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Restarted FOM Augmented with Ritz Vectors for Shifted Linear Systems†

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Abstract. The restarted FOM method presented by Simoncini [7] according to the natural collinearity of all residuals is an efficient method for solving shifted systems, which generates the same Krylov subspace when the shifts are handled simultaneously. However, restarting slows down the convergence. We present a practical method for solving the shifted systems by adding some Ritz vectors into the Krylov subspace to form an augmented Krylov subspace. Numerical experiments illustrate that the augmented FOM approach (restarted version) can converge more quickly than the restarted FOM method.

Key words: Augmented Krylov subspace; FOM; restarting; shifted systems.

AMS subject classifications: 65F10, 65Y20

1 Introduction

Given a real large nonsymmetric matrix A, we are interested in solving the following shifted systems

$$Ax = b \tag{1}$$

and

$$\hat{A}x = b, \tag{2}$$

where $\hat{A} = A + \sigma I$ for several (say a few hundreds; see e.g. [7]) σ, $\sigma \in R$. These kinds of linear systems arise in many fields. For instance, in image restorations, numerical methods for integral equations, structural dynamics, and QCD problems.

The system (1) can be called seed system and (2) called add system. It is well known that the Krylov subspace $K_m(A, r_0) = \text{span}\{r_0, Ar_0, \cdots, A^{m-1}r_0\}$ is the same as $K_m(\hat{A}, \hat{r}_0) = \text{span}\{\hat{r}_0, \hat{A}\hat{r}_0, \cdots, \hat{A}^{m-1}\hat{r}_0\}$ with $\hat{r}_0 = \beta_0 r_0$. Therefore, if we apply a Krylov subspace method to

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solve (1) and (2) simultaneously, the basis has to be calculated only once. Then the iterative solution of the add system may be calculated at a very low extra expense.

However, the Krylov subspace required to satisfactorily approximate (1) and (2) appears to be too large, and the computational cost is expensive, so the method needs to be restarted, taking the current system residual as a new generating vector. If the new Krylov subspace is the same for all shifted systems, the computational efficiency can be maintained. We want to get the identical basis vectors for $K_m(A, r_m)$ and $K_m(\hat{A}, \hat{r}_m)$, so the collinearity of residuals r_m and $\hat{r}_m$ is required. Simoncini[7] gave the natural collinearity of r_m and $\hat{r}_m$ for FOM by computing

$$r_m = b - Ax_m = r_0 - AV_m d_m = -h_{m+1,m} v_{m+1} e_m^T d_m = \beta v_{m+1}, \quad (3)$$

$$\hat{r}_m = b - \hat{A}\hat{x}_m = \hat{r}_0 - \hat{A} V_m \hat{d}_m = -\hat{h}_{m+1,m} v_{m+1} e_m^T \hat{d}_m = \hat{\beta} v_{m+1}. \quad (4)$$

So restarting can also be employed in the shifted case. For GMRES, the natural collinearity of residuals are not satisfied. Frommer and Glassner [1] give a variant of GMRES by forcing the residual $\hat{r}_m$ to be collinear to r_m, so restarting can also be employed. However restarting will slow down the convergence since some information is lost when restarting.

In [3,4], we have presented restarted GMRES and restarted FOM augmented with exact eigenvectors to solve system (1) and (2) based on the Morgan's augmented method [5] and the idea of Frommer and Glassner [1]. However, these methods are generally impractical since the exact eigenvectors are difficult or impossible to obtain. In this paper, we show that FOM augmented by adding some Ritz vectors, instead of exact eigenvectors, can also be used to solve the shifted systems (1) and (2). This version of augmented FOM (denoted as shifted FOM-R) can practically be implemented since the Ritz vectors can be easily derived. Numerical experiments illustrate the efficiency of the method.

2 Review of some known facts

In [5], Morgan presented an augmented Krylov subspace method by adding some eigenvectors z_i associated with a few of the smallest eigenvalues of A into the standard Krylov subspace to form an augmented Krylov subspace

$$K_{m,l}(A, r_0, z_i) = \text{span}\{r_0, Ar_0, \cdots, A^{m-1}r_0, z_1, \cdots, z_l\}.$$

Let m be the dimension of the standard Krylov subspace$K_m(A, r_0)$ and $V_m = [v_1, \cdots, v_m]$ is the basis of the subspace. Suppose l eigenvectors $z_1, \cdots, z_l$ are added into the subspace. Let $W_s = [v_1, \cdots, v_m, z_1, \cdots, z_l]$, $Q_{s+1} = [v_1, \cdots, v_{m+1}, q_1, \cdots, q_l]$, where q_i is formed by orthogonalizing the vectors Az_i against the previous columns of Q_{s+1}. By the augmented Arnoldi process [5,6], we have the Arnoldi factorization

$$AW_s = Q_{s+1}\bar{H}_s \quad (s = m + l), \quad (1)$$

where $\bar{H}_s$ is an $(s + 1) \times s$ upper-Hessenberg matrix. An augmented Krylov subspace method is a project process on the augmented subspace $K_{m,l}(A, r_0, z_i)$.

