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Restarted Full Orthogonalization Method with Deflation for Shifted Linear Systems

Jun-Feng Yin[1] and Guo-Jian Yin[2,*]

[1] *Department of Mathematics, Tongji University, 1239 Siping Road, Shanghai 200092, P. R. China.*
[2] *Department of Mathematics, The Chinese University of Hong Kong, Shatin, NT, Hong Kong.*

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Abstract. In this paper, we study shifted restated full orthogonalization method with deflation for simultaneously solving a number of shifted systems of linear equations. Theoretical analysis shows that with the deflation technique, the new residual of shifted restarted FOM is still collinear with each other. Hence, the new approach can solve the shifted systems simultaneously based on the same Krylov subspace. Numerical experiments show that the deflation technique can significantly improve the convergence performance of shifted restarted FOM.

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Key words: Shifted linear systems, full orthogonalization method, restarted Arnoldi process, deflation, collinear.

1. Introduction

Given a large sparse nonsymmetric matrix $A \in \mathbb{R}^{n\times n}$ and the right-hand side $b \in \mathbb{R}^n$, we want to simultaneously solving a sequence of shifted systems as follow

$$(A - \sigma_i I)x = b,\ \sigma_i \in \mathbb{R}, \quad i = 1, \cdots, s, \tag{1.1}$$

where I denotes the $n \times n$ identity matrix. Such shifted systems arise in many scientific and engineering fields, such as control theory, image restorations, structural dynamics, and QCD problems, and thus attract a number of attention of many researchers, see [5, 8, 12, 13]. Among all the systems, when $\sigma = 0$, the system $Ax = b$ is treated as the seed system.

*Corresponding author. *Email addresses:* `yinjf@tongji.edu.cn` (J.-F. Yin), `gjyin@math.cuhk.edu.hk` (G.-J. Yin)

Krylov subspace methods, for instance, FOM and GMRES, are popular choices for solving large sparse system of linear equations, which construct an orthonormal basis of Krylov subspace of the form,

$$\mathcal{K}_m(A,v) = \operatorname{span}\{v, Av, \cdots, A^{m-1}v\}.$$

Since the storage requirement and computational cost of FOM and GMRES will become expensive as m increases, restarting is often taken into use.

Let x_0 be an initial vector, in order to solve a sequence of shifted systems (1.1), a number of Krylov subspaces

$$\mathcal{K}_m(A-\sigma_i I, r_0^{(i)}) = \operatorname{span}\{r_0^{(i)}, (A-\sigma_i I)r_0^{(i)}, \cdots, (A-\sigma_i I)^{m-1}r_0^{(i)}\}, \quad i = 1, \cdots, s, \tag{1.2}$$

will be considered where $r_0^{(i)} = b - (A - \sigma_i I)x_0$ are the initial residuals, $i = 1, \cdots, s$.

It is shown in [3] that Krylov subspace is shift invariant, i.e.,

$$\mathcal{K}_m(A,v) = \mathcal{K}_m(A - \sigma I, v), \quad \forall\, \sigma. \tag{1.3}$$

It shows that the Krylov subspaces $\mathcal{K}_m(A - \sigma I, v)$ can be spanned by the same basis regardless of the choice of parameter σ, which shed a light that the shifted systems (1.1) can be solved simultaneously based on only one Krylov subspace.

From formula (1.2), it is seen that when the initial residual $r_0^{(i)}, i = 1, \cdots, s$, are parallel to each other, FOM and GMRES can be applied to solve (1.1) simultaneously at the first cycle. Usually, the initial vector for the next cycle is the current residual vector associated with an approximate solution. This means that all residual vectors formed at the end of a cycle are required to be collinear with each other, so that even in restarted scheme, the shifted systems (1.1) can always be solved based on the same Krylov subspace.

For GMRES, the collinearity of residuals are lost after the first restart, a variant of GMRES has been presented in [8] for (1.1) by forcing the residuals to be parallel. Note that in this case, only the base system has the minimum residual property, the solution of the other shifted systems is not equivalent to GMRES applied to those systems.

Note that the collinearity of residuals are satisfied automatically for FOM. Hence, Simoncini [5] gave an effective restarted FOM to solve all shifted linear systems simultaneously. Jing and Huang in [13] further accelerated this method by introducing a weighted norm.

In this paper, we study restarted FOM with the deflation technique for solving all shifted linear systems simultaneously. Due to Restarting generally slows the convergence of FOM by discarding some useful information at the restart, the deflation technique can compensate this disadvantage in some sense by keeping the Ritz vectors from the last cycle. This idea was first proposed by Morgan in [10] and then widely studied in [4, 9, 11].

Theoretical analysis show that the advantage of deflated restarted FOM is that the collinearity property of residual vectors by the deflated Arnoldi process are still maintained. Thus, the restart technique can be applied and finding the solution of the shifted systems (1.1) simultaneously is also possible. Numerical experiments further confirm that the deflation techniques can greatly improve the convergence performance of the restarted FOM.

