

PERFORMANCE ANALYSIS OF A FLEXIBLE RESTARTED FOM(k) ALGORITHM

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ABSTRACT. This paper contains a convergence analysis of a flexible restarted FOM(k)(FFOM(k)), and its performance is compared with FGMRES(k). Performances of these two algorithms with variable preconditioners are also compared with those of preconditioned FOM(k) and GMRES(k). Numerical experiments show that FFOM(k) performs as well as, or better than for some problems, FGMRES(k).

1. Introduction

Many iterative methods based on the Krylov subspace techniques for solving large sparse nonsymmetric linear systems have been proposed in the last decades. Although iterative methods lack the robustness of direct methods, they are effective for the large class of problems arising from the elliptic partial differential equations. For the robustness and acceleration of convergence of iterative methods, preconditioning techniques such as incomplete factorization preconditioners have been presented in the mid-seventies [1, 3].

In order to be able to enhance robustness of iterative methods, we should be able to change preconditioner if a given preconditioner is not suitable for the problem at hand. To this end, Saad [5] proposed the *flexible GMRES*(FGMRES) which allows changes in the preconditioning at every step. An important property of FGMRES is that it satisfies the residual norm minimization property over the preconditioned Krylov subspace just as in the standard GMRES algorithm [6].

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Saad [4] also proposes the Full Orthogonalization Method(FOM) which uses the Galerkin property rather than the residual norm minimization property of GMRES. In this paper, we introduce a *flexible restarted FOM(k)*(FFOM(k)) which can be derived from the right-preconditioned FOM(k) in the similar way as was done in the restarted FGMRES(k) [5]. It is well-known that GMRES(k) can not break down unless it has already converged, while FGMRES(k) and FOM(k) may break down without convergence. To this end, we analyze convergence and break-down properties of FFOM(k), and then numerical results of FFOM(k) with a certain criterion are compared with those of FGMRES(k).

Throughout the paper, we consider a linear system $Ax = b$, where $A \in R^{n \times n}$ is a large sparse nonsymmetric nonsingular matrix, $x \in R^n$, and $b \in R^n$. Given a set of vectors $\{p_0, p_1, \dots, p_k\}$, let $\langle p_0, p_1, \dots, p_k \rangle$ denote the subspace spanned by $\{p_0, p_1, \dots, p_k\}$. For a given vector c_0 , let the m -th *Krylov subspace* $K_m(A, c_0)$ denote the subspace $\langle c_0, Ac_0, \dots, A^{m-1}c_0 \rangle$. (\cdot, \cdot) denotes the Euclidean inner product on $R^n \times R^n$, and $\|\cdot\|$ denotes the Euclidean vector norm on R^n as well as matrix norm associated with the Euclidean vector norm.

2. A flexible restarted FOM(k) algorithm(FFOM(k))

The FOM algorithm introduced in [4] for solving a linear system $Ax = b$ uses the Galerkin condition on the Krylov subspace to generate a sequence of approximate solutions. The right preconditioning technique is to apply a Krylov subspace method to a modified linear system $AM^{-1}(Mx) = b$, where M is a right preconditioner that approximates A and can be easily inverted. The restarted FOM(k) algorithm with a fixed right preconditioner M is obtained by applying FOM(k) to $AM^{-1}y = b$, where $y = Mx$. As was done in FGMRES(k) [5], a *flexible FOM(k)*(FFOM(k)) algorithm which uses a variable preconditioner M_j at the j -th step can be easily derived from FOM(k) algorithm with a fixed right preconditioner M :

ALGORITHM 2.1 : FFOM(k) algorithm

1. Choose x_0 and compute $r_0 = b - Ax_0$
 Compute $v_1 = r_0 / \|r_0\|$ and set $\beta = \|r_0\|$
2. for $j = 1, 2, \dots, k$

