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RESTARTED FULL ORTHOGONALIZATION METHOD FOR SHIFTED LINEAR SYSTEMS *

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Abstract.

Restarted GMRES is known to be inefficient for solving shifted systems when the shifts are handled simultaneously. Variants have been proposed to enhance its performance. We show that another restarted method, restarted Full Orthogonalization Method (FOM), can effectively be employed. The total number of iterations of restarted FOM applied to all shifted systems simultaneously is the same as that obtained by applying restarted FOM to the shifted system with slowest convergence rate, while the computational cost grows only sub-linearly with the number of shifts. Numerical experiments are reported.

AMS subject classification: 65F10, 65F15, 15A06, 15A18.

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1 Introduction.

Given a real large $n \times n$ nonsymmetric matrix A, we are interested in the simultaneous solution of the *shifted* nonsingular linear system

$$(A - \sigma I)x = b, \tag{1.1}$$

for several (say a few hundreds; see, e.g., [2]) tabulated values of the parameter σ. (I stands for the identity matrix.) This type of problem arises in many applications, such as control theory, structural dynamics, time–dependent PDEs and quantum chromodynamics; see [1, 2, 5, 6] and references therein. One such application is discussed in the experiments section. Krylov subspace techniques are particularly appealing since they rely on a shift–invariance property, which allows to obtain approximation iterates for all parameter values by only constructing one approximation subspace. Indeed, the Krylov subspace $\mathcal{K}_m(A, v) = \text{span}\{v, Av, \ldots, A^{m-1}v\}$ satisfies $\mathcal{K}_m(A, v) = \mathcal{K}_m(A - \sigma I, v)$. In the linear system setting, the *generating* vector v is the residual associated with a starting approximate solution. A widely known and appreciated scheme, the Generalized Minimum residual method (GMRES), has been shown to be effective on (1.1), see [1]. However, in several circumstances, the approximation

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space required to satisfactorily approximate all shifted systems appears to be too large, and the method needs to be restarted, taking the current system residual as new generating vector. Computational efficiency can be maintained after restart if the new Krylov subspace is the same for all shifted systems. This happens when the generating vectors, in our case the current residuals, are collinear. Since in general the computed GMRES shifted residuals are not collinear, after the first restart, restarted GMRES can only be applied to each shifted system separately. Several alternative strategies can be considered within the Krylov subspace setting with restarting:

1) Run GMRES on a *seed* system, e.g. the system with zero shift, and then generate the approximate solutions to the shifted systems imposing collinearity with the computed seed residual. This idea was investigated in [5]. Note that only the seed system residual is minimized, whereas no minimization property is satisfied by the shifted systems residuals.

2) Take as seed system one of the shifted systems, on which restarted GMRES is applied, and generate approximate solutions to the remaining shifted systems imposing collinearity. Possibly a new seed is selected at each restart, choosing as seed the system with larger residual norm. This is a simple variant of the previous scheme, which was used in [2] to cure misconvergence of the original approach in [5]. Note that in general, at each restarting phase a different system residual is minimized.

3) Use a restarted Krylov subspace method other than restarted GMRES, that naturally generates collinear residuals.

To the best of our knowledge, the third option above has not been considered in the past. The aim of this contribution is to draw attention to the fact that another restarted method, the Full Orthogonalization method (FOM), can be naturally applied to shifted systems since all residuals are naturally collinear. It will become apparent that the convergence history is the same as that obtained by applying restarted FOM to each shifted system independently, while computational cost and memory requirements[1] are substantially reduced, since a single approximation space is constructed for all shifted systems.

Alternative approaches that do not require restarting are based on CG and Lanczos recurrences. These include the shifted TFQMR method, proposed by R. Freund [4], and the Shifted two-sided Lanczos method [9]. Memory requirements however may limit their applicability to general shifted problems, since additional long vectors need to be stored for each shifted system simultaneously handled. We refer to [2, 9] for numerical experiences on applications on which variants of these solvers are particularly effective. We refer to [6] for a comparison of unrestarted FOM and GMRES in the symmetric shifted case.