The outline of the paper is as follows. In the next section we review the restarted FOM for the seed system, as well as the shifted restarted FOM for simultaneously solving the shifted systems. In Section 3, we propose the deflated shifted restarted FOM and discuss its implementation and theoretical properties in detail. Finally, numerical experiments are reported in Section 4 and some concluding remarks are given in Section 5.

2. Shifted restarted FOM for shifted linear systems

In this section, we briefly review restarted FOM for the seed system $Ax = b$ and the shifted restarted FOM method proposed in [5] for simultaneously solving shifted systems (1.1).

In the following, e_i denotes the ith column of the identity matrix whose dimension is clear from the context.

Let x_0 be an initial vector, $r_0 = b - Ax_0$ be the corresponding residual and $\beta_0 = \|r_0\|_2$. An orthonormal basis $\{v_1, v_2, \cdots, v_m\}$ of Krylov subspace $\mathcal{K}_m(A, r_0)$ can be constructed by Arnoldi process. Denote $V_m = [v_1, v_2, \cdots, v_m]$, then we have $V_m^T V_m = I$ and

$$AV_m = V_m H_m + h_{m+1,m} v_{m+1} e_m^T, \tag{2.1}$$

where $H_m = V_m^T A V_m$ is an upper Hessenberg matrix.

Let x_m and r_m be the approximation solution and the corresponding residual vector given by the mth Arnoldi process. By imposing the Galerkin condition

$$r_m \perp \mathcal{K}_m(A, r_0), \tag{2.2}$$

the approximation solution x_m can be represented by

$$x_m = x_0 + V_m d \in x_0 + \mathcal{K}_m(A, r_0)$$

where $d \in \mathbb{R}^{m \times 1}$ is the solution of a small system of linear equation

$$H_m d = \beta_0 e_1. \tag{2.3}$$

Then, it follows that

$$\begin{aligned} r_m &= b - A(x_0 + V_m d) \\ &= r_0 - AV_m d \\ &= -h_{m+1,m} d_m v_{m+1}, \end{aligned}$$

where d_m represents the last element of d. Denote $\beta = -h_{m+1,m} d_m$, then we have $r_m = \beta v_{m+1}$, which indicates that r_m is collinear with v_{m+1}.

If the approximate solution is not sufficiently accurate, then the Arnoldi process can be restarted again and again by taking the r_m as the new initial vector, and the corresponding approach is called restarted FOM.

Then, we review the shifted restarted FOM in [5] for simultaneously solving the shifted systems.

For the shifted systems (1.1), the above relation (2.1) becomes

$$(A - \sigma_i I)V_m = V_m(H_m - \sigma_i I_m) + h_{m+1,m}v_{m+1}e_m^T, \quad i = 1, 2, \cdots, s, \tag{2.4}$$

where I_m is the identity matrix of size m.

Let $\mathcal{I} = \{1, 2, \cdots, s\}$ denote an index set. If the solution of the ith shifted system satisfies the stopping rule, we remove the index i from the index set $\mathcal{I}$.

Let $x_0 = 0$, then all the systems have the same initial residual, $r_0^{(i)} = b,\ i \in \mathcal{I}$. As mentioned in the above section, the Krylov subspace is shift invariant, thus the approximation subspaces for the shifted systems can be constructed on

$$\mathcal{K}_m(A, b) = \mathrm{span}\{b, Ab, \cdots, A^{m-1}b\}. \tag{2.5}$$

Therefore, we only need perform the Arnoldi process once to construct the orthogonal basis V_m for $\mathcal{K}_m(A, b)$.

Then, the approximation solutions $x^{(i)} = V_m d^{(i)}$ are obtained by solving a sequence of reduced shifted systems

$$(H_m - \sigma_i I_m)d_i = \beta_0 e_1, \quad i \in \mathcal{I}. \tag{2.6}$$

It should be pointed out that the residuals of shifted systems satisfy

$$r_m^{(i)} = \beta^{(i)} v_{m+1}, \quad i \in \mathcal{I}, \tag{2.7}$$

where $\beta^{(i)} = -h_{m+1,m}d_m^{(i)}$ and $d_m^{(i)}$ denotes the mth element of $d^{(i)}$.

It is observed that all the residuals $r_m^{(i)}$ $(i \in \mathcal{I})$ are collinear with v_{m+1}, and thus they are collinear with each other. This property is excellent so that we could restart the shifted FOM by taking the common vector v_{m+1} as the new initial vector, and the corresponding approximate Krylov subspace is $\mathcal{K}_m(A, v_{m+1})$.

Just as the first cycle, all the new residuals still satisfy the formula (2.7), and the restarted Arnoldi process can be repeated until convergence. This leads to the shifted restarted FOM method for simultaneously solving shifted systems (1.1).

We described this method in detail as follows.

Method 2.1. Shifted restarted FOM(m) for shifted systems

1. Set $x_0^{(i)} = 0,\ i \in \mathcal{I}$ and $r_0 = b$.
2. Compute $\beta_0^{(i)} = \|r_0\|, v_1 = r_0/\beta_0^{(i)}$.
3. For $l = 1, 2, \cdots$. Do*:*
4. Compute $AV_m = V_m H_m + h_{m+1,m}v_{m+1}$.

