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Linear systems with a quadratic parameter and application to structural dynamics

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Abstract

The numerical solution of the linear system $(\sigma^2 A + \sigma B + C)x = b$, where A, B and C are large complex Hermitian or symmetric matrices of size n, b, x vectors of length n and $\sigma \in \mathbb{C}$, arises in important applications. In this paper we explore a symmetric formulation that allows to efficiently solve the system for several values of σ simultaneously, by means of a short-term recurrence method. Numerical experiments on structural dynamic problems report on the improvement of the new approach over existing methods.

Keywords: Iterative methods, quadratic parameter, QMR, J–symmetric linear systems, complex symmetric matrices.

1 Introduction

We are interested in the numerical solution of the linear system

$$(\sigma^2 A + \sigma B + C)x = b, \tag{1}$$

where A, B and C are large complex Hermitian or symmetric matrices of size n; b, x are vectors of length n and $\sigma \in \mathbb{C}$. The complex parameter σ is allowed to vary, while the matrices and the right-hand side are fixed, therefore the solution x will depend on σ, that is $x = x(\sigma)$. We shall assume throughout the paper that $\sigma \neq 0$ and that at least one of the two matrices A, C is nonsingular. From now on we shall assume A nonsingular; otherwise, the reverse formulation with coefficient matrix $(\omega^2 C + \omega B + A)$ can be employed, with $\omega = \sigma^{-1}$.

Problem (1) has been extensively studied in connection with the solution of certain difference and ordinary differential equations, for which a wide literature is available that relies on the properties of matrix polynomials; see for instance [11]. Unfortunately, important applications such as electromagnetic scattering [18], wave propagation in porous media [24] and structural dynamics [3] require the solution to (1) with very large size matrices, on which the theory developed in [11] is not applicable.

Equation (1) can be treated as a general nonlinear equation; Power series and Padé series expansions have shown good performance when analyzing neighborhoods of a given value σ_0 [18]. Different algebraic strategies can be adopted, most of which resort to methods that have been successfully applied to the solution of the corresponding large *quadratic* eigenvalue problem $(\sigma^2 A + \sigma B + C)x = 0$ with σ also unknown; see for instance [22, 25, 13] and their references.

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In this paper we explore a matrix formulation that can efficiently exploit the symmetry of the problem. This approach will allow us to: (i) Employ an efficient implementation of Krylov subspace linear system solvers; (ii) Solve (1) for several σ's simultaneously at a cost per iteration that is slightly higher than that for solving one system. We shall focus on the case of complex symmetric matrices[1] (see [3, 18]), and we shall report on numerical experiments carried out on structural dynamic problems.

In [3] experiments with a nonsymmetric matrix formulation were carried out. The high non–symmetry of the formulation penalized the performance of short–term recurrence methods, so that long–term recurrence schemes with restarting were preferred. On the other hand, these latter schemes are very memory demanding, and necessitate a lot of tuning for the selection of the optimal restarting parameter [3]. Therefore, the efficient solution of these large application problems really calls for effective and robust short-term recurrence procedures. In this paper we show a possible way of exploiting these methods when a symmetric formulation of the original problem is derived.

In section 2 we shall recall some standard matrix formulations of (1) that lead to the solution of a $2n \times 2n$ linear system $(T + \sigma S)z = d$. Known methods for solving this system are reviewed in section 3; in there, the strategy for solving $(T + \sigma S)z = d$ exploiting symmetry is also presented. In section 4 the Krylov subspace iterative solver employed is described, together with the simplifications that the new approach entail. Section 5 discusses some implementation aspects for dealing with singular matrices and for stopping the iterative procedure. In section 6.1 the computational cost and the memory requirements of the new approach are discussed, while in section 6.2 results on numerical experiments on real applications are presented. Finally, comments on future work are provided in section 7.

Matlab notation will be used throughout the paper. For a given $x = [x_1, \ldots, x_n] \in \mathbb{C}^n$, $\|\cdot\|$ denotes the vector 2-norm, $\|x\|^2 := \sum_{i=1}^n |x_i|^2$, $\|\cdot\|_2$ denotes the induced matrix norm and $\|\cdot\|_\infty$ denotes the infinity norm, the largest matrix row sum. For a given complex matrix M, M^t denotes the transpose matrix (without conjugation), and $M^H = \overline{M}^t$, where $\overline{M}$ is the conjugate of M.