All experiments were run using Matlab 6 on one processor of a Sun Enterprise 4500. Exact arithmetic is assumed throughout the paper.

[1]Order n memory requirements are the same as for standard restarted FOM if this is applied to each shifted system sequentially.

2 The algorithm.

Given a nonsymmetric linear system $Ax = b$ and a starting guess x_0, consider the Krylov subspace $\mathcal{K}_m(A, r_0)$, where $r_0 = b - Ax_0$. Letting V_m be an orthogonal basis of $\mathcal{K}_m(A, r_0)$ and H_m be the projection and restriction of A onto $\mathcal{K}_m(A, r_0)$, then the FOM approximation $x_m = x_0 + z_m$ to x is determined in $x_0 + \mathcal{K}_m(A, r_0)$ so that the associated residual $r_m = b - Ax_m$ is orthogonal to the approximation space $\mathcal{K}_m(A, r_0)$. More precisely, $x_m = x_0 + V_m y_m$, where y_m solves the reduced system $H_m y = \beta_0 e_1$, with $\beta_0 = \|r_0\|$ [7]. Here and below, e_i denotes the ith column of the identity matrix, whose dimension is clear from the context; $\|\cdot\|$ is the vector 2–norm. If the obtained approximate solution is not sufficiently accurate, then the FOM method is restarted, by using $r_m = b - Ax_m$ as new starting residual. The generation of the Krylov subspace can be carried out by means of the Arnoldi algorithm, which constructs V_m, H_m so that the first basis vector v_1 is $v_1 = r_0/\beta_0$, and

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

e_m^T indicates the real transpose of e_m.

Consider now the shifted system (1.1). Shifting transforms (2.1) into

$$(A - \sigma I)V_m = V_m(H_m - \sigma I_m) + h_{m+1,m} v_{m+1} e_m^T, \tag{2.2}$$

where I_m is the identity matrix of size m. Thanks to (2.2), the only difference in FOM is that y_m is computed by solving the reduced shifted system $(H_m - \sigma I_m)y = \beta_0 e_1$. Therefore, the expensive step of constructing the orthogonal basis V_m is performed only once for all values of σ of interest, $\sigma \in \{\sigma_1, \ldots, \sigma_s\}$, whereas s reduced systems of size m need be solved. This is the case if the right–hand sides are collinear. In the following, we shall assume that $x_0 = 0$ so that all shifted systems have the same right-hand side.

Restarting can also be employed in the shifted case. The key fact is that the FOM residual r_m is a multiple of the basis vector v_{m+1}, that is $r_m = -h_{m+1,m} v_{m+1} (y_m)_m$; see e.g. [7]. In the last expression, $(y_m)_m$ is the mth component of the vector y_m. The next proposition shows that collinearity still holds in the shifted case when FOM is applied.

PROPOSITION 2.1. *For each $i = 1, \ldots, s$, let $x_m^{(i)} = V_m y_m^{(i)}$ be a FOM approximate solution to $(A - \sigma_i I)x = b$ in $\mathcal{K}_m(A - \sigma_i I, b)$, with V_m satisfying* (2.2) *with $\sigma = \sigma_i$. Then there exists $\beta_m^{(i)} \in \mathbb{R}$ such that $r_m^{(i)} = b - (A - \sigma_i I)x_m^{(i)} = \beta_m^{(i)} v_{m+1}$.*

PROOF. For $i = 1, \ldots, s$, we have

$$\begin{aligned} r_m^{(i)} &= b - (A - \sigma_i I)x_m^{(i)} = r_0 - (A - \sigma_i I)V_m y_m^{(i)} \\ &= V_m \beta_0 e_1 - V_m H_m y_m^{(i)} + \sigma_i V_m y_m^{(i)} - h_{m+1,m} v_{m+1} (y_m^{(i)})_m \\ &= -h_{m+1,m} v_{m+1} (y_m^{(i)})_m. \end{aligned}$$

Setting $\beta_m^{(i)} = -h_{m+1,m}(y_m^{(i)})_m$, $i = 1, \ldots, s$, we have $r_m^{(i)} = \beta_m^{(i)} v_{m+1}$. □