5. Compute $d^{(i)} = (H_m - \sigma_i I_m)^{-1} e_1 \beta_{l-1}^{(i)},\ i \in \mathcal{I}$.
6. Compute $x_l^{(i)} = x_{l-1}^{(i)} + V_m d^{(i)},\ i \in \mathcal{I}$.
7. Update $\mathcal{I}$. If $\mathcal{I} = \emptyset$, exit. EndIf.
8. Set $\beta_l^{(i)} = -h_{m+1,m} d_m^{(i)},\ i \in \mathcal{I}$.
9. Set $v_1 = v_{m+1}$.
10. EndDo

It was shown in [5] that the information sharing does not cause any degradation of convergence performance, and the convergence history of shifted FOM on each system is the same as that of the usual restarted FOM method applied individually to each shifted system.

We should point out that an outstanding advantage of this approach is that the base $\{v_1, \cdots, v_m\}$ is only required to be computed once for solving all shifted systems in each cycle, so that a number of computational cost can be saved.

3. Shifted deflated FOM for shifted linear systems

In this section, we propose shifted restarted FOM with deflation for simultaneously solving a sequence of shifted systems (1.1), and discuss the implementation in detail. Theoretical analysis shows that with the deflation, the new residuals of all shifted systems are still collinear so that restarted technique can be applied.

Since the restart technique usually leads to the lost of projection information of Krylov subspace, it often slows down the convergence of FOM. A compensation technique is to save some approximate eigenvectors from the previous subspace, and add them into the new approximation subspace to deflate the smallest eigenvalues of A.

The first cycle of shifted deflated FOM is standard shifted restarted FOM with $x_0 = 0$ and $r_0 = b$, as discussed in the above section. Let $V_m = [v_1, v_2, \cdots, v_m]$ be the orthonormal matrix whose columns span the subspace $\mathcal{K}_m(A, r_0)$, and H_m be the corresponding upper Hessenberg matrix, then formula (2.4) is still valid. After this cycle, we get the approximation solutions $x^{(i)} = V_m d^{(i)},\ i \in \mathcal{I}$ and the corresponding residual vectors $r^{(i)}$ that satisfy (2.7).

Let $\theta_1, \theta_2, \cdots, \theta_k$ and $z_1, z_2, \cdots, z_k$ be the k smallest (in absolute value) eigenvalues and the corresponding eigenvectors of H_m respectively. In the following, without additional explanation, we always assume that $k \le m$.

Denote $y_i = V_m z_i$ $(i = 1, 2, \cdots, k)$ be the Ritz vectors of A corresponding to the k smallest eigenvalues, then the new approximation subspace for all shifted systems is chosen as

$$\mathcal{K}_{m,k}(A, v_{m+1}) = \mathrm{span}\{y_1, \cdots, y_k, v_{m+1}, Av_{m+1}, \cdots, A^{m-k-1} v_{m+1}\}, \tag{3.1}$$

where v_{m+1} represents the last orthonormal vector from the previous cycle. It is clear that $v_{m+1} \perp y_i, i = 1, 2, \cdots, k$ due to $v_{m+1} \perp V_m$. Here, the Ritz vectors are put at the beginning in the next approximation subspace, so that the new project matrix will have very simple structure; for details, we refer the reader to [9, 14].

Note that the Ritz vectors $y_1, \cdots, y_k$ of A also belong to matrices $A - \sigma_i I, i \in \mathcal{I}$. We expect that keeping these vector in the next approximation subspace can accelerate the convergence performance of FOM simultaneously, since it was shown in [9, 10] that keeping several approximate eigenvectors in the approximation subspace can improve the convergence performance of FOM/GMRES, even if these eigenvectors are not extremely accurate.

Since H_m is not symmetric, its eigenvalues and eigenvectors could be complex. However, it is noted that if $\theta = a + bi$ was one of the eigenvalues of H_m with the eigenvector $w + ui$, then $\overline{\theta} = a - bi$ is also the eigenvalues of H_m with the eigenvector $w - ui$, and satisfy

$$H_m \begin{pmatrix} w & u \end{pmatrix} = \begin{pmatrix} w & u \end{pmatrix} \begin{pmatrix} a & b \\ -b & a \end{pmatrix}.$$

Hence, if θ_i and $\overline{\theta}_i$ are complex eigenvalues in $\theta_1, \theta_2, \cdots, \theta_k$, we replace them by a and b, the corresponding eigenvectors by w and u, so that all the θ_i and z_i $(i = 1, 2, \cdots, k)$ are real and satisfy

$$H_m Z_k = Z_k \Theta_k, \tag{3.2}$$

where $Z_k = [z_1, z_2, \cdots, z_k]$ and Θ_k is a block diagonal matrix, whose diagonal blocks are either 1 by 1 or 2 by 2.

We should remark that, if there is odd complex eigenvalue in the kth smallest eigenvalues, we can change k by increasing 1 or decreasing 1, so that both the complex eigenvalue and its complex conjugate are include and the above transform can be done.