In [4], we have shown that the restarted FOM method augmented with exact eigenvectors (denoted as shifted FOM-E) can be used to solve the shifted systems (1) and (2). In that case, we want to derive the approximate solution of the seed system and the add system in the augmented Krylov subspace $K_{m,l}(A, r_0, z_i)$. According to FOM , the approximate solution of the seed system $x_s = x_0 + W_s d_s$ can be obtained with $d_s = H_s^{-1}\|r_0\|_2 e_1$, and by forcing the residual of the add system $\hat{r}_s$ to be collinear to the residual of the seed system r_s, the approximate solution of the add system $\hat{x}_s = \hat{x}_0 + W_s\hat{d}_s$ can be obtained by solving the following linear system

$$\left(\begin{array}{ccc} \hat{H}_m & G_1(I+\sigma\Lambda_l^{-1}) & 0 \\ 0 & G_2(I+\sigma\Lambda_l^{-1}) & -h_{s+1,s}e_l e_s^T d_s \end{array}\right)\left(\begin{array}{c} \hat{d}_m \\ \hat{\alpha} \\ \beta_s \end{array}\right) = \left(\begin{array}{c} \beta_0\|r_0\|_2 e_1 \\ 0 \end{array}\right), \tag{2}$$

where $\hat{H}_m = \bar{H}_m + \sigma\left[\begin{array}{c} I_m \\ 0 \end{array}\right]$, $\Lambda_l = \mathrm{diag}(\lambda_1, \cdots, \lambda_l)$, $\lambda_1, \cdots, \lambda_l$ are the l smallest eigenvalues of A, and $\hat{d}_s = \left[\begin{array}{c} \hat{d}_m \\ \hat{\alpha} \end{array}\right]$.

In [4], we show that the above equation (2) has a unique solution under some conditions.

Theorem 2.1 ([4]). *Assume that $K_{m+1,l}(A, r_0, z_i)$ is the subspace with dimension $s+1$, $\beta_0 \neq 0$ and $\lambda_i + \sigma \neq 0$. Then the system (2) has a unique solution $(\hat{d}_m, \hat{\alpha}, \beta_s)$ if and only if $p_m(-\sigma) \neq 0$. where p_m is a residual polynomial with degree m, i.e., $r_m = p_m(A)r_0$.*

3 Augmented FOM with Ritz vectors

In practice, the eigenvalues and the eigenvectors are difficult or impossible to obtain, and what we can get is only the approximate eigenvalues and eigenvectors, for example, the Ritz values and Ritz vectors. In this section, we show that the restarted FOM method augmented with the Ritz vectors can be used to solve the shifted systems (1) and (2).

By the Arnoldi process, we have the following relation

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

Assume that $H_m p_i = \theta_i p_i$, $i = 1, \cdots, l$ and $\theta_1, \cdots, \theta_l$ are the l smallest eigenvalues of H_m, and $p_1, \cdots, p_l$ are the corresponding eigenvectors. Then the Ritz value θ_i is the approximate eigenvalue of A, and the Ritz vector $y_i = V_m p_i$ is the approximate eigenvector. According to (1), we get

$$\begin{aligned} Ay_i - \theta_i y_i &= AV_m p_i - \theta_i V_m p_i \\ &= V_m H_m p_i - \theta_i V_m p_i + v_{m+1}h_{m+1,m}e_m^T p_i \\ &= V_m(H_m p_i - \theta_i p_i) + v_{m+1}h_{m+1,m}e_m^T p_i \\ &= v_{m+1}h_{m+1,m}e_m^T p_i \\ &= \delta_i v_{m+1} \end{aligned} \tag{2}$$

where $\delta_i = h_{m+1,m}e_m^T p_i$. The matrix form of (2) is

$$AY_l = Y_l\Theta_l + v_{m+1}\Delta_l, \tag{3}$$

where $Y_l = [y_1, \cdots, y_l]$, $\Theta_l = \mathrm{diag}(\theta_1, \cdots, \theta_l)$ and $\Delta_l = [\delta_1, \cdots, \delta_l]$.

Suppose that we have obtained the approximate solution $x_s^{(k)}$ of the seed system and the l Ritz vectors $y_1^{(k)}, \cdots, y_l^{(k)}$ associated with the l smallest Ritz values in the Krylov subspace $K_m(A, r_0^{(k)})$, where the superscript (k) denotes the restart number, $k = 1, 2, \cdots$. When the residual norm does not reach the tolerance, we consider restarting in the Krylov subspace $K_{m,l}(A, r_0^{(k+1)}, y_i^{(k)})$, that is, we compute an approximate solution $x_s^{(k+1)}$ such that $x_s^{(k+1)} - x_0^{(k+1)} \in K_{m,l}(A, r_0^{(k+1)}, y_i^{(k)})$ with $r_0^{(k+1)} = r_s^{(k)}$ and $x_0^{(k+1)} = x_s^{(k)}$. Thus $x_s^{(k+1)}$ can be written as