2 Matrix formulations

If A is nonsingular, the most natural matrix formulation can be written by exploiting the block companion matrix of the matrix polynomial in (1), so that, by means of a left multiplication with A^{-1} we have [11]

$$\left[\begin{pmatrix} 0 & I \\ -A^{-1}C & -A^{-1}B \end{pmatrix} - \sigma \begin{pmatrix} I & \\ & I \end{pmatrix}\right] \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 0 \\ -A^{-1}b \end{bmatrix} \tag{2}$$

or, by a right multiplication,

$$\left[\begin{pmatrix} 0 & I \\ -CA^{-1} & -BA^{-1} \end{pmatrix} - \sigma \begin{pmatrix} I & \\ & I \end{pmatrix}\right] \begin{bmatrix} x \\ \widehat{y} \end{bmatrix} = \begin{bmatrix} 0 \\ -b \end{bmatrix}.$$

Both formulations are mathematically equivalent to

$$\left[\begin{pmatrix} 0 & I \\ -C & -B \end{pmatrix} - \sigma \begin{pmatrix} I & \\ & A \end{pmatrix}\right] \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 0 \\ -b \end{bmatrix} \tag{3}$$

[1]A complex matrix M is symmetric when its real and imaginary parts are real symmetric.

where the first addend in the coefficient matrix is in general nonhermitian. When A, B and C are complex Hermitian or symmetric, the problem (3) can be transformed into a corresponding Hermitian or symmetric problem by multiplying the first block row by $-C^*$. Here C^* stands for C or $\overline{C}$, depending on the symmetry properties of the coefficient matrices. Reordering rows and columns, we obtain ([3])

$$\left[\begin{pmatrix} B & C \\ C^* & 0 \end{pmatrix} + \sigma \begin{pmatrix} A & \\ & -C^* \end{pmatrix}\right]\begin{bmatrix} y \\ x \end{bmatrix} = \begin{bmatrix} b \\ 0 \end{bmatrix}. \tag{4}$$

We refer to [26] for a recent backward error analysis when using these different formulations in the eigenvalue context. The system (4) is of the type

$$(T + \sigma S)z = d \tag{5}$$

with T and S both Hermitian or symmetric. The block companion formulation (2) is a particular case of the system above, with $S = I$ and T nonsymmetric. From now on we shall focus on the case in which the matrices A, B and C are complex symmetric. As a consequence, the matrices T and S are complex symmetric in the formulation (4). All statements will hold for Hermitian matrices with the obvious change of notation.

The formulation in (4) has been derived assuming C nonsingular. Nevertheless, if C is singular it can still be shown that the solution to (5) is also a solution to (1). Indeed, if $[y; x]$ is a solution to (5) then the second block equation in (4) ensures that $C(y - \sigma x) = 0$, that is $Cy = \sigma Cx$. Substituting in the first block equation $By + \sigma Ay + Cx = b$, we get $By + \sigma Ay + \sigma^{-1}Cy = b$, which shows that $\sigma^{-1}y$ is a solution to (1). In section 5 we will describe how to practically deal with the case of singular C.

3 Solution methods

The *generalized* linear system

$$(T + \sigma S)z = d \qquad \sigma \in \mathbb{C} \tag{6}$$

also arises in the solution of generalized eigenvalue problems [2, 12, 23, 20], and in the computation of the frequency-domain transfer function [6, 7]. In our application, we are interested in solving (5) for several σ's possibly at the same time. Krylov subspace approaches can efficiently handle several simultaneous σ's if the coefficient matrix has a shifted structure of the type $T + \sigma I$ [23, 10, 5, 3]. This can be obtained by simply inverting S in (6), so that

$$(TS^{-1} + \sigma I)\widehat{z} = d \qquad z = S^{-1}\widehat{z}. \tag{7}$$

If carried out explicitly, this approach destroys any possible symmetry of the original problem. Symmetry may be maintained if the nonsingular matrix S has some additional properties. If S is Hermitian positive definite and T is Hermitian then the Cholesky factorization $S = LL^H$ allows to transform the original generalized problem into the shifted Hermitian system

$$(L^{-1}TL^{-H} + \sigma I)\widehat{z} = L^{-1}d \qquad z = L^{-H}\widehat{z}.$$

If T and S are complex symmetric and S has both positive (or negative) real and imaginary parts, a similar strategy can be adopted. By writing $S = LDL^t$ with L lower triangular and D diagonal with positive entries [15], we obtain the symmetric problem

$$\left(D^{-\frac{1}{2}}L^{-1}TL^{-t}D^{-\frac{1}{2}} + \sigma I\right)\widehat{z} = D^{-\frac{1}{2}}L^{-1}d \qquad z = L^{-t}D^{-\frac{1}{2}}\widehat{z}. \tag{8}$$

Unfortunately, current factorization codes do not seem to exploit the fact that S has definite real and imaginary parts, therefore the code may deliver a factorization with D *block* diagonal with 2 by 2 blocks [15]. This would not allow the derivation of the formulation (8).