The Shifted FOM method can be restarted by using any of the shifted system residuals $r_m^{(i)}$, $i = 1, \ldots, s$ as new generating vector. Let thus $\hat{v}_1$ be the first vector of the new basis $\hat{V}_m$ after restart[2]. Note that

$$\hat{v}_1 = r_m^{(i)}/\beta_m^{(i)} = \pm v_{m+1}, \quad i = 1, \ldots, s.$$

Hence the new problem reads: For each $i = 1, \ldots, s$, find $\hat{x}_m^{(i)} = x_m^{(i)} + \hat{V}_m \hat{y}_m^{(i)}$ with $\mathrm{Range}(\hat{V}_m) = \mathcal{K}_m(A, \hat{v}_1)$ where $\hat{y}_m^{(i)}$ solves the reduced system

$$(\hat{H}_m - \sigma_i I_m)\hat{y} = \beta_m^{(i)} e_1.$$

For each shifted system, the new residual can be computed as

$$\hat{r}_m^{(i)} = r_m^{(i)} - (A - \sigma_i I)\hat{V}_m \hat{y}_m^{(i)} = -\hat{h}_{m+1,m}\hat{v}_{m+1}(\hat{y}_m^{(i)})_m,$$

showing that all new residuals are collinear to the $m+1$st basis vector, hence the process can be repeated. In particular, we have shown that collinearity holds also when the original right-hand sides are different but collinear. The final algorithm can be written as follows.

Algorithm. Restarted Shifted FOM:

Given $A, b, x_0 = 0, m, \{\sigma_1, \ldots, \sigma_s\}$, $\mathcal{I} = \{1, \ldots, s\}$:

1. Set $r_0 = b$, $\beta_m^{(i)} = \|r_0\|, x_m^{(i)} = x_0$, $i = 1, \ldots, s$. Set $v_1 = r_0/\beta_m^{(i)}$.
2. Generate V_m, H_m associated with $\mathcal{K}_m(A, v_1)$
3. For each $i \in \mathcal{I}$
   $y_m^{(i)} = (H_m - \sigma_i I_m)^{-1} e_1 \beta_m^{(i)}$
   Update $x_m^{(i)} \leftarrow x_m^{(i)} + V_m y_m^{(i)}$
4. Eliminate converged systems. Update $\mathcal{I}$. If $\mathcal{I} = \emptyset$ exit.
5. Set $\beta_m^{(i)} = -h_{m+1,m}(y_m^{(i)})_m$ for each $i \in \mathcal{I}$
6. Set $v_1 \leftarrow v_{m+1}$. Goto 2

The convergence history of the shifted restarted method on each system is the same as the convergence of the usual restarted method applied individually to each shifted system. This can be clearly observed by noticing that both the sequence of Krylov subspace systems and approximation iterates are the same as those computed by standard restarted FOM. In particular, this implies that Shifted Restarted FOM only generates one sequence of bases $\{V_m\}$ for all shifted systems simultaneously solved and that no degradation of performance is caused by the information sharing.

3 Numerical experiments.

In this section we report the results of some numerical experiments we have carried out. We compare the Frommer and Glässner correction of restarted GMRES(m) for shifted systems (hereafter $gm_s(m)$), its variant proposed in [2] (hereafter $gm_{sv}(m)$) and restarted FOM(m). Restarted Arnoldi-type methods

[2] To avoid indexing overwhelming we shall adopt the hat symbol ˆ for the computed quantities after restart.

are known to suffer when A is indefinite. The presence of the shift may exacerbate the situation making the shifted system particularly hard to solve when the spectrum of the coefficient matrix $A - \sigma I$ surrounds the origin. Numerical experiments with restarted FOM are less common in the literature than with restarted GMRES; see e.g. [8, 7]. Performance evaluation of $gm_s(m)$ and $gm_{sv}(m)$ can be found in [5] and in [2], respectively. Far from being exhaustive, our numerical experiments aim to describe typical convergence behavior of the discussed methods in situations where the shift may deteriorate convergence. Our convergence stopping criterion is based on the residual norm, $\|r_m^{(i)}\|$. Depending on the problem at hand, different strategies may be more relevant; see the discussion below on the structural dynamics problem.