$$x_s^{(k+1)} = x_0^{(k+1)} + q_{m-1}^{(k+1)}(A)r_0^{(k+1)} + \sum_{i=1}^{l}\alpha_i^{(k)}y_i^{(k)},$$

where $q_{m-1}^{(k+1)}(t)$ is a polynomial of degree $\leq m-1$. The residual $r_s^{(k+1)} = b - Ax_s^{(k+1)}$ is

$$r_s^{(k+1)} = r_0^{(k+1)} - Aq_{m-1}^{(k+1)}(A)r_0^{(k+1)} - \sum_{i=1}^{l} \alpha_i^{(k)} Ay_i^{(k)} = p_m^{(k+1)}(A)r_0^{(k+1)} - \sum_{i=1}^{l} \alpha_i^{(k)} Ay_i^{(k)},$$

where $p_m^{(k+1)}(t) = 1 - tq_{m-1}^{(k+1)}(t)$ with $p_m^{(k+1)}(0) = 1$. For the add system (2), we similarly have

$$\hat{x}_s^{(k+1)} = \hat{x}_0^{(k+1)} + \hat{q}_{m-1}^{(k+1)}(\hat{A})\hat{r}_0^{(k+1)} + \sum_{i=1}^{l} \hat{\alpha}_i^{(k)} y_i^{(k)},$$

and

$$\hat{r}_s^{(k+1)} = b - \hat{A}\hat{x}_s^{(k+1)} = \hat{p}_m^{(k+1)}(\hat{A})\hat{r}_0^{(k+1)} - \sum_{i=1}^{l} \hat{\alpha}_i^{(k)} \hat{A}y_i^{(k)},$$

where $\hat{p}_m^{(k+1)}(t)$ is the polynomial of degree $\leq m$ with $\hat{p}_m^{(k+1)}(0) = 1$.

Now assume the initial residuals are collinear $\hat{r}_0^{(k+1)} = \beta_0^{(k+1)} r_0^{(k+1)}$, $\beta_0^{(k+1)} \in R$. Then we require that

$$\hat{r}_s^{(k+1)} = \beta_s^{(k+1)} r_s^{(k+1)}, \qquad \beta_s^{(k+1)} \in R. \tag{4}$$

Equivalently, we have

$$\beta_0^{(k+1)}\hat{p}_m^{(k+1)}(A+\sigma I)r_0^{(k+1)} - \sum_{i=1}^{l} \hat{\alpha}_i^{(k)}(A+\sigma I)y_i^{(k)} = \beta_s^{(k+1)}(p_m^{(k+1)}(A)r_0^{(k+1)} - \sum_{i=1}^{l} \alpha_i^{(k)} Ay_i^{(k)}).$$

It follows from $Ay_i^{(k)} = \delta_i^{(k)} v_{m+1}^{(k)} + \theta_i^{(k)} y_i^{(k)}$, $(A+\sigma I)y_i^{(k)} = \delta_i^{(k)} v_{m+1}^{(k)} + (\theta_i^{(k)} + \sigma)y_i^{(k)}$, (3) and $r_0^{(k+1)} = r_m^{(k)} = \beta^{(k+1)} v_{m+1}^{(k)}$ that

$$\begin{aligned} & \beta_0^{(k+1)}\hat{p}_m^{(k+1)}(A+\sigma I)r_0^{(k+1)} - \sum_{i=1}^{l} \hat{\alpha}_i^{(k)}(\delta_i^{(k)} \frac{r_0^{(k+1)}}{\beta^{(k+1)}} + (\theta_i^{(k)}+\sigma)y_i^{(k)}) \\ = \quad & \beta_s^{(k+1)}(p_m^{(k+1)}(A)r_0^{(k+1)} - \sum_{i=1}^{l} \alpha_i^{(k)}(\delta_i^{(k)} \frac{r_0^{(k+1)}}{\beta^{(k+1)}} + \theta_i^{(k)} y_i^{(k)})). \end{aligned}$$

By assumption that the vectors $r_0^{(k+1)}, Ar_0^{(k+1)}, \cdots, A^{m-1}r_0^{(k+1)}, y_1^{(k)}, \cdots, y_l^{(k)}$ are linearly independent, we can deduce that

$$\beta_0^{(k+1)}\hat{p}_m^{(k+1)}(t+\sigma) - \sum_{i=1}^{l} \frac{\delta_i^{(k)}}{\beta^{(k+1)}}(\hat{\alpha}_i^{(k)} - \beta_s^{(k+1)}\alpha_i^{(k)}) - \beta_s^{(k+1)} p_m^{(k+1)}(t) = 0, \tag{5}$$

$$\hat{\alpha}_i^{(k)}(\theta_i^{(k)} + \sigma) = \beta_s^{(k+1)}\alpha_i^{(k)}\theta_i^{(k)}, \qquad i = 1, \cdots, l. \tag{6}$$