We next present an alternative approach which does not put other constraint on S other than being symmetric and nonsingular. We first need to recall the notion of J–symmetry [16, 17, 9]:

Definition 3.1 ([9]) *A matrix M is J–symmetric (resp. J-Hermitian) if $JM = M^tJ$ (resp. $JM = M^HJ$) where J is a symmetric (resp. Hermitian) nonsingular matrix.*

In the remaining of this paper we shall focus on the case of J–symmetric matrices; we refer to [9] for the treatment of J-Hermitian matrices. We will see in section 4 that the Lanczos method can appropriately exploit this particular symmetry so as to drastically lower the computational cost per iteration.

For any complex matrix M there always exists a nonsingular matrix J for which M is J–symmetric [16, 17]. However, finding such J may be extremely expensive, so that this property is often of little practical use unless J is known explicitly. It was shown in [9] that J can be naturally computed in some common structured problems. A convenient J can also be explicitly determined in our case by first appropriately adjusting the coefficient matrix; see also [6, 7] for analogous applications.

Let J be any nonsingular complex symmetric matrix. Then, it can be easily shown that the matrix $M \equiv (T + \sigma S)J$ is J–symmetric; for such J we can consider the system

$$(T + \sigma S)J\widehat{z} = d \qquad z = J\widehat{z},$$

which can be solved with the simplified Lanczos algorithm reviewed in Section 4. By choosing $J := S^{-1}$ we derive a formulation that is mathematically equivalent to that in (7). In practice, we implicitly solve the system $(TS^{-1} + \sigma I)\widehat{z} = d$ by actually using the S^{-1}–symmetry of $(T + \sigma S)S^{-1}$. Moreover, by choosing $J = S^{-1}$ we can isolate the shift so as to exploit the Krylov subspace properties.

4 Simplified Lanczos and QMR methods for shifted systems

In this section we briefly recall some known facts about the Lanczos process and its simplification in case of J–symmetric matrices [9]. Given two vectors $v, w \in \mathbb{C}^n$ and the complex matrix $M \in \mathbb{C}^{n\times n}$, the classical Lanczos process generates two vector sequences $\{v_1, v_2, \dots, v_k\}$, $\{w_1, w_2, \dots, w_k\}$ with $v_1 \equiv v$ and $w_1 \equiv w$ that span the Krylov subspaces

$$K_k(M, v) = \text{span}\{v, Mv, \dots, M^{k-1}v\}, \qquad K_k(M^H, w) = \text{span}\{w, M^Hw, \dots, (M^H)^{k-1}w\}$$

for $k \geq 1$ [19, 23]. The matrices $V_k = [v_1, v_2, \dots, v_k]$, $W_k = [w_1, w_2, \dots, w_k]$ are computed so as to satisfy the bi-orthogonality condition, $W_k^HV_k = \Omega$, with Ω diagonal matrix. The Lanczos process can proceed as long as the matrix Ω is nonsingular. It was first observed[2] in [17] for real matrices and then investigated in [9] in the general case that the Lanczos process simplifies when using J–symmetric matrices. If M is J–symmetric then the auxiliary subspace $K_k(M^t, w_1)$ can be generated instead of $K_k(M^H, w_1)$; setting $w_1 := Jv_1$, then

$$w_i = \xi_i J v_i, \quad i = 2, 3, \dots, \quad \xi_i \in \mathbb{C}^n$$

[2]We thank M. Gutknecht for pointing to this reference.

where ξ_i depends on the normalization used in the Lanczos process. Moreover, it can be shown that the generated vectors satisfy the relation $v_i^t J v_j = \delta_{i,j}$, for $i, j = 1, \dots, k$ [9]. The procedure simplifies in that matrix–vector multiplications with M^t need not be carried out in order to generate the $\{w_i\}$ sequence, therefore the cost per iteration is highly reduced.