It should be mentioned that after this transformation, the columns of Z_k are no more orthonormal, so does the columns of Y_k. Hence, a modified Gram-Schmidt can be applied to $z_i (i = 1, 2, \cdots, k)$, so that

$$Z_k^{\rm new} = Z_k P,$$

where $Z_k^{\rm new}$ is column orthonormal and $P \in \mathbb{R}^{k \times k}$ is nonsingular. Then, we have

$$H_m Z_k^{\rm new} = Z_k^{\rm new} \Theta_k^{\rm new}, \tag{3.3}$$

where $\Theta_k^{\rm new} = P^{-1} \Theta_k P$ so that $Y_k = V_m Z_k^{\rm new}$ is column orthonormal.

Let $\tilde{V}_m$ denote the orthonormal matrix of the second cycle, whose first k columns are formed by the orthonormal vectors $y_i, i = 1, 2, \cdots, k$, and the rest can be generated by the usual Arnoldi approach with initial vector v_{m+1} obtained from the previous cycle.

At the end of this cycle, the recurrence formula similar to the Arnoldi recurrence (2.1) is held. We describe this property as follow.

Proposition 3.1. *Denote $\tilde{V}_m$ and $\tilde{H}_m$ be the orthonormal matrix and projection matrix of the second cycle of deflated restarted FOM, then the following relation holds*

$$A \tilde{V}_m = \tilde{V}_m \tilde{H}_m + \tilde{h}_{m+1,m} \tilde{v}_{m+1} e_m^T \tag{3.4}$$

and the projection matrix $\tilde{H}_m$ has the form

$$\tilde{H}_m = \begin{bmatrix} \Theta_k & \vdots & \cdots & \cdots & \vdots \\ h_{m+1,m}f^T & \tilde{h}_{k+1,k+1} & \cdots & \cdots & \tilde{h}_{k+1,m} \\ & \tilde{h}_{k+2,k+1} & \tilde{h}_{k+2,k+2} & \cdots & \tilde{h}_{k+2,m} \\ & & \ddots & \ddots & \vdots \\ & & & \tilde{h}_{m,m-1} & \tilde{h}_{m,m} \end{bmatrix}, \tag{3.5}$$

where $f = Z_k^T e_m$.

Proof. Under the above definitions, it follows from (2.1) and (3.2) that

$$\begin{aligned} A\tilde{V}_k &= AV_m Z_k \\ &= (V_m H_m + h_{m+1,m} v_{m+1} e_m^T) Z_k \\ &= V_m Z_k \Theta_k + h_{m+1,m} v_{m+1} e_m^T Z_k \\ &= \tilde{V}_k \Theta_k + h_{m+1,m} v_{m+1} f^T \\ &= \tilde{V}_{k+1} \begin{bmatrix} \Theta_k \\ h_{m+1,m} f^T \end{bmatrix}, \end{aligned}$$

where $h_{m+1,m}$ is from previous cycle and $f = Z_k^T e_m$.

Because the rest are the standard Arnoldi process, it is obvious that the relation (3.4) is satisfied and $\tilde{H}_m$ has an upper-Hessenberg portion of the form (3.5). □

Now, we are in a position to simultaneously form the solution of the shift systems (1.1) by solving a sequence of small reduced systems. The following proposition gives the details for solving the approximate solution of the shift systems in the deflated restarted FOM.

Proposition 3.2. *Denote $\tilde{V}_m$ and $\tilde{H}_m$ be the orthonormal matrix and project matrix of the current cycle of deflated restarted FOM, and $x^{(i)}$ be the approximate solution of $(A - \sigma_i I)x = b,\ i \in \mathcal{I}$ in precious cycle, then the new approximate solution $\tilde{x}^{(i)}$ can be computed by*

$$\tilde{x}^{(i)} = x^{(i)} + \tilde{V}_m \tilde{d}^{(i)}, \quad i \in \mathcal{I},$$

where $\tilde{d}^{(i)}$ solves the reduced system

$$(\tilde{H}_m - \sigma_i I_m)\tilde{d}^{(i)} = -h_{m+1,m} d_m^{(i)} e_{k+1}, \quad i \in \mathcal{I}. \tag{3.6}$$

Proof. From the definition of FOM, the associated residual $\tilde{r}^{(i)} = b - (A - \sigma_i I)\tilde{x}^{(i)}$ is orthogonal to the approximation subspace $\mathcal{K}_{m,k}(A, v_{m+1})$, i.e.,

$$\tilde{r}^{(i)} \perp \tilde{V}_m^T, \quad i \in \mathcal{I},$$

thus,

$$\begin{aligned}\tilde{V}_m^T\tilde{r}^{(i)} &= \tilde{V}_m^T(b-(A-\sigma_iI)(x^{(i)}+\tilde{V}_m\tilde{d}^{(i)}))\\ &= \tilde{V}_m^T(r^{(i)}-(A-\sigma_iI)\tilde{V}_m\tilde{d}^{(i)})\\ &= \tilde{V}_m^T(-h_{m+1,m}d_m^{(i)}v_{m+1}-V_m\tilde{H}_m-\sigma_iI_m)\tilde{d}^{(i)})\\ &= -h_{m+1,m}d_m^{(i)}\tilde{V}_m^Tv_{m+1}-(\tilde{H}_m-\sigma_iI_m)\tilde{d}^{(i)}\\ &= 0, \quad i\in\mathcal{I}.\end{aligned}$$

Note that $\tilde{v}_{k+1}=v_{m+1}$, it follows that

$$-h_{m+1,m}d_m^{(i)}e_{k+1}-(\tilde{H}_m-\sigma_iI_m)\tilde{d}^{(i)}=0, \quad i\in\mathcal{I}.$$

Therefore, the results of (3.6) is obtained. □

From Proposition 3.2, it can be seen that the reduced systems we solved in deflated restarted FOM are similar to those in shifted FOM, except that e_1 in (2.6) is replaced by e_{k+1} in formula (3.6).