Compute $z_j = M_j^{-1}v_j$

Compute $\hat{v}_{j+1} = Az_j$

for $i = 1, 2, \dots, j$

$h_{ij} = (\hat{v}_{j+1}, v_i)$

$\hat{v}_{j+1} = \hat{v}_{j+1} - h_{ij}v_i$

Compute $h_{j+1,j} = \|\hat{v}_{j+1}\|$ and $v_{j+1} = \hat{v}_{j+1}/h_{j+1,j}$

3. Form the approximate solution:

Compute $x_k = x_0 + Z_k y_k$, where $y_k = H_k^{-1} \beta e_1$,

$Z_k = [z_1, z_2, \dots, z_k]$ is the $n \times k$ matrix, H_k is the upper $k \times k$ Hessenberg matrix whose entries are the scalars

h_{ij} , and $e_1 = [1, 0, \dots, 0]^T \in R^k$

4. Restart:

Compute $r_k = b - Ax_k$. If $\|r_k\| / \|r_0\| < (\text{tolerance})$,

stop. Otherwise, set $x_0 = x_k$ and $v_1 = r_k / \|r_k\|$, and

then go to 2

If $M_j = M$ for all j , then Algorithm 2.1 is equivalent to the FOM(k) with a fixed right preconditioner M . It is easy to see that FFOM(k) satisfies

$$(1) \quad AZ_l = V_{l+1} \hat{H}_l = V_l H_l + \hat{v}_{l+1} e_l^T \quad \text{for } 1 \leq l \leq k,$$

where $V_{l+1} = [v_1, \dots, v_{l+1}]$ is the $n \times (l+1)$ matrix with orthonormal columns and \hat{H}_l is the upper $(l+1) \times l$ Hessenberg matrix whose only nonzero entries are the scalars h_{ij} generated by the FFOM(k) algorithm. From equation (1), one can obtain

$$(2) \quad V_l^T AZ_l = H_l.$$

Equation (2) shows that x_l in the FFOM(k) is chosen so that $r_l = r_0 - AZ_l y_l$ is orthogonal to $\langle v_1, v_2, \dots, v_l \rangle$. Notice that x_l in FGMRES(k) is chosen so that r_l is orthogonal to $\langle Az_1, Az_2, \dots, Az_l \rangle$. Instead of forming a preconditioner M_j at the j -th step explicitly and then computing $z_j = M_j^{-1}v_j$, z_j is chosen so that z_j is an approximate solution to $Ax = v_j$. An approximate solution z_j to $Ax = v_j$ can be obtained using any iterative methods available, e.g., SOR, GMRES, CGNR, BiCGSTAB, etc.

If H_l is nonsingular, FFOM(k) does not break down, i.e., $x_l = x_0 + Z_l y_l$ exists. Moreover, if H_l is nonsingular and $h_{l+1,l} = 0$, then it can be easily shown that x_l in the FFOM(k) will be the exact solution to $Ax = b$. The

preconditioner M_j at the j -th step so that FFOM(k) converges fast to the exact solution without breakdown and stagnation.

3. Convergence analysis of FFOM(k)

Notice that in the FFOM(k) a variable preconditioner M_j is not formed explicitly, but $z_j (= M_j^{-1}v_j)$ is directly chosen as an approximate solution to $Ax = v_j$.

LEMMA 3.1. *Suppose that $\|Az_j - v_j\| = \|A(M_j^{-1}v_j) - v_j\| \leq \varepsilon$ for $1 \leq j \leq l$. Then, for each $1 \leq j \leq l$*

$$(6) \quad \begin{aligned} 1 - \varepsilon &\leq h_{jj} \leq 1 + \varepsilon \\ |h_{ij}| &\leq \varepsilon \quad (i \neq j, 1 \leq i \leq j - 1) \end{aligned}$$

Moreover, if $\varepsilon < \frac{1}{e+1}$ for a positive number e , then $0 \leq \frac{h_{j+1,j}}{h_{jj}} < \frac{1}{e}$ for $1 \leq j \leq l$.