Krylov subspace methods are invariant under shift, that is $K_k(M, v) = K_k(M + \sigma I, v)$. In the Lanczos process, the relation $MV_k = V_{k+1}H_k$, with $H_k \in \mathbb{C}^{(k+1)\times k}$ tridiagonal, implies $(M+\sigma I)V_k = V_{k+1}(H_k+\sigma\tilde{I}_k)$, where $\tilde{I}_k$ is the $(k+1)\times k$ principal portion of the identity matrix. The solution to a shifted system $(M + \sigma I)\hat{z} = d$ can be approximated as $z_k(\sigma) = V_k g_k(\sigma)$, for some g_k, and the residual is given by $s_k = d - (M + \sigma I)V_k g_k = V_{k+1}(\beta_0 e_1 - (H_k + \sigma\tilde{I})g_k)$, with $v_1 = d/\beta_0$. In a quasi–minimum residual approach (QMR), $g_k(\sigma)$ is computed so as to minimize

$$\|\beta_0 e_1 - (H_k + \sigma\tilde{I}_k)g\|. \tag{9}$$

Owing to the tridiagonal structure of H_k, the vector g_k can be computed by means of a short–term recurrence [8, 5]. Therefore, for each shifted system, only the cost of solving (9) and updating $x_k(\sigma)$ is needed, while the expensive step of generating the Lanczos vectors is done only once for all σ's.

In practical implementations, it is known that the coupled two-term recurrence version of the Lanczos process should be preferred [8, 14]. Such variant requires the updating of two additional recurrences that are coupled as shown above [9]. In our tests, we have implemented the coupled two-term QMR recurrence for shifted complex J–symmetric systems using $M = (T + \sigma S)J$ with $J = S^{-1}$.

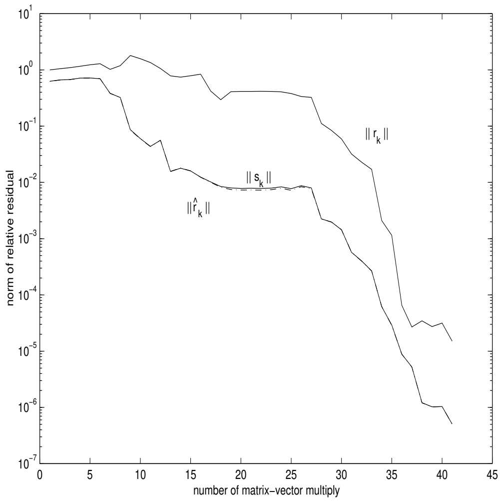

Figure 1: Comparison of residual norms

5 Residual analysis and singularity

The simplified QMR method determines an approximate solution to (5). However, the original system (1) in general will not be solved with the same accuracy as (5). By setting $r_k = b - (\sigma^2 A + \sigma B + C)x_k$ and $s_k = d - (T + \sigma S)z_k$, with $z_k = [y_k; x_k]$, then

$$r_k = \left[I, \quad -(B + \sigma A)C^{-1}\right] s_k \quad \text{and} \quad \|r_k\| \le \left(1 + \|(B + \sigma A)C^{-1}\|_2\right) \|s_k\|.$$

A more interesting relation can be obtained by considering the residual

$$\widehat{r}_k = b - (\sigma^2 A + \sigma B + C)\left(\frac{1}{\sigma} y_k\right)$$

as a function of the approximate solution $\frac{1}{\sigma} y_k$. Then, by writing $s_k = [s_{k,1}; s_{k,2}]$ we obtain

$$\widehat{r}_k = s_{k,1} + \frac{1}{\sigma} s_{k,2} = \left[I, \frac{1}{\sigma} I\right] s_k \quad \text{and} \quad \|\widehat{r}_k\| \leq \left(1 + \frac{1}{|\sigma|}\right) \|s_k\|.$$

Note that the upper bound for the ratio $\|\widehat{r}_k\|/\|s_k\|$ only depends on the shift, and not on the coefficient matrices. Figure 1 shows the behavior of $\|r_k\|, \|s_k\|$ and $\|\widehat{r}_k\|$ for the structural dynamic problem of size 3627. The norm of the residual $\widehat{r}_k$ overlaps that of the generalized system residual, also suggesting that for this problem the vector $\frac{1}{\sigma} y_k$ is a much better approximation than x_k to the solution of (1). Note that for this problem, $\|A + \sigma B\|_\infty \approx 10^8$ and $\|C^{-1}\|_2 \approx 40$. This shows that the bound for $\|r_k\|$ is not tight, and that, as shown in the plot, a difference from $\|s_k\|$ of a few orders of magnitude may be expected. The residual s_k need not be explicitly computed at each iteration. Setting $\varrho_k(\sigma) = \|\beta_0 e_1 - (H_k + \sigma \tilde{I}_k) y_k(\sigma)\|$, an approximation to $\|s_k\|$ can be obtained as ([8])

$$\|s_k\| \leq \sqrt{k+1}\, \varrho_k(\sigma).$$

The implementation of the algorithm when C is singular requires some care, since S becomes singular. The following proposition describes how to circumvent the problem.