From the previous section, we know that if the residual vectors of all shifted systems are parallel to each other, the FOM can be restarted in the same subspace corresponding to the seed system. It is noticed that the new approximation subspace (3.1) contains a Krylov portion

$$\mathrm{span}\{v_{m+1},Av_{m+1},\cdots,A^{m-k-1}v_{m+1}\},$$

we expect that the advantage of shifted restarted FOM can be kept here, that is, the current residuals of all shifted systems are still collinear with $\tilde{v}_{m+1}$.

We states this property as follows.

Proposition 3.3. *Denote $\tilde{V}_m$ and $\tilde{H}_m$ be the orthonormal matrix and projection matrix of the current cycle of deflated restarted FOM, and the approximate solutions of $(A-\sigma_iI)x=b,\ i\in\mathcal{I}$ be $\tilde{x}^{(i)}=x^{(i)}+\tilde{V}_m\tilde{d}^{(i)},\ i\in\mathcal{I}$, then, there exists $\tilde{\beta}^{(i)}\in\mathbb{R}$ such that*

$$\tilde{r}^{(i)}=b-(A-\sigma_iI)\tilde{x}^{(i)}=\tilde{\beta}^{(i)}\tilde{v}_{m+1}. \tag{3.7}$$

Proof. It follows from the result in Proposition 3.2 that

$$\begin{aligned}\tilde{r}^{(i)} &= b-(A-\sigma_iI)\tilde{x}^{(i)}\\ &= b-(A-\sigma_iI)(x^{(i)}+\tilde{V}_m\tilde{d}^{(i)})\\ &= r^{(i)}-(A-\sigma_iI)\tilde{V}_m\tilde{d}^{(i)}\\ &= -h_{m+1,m}d_m^{(i)}v_{m+1}-\tilde{V}_m(\tilde{H}_m-\sigma_iI_m)\tilde{d}^{(i)}-\tilde{h}_{m+1,m}\tilde{v}_{m+1}e_m^T\tilde{d}^{(i)}\\ &= -\tilde{h}_{m+1,m}\tilde{v}_{m+1}\tilde{d}_m^{(i)},\end{aligned}$$

where $\tilde{d}_m^{(i)}$ represents the last element of $\tilde{d}^{(i)}$. By defining $\tilde{\beta}^{(i)}=-\tilde{h}_{m+1,m}\tilde{d}_m^{(i)}$, the result (3.7) is obtained immediately. □

From (3.7), it is seen that all current residuals are collinear with $\tilde{v}_{m+1}$ at the end of the second cycle, hence the process can also be restarted again until convergence.

The implementation of shifted deflated restarted FOM can now be given in detail as follows.

Method 3.1. s-DFOM(m) for shifted systems

1. Set $x_0^{(i)} = 0,\ i \in \mathcal{I}$ and $r_0 = b$.
2. Compute $\beta_0^{(i)} = \|r_0\|, v_1 = r_0/\beta_0^{(i)}$.
3. Compute $AV_m = V_m H_m + h_{m+1,m} v_{m+1}$.
4. Compute $d^{(i)} = (H_m - \sigma_i I_m)^{-1} \beta_0^{(i)} e_1,\ i \in \mathcal{I}$.
5. Compute $x_1^{(i)} = x_0^{(i)} + V_m d^{(i)},\ i \in \mathcal{I}$.
6. For $l = 2, 3, \cdots$ Do*:*
7. Set $\beta_{l-1}^{(i)} = -h_{m+1,m} d_m^{(i)},\ i \in \mathcal{I}$.
8. Compute the matrices Z_k and Θ_k corresponding to the kth smallest eigenvalues of H_m.
9. Compute $V_k = V_m Z_k$ and $v_{k+1} = v_{m+1}$.
9. Compute $AV_m = V_m H_m + h_{m+1,m} v_{m+1}$.
10. Compute $d^{(i)} = (H_m - \sigma_i I_m)^{-1} \beta_{l-1}^{(i)} e_{k+1},\ i \in \mathcal{I}$.
11. Compute $x_l^{(i)} = x_{l-1}^{(i)} + V_m d^{(i)},\ i \in \mathcal{I}$.
12. Update $\mathcal{I}$. If $\mathcal{I} = \emptyset$, exit. EndIf.
13. EndDo

It is seen from the above Method 3.1 that the first cycle of new approach, i.e., from Step 2 to Step 5, is the same as the standard shifted FOM. In the new cycle, we firstly compute out Z_k and Θ_k and apply the Arnoldi iteration from v_{k+1} to form the rest of V_{m+1} and $\bar{H}_m$.