For $\hat{p}_m^{(k+1)}(0) = 1$, (5) and (6) can be written as the following system,

$$\begin{pmatrix} \beta^{(k+1)}p_m^{(k+1)}(-\sigma) - \sum_{i=1}^{l} \delta_i^{(k)}\alpha_i^{(k)} & \delta_1^{(k)} & \cdots & \delta_l^{(k)} \\ \alpha_1^{(k)}\theta_1^{(k)} & \theta_1^{(k)} + \sigma & \cdots & 0 \\ \vdots & \vdots & \cdots & \vdots \\ \alpha_l^{(k)}\theta_l^{(k)} & 0 & \cdots & \theta_l^{(k)} + \sigma \end{pmatrix} \begin{pmatrix} \beta_s^{(k+1)} \\ \hat{\alpha}_1^{(k)} \\ \vdots \\ \hat{\alpha}_l^{(k)} \end{pmatrix} = \begin{pmatrix} \hat{\beta}^{(k+1)} \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \tag{7}$$

where $\hat{\beta}^{(k+1)} = \beta_0^{(k+1)}\beta^{(k+1)}$. Thus, we get the following theorem.

Theorem 3.1. *Assume that* $K_{m+1,l}(A, r_0^{(k+1)}, y_i^{(k)})$ *is the subspace with dimension* $s+1$, $\hat{\beta}^{(k+1)} \neq 0$. *Then there exists a polynomial* $\hat{p}_m^{(k+1)}$ *and number* $\beta_s^{(k+1)}, \hat{\alpha}_1^{(k)}, \cdots, \hat{\alpha}_l^{(k)}$ *satisfying (7) if and only if* $\theta_i^{(k)} + \sigma \neq 0, \quad i = 1, \cdots, l$ *and* $\sum_{i=1}^{l} \alpha_i^{(k)} \delta_i^{(k)} (\frac{2\theta_i^{(k)} + \sigma}{\theta_i^{(k)} + \sigma}) \neq \beta^{(k+1)} p_m^{(k+1)}(-\sigma)$. *In that case,*

$$\hat{p}_m^{(k+1)}(t) = [\beta^{(k+1)} \beta_s^{(k+1)} p_m^{(k+1)}(t-\sigma) - \sum_{i=1}^{l} \delta_i^{(k)} (\hat{\alpha}_i^{(k)} - \beta_s^{(k+1)} \alpha_i^{(k)})] / \hat{\beta}^{(k+1)}.$$

For a given Krylov subspace method, the polynomial p_m is usually not calculated in practice. We now work out how the iterates for (2) satisfying (4) can be practically computed when the augmented FOM iterates is performed on (1).

Suppose that the Arnoldi vectors $v_1^{(k)}, \cdots, v_{m+1}^{(k)}$ have been produced by the Arnoldi process with $v_1^{(k)} = r_0^{(k)} / \|r_0^{(k)}\|_2$, then we get the l Ritz vectors $y_1^{(k)}, \cdots, y_l^{(k)}$ associated with the l smallest Ritz values and the approximate solution $x_m^{(k)}$ in the Krylov subspace $K_m(A, r_0^{(k)})$. The relation (3) holds for k. When the residual norm $r_m^{(k)}$ does not reach the tolerance, we consider restarting with

$$r_0^{(k+1)} = r_m^{(k)}, \; v_1^{(k+1)} = r_0^{(k+1)} / \|r_0^{(k+1)}\|_2 \quad \text{and} \; x_0^{(k+1)} = x_m^{(k)}.$$

By (3), $r_0^{(k+1)} = \beta^{(k+1)} v_{m+1}^{(k)}$, we have $v_1^{(k+1)} = v_{m+1}^{(k)}$. We add the l Ritz vectors into the Krylov subspace. Denote

$$W_s^{(k+1)} = [v_1^{(k+1)}, \cdots, v_m^{(k+1)}, y_1^{(k)}, \cdots, y_l^{(k)}], \; Q_{s+1}^{(k+1)} = [v_1^{(k+1)}, \cdots, v_{m+1}^{(k+1)}, q_1^{(k)} \cdots, q_l^{(k)}],$$

where $q_i^{(k)}$ is formed by orthogonalizing the vectors $Ay_i^{(k)}$ against the previous columns of $Q_{s+1}^{(k+1)}$. Then,we have

$$AW_s^{(k+1)} = Q_{s+1}^{(k+1)} \bar{H}_s^{(k+1)} = Q_s^{(k+1)} H_s^{(k+1)} + h_{s+1,s}^{(k+1)} q_l^{(k)} e_l^T,$$

where $\bar{H}_s^{(k+1)}$is an $(s+1) \times s$ upper-Hessenberg matrix and $H_s^{(k+1)}$ obtained from $\bar{H}_s^{(k+1)}$ by deleting its last row.