Proposition 5.1 *Let $P \in \mathbb{C}^{n \times m}$ be a full column rank basis for the orthogonal complement to the null space of the symmetric matrix $C \in \mathbb{C}^{n \times n}$ and assume that $\sigma \neq 0$. If $[y; \widehat{x}]$ solves*

$$\left[\begin{pmatrix} B & CP \\ P^t C & 0 \end{pmatrix} + \sigma \begin{pmatrix} A & \\ & -P^t C P \end{pmatrix}\right] \begin{bmatrix} y \\ \widehat{x} \end{bmatrix} = \begin{bmatrix} b \\ 0 \end{bmatrix} \tag{10}$$

then $\frac{1}{\sigma} y$ solves $(\sigma^2 A + \sigma B + C)x = b$.

Proof. We first observe that the nonsingularity of $P^t C P$ follows from the properties of complex symmetric matrices. Indeed, if C is complex symmetric, then there exists a unitary matrix U such that $C = U \Sigma U^t$, with Σ diagonal with non–negative decreasingly ordered real entries [16]. Partitioning U as $U = [U_1, U_2]$ with $C\overline{U}_2 = 0$ and $C\overline{U}_1$ full rank, we can choose $P = \overline{U}_1$, so that $P^t C P$ is the principal nonsingular portion of Σ.

From the second block equation in (10) we have

$$P^t C y - \sigma P^t C P \widehat{x} = 0. \tag{11}$$

The matrix-vector product Cy can be written as $Cy = CPz$ for some $z \in \mathbb{C}^m$. If $z \neq 0$ then (11) implies $z = \sigma \widehat{x}$. Substituting into the first block $By + \sigma Ay + CP\widehat{x} = b$, and using $CP\widehat{x} = \frac{1}{\sigma} CPz = \frac{1}{\sigma} Cy$, we obtain

$$By + \sigma Ay + C\frac{1}{\sigma} y = b$$

which proves the assertion. If $z = 0$, then $Cy = 0$ so that $P^t C P \widehat{x} = 0$ and $\widehat{x} = 0$, hence $By + \sigma Ay = b$. Therefore, $\frac{1}{\sigma} y$ satisfies the wanted relation for $Cy = 0$. ∎

In the application we propose in section 6.2 the problem can be solved in a simple manner, since C is diagonal. A basis P can thus be obtained as the portion of the identity matrix $I = [e_1, e_2, \ldots, e_n]$ corresponding to the m nonzero diagonal elements of C, that is $P = [e_{\tau_1}, e_{\tau_2}, \ldots, e_{\tau_m}]$, where $\{\tau_1, \ldots, \tau_m\}$ is an increasingly ordered subset of $\{1, 2, \ldots, n\}$. Then the matrix CP is rectangular and full rank, with one nonzero entry per column. The convergence of the approximate solution to the original problem when C is singular can be naturally monitored by using the residual $\widehat{r}_k$.

6 Numerical results

6.1 Computational cost and memory considerations

The approach described in the previous sections aims at solving the system $(T + \sigma_j S)z = d$, for $j = 1, \ldots, s$, by implicitly transforming the problem into $(TS^{-1} + \sigma I)\widehat{z} = d$. This requires one solve with S at each iteration of the Lanczos process, so that minimizing the total number of iterations becomes crucial. If the matrix S is very sparse, it can be efficiently factorized before starting the iterative process and then triangular solves with its factors need be performed at each iteration. We have used the Harwell code ME47 in our fortran tests ([1]). If the factorization of S is too expensive then the solution to $Sy = q$ can be approximated by means of an iterative solver, giving rise to a so–called inner–outer iteration. This approach is currently under investigation.

In addition to the memory requirements for the generation of the Lanczos recurrence vectors of length $2n$, the approach necessitates the storage of two long vectors for each parameter σ_j, $j = 1, \ldots, s$, that are used to update the approximate solution with a short-term recurrence. Since only half solution vector is needed for solving the original problem, each σ_j only requires two additional vectors of length n, as well as the solution vector $\frac{1}{\sigma_j} y_k(\sigma_j)$.

6.2 Experimental results

In this section we report on some experiments where the performance of simplified QMR (SQMR) is compared to that of another short-term recurrence method for shifted system, TFQMR, applied on the nonsymmetric system (7). We first describe an experiment on a system directly generated in the form (5) in order to show that the new approach is indeed superior to an alternative method that does not take symmetry into account. Results on tests performed on data originating from the solution to (1) in structural dynamic problems are then reported.

In all plots, the true residual of the generalized system is monitored and the iteration is stopped when $\|s_k\| \leq 10^{-8}\|s_0\|$ for all systems. The figures show the convergence history of the methods versus the number of matrix–vector multiplications, which represent the major computational cost per iteration, since they also include solving with S.