The most important part of Method 3.1 is to choose the deflation terms, Z_k and Θ_k. For numerical stability, in practical, we can also reorthogonalize v_{k+1} against the former Ritz vectors to construct new H_k.

The memory requirement of shifted deflated restarted FOM is the same as that of shifted restarted FOM without deflation. From the viewpoint of computational cost, the shifted deflated restarted FOM can save some operation in Gram-Schmidt process, but require additional computation for the k smallest eigenvalues and eigenvectors of H_m. The main potential advantage of s-DFOM compared to shifted restarted FOM is the convergence performance, which will be illustrated in the next section.

4. Numerical experiments

In this section, we present some numerical experiments to illustrate the convergence performance of shifted restarted FOM with deflation, compared with the restarted shifted FOM proposed by Simoncini in [5].

The initial guess solution x_0 and the right-hand side vector b are taken as $x_0 = (0,0,\cdots,0)^T$ and $b = (1,1,\cdots,1)^T$ respectively. Suppose x_k is the approximate solution in the kth cycle, we stop the procedure if x_k satisfies

$$\frac{\|b-(A-\sigma_i I)x_k\|_2}{\|b-(A-\sigma_i I)x_0\|_2} < 10^{-8}, \quad i \in \mathcal{I},$$

or the number of maximal iteration, e.g., 5000, is reached. Numerical experiments were done in Matlab 6.5 on a computer with 2.10 GHz CPU and 3G memory.

In our numerical experiments, two shifted values, $\sigma_1 = -0.5, \sigma_2 = 0.5$, for shifted systems are considered. The dimension of approximation subspace is chosen to be $m = 20$.

We firstly described the test examples as follow.

Example 1. Let A is a 500×500 upper bidiagonal matrix, with entries $0.01, 0.02, 0.03, 0.04, 10, 11, \cdots, 505$ on the main diagonal and all ones on the super diagonal.

Example 2. The matrix is ORSIRR2 from the Harwell-Boeing sparse matrix collection [2], whose dimension is 886.

Example 3. The matrix $A \in \mathbb{R}^{2000\times 2000}$ is of the form

$$A = \begin{bmatrix}
1 & 0.21 & 1.2 & 0 & 0.13 & 1.42 & & & & \\
0.45 & 2 & 0.21 & 1.2 & 0 & 0.13 & 1.42 & & & \\
0 & 0.45 & 3 & 0.21 & 1.2 & 0 & 0.13 & & & \\
0.12 & 0 & 0.45 & 4 & 0.21 & & & \ddots & & \\
0.11 & 0.12 & 0 & 0.45 & & & \ddots & & 0.13 & 0.42 \\
 & 0.11 & 0.12 & & & \ddots & & 1.2 & 0 & 0.13 \\
 & & & & \ddots & & 1997 & 0.21 & 1.2 & 0 \\
 & & & \ddots & & 0 & 0.45 & 1998 & 0.21 & 1.2 \\
 & & & & 0.11 & 0.12 & 0 & 0.45 & 1999 & 0.21 \\
 & & & & & 0.11 & 0.12 & 0 & 0.45 & 2000
\end{bmatrix}.$$

Example 4. The test matrix A is ORSREG1 from the Harwell-Boeing sparse matrix collection [2]. The size of this matrix is 2205.

4.1. Choice of the number of deflation vectors

In this section, we give an example to illustrate how the number of deflation vectors influent the performance of shifted restarted FOM. Then, we give some comments and suggestion on the choice of the deflation vectors.

We focus our attention on Example 3, since it is a standard test example, which was also tested in [5, 13].

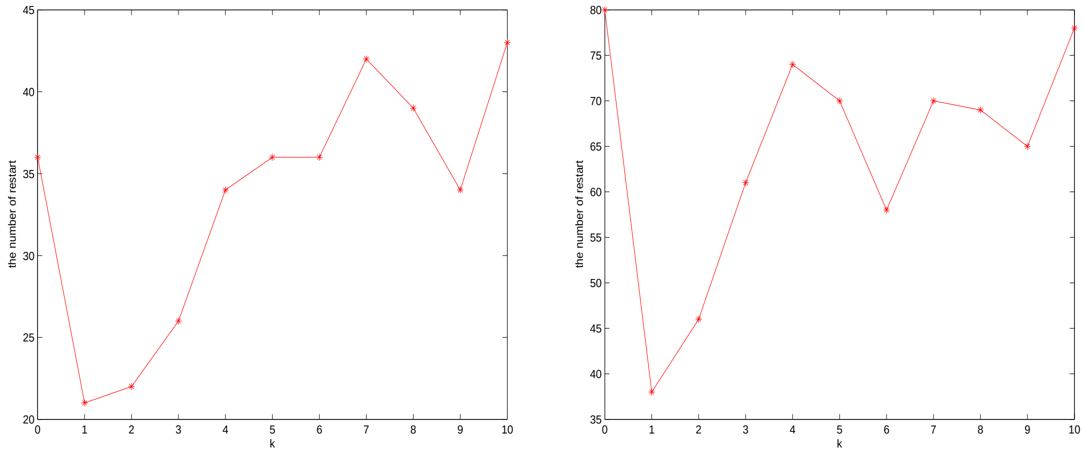

Figure 1: Example 3. Left: $\sigma_1 = -0.5$; Right: $\sigma_2 = 0.5$.