The augmented FOM approximate solution $x_s^{(k+1)}$ will be derived by

$$x_s^{(k+1)} = x_0^{(k+1)} + W_s^{(k+1)} d_s^{(k+1)},$$

where

$$d_s^{(k+1)} = (H_s^{(k+1)})^{-1} \beta^{(k+1)} e_1 \quad \text{with} \quad \beta^{(k+1)} = \|r_0^{(k+1)}\|_2.$$

The residual

$$r_s^{(k+1)} = b - Ax_s^{(k+1)} = r_0^{(k+1)} - AW_s^{(k+1)} d_s^{(k+1)}$$

has the following expression

$$r_s^{(k+1)} = Q_s^{(k+1)} \beta^{(k+1)} e_1 - Q_s^{(k+1)} H_s^{(k+1)} d_s^{(k+1)} - h_{s+1,s}^{(k+1)} q_l^{(k)} e_s^T d_s^{(k+1)} = -h_{s+1,s}^{(k+1)} q_l^{(k)} e_s^T d_s^{(k+1)}.$$

Let

$$W_s^{(k+1)} = [V_m^{(k+1)}, Y_l^{(k)}], \quad Q_{s+1}^{(k+1)} = [V_{m+1}^{(k+1)}, Q_l^{(k)}], \quad \bar{H}_s^{(k+1)} = \begin{bmatrix} \bar{H}_m^{(k+1)} & G_1^{(k+1)} \\ 0 & G_2^{(k+1)} \end{bmatrix},$$

where

$$V_m^{(k+1)} = [v_1^{(k+1)}, \cdots, v_m^{(k+1)}], \quad Y_l^{(k)} = [y_l^{(k)}, \cdots, y_l^{(k)}], \quad Q_l^{(k)} = [q_1^{(k)}, \cdots, q_l^{(k)}].$$

Since $AW_s^{(k+1)} = Q_{s+1}^{(k+1)} \bar{H}_s^{(k+1)}$ and $AY_l^{(k)} = Y_l^{(k)} \Theta_l^{(k)} + v_1^{(k+1)} \Delta_l^{(k)}$, we have i

$$\begin{aligned} AV_m^{(k+1)} &= V_{m+1}^{(k+1)} \bar{H}_m^{(k+1)}, \\ AY_l^{(k)} &= V_{m+1}^{(k+1)} G_1^{(k+1)} + Q_l^{(k)} G_2^{(k+1)} = Y_l^{(k)} \Theta_l^{(k)} + v_1^{(k+1)} \Delta_l^{(k)}. \end{aligned} \tag{8}$$

Then

$$\hat{A} Y_l^{(k)} = (A + \sigma I) Y_l^{(k)} = Y_l^{(k)} (\Theta_l^{(k)} + \sigma I) + v_1^{(k+1)} \Delta_l^{(k)}. \tag{9}$$

For the add system (2), the following relation holds

$$\hat{A} V_m^{(k+1)} = V_{m+1}^{(k+1)} \hat{H}_m^{(k+1)},$$

where

$$\hat{H}_m^{(k+1)} = \bar{H}_m^{(k+1)} + \sigma \begin{bmatrix} I_m \\ 0 \end{bmatrix}.$$

We want to calculate $\hat{x}_s^{(k+1)} = \hat{x}_0^{(k+1)} + W_s^{(k+1)} \hat{d}_s^{(k+1)}$ by requiring the collinearity of $r_s^{(k+1)}$ and $\hat{r}_s^{(k+1)}$. Let $\hat{d}_s^{(k+1)} = \left[\hat{d}_m^{(k+1)}, \hat{\alpha}^{(k+1)} \right]^T$. According to the collinearity, we have

$$\begin{aligned} \hat{r}_s^{(k+1)} &= \beta_s^{(k+1)} r_s^{(k+1)}, \\ b - \hat{A}(\hat{x}_0^{(k+1)} + V_m^{(k+1)} \hat{d}_m^{(k+1)} + Y_l^{(k)} \hat{\alpha}^{(k+1)}) &= \beta_s^{(k+1)} (-h_{s+1,s}^{(k+1)} q_l^{(k)} e_s^T d_s^{(k+1)}), \\ \beta_0^{(k+1)} r_0^{(k+1)} - \hat{A} V_m^{(k+1)} \hat{d}_m^{(k+1)} - \hat{A} Y_l^{(k)} \hat{\alpha}^{(k+1)} &= \beta_s^{(k+1)} (-h_{s+1,s}^{(k+1)} q_l^{(k)} e_s^T d_s^{(k+1)}), \\ V_{m+1}^{(k+1)} \hat{H}_m^{(k+1)} \hat{d}_m^{(k+1)} - \beta_s^{(k+1)} h_{s+1,s}^{(k+1)} q_l^{(k)} e_s^T d_s^{(k+1)} &= \beta_0^{(k+1)} \| r_0^{(k+1)} \|_2 v_1^{(k+1)} - \hat{A} Y_l^{(k)} \hat{\alpha}^{(k+1)}. \end{aligned}$$

