma I_m, z] = QR$. Solve $Ry_i = \beta_i Q^T c - \beta_i^{new}Q^T z$, using the last row to solve for β_i^{new} and the first m rows for y_i.
5: The new approximate solution of the ith system is $X_i = X_{i,1} + \mathcal{V}_m(y_i\otimes I_p)$, and the new residual is $R_i = \beta_i^{new}R_1$
6: Test the residual norms for convergence. If not satisfied, for $i=2,\ldots,s$, set $\beta_i = \beta_i^{new}$ and for $i=1,\ldots,s$, set $X_{0,i} = X_i$ and $R_{0,i} = R_i$. Then go back to Step 1.

V. Numerical results

In this section, some numerical experiments will be described. The goal of these experiments is to examine the the effectiveness of GLGMRESIRsh (Algorithm 3).

In all of our runs we use a $\mathbf{0}_{n\times p}$ initial guess and choose different values for σ. Here, m and k denote the number of iterations for each restart and the number of harmonic Ritz vectors, respectively. The parameters are taken as $m = 30$, $k = 15$ for all the experiments. The stopping criterion in all iterative methods is $\frac{||R_k||_F}{||R_0||_F} \leq 10^{-6}$.

All the numerical experiments were performed in MATLAB 2011b. The machine we have used is a PC Pentium(R), CPU 2.80 GHz, 2.00 GB of RAM.

Example 1. Following [11], the first test matrix is a tridiagonal matrix with entries 0.01, 0.02, 0.03, 0.04, 0.05, 6, 7, ..., 1000 on the main diagonal, subdiagonal entries all 1 and superdiagonal entries all -1. The shifts are taken six different values $\{0, 0.9i, i, 0.6, -i, -1\}$. The right hand sides are chosen to be random vectors with $p = 5$ or 10.

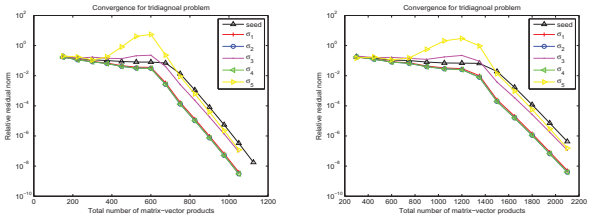

Fig. 1. Convergence history of GLGMRESIRsh for tridiagonal problem. Left: $p = 5$, Right: $p = 10$.

The results in Fig. 1 highlight the interest of performing GLGMRESIRsh which could simultaneously solve all the linear systems at the expense of just the matrix vector multiplications for the seed systems.

Example 2. We test GLGMRESIRsh on the reaction diffusion Brusselator model matrices RDB1250 and RDB2048 from Matrix Market [2]. For the examples, we take six values for the shift, $\sigma = \{0, \frac{1}{2} + \frac{1}{5}i, \frac{1}{2} - \frac{1}{5}i, 2, 1 - \frac{1}{2}i, 1 - \frac{1}{2}i\}$. As right hand sides we choose B = $rand(n, p)$ with $p = 10$.

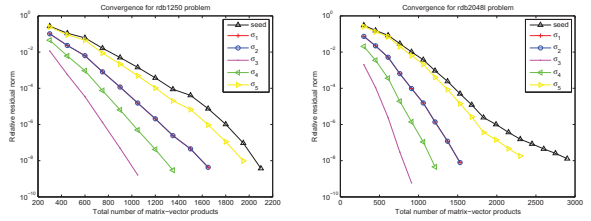

Fig. 2. Convergence history of GLGMRESIRsh for RDB1250 and RDB2048.

Fig. 2 depict the residual history of examples using the GLGMRESIRsh method. GLGMRESsh can simultaneously compute solutions for the seed and shifted systems without any additional matrix vector for iterates of the shifted systems. And the shifted systems enjoy a faster convergence.

Example 3. Convection diffusion problem

The third example is the convection diffusion problem with Dirichlet boundary conditions in the unit square $[0, 1]^2 = \Omega \bigcap \partial\Omega$, where $\Omega = (0, 1)^2$,

$$\begin{cases} -\varepsilon\triangle u + cu_x + du_y = g \quad in \quad \Omega \\ u = 0 \quad on \quad \partial\Omega \end{cases}$$

This problem is discretized with a second order finite difference scheme for a vertex centered location of unknowns. We adopt $\frac{h}{\varepsilon}max(|c|, |d|) = 2$ to satisfy the Péclet condition, where $h = \frac{1}{N-1}$ is the mesh size and N is the number of points per direction. Here, $h = 1/128(1/256)$, $c = d = 256(512)$ and $\varepsilon = 1$ are taken, then the problem size is $129^2(257^2) = 16641(66049))$ and has 80137(324105) non zero entries, which is real, sparse and nonsymmetric. The right hand sides have normally distributed rand elements with $p = 10$. The numerical behaviour of the GLGMRESIRsh approaches are plotted in Fig. 3.

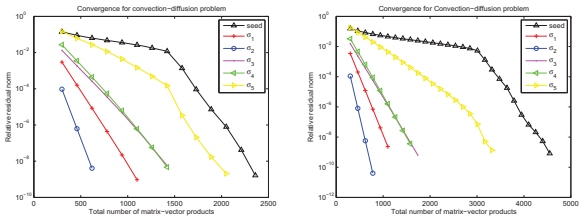

Fig. 3. Convergence history of GLGMRESIRsh for convection diffusion problem. Left: $n = 16641$, Right: $n = 66049$.

The curves in Fig. 3 highlight interest of performing shift invariance with GLGMRESIR at each iteration. The curves for shifted systems enjoys a significant decrease in the number of matrix vector products than the one for seed system. In addition, GLGMRESIRsh simultaneously solve all shifted linear systems in only one global Krylov subspace, leading to large saving in storage and time. Thus, it is demonstrated that the potential effectiveness of our algorithm for the shift systems with multiple shifts and multiple right hand sides.

VI. Conclusions

In this paper, we have derived the extension of GLGMRESIRsh for shifted linear systems with multiple shifts and multiple right hand sides (1). We use a strategy to make the residuals of the shift systems collinear. With this condition, our method not only enjoys the benefits of using deflation technique, but also can exploit the shift invariance, without computing additional matrix vector products for solving the shifted systems. Numerical examples also confirm the effectiveness of our method. Therefore, it is concluded that the GLGMRESIRsh is a competitive method for solving the linear systems with multiple right hand sides and multiple shifts.

Acknowledgments

This research is supported by YBXSZC20131070, the the National Natural Science Foundation of China (11026085, 11101071, 51175443) and OATF, UESTC.

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