In Fig. 1, the curves of the number of restart versus the number of preserved Ritz vector for s-DFOM is depicted when $\sigma = -0.5$ and 0.5 respectively.

From Fig. 1, it is observed that the number of restart is different for different k when $\sigma = -0.5$ and 0.5. This implies that the convergence performance of s-DFOM is influenced by the number of preserved Ritz vector.

On the other hand, it is observed from Fig. 1 that when $\sigma = -0.5$, s-DFOM can converge faster than s-FOM for $k = 1, 2, 3, 4, 9$, while when $\sigma = 0.5$, s-DFOM is faster than s-FOM for all k. This shows that the accelerate performance of deflation is different for different k.

The convergence curves demonstrate that the deflated restating technique is effective in achieving fast convergence.

From Fig. 1, it is seen that $k = 1$ is the optimal choice of k, since in this case s-DFOM converges the fastest for both $\sigma_1 = -0.5$ and $\sigma_2 = 0.5$.

We should remark that the optimal choice for k is problem dependent, and is difficult to analyze from the theoretical viewpoint. However, in practical, we can test the efficiency of deflation technique by some small k, for instance, k is from 1 to 5.

4.2. Numerical comparison with shifted FOM

In this section, we compare the total computational costs of s-DFOM with those of s-FOM. Since $m = 20$ is taken for all the examples, the total iteration number of both methods can be counted by the number of restart.

In Figs. 2-5, the curves of residual norms versus the number of restarts of both s-DFOM and s-FOM are plotted for examples 1-4 respectively, when $\sigma_1 = -0.5$ and $\sigma_2 = 0.5$. Here, the number for k is the same for different σ, which is also listed in Figs. 2-5.

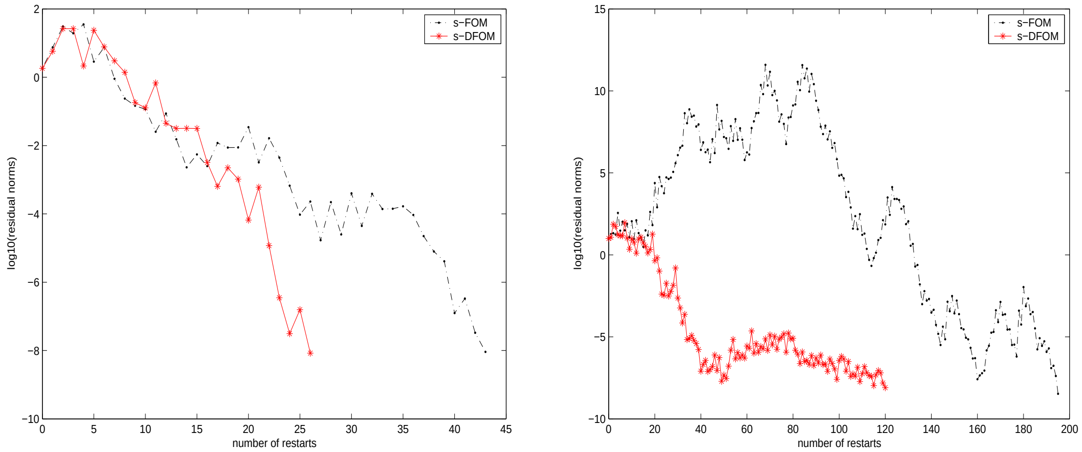

Figure 2: Example 1 ($k = 2$). Left: $\sigma_1 = -0.5$; Right: $\sigma_2 = 0.5$.

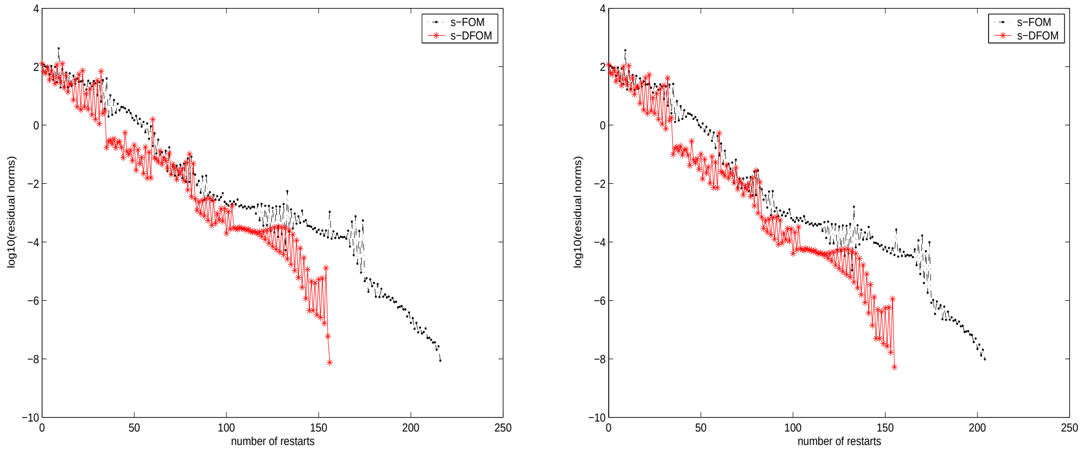

Figure 3: Example 2 ($k = 5$). Left: $\sigma_1 = -0.5$; Right: $\sigma_2 = 0.5$.