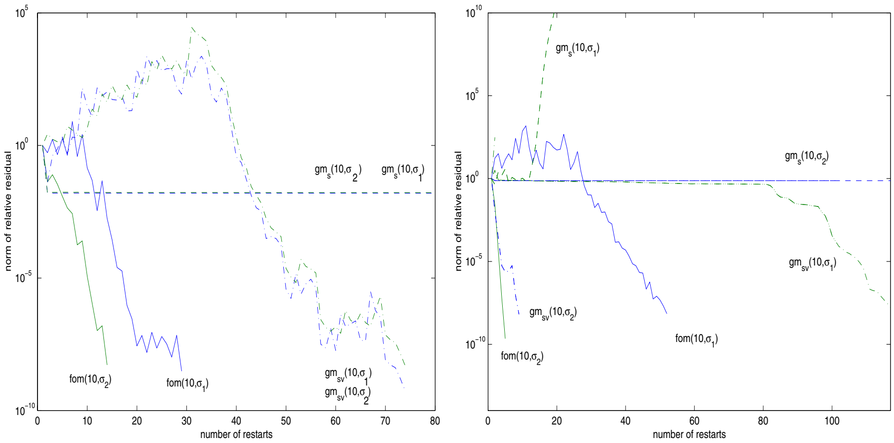

Figure 3.1: Left: Example with bidiagonal matrix and $\sigma_1 = 1$, $\sigma_2 = -1$. Right: Example with operator $L(u)$ and $\sigma_1 = 0.5$, $\sigma_2 = -0.5$.

The first example considers a 100×100 upper bidiagonal matrix A with diagonal the vector $d = [0.01, 0.02, 0.03, 0.04, 10, 11, \cdots, 105]$ and super-diagonal the vector of all ones; see e.g. [8]. The right–hand side is the vector of all ones, normalized to have unit norm, and we consider two values for the shift parameter, $\sigma = -1, 1$. The results are reported in the left plot of Figure 3.1 for $m = 10$ and stopping tolerance $\varepsilon = 10^{-8}$. While $gm_s(10)$ stagnates on both shifted systems, its variant is able to converge, although the convergence is slowed down, compared with running restarted GMRES on each shifted system separately. Indeed, restarted GMRES with $m = 10$ would converge in 16 restarts on $A + I$ and in 22 restarts on $A - I$. Therefore, the restarting strategy that chooses as seed the slower converging shifted system in practice affects the convergence of all systems. Note also that a different ordering of the shifts at start time (when all residuals equal the right–hand side b) would yield a quite different convergence history of gm_{sv} on the two systems.

We next consider the 100×100 matrix corresponding to the discretization of the operator $L(u) = -\Delta u + 10u_x$ on the unit square with Dirichlet boundary conditions. We set b and stopping tolerance as before, and $\sigma = -0.5, 0.5$. Results are summarized in the right plot of Figure 3.1. Standard restarted GMRES applied to each shifted system separately with $m = 10$ would converge in 4 restarts on $A + 0.5\,I$ and in 172 restarts on $A - 0.5\,I$. The difference in performance is more pronounced on this example. Note that gm_{sv} converges very rapidly on σ_2 so that only σ_1 is processed in later restarts.

The matrices in our next example stem from a structural dynamics engineering problem, whose algebraic formulation was discussed in detail in [9]. Direct frequency analysis leads to the solution of the following algebraic linear system

$$(\sigma^2 A + \sigma B + C)x = b, \tag{3.1}$$

for several values of the frequency-related parameter σ. Here A, B and C are complex symmetric. Linearization yields the system

$$\left[\begin{pmatrix} B & C \\ C^T & 0 \end{pmatrix} + \sigma \begin{pmatrix} A & 0 \\ 0 & -C^T \end{pmatrix}\right] \begin{bmatrix} y \\ x \end{bmatrix} = \begin{bmatrix} b \\ 0 \end{bmatrix} \quad \Leftrightarrow \quad (T - \sigma S)z = f.$$

Note that only a portion of the approximation to z is employed to approximate x in (3.1). We refer to [9] for a detailed analysis of the connections between the two algebraic approximation problems and for stopping criteria that take the original problem (3.1) into account.