Proof. For each $1 \leq j \leq l$, $Az_j = \sum_{i=1}^j h_{ij}v_i + h_{j+1,j}v_{j+1}$. Since the vectors v_1, v_2, \dots, v_{j+1} are orthonormal,

$$\|Az_j - v_j\|^2 = \sum_{i=1}^{j-1} h_{ij}^2 + (h_{jj} - 1)^2 + h_{j+1,j}^2.$$

Since $\|Az_j - v_j\| \leq \varepsilon$, $|h_{ij}| \leq \varepsilon$ for $i \neq j$ and $1 \leq i \leq j + 1$, and $|h_{jj} - 1| \leq \varepsilon$. Thus, (6) is proved. if $\varepsilon < \frac{1}{e+1}$ for a positive number e , from (6) $h_{jj} > \frac{e}{e+1} > e\varepsilon$. Since $0 \leq h_{j+1,j} \leq \varepsilon$, $0 \leq \frac{h_{j+1,j}}{h_{jj}} < \frac{1}{e}$ is obtained. \square

For simplicity of exposition, we define new scalars \hat{h}_{ij} which are generated from the following algorithm:

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for  $j = 1, 2, \dots, k$ 
     $\hat{h}_{1j} = h_{1j}$ 
for  $i = 2, \dots, k$ 
    for  $j = i, \dots, k$ 
         $\hat{h}_{ij} = s_{i-1}\hat{h}_{i-1,j} + c_{i-1}h_{ij}$ 
    
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where h_{ij} 's are scalars generated from FFOM(k) algorithm, and c_i and s_i are scalars defined by equation (3). Then, it is easy to show that for each $1 \leq i \leq k$, \hat{h}_{ii} generated from the above algorithm is the i -th diagonal element of the upper triangular matrix R_i such that $H_i = Q_i^T R_i$.

LEMMA 3.2. Let α and e be positive numbers. Suppose that $s^2 + c^2 = 1$, where $0 \leq s \leq \frac{1}{\sqrt{1+e^2}}$ and $c \geq 0$. Then, $s + \alpha c$ has a maximum value

$$\begin{cases} \sqrt{1 + \alpha^2} & \text{if } \alpha \geq e \\ \frac{1+\alpha e}{\sqrt{1+e^2}} & \text{if } \alpha \leq e \end{cases}$$

Proof. Let $f(s) = s + \alpha c = s + \alpha\sqrt{1 - s^2}$, where $0 \leq s \leq \frac{1}{\sqrt{1+e^2}}$. By simple calculus, the lemma can be easily shown. \square

THEOREM 3.3. Let e be a given number such that $1 \leq e \leq 2$, $d = 2e^3 + e + 1$, $\beta = \frac{1}{\sqrt{1+e^2}}$, and $f(e) = \frac{2e^3}{\sqrt{5e^2+d+(2e^5+d)\beta}}$. If $\|Az_j - v_j\| \leq \varepsilon$ for $1 \leq j \leq l$ and $\varepsilon < f(e)$, then $0 \leq \frac{h_{j+1,j}}{h_{jj}} < \frac{1}{e}$ for $1 \leq j \leq l$, i.e., H_j 's are nonsingular for $1 \leq j \leq l$.

Proof. For $l = 1$, $\hat{h}_{11} = h_{11}$. Since $\varepsilon < f(e) < \frac{1}{1+e}$, by Lemma 3.1 $0 \leq \frac{h_{21}}{h_{11}} < \frac{1}{e}$. Suppose that the theorem holds for $l = m$. Then, we must show that the theorem holds for $l = m + 1$. By induction hypothesis, one obtains

$$|s_j| = \frac{h_{j+1,j}}{\sqrt{\hat{h}_{jj}^2 + h_{j+1,j}^2}} < \beta \text{ and } e\beta < |c_j| \leq 1 \text{ for } 1 \leq j \leq m.$$