Academic example: Our first experiments were done in Matlab [21] with a matrix $T \in \mathbb{R}^{n \times n}$, $n = 100$, generated by the 5-point stencil finite difference discretization of the 2D Laplacian on the unit square, with homogeneous boundary conditions. The two matrices

$$S_1 = \begin{pmatrix} I & \\ & -I \end{pmatrix}, \qquad S_2 = \text{tridiag}(1, \underline{1}, 1)$$

have been used, for which the matrix TS^{-1} is highly indefinite. The right-hand side was chosen with real random entries uniformly distributed in $[0, 1]$ (Matlab function `rand`), while the complex shift $\sigma = \imath$ was used. The performance of the two algorithms with S_1 and S_2 is reported in Figure 2(left) and Figure 2(right), respectively. The improvement of SQMR over TFQMR is clearly noticeable.

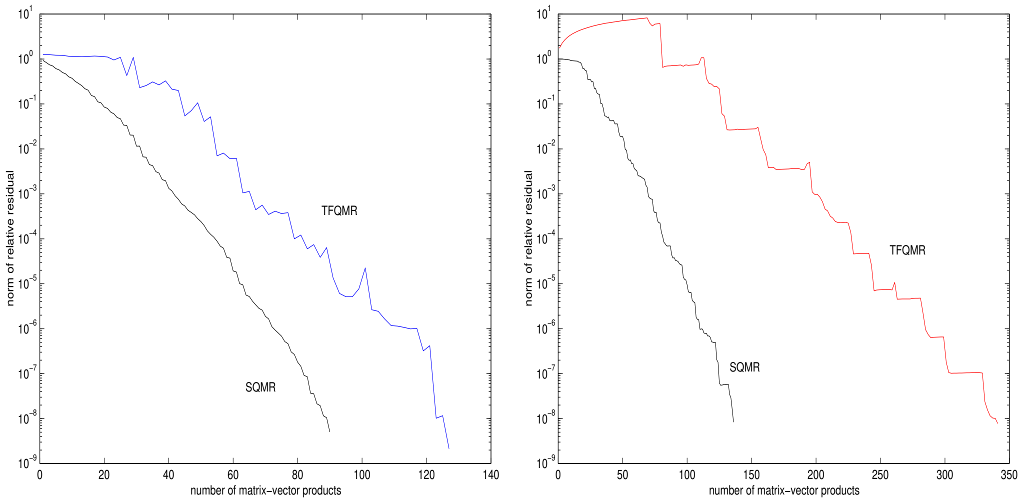

Figure 2: First set of experiments. Matrix T is the Laplacian. Left: $S = S_1$. Right: $S = S_2$.

Real application: Next reported experiments aimed at solving (1) for a linear system arising in the direct frequency domain analysis of two linearized structural dynamic problems [3] and were done in Fortran. The original equation of motion can be written in matrix form as

$$M\ddot{q} + \widehat{C}\dot{q} + Kq = p$$

where M and K are the inertia and stiffness matrices, respectively, and $\widehat{C}$ is the viscous damping matrix. Under complex harmonic excitations of type $p(t) = fe^{\imath\omega t}$, the steady-state solution is given by $q(t) = \tilde{q}(\omega)e^{\imath\,\omega t}$, yielding the system

$$E(\omega)\tilde{q}(\omega) = f \qquad \text{with} \qquad E(\omega) = -\omega^2 M + \imath\omega\widehat{C} + K,$$

where $E(\omega)$ is the dynamic impedance matrix. In case of hysteretic damping, we can write $\widehat{C} = C_V + \frac{1}{\omega}C_H$, leading to the impedance matrix formulation $E(\omega) = -\omega^2 M + \imath\omega C_V + (K + \imath C_H)$. In both our tests, we consider the reverse matrix formulation [3], which gives the linear system

$$\left(-\sigma^2(K + \imath C_H) - \sigma\imath C_V + M\right) x = b, \qquad \sigma := \frac{1}{\omega}.$$

The system corresponds to (1) for $A := -(K+\imath C_H)$, $B := -\imath C_V$ and $C := M$. In both problems the matrix C is diagonal, therefore system solutions with S only entail the factorization of A.