Let $\alpha = -h_{s+1,s}^{(k+1)} q_l^{(k)} e_s^T d_s^{(k+1)}$ and $\hat{\beta}^{(k+1)} = \beta_0^{(k+1)} \| r_0^{(k+1)} \|_2$. It follows from (8) that

$$Y_l^{(k)} = (V_{m+1}^{(k+1)} G_1^{(k+1)} + Q_l^{(k)} G_2^{(k+1)} - v_1^{(k+1)} \Delta_l^{(k)}) (\Theta_l^{(k)})^{-1}.$$

Consequently,

$$\hat{A} Y_l^{(k)} = (V_{m+1}^{(k+1)} G_1^{(k+1)} + Q_l^{(k)} G_2^{(k+1)}) (I + \sigma (\Theta_l^{(k)})^{-1}) - \sigma v_1^{(k+1)} \Delta_l^{(k)} (\Theta_l^{(k)})^{-1}.$$

Therefore, we obtain

$$\begin{aligned} &V_{m+1}^{(k+1)} \hat{H}_m^{(k+1)} \hat{d}_m^{(k+1)} + \beta_s^{(k+1)} \alpha + \hat{\alpha}^{(k+1)} [(V_{m+1}^{(k+1)} G_1^{(k+1)} \\ &\quad + Q_l^{(k)} G_2^{(k+1)}) (I + \sigma (\Theta_l^{(k)})^{-1}) - \sigma v_1^{(k+1)} \Delta_l^{(k)} (\Theta_l^{(k)})^{-1}] = \hat{\beta}^{(k+1)} v_1^{(k+1)}. \end{aligned} \tag{10}$$

Multiplying (10) from left by $Q_{s+1}^T = \begin{bmatrix} (V_{m+1}^{(k+1)})^T \\ (Q_l^{(k)})^T \end{bmatrix}$, and noting that $(V_{m+1}^{(k+1)})^T Q_l^{(k)} = 0$, we have

$$\begin{cases} \hat{H}_m^{(k+1)} \hat{d}_m^{(k+1)} + [G_1^{(k+1)} (I + \sigma (\Theta_l^{(k)})^{-1}) - \sigma e_1 \Delta_l^{(k)} (\Theta_l^{(k)})^{-1}] \hat{\alpha}^{(k+1)} &= \hat{\beta}^{(k+1)} e_1 \\ \qquad G_2^{(k+1)} (I + \sigma (\Theta_l^{(k)})^{-1}) \hat{\alpha}^{(k+1)} + \beta_s^{(k+1)} \alpha &= 0, \end{cases}$$

which can be written as the following linear system with unknowns $\hat{d}_m^{(k+1)}$, $\hat{\alpha}^{(k+1)}$ and $\beta_s^{(k+1)}$:

$$\begin{pmatrix} \hat{H}_m^{(k+1)} & G_1^{(k+1)}(I+\sigma(\Theta_l^{(k)})^{-1}) - \sigma e_1 \Delta_l^{(k)}(\Theta_l^{(k)})^{-1} & 0 \\ 0 & G_2^{(k+1)}(I+\sigma(\Theta_l^{(k)})^{-1}) & \alpha \end{pmatrix} \begin{pmatrix} \hat{d}_m^{(k+1)} \\ \hat{\alpha}^{(k+1)} \\ \beta_s^{(k+1)} \end{pmatrix} = \begin{pmatrix} \hat{\beta}^{(k+1)} e_1 \\ 0 \end{pmatrix}. \tag{11}$$

Theorem 3.2. *Assume that $K_{m+1,l}(A, r_0^{(k+1)}, y_i^{(k)})$ is the subspace with dimension $s+1$, $\hat{\beta}^{(k+1)} \neq 0$. Then the system* (11) *has a unique solution $(\hat{d}_m^{(k+1)}, \hat{\alpha}^{(k+1)}, \beta_s^{(k+1)})$ if and only if $\theta_i^{(k)} + \sigma \neq 0, \quad i = 1, \cdots, l$ and*

$$\sum_{i=1}^{l} \alpha_i^{(k)} \delta_i^{(k)} \left(\frac{2\theta_i^{(k)} + \sigma}{\theta_i^{(k)} + \sigma}\right) \neq \beta^{(k+1)} p_m^{(k+1)}(-\sigma).$$

In the augmented Krylov subspace, the relation (2) does not hold any more, so we consider dividing the algorithm into two parts: for odd restarting number, we use the original method presented by Simoncini [7], then we calculate the Ritz values and the Ritz vectors of A in the Krylov subspace $K_m(A, r_0)$; for even restarting number, we add the Ritz vectors into the Krylov subspace to form an augmented Krylov subspace $K_{m,l}(A, r_0, y_i)$, then we use the augmented FOM method to solve the shifted systems.

We now present the algorithm as the following for solving the shifted system (1) and (2).