Applying Givens rotations to the upper Hessenberg matrix H_{m+1} of order $m + 1$,

$$\begin{aligned} \hat{h}_{m+1,m+1} &= s_m \hat{h}_{m,m+1} + c_m h_{m+1,m+1} \\ &= s_m (s_{m-1} \hat{h}_{m-1,m+1} + c_{m-1} h_{m,m+1}) + c_m h_{m+1,m+1} \\ &= s_m s_{m-1} \hat{h}_{m-1,m+1} + s_m c_{m-1} h_{m,m+1} + c_m h_{m+1,m+1} \\ &\quad \vdots \\ &= s_m \cdots s_2 s_1 h_{1,m+1} + s_m \cdots s_2 c_1 h_{2,m+1} + s_m \cdots s_3 c_2 h_{3,m+1} + \\ &\quad \cdots + s_m s_{m-1} c_{m-2} \hat{h}_{m-1,m+1} + s_m c_{m-1} h_{m,m+1} + c_m h_{m+1,m+1}. \end{aligned}$$

Since $|h_{i,m+1}| \leq \varepsilon$ for $i \leq m$,

$$\begin{aligned} & |\hat{h}_{m+1,m+1} - c_m h_{m+1,m+1}| \\ & \leq \varepsilon |s_m| (|s_{m-1} \cdots s_2 s_1| + |s_{m-1} \cdots s_2 c_1| + \dots + |s_{m-1} c_{m-2}| + |c_{m-1}|) \\ & = \frac{\varepsilon}{2} |s_m| (|s_{m-1} \cdots s_1| + |s_{m-1} \cdots s_2| (|s_1| + |c_1|) + |s_{m-1} \cdots s_3| (|c_1| \cdot \\ & \quad |s_2| + |c_2|) + \dots + |s_{m-1}| (|c_{m-3}| |s_{m-2}| + |c_{m-2}|) + (|c_{m-2}| |s_{m-1}| \\ & \quad + 2|c_{m-1}|)) \\ & \leq \frac{\varepsilon}{2} |s_m| (|s_{m-1} \cdots s_1| + |s_{m-1} \cdots s_2| (|s_1| + |c_1|) + |s_{m-1} \cdots s_3| (|s_2| \\ & \quad + |c_2|) + \dots + |s_{m-1}| (|s_{m-2}| + |c_{m-2}|) + (|s_{m-1}| + 2|c_{m-1}|)). \end{aligned}$$

Using Lemma 3.2 and $|s_j| < \beta$ for $1 \leq j \leq m$,

$$\begin{aligned} (7) \quad & |\hat{h}_{m+1,m+1} - c_m h_{m+1,m+1}| \leq \frac{\varepsilon}{2} \beta (\beta^{m-1} + \beta^{m-1}(1+e) + \dots \\ & \quad + \beta^2(1+e) + \sqrt{5}) \\ & < \frac{\varepsilon}{2} \beta \left(\frac{\beta^2}{1-\beta} (1+e) + \sqrt{5} \right). \end{aligned}$$

Using (7) and Lemma 3.1,

$$\begin{aligned} \hat{h}_{m+1,m+1} & \geq c_m h_{m+1,m+1} - \frac{\varepsilon}{2} \beta \left(\frac{\beta^2}{1-\beta} (1+e) + \sqrt{5} \right) \\ & > \beta e (1-\varepsilon) - \frac{\varepsilon}{2} \beta \left(\frac{\beta^2}{1-\beta} (1+e) + \sqrt{5} \right) \\ & = \beta \left(e - \varepsilon \left(\frac{\beta^2}{1-\beta} \frac{1+e}{2} + e + \frac{\sqrt{5}}{2} \right) \right). \end{aligned}$$

If $\varepsilon < f(e)$, then $\beta \left(e - \varepsilon \left(\frac{\beta^2}{1-\beta} \frac{1+e}{2} + e + \frac{\sqrt{5}}{2} \right) \right) > e\varepsilon$. Since $0 \leq h_{m+2,m+1} < \varepsilon$, $\hat{h}_{m+1,m+1} > eh_{m+2,m+1}$ and so $0 \leq \frac{h_{m+2,m+1}}{\hat{h}_{m+1,m+1}} < \frac{1}{e}$. Therefore, the proof is complete. \square