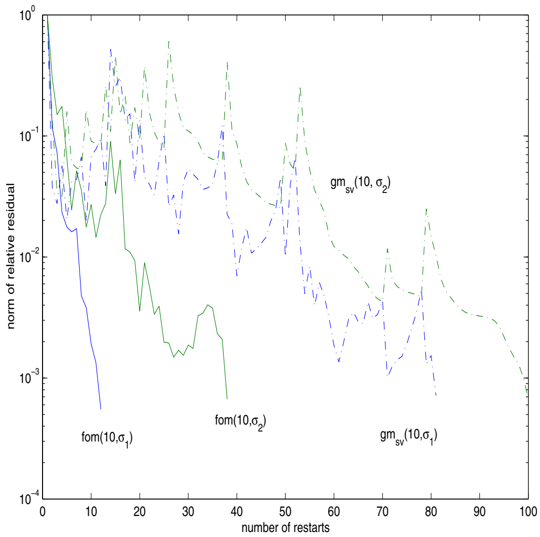

Figure 3.2: Example from structural dynamics. $\sigma_1 = (5 \cdot 2\pi)^{-1}, \sigma_2 = (8 \cdot 2\pi)^{-1}$.

Whenever S is nonsingular, we can write the problem above as in (1.1), namely $(TS^{-1} - \sigma I)\hat{z} = f$, $S\,z = \hat{z}$. We consider test case **C** in [9] and for the sake of simplicity, we only report results for two parameters $\sigma_1 = (5 \cdot 2\pi)^{-1}, \sigma_2 = (8 \cdot 2\pi)^{-1}$. The linearized problem has dimension 3947 and the right-hand side is $f = e_{1160} + e_{2298}$. Convergence curves with shifted restarted FOM and with gm_{sv} and $m = 10$ are displayed in Figure 3.2. The stopping tolerance was set to $\varepsilon = 10^{-3}$, a loose value which is typical in this kind of applications [9]. FOM is faster than gm_{sv} with both shifts. Again, different shifting affects the whole computation in gm_{sv}: restarted GMRES with $m = 10$ would converge in 9 restarts for σ_1 and in 29 restarts for σ_2. This suggests that in gm_{sv} other strategies should be devised to select the seed system, to prevent convergence delay.

4 Conclusions and further remarks.

We have shown that a known Arnoldi-based method, the restarted Full Orthogonalization Method, can efficiently solve shifted algebraic linear systems, at the cost that grows only modestly as the number of shifts increases. Limited numerical experiments seem to show its competitiveness with respect to other restarted methods. Note also that the various methods can be combined by switching to any of the strategies at restart time. Our experience seems to show that known problems associated with restarting (see, e.g., [8]), are exacerbated in the shifting setting in GMRES-based methods; other strategies to select the collinearity restarting vector should perhaps be considered.

The natural implementation of FOM in the shifted context is particularly attractive when both A and b are real, while the shift is complex. More precisely, let $\sigma \in \mathbb{C}$ and consider

$$(A - \sigma I)x = b \qquad A \in \mathbb{R}^{n\times n}, b \in \mathbb{R}^n.$$

The subspace $\mathcal{K}_m(A, b)$ as well as H_m and V_m are real, whereas only the approximate solution in the projected space, $y_m = (H_m - \sigma I)^{-1} e_1 \beta_m$, has complex entries; see [3] for similar considerations. At restart time, all (complex) residuals are collinear to the $m + 1$st basis vector, which is real. Therefore, the new approximation basis after restart can still be imposed to be real, while the collinearity coefficients $\beta_m^{(i)}$ are complex. As a consequence, at each restart, the expensive step of constructing the orthogonal basis is done in real arithmetic, whereas most of the remaining computation, of order m, is done in complex arithmetic.

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