From Figs. 2-5, it is seen that the s-DFOM converges faster than s-FOM for these four examples when $\sigma_1 = -0.5$ and $\sigma_2 = 0.5$ respectively.

For instance, in Example 3 when $\sigma_2 = 0.5$, the s-FOM requires 80 restarts to obtain the desired accuracy, but the new method need only 46 restarts to reach the stopping criteria. This show that the deflation technique can accelerate the convergence considerably.

5. Conclusion

We have presented and implemented shifted restarted FOM with deflation for simultaneously solving shifted systems (1.1).

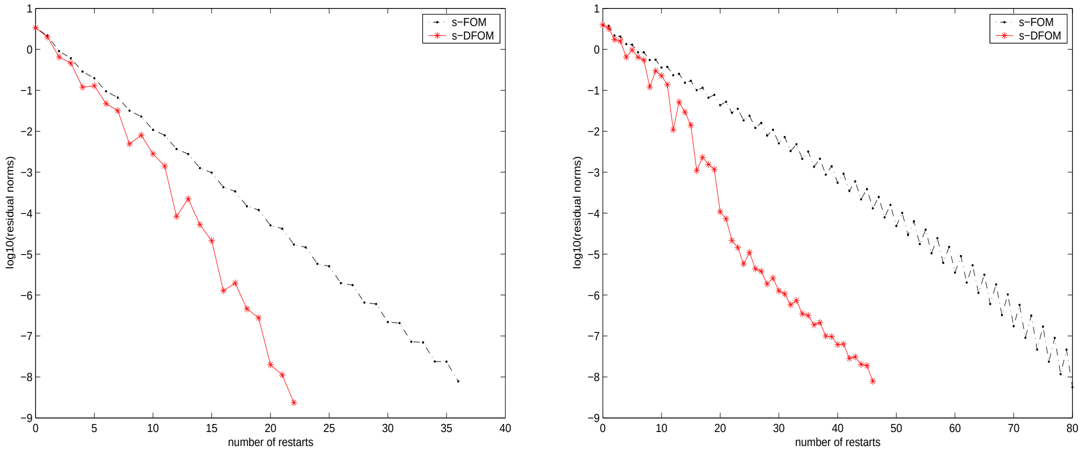

Figure 4: Example 3 ($k = 2$). Left: $\sigma_1 = -0.5$; Right: $\sigma_2 = 0.5$.

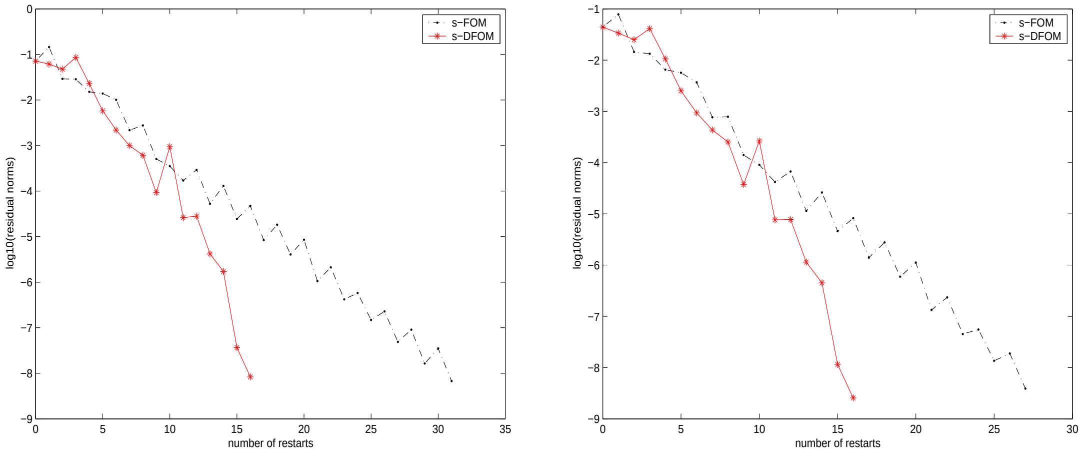

Figure 5: Example 4 ($k = 5$). Left: $\sigma_1 = -0.5$; Right: $\sigma_2 = 0.5$.

Theoretical analysis showed that with the deflation technique, the new residual of shifted restarted FOM is still collinear with each other so that the shifted systems can be solved simultaneously only based on one restarted Arnoldi process.

Numerical experiment further proved that the deflation technique can greatly improve the convergence performance of shifted restarted FOM.

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