THEOREM 3.4. *Let e be a given number such that $e \geq 2$, $\hat{d} = 2e^5 + 3e^3 + e^2 + e + 1$, $\beta = \sqrt{1+e^2}$, and $f(e) = \frac{2e^3\sqrt{1+e^2}}{e^3+(1+\beta)\hat{d}}$. If $\|Az_j - v_j\| \leq \varepsilon$ for $1 \leq j \leq l$ and $\varepsilon < f(e)$, then $0 \leq \frac{h_{j+1,j}}{h_{j,j}} < \frac{1}{e}$ for $1 \leq j \leq l$.*

Proof. For $l = 1$, $\hat{h}_{11} = h_{11}$. Since $\varepsilon < f(e) < \frac{1}{1+e}$, by Lemma 3.1 $0 \leq \frac{h_{21}}{h_{11}} < \frac{1}{e}$. Suppose that the theorem holds for $l = m$. Then, we must show that the theorem holds for $l = m + 1$. In the similar way as was done in Theorem 3.3, one obtains the following inequality

$$\begin{aligned}
 |\hat{h}_{m+1,m+1} - c_m h_{m+1,m+1}| &\leq \frac{\varepsilon}{2} \beta (\beta^{m-1} + \beta^{m-1}(1+e) + \dots \\
 &\quad + \beta^2(1+e) + \beta(1+2e)) \\
 (8) \qquad \qquad \qquad &< \frac{\varepsilon}{2} \beta^2 \left(\frac{1+e}{1-\beta} + e \right).
 \end{aligned}$$

Using (8) and Lemma 3.1,

$$\begin{aligned}
 \hat{h}_{m+1,m+1} &> \beta e(1-\varepsilon) - \frac{\varepsilon}{2} \beta^2 \left(\frac{1+e}{1-\beta} + e \right) \\
 &= \beta \left(e - \varepsilon \left(\frac{\beta}{1-\beta} \frac{1+e}{2} + \frac{\beta}{2} e + e \right) \right)
 \end{aligned}$$

If $\varepsilon < f(e)$, then $\beta \left(e - \varepsilon \left(\frac{\beta}{1-\beta} \frac{1+e}{2} + \frac{\beta}{2} e + e \right) \right) > e\varepsilon$. Since $0 \leq h_{m+2,m+1} < \varepsilon$, the proof is complete. □

By a routine calculus, it can be shown that $f(e)$ is a decreasing function for $e \geq 2$. Table 1 shows the values of $f(e)$ for $e \geq 1$ which is defined in Theorems 3.3 and 3.4. The larger e is, the faster FFOM(k) converges to the exact solution. So, the estimation $f(e)$ for ε should be larger for smaller number of e . From this point of view, it can be said that $f(e)$ is not a good estimation for ε when $e < 1.8$.

e	$f(e)$	e	$f(e)$
1.0	0.1909	2.0	0.2459
1.5	0.2425	3.0	0.2160
1.7	0.2473	4.0	0.1837
1.75	0.2476	5.0	0.1576
1.8	0.2477	6.0	0.1374
1.85	0.2476	7.0	0.1214
1.9	0.2472	8.0	0.1086
2.0	0.2459	9.0	0.0982

TABLE 1: Values of $f(e)$ for $e \geq 1$

From Table 1, it can be seen that the maximum of $f(e)$ for $e \geq 1$ is about 0.2477 when e is equal to about 1.8. Hence, the following corollary can be obtained from (5).

COROLLARY 3.5. *Suppose that $\|Az_j - v_j\| \leq \varepsilon$ for $1 \leq j \leq k$. If $\varepsilon < f(1.8) \approx 0.2477$, then FFOM(k) converges to the exact solution without breakdown and stagnation, and $\frac{\|r_n\|}{\|r_{j-1}\|} < \frac{1}{1.8}$ for $1 \leq j \leq k$.*

4. Numerical results

We report some numerical experiments comparing performances of FFOM(20) with those of FGMRES(20). These algorithms using variable preconditioners are also compared with standard ILU(0) right-preconditioned FOM(20) and GMRES(20) which are called PFOM(20) and PGMRES(20), respectively. The tests were performed using 64-bit arithmetics. In all cases, the iteration was started with $x_0 = 0$ and the iterations were terminated when $\frac{\|r_n\|}{\|r_0\|} < 10^{-8}$.