The first test (case B in [3]) comes from the finite element modelization of a machine foundation resting on ground. The frequency response is determined in the range $[.1Hz, 60.1Hz]$, giving $\sigma^{-1} \in 2\pi[.1Hz, 60.1Hz]$. The interval can then be split so as to have up to a few hundred frequencies to solve with [3]; we shall only report on experiments with the simultaneous solution of systems for the two values $\sigma_1 = 1/(100.1\pi)$ and $\sigma_2 = 1/(80.1\pi)$. The problem size is $n = 3627$, yielding a generalized linear system of size 7254. After an initial similar convergence history, the convergence of simplified QMR clearly outperforms that of TFQMR for both values

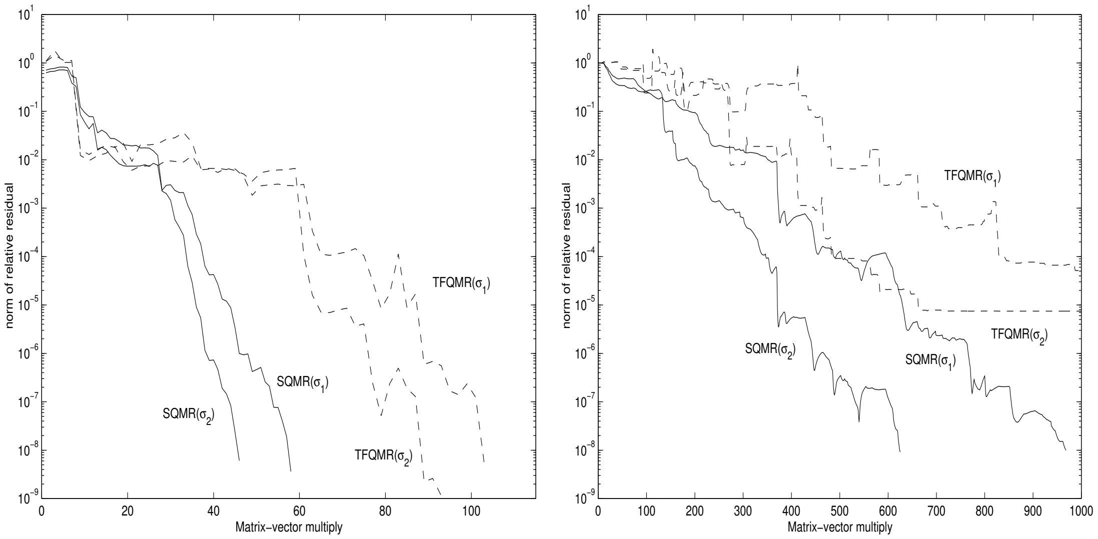

Figure 3: Convergence history on the structural dynamic problem with parameters $\sigma_1 = (100.1\pi)^{-1}, \sigma_2 = (80.1\pi)^{-1}$. Left: Problem size $n = 3627$. Right: Problem size $n = 11957$.

of the parameters, yielding a total number of matrix-vector products that is half that required by TFQMR.

The second test (case F in [3]) comes from the 3D finite element modeling of a soil structure interaction problem. In the reverse formulation, the matrix C is diagonal and semi–definite, therefore the procedure described in section 5 was implemented. The problem size is 11957. Taking into account that 50 diagonal elements of C are zero, the final size of the generalized linear system (10) is 23864. The frequency analysis led to consider $\sigma^{-1} \in 2\pi[10Hz, 50Hz]$; the two shifts $\sigma_1 = 1/(100.1\pi)$ and $\sigma_2 = 1/(80.1\pi)$ were used. The problem is more sensitive to the choice of the parameter and the convergence curve differs substantially for σ_1 and σ_2. In both cases SQMR is able to reach convergence. TFQMR shows a much slower convergence history, together with lack of successful termination to the required accuracy.

7 Conclusions and future work

In this paper we have addressed the problem of solving (1) by using a complex symmetric matrix formulation of the original problem. We have shown how to adapt a known iterative process so as to exploit the symmetry and lower the computational cost per iteration by also solving for several σ's simultaneously. The performance of the approach is very promising; the implementation of a look-ahead strategy will make the method more robust [4]. For large problems such as the second application above, preconditioning becomes mandatory. Although few effective preconditioning techniques are available for shifted and generalized problems, we believe that the particular structure of the problem could be further exploited to that end. The convergence analysis relating the iterative solutions to (5) and (1) is currently under investigation.

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References

[1] AEA Technology, *Harwell subroutine library*, Harwell Laboratory, Oxfordshire, England, Dec. 1995.

[2] T. Ericsson and A. Ruhe, *The spectral transformation Lanczos method for the numerical solution of large sparse generalized symmetric eigenvalue problem*, Math. Comp., 35 (1980), pp. 1251–1268.