Algorithm: Shifted FOM-R (restarted version)
Give a initial guess x_0, and $\hat{x}_0 = x_0$.
$r_0 = b - Ax_0$, $\hat{r}_0 = r_0$, $\beta_0 = 1$.
$k = 1, 2, \cdots$ until converge

If the step k is odd,

1. Set $v_1 = r_0/\|r_0\|_2$.
2. Arnoldi procedure with v_1 generates $V_s = [v_1, \cdots, v_s]$ and $\bar{H}_s$: $AV_s = V_{s+1}\bar{H}_s$.
3. Compute $d_s = H_s^{-1}\|r_0\|_2 e_1$ and $x_s = x_0 + V_s d_s$.
4. Set $\check{H}_s = H_s + \sigma I$.
5. Compute $\hat{d}_s = \check{H}_s^{-1}\beta_0\|r_0\|_2 e_1$ and $\hat{x}_s = \hat{x}_0 + V_s\hat{d}_s$.
6. Compute $r_s = b - Ax_s$.
7. If $\|r_s\|_2 < \epsilon$ stop, else go to next step.
8. Seek the l eigenvectors $P_l = [p_1, \cdots, p_l]$ associated with the l smallest eigenvalues $\theta_1, \cdots, \theta_l$ from H_s: $H_s p_i = \theta_i p_i$, compute $Y_l = [y_1, \cdots, y_l] = V_s P_l$.
9. Set $r_0 = r_s$, $\hat{r}_0 = \hat{r}_s$ and $\beta_0 = e_s^T\hat{d}_s / e_s^T d_s$.

End for odd k.

If the step k is even,

1. Set $v_1 = r_0/\|r_0\|_2$.
2. Augmented Arnoldi procedure with v_1 and $y_1, \cdots, y_l$ generates

$$W_s = [v_1, \cdots, v_m, y_1, \cdots, y_l] \text{ and } \bar{H}_s : AW_s = Q_{s+1}\bar{H}_s.$$

3. Compute $d_s = H_s^{-1}\|r_0\|_2 e_1$ and $x_s = x_0 + W_s d_s$.

Table 1: Example 1: Number of restarts to convergence of the seed system and the residual norm of the add system when the residual norm of seed system reaches the tolerance

	shifted FOM($s=20$)	shifted FOM-E($m=16, l=4$)	shifted FOM-R($m=16, l=4$)
k	26	12	19
$\|\hat{r}_m\|_2$	5.946822e-012	1.966866e-009	5.673352e-012

Table 2: Example 1: Number of restarts to convergence of the seed system and the add system respectively (i.e. the residual norm reached the tolerance).

	shifted FOM($s=20$)	shifted FOM-E($m=16, l=4$)	shifted FOM-R($m=16, l=4$)
$k(\|r_m\|_2)$	26	12	19
k($\|\hat{r}_m\|_2$)	16	11	13

4. Compute $\alpha = -h_{s+1,s} e_l e_s^T d_s$.
5. Solve

$$\begin{pmatrix} \hat{H}_m & G_1(I+\sigma\Theta_l^{-1}) - \sigma e_1 \Delta_l \Theta_l^{-1} & 0 \\ 0 & G_2(I+\sigma\Theta_l^{-1}) & \alpha \end{pmatrix} \begin{pmatrix} \hat{d}_m \\ \hat{\alpha} \\ \beta_s \end{pmatrix} = \begin{pmatrix} \beta_0 \|r_0\|_2 e_1 \\ 0 \end{pmatrix}.$$

6. $\hat{x}_s = \hat{x}_0 + W_s \hat{d}_s$, where $\hat{d}_s = \begin{bmatrix} \hat{d}_m \\ \hat{\alpha} \end{bmatrix}$.
7. $r_s = b - Ax_s$.
8. If $\|r_s\|_2 < \varepsilon$ stop, else go to next step.
9. Set $r_0 = r_s$, $\hat{r}_0 = \hat{r}_s$ and $\beta_0 = \beta_s$.

End for even k.

4 Numerical experiments

In this section ,we give some numerical experiments to illustrate the convergence behavior of three methods (shifted FOM presented by Simoncini [7], shifted FOM-E, and shifted FOM-R) and to compare their performance. In order to make the comparison, the sizes of Krylov subspace for the same example are identical. The tests start with $x_0 = \hat{x}_0 = 0$ and $\sigma = 1$, and stop when the residual norm reach the tolerance ($tol = 10^{-7}$).

Example 1 Let A is an upper bidiagonal matrix. The entries on the main diagonal are $1, 2, \cdots, 1000$ and the superdiagonal are 0.1, so the eigenvalues of A are $1, 2, \cdots, 1000$.