The preconditioned vectors $z_j = M_j^{-1}v_j$ were computed using m iteration steps of the right-preconditioned BiCGSTAB[7] with minimal residual smoothing technique which is called PBSTABMR. PBSTABMR was also started with zero initial vector. Minimal residual smoothing technique is used to avoid an irregular convergence behavior of BiCGSTAB. An advantage of using BiCGSTAB to compute preconditioned vectors z_j is that it uses less storages than other GMRES-type methods. It was shown in Corollary 3.5 that ε set to $f(1.8) \approx 0.2477$ guarantees the convergence of FFOM(k) to the exact solution. For most problems PBSTABMR yields z_j satisfying $\|v_j - Az_j\| \leq \varepsilon$ within a few iteration steps, but for some problems it converges too slow, so that its execution is limited to m iteration steps for efficient performance, where m is a fixed number. Performance of FFOM(k) varies depending upon m , and an optimal number of m depends upon problems to be considered. Numerical experiments show that the optimal number of m ranges from 2 to 5. *Matrix-vector products*(SPMV) for computing Ay and *preconditioner solves*(SPSV) for computing $M^{-1}y$ are counted for performance evaluation of each algorithm. Vector updates and inner products are neglected since their execution time is relatively small compared with SPMV and SPSV.

Performance analysis of a flexible FOM(k) algorithm

n	δ	PFOM(20)	FFOM(20)	PGMRES(20)	FGMRES(20)
2500	0.2	$57 + 57 = 114$	$62 + 46 = 108$	$58 + 58 = 116$	$62 + 46 = 108$
	0.5	$25 + 25 = 50$	$39 + 28 = 67$	$25 + 25 = 50$	$39 + 28 = 67$
4900	0.2	$101 + 101 = 202$	$81 + 66 = 147$	$101 + 101 = 202$	$81 + 66 = 147$
	0.5	$39 + 39 = 78$	$47 + 36 = 83$	$39 + 39 = 78$	$47 + 36 = 83$

TABLE 2: Numerical results for Example 4.1

n	β	γ	PFOM(20)	FFOM(20)	PGMRES(20)	FGMRES(20)
1024	-100	10	NC	$123 + 92 = 215$	NC	$131 + 98 = 229$
	10	1000	$209 + 209 = 418$	$595 + 470 = 1065$	$224 + 224 = 448$	$686 + 542 = 1228$
2304	-100	10	NC	$157 + 118 = 275$	NC	$159 + 120 = 279$
	10	1000	$167 + 167 = 334$	$592 + 468 = 1060$	$158 + 158 = 316$	$688 + 544 = 1232$

TABLE 3: Numerical results for Example 4.2

5. Concluding Remarks

Most of the existing preconditioned iterative methods use a fixed preconditioner which can be usually found using various incomplete factorization techniques, see [1, 3] for details. For indefinite and/or highly non-symmetric matrices, the performance of an iterative method with a fixed preconditioner can be unpredictable, see the performances of PFOM(20) and PGMRES(20) in Table 3. It was shown that FFOM(k) yields a sequence of approximate solutions which converges to the exact solution by choosing a suitable preconditioner every iteration. Hence, a big advantage of FFOM(k) with a variable preconditioner is its robustness. However, PFOM(k) can fail to yield a sequence of approximate solutions which converges to the exact solution.

If PFOM(k) with a fixed preconditioner does not perform well, then we need to use another preconditioner for which it performs well. Finding a good preconditioner for PFOM(k) requires complicated computational steps, while a good variable preconditioner for FFOM(k) can be easily obtained by using any iterative methods available. Numerical experiments show that FFOM(k) performs as well as, or better than for some problems, FGMRES(k). Hence, it may be concluded that FFOM(k) can be used as a good substitute for FGMRES(k).

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