[3] A. Feriani, F. Perotti, and V. Simoncini, *Iterative system solvers for the frequency analysis of linear mechanical systems*, Tech. Rep. 1077, Istituto di Analisi Numerica del CNR, Pavia, Italy, March 1998.

[4] R. Freund, M. Gutknecht, and N. Nachtigal, *An implementation of the look-ahead Lanczos algorithm for non-Hermitian matrices*, SIAM J. Sci. Comput., 14 (1993), pp. 137–158.

[5] R. F. Freund, *Solution of shifted linear systems by quasi-minimal residual iterations*, in Numerical Linear Algebra, L. Reichel, A. Ruttan, and R. S. Varga, eds., Berlin, 1993, W. de Gruyter, pp. 101–121.

[6] R. W. Freund and P. Feldmann, *The SyMPVL algorithm and its applications to interconnect simulation*, in Proceedings of the 1997 International Conference on Simulation of Semiconductor Processes and Devices, IEEE, 1997, pp. 113–116.

[7] ——, *Reduced-order modeling of large linear passive multi-terminal circuits using matrix-Padé approximation*, in Proceedings of the Design, Automation and Test in Europe Conference 1998, IEEE Computer Society Press, 1998, pp. 530–537.

[8] R. W. Freund and N. M. Nachtigal, *An implementation of the QMR method based on coupled two-term recurrences*, SIAM J. Sci. Comput., 15 (1994).

[9] ——, *Software for simplified Lanczos and QMR algorithms*, Applied Numerical Mathematics, 19 (1995), pp. 319–341.

[10] A. Frommer and U. Glässner, *Restarted GMRES for shifted linear systems*, SIAM J. Sci. Comput., 19 (1998), pp. 15–26.

[11] I. Gohberg, L. Rodman, and P. Lancaster, *Matrix Polynomials*, Academic Press, New York, 1982.

[12] R. Grimes, J. Lewis, and H. Simon, *A shifted block Lanczos algorithm for solving sparse symmetric generalized eigenproblems*, SIAM J. Matrix Anal. Appl., 15 (1994), pp. 228–272.

[13] P. Guillaume, *Nonlinear eigenproblems*, Tech. Rep. 97.14, CNRS-INSA- Universitè Paul Sabatier, Toulouse, France, 1997.

[14] M. H. Gutknecht and Z. Strakos, *Accuracy of three-term and two-term recurrences for Krylov space solvers*, Tech. Rep. TR-97-21, ETH, Zurich, December 1997.

[15] N. J. Higham, *Factorizing complex symmetric matrices with positive definite real and imaginary parts*, Math. Comput., 67 (1998), pp. 1591–1599.

[16] R. A. Horn and C. R. Johnson, *Matrix Analysis*, Cambridge University Press, Cambridge, 1985.

[17] K. C. Jea and D. M. Young, *On the simplification of generalized conjugate-gradient methods for nonsymmetrizable linear systems*, Lin. Alg. Appl., 52–53 (1983), pp. 399–417.

[18] M. Kuzuoglu and R. Mittra, *Finite element solution of electromagnetic problems over a wide frequency range via the Padé approximation*, tech. rep., Applied Res. Lab., PennState Univ., State College PA, 1998.

[19] C. Lanczos, *An Iteration Method for the Solution of the Eigenvalue Problem of Linear Differential and Integral Operators*, J. Res. Natl. Bur. Stand., 45 (1950), pp. 255–282.

[20] R. Lehoucq and K. Meerbergen, *Using generalized Cayley transformations within an inexact rational Krylov sequence method*, SIAM J. Matrix Anal. Appl., 20 (1999), pp. 131–148.

[21] The MathWorks, Inc., *MATLAB User's Guide*, Natick, Mass. 01760, Jan 1998.

[22] B. N. Parlett and H. C. Chen, *Use of indefinite pencils for computing damped natural modes*, Lin. Alg. Appl., 140 (1990), pp. 53–88.

[23] Y. Saad, *Iterative methods for sparse linear systems*, The PWS Publishing Company, 1996.

[24] J. E. Santos and P. M. Gauzellino, *Parallel algorithms for wave propagation in fluid-saturated porous media*, in Computational Mechanics, New trends and applications, CINME, Barcelona, Spain, 1998, pp. 1–13.

[25] G. Sleijpen, A. Booten, D. Fokkema, and H. V. der Vorst, *Jacobi-Davidson type methods for generalized eigenproblems and polynomial eigenproblems*, BIT, 36 (1996), pp. 595–633.

[26] F. Tisseur, *Backward error and condition of polynomial eigenvalue problems*, Numerical Analysis Report No. 332, Manchester Centre for Computational Mathematics, Manchester, England, Aug. 1998.

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