Fig. 1 plots the convergence history of the seed system and add system by using the three methods. The tests are stopped when the residual norm of the seed system and the add system have reached 10^{-7} respectively. Table 1 shows the residual accuracy of the add system when the residual norm of the seed system has reached the tolerance. Table 2 shows the restart number when the residual norm of the seed system and that of the add system have reached the tolerance(10^{-7}) respectively. We observed that the add system has good convergence than the seed system when the two systems are handled simultaneously. This is because the smallest eigenvalue of $A + \sigma I$ is larger than the smallest eigenvalue of A. Shifted FOM-E is the best but

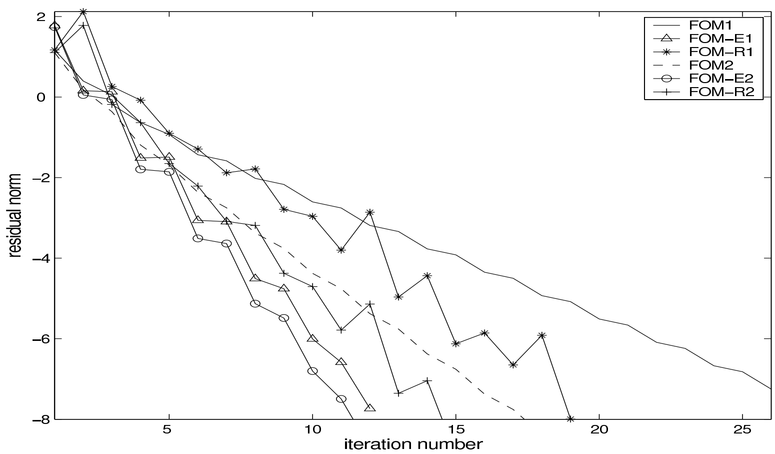

Figure 1: Example 1: Convergence history of the residual for both the seed system and the add system of three methods. The notation FOM1 denote the residual of the seed system by the FOM method and FOM2 denote the residual of the add system by the FOM method.

the method is impractical since the exact eigenvectors can not be obtained, and shifted FOM-R is efficient than shifted FOM.

Example 2 Let A be an upper bidiagonal matrix with the entries $0.01, 0.02, 3, 4, 5, 6, \cdots, 1000$ on the main diagonal, and 0.1 on the superdiagonal.

For the Example 2, the shifted FOM method does not converge after 100 iterations, but the shifted FOM-E method and the shifted FOM-R still keep a good convergence. The numerical results are provided in Table 3. The notation $*$ means the residual norm of the seed system have not reached the tolerance after 100 iterations.

Example 3 We consider the partial differential equation

$$-u_{xx} - u_{yy} + \gamma(u_x + u_y) = f \quad (\gamma \geq 0) \tag{1}$$

on the unit square with homogeneous Dirichlet boundary condition.

The five-point centered difference is used to discretize (1) on 45×45 grid with mesh size $h = 1/46$ and natural ordering. The resulting linear system has a coefficient matrix A of order $n = 2025$. It is well known that the matrix A has the eigenvalues

$$\lambda_{p,q} = 2[2 - \sqrt{1 - (\gamma h/2)^2}(\cos ph\pi + \cos qh\pi)], \quad p, q = 1, \cdots, 45.$$

and for $\gamma = 0$, the matrix A has the eigenvectors

$$v_{p,q} = \sqrt{2h}(\sin qh\pi \cdot z_p^T, \sin 2qh\pi \cdot z_p^T, \cdots, \sin 45qh\pi \cdot z_p^T)^T, \quad p, q = 1, 2, \cdots, 45,$$

where

$$z_p = \sqrt{2h}(\sin ph\pi, \sin 2ph\pi, \cdots, \sin 45ph\pi)^T, \quad p = 1, \cdots, 45.$$

We only consider the case $\gamma = 0$, because in that case we have the exact eigenvalues and eigenvectors.

We can see from Table 4 and Table 5 that both the shifted FOM-E method and the shifted FOM-R method enjoy a good convergence behaviors for both the seed system and the add system.

Table 3: Example 2: Number of restarts to convergence of the seed system and the residual norm of the add system when the residual norm of seed system reached the tolerance.

	shifted FOM($s = 70$)	shifted FOM-E($m = 67, l = 3$)	shifted FOM-R($m = 67, l = 3$)
k	$*$	3	11
$\|\hat{r}_m\|_2$	$*$	5.511425e-011	1.297446e-011

Table 4: Example 3: Number of restarts of the seed system and the residual norm of the add system when the residual norm of seed system reached the tolerance.

	shifted FOM(s=25)	shifted FOM-E($m = 24, l = 1$)	shifted FOM-R($m = 24, l = 1$)
k	12	5	8
$\|\hat{r}_m\|_2$	3.799690e-012	2.400136e-014	3.117452e-013

Table 5: Example 3: Number of restarts to convergence of the seed system and the add system respectively (i.e. the residual norm reached the tolerance).

	shifted FOM($s = 25$)	shifted FOM-E($m = 24, l = 1$)	shifted FOM-R($m = 24, l = 1$)
$k(\|r_m\|_2)$	12	5	8
k($\|\hat{r}_m\|_2$)	2	2	2

The shifted FOM-E method is the best and the shifted FOM-R method is better. However, the shifted FOM-E is an impractical approach.

5 Conclusion

In this paper we presented a restarted FOM method augmented with some Ritz vectors for solving the shifted systems simultaneously. The numerical experiments show that the augmented FOM method can converge more quickly than the original FOM method. The shifted FOM-R is a practical method, and the Shifted FOM-E has the best convergence but is impractical.

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