A SUBSPACE APPROXIMATION METHOD FOR THE QUADRATIC EIGENVALUE PROBLEM

U. B. HOLZ, G. H. GOLUB AND K. H. LAW

Abstract. Quadratic eigenvalue problems involving large matrices arise frequently in areas such as the vibration analysis of structures, MEMS simulation, and the solution of quadratically constrained least squares problems. The typical approach is to solve the quadratic eigenvalue problem using a mathematically equivalent linearized formulation, resulting in a doubled dimension and a lack of backward stability.

This paper introduces a method that uses perturbation subspaces for block eigenvector matrices to reduce the modified problem to a sequence of problems of smaller dimension. These perturbation subspaces are shown to be contained in certain generalized Krylov subspaces of the n-dimensional space, where n is the undoubled dimension of the matrices in the quadratic problem. The method converges at least as fast as the corresponding Taylor series, and the convergence can be accelerated further by applying a block generalization of the quadratically convergent Rayleigh quotient iteration. Numerical examples are presented to illustrate the applicability of the method.

1. Introduction.

The quadratic eigenvalue problem

$$(\lambda^2 \mathrm{M} + \lambda \mathrm{C} + \mathrm{K})\mathbf{x} = 0 \tag{1.1}$$

commonly arises during the solution of systems of second order ordinary differential equations found in scientific and engineering applications. Gohberg, Lancaster, and Rodman [6] and Lancaster [11] provided an extensive theoretical background on quadratic and other polynomial eigenvalue problems. For a current review of numerical methods for quadratic eigenvalue problems along with a broad discussion of application areas, see Tisseur and Meerbergen [14]. The most common approach is to linearize (1.1), for example as

$$\left[\begin{pmatrix} 0 & \mathrm{N} \\ -\mathrm{K} & -\mathrm{C} \end{pmatrix} - \lambda \begin{pmatrix} \mathrm{N} & 0 \\ 0 & \mathrm{M} \end{pmatrix}\right] \mathbf{z} = 0 \quad \text{or} \quad \left[\begin{pmatrix} -\mathrm{C} & -\mathrm{K} \\ \mathrm{N} & 0 \end{pmatrix} - \lambda \begin{pmatrix} \mathrm{M} & 0 \\ 0 & \mathrm{N} \end{pmatrix}\right] \mathbf{w} = 0, \tag{1.2}$$

where N is any nonsingular matrix. Not only does the linearized problem have twice the dimension of the quadratic problem, but also, in general, even if a backward stable method is used for the linear eigenvalue problem, that stability is not guaranteed for the quadratic eigenvalue problem, as shown by Tisseur [13]. This paper introduces a method that uses subspace approximation and perturbation techniques for the quadratic eigenvalue problem.

1.1. Subspace approximation method for linear eigenvalue problems.

Zhang, Golub, and Law [16] presented a generalized Krylov subspace method for the perturbed symmetric standard eigenvalue problem, $(\mathrm{A} + \Delta\mathrm{A})\mathbf{x} = \lambda\mathbf{x}$ given the known solution for $\mathrm{A}\mathbf{x} = \lambda\mathbf{x}$. The method is based on the following theorem.

THEOREM 1.1. [16] *Assume $Q = [Q_1\ Q_2]$ is orthogonal, with each Q_i representing an eigenspace, and assume $\Lambda_1 = Q_1^T \mathrm{A} Q_1 = \lambda_1 \mathrm{I}$. Let $\Lambda_2 = Q_2^T \mathrm{A} Q_2$, $E = Q_2(\Lambda_2 - \lambda_1 \mathrm{I})Q_2^T$, and $F = E\Delta\mathrm{A}$. Let Q_1^m be the eigenspace of $\mathrm{A} + \Delta\mathrm{A}$ (as a perturbation of Q_1) obtained by the mth order Taylor series expansion. Then Q_1^m belongs to the subspace $\mathcal{K}(E, F, Q_1, m)$, where*

$$\mathcal{K}(E, F, Q_1, m) = \mathcal{R}([P_0(E, F)Q_1, \ldots, P_m(E, F)Q_1]).$$

Here $P_k(E,F)$ is the space spanned by all the homogeneous polynomials in E and F of order k, and $\mathcal{R}(Y)$ denotes the range of Y.

The method computes the spaces $\mathcal{K}(E,F,Q_1,m)$, $m = 1,2,3,\ldots$, and solves the reduced problems in these spaces until convergence of the eigenpairs. The method is at least as fast as the convergence of the corresponding Taylor polynomials. The subspace approximation concept is employed here for solving the quadratic eigenvalue problem.

1.2. The perturbed quadratic eigenvalue problem. Consider computing a few eigenpairs for the perturbed problem

$$(\lambda^2(\mathrm{A}+\Delta\mathrm{A})+\lambda(\mathrm{B}+\Delta\mathrm{B})+(\mathrm{C}+\Delta\mathrm{C}))\mathbf{x}=0, \tag{1.3}$$

assuming that corresponding eigenpairs for the unperturbed problem, $(\lambda^2\mathrm{A}+\lambda\mathrm{B}+\mathrm{C})\mathbf{x}=0$, are known [8]. For the special case of the quadratic eigenvalue problem discussed in this paper, we consider the case with $\Delta\mathrm{A}=\mathrm{B}=\Delta\mathrm{C}=0$ and at least one of A and C nonsingular. That is, we consider the quadratic eigenvalue problem as a special case of the perturbed quadratic eigenvalue problem. Specifically, in (1.3), A,C, and $\Delta\mathrm{B}$ correpsond to M,K, and C, respectively, in (1.1).

This paper is organized as follows: In Section 2 a block perturbation form of (1.3) is introduced and a subspace approximation theorem is proved. Then in Section 3 the computation of perturbation subspaces is described, both in terms of generalized Krylov subspaces and in terms of smaller, directly computed subspaces. Section 4 gives a first order error analysis and develops a stopping criterion. In Section 5 a hybrid algorithm is developed using perturbation subspaces and block Rayleigh quotients, and in Section 6 the complexity of the subspace approximation computations is considered. Finally, Section 7 illustrates the subspace approximation method, using numerical examples drawn from structural dynamics applications.

The numerical examples are performed using MATLAB 6.1.0 on a 1GHz Sun Blade 2000 with 2GB of main memory, running Solaris 8. Examples involving flop counts are performed on the same machine using MATLAB 5.3.1.

2. Block quadratic equation. Given M, C, and K in $\mathbf{R}^{\mathrm{n}\times\mathrm{n}}$, with M nonsingular, let $P(\lambda,t)=\lambda^2\mathrm{M}+\lambda t\mathrm{C}+\mathrm{K}$ for $\lambda\in\mathbf{C}$ and $0\le t\le 1$. Consider the eigenvalue problem

$$P(\lambda(t),t)\mathbf{x}(t)=0,\ t\in[0,1]. \tag{2.1}$$

Because M is nonsingular for t in $[0,1]$, there exist continuous eigenvalue paths $\lambda_1(t),\lambda_2(t),\ldots,\lambda_{2n}(t)$. (See e.g. Ahlfors [1, Sec. 8.2].) If, instead, M is singular but K is nonsingular, all the theory of this section still applies to the problem rearranged as $P(\mu(t),t)\mathbf{x}(t)=0,\ t\in[0,1]$, with $P(\mu,t)\equiv\mathrm{M}+\mu t\mathrm{C}+\mu^2\mathrm{K}$ and $\lambda(t)=\frac{1}{\mu(t)}$ for $\mu(t)\neq 0$.

When the eigenvalues $\lambda(t)$ of interest are nondefective, it is useful to compute a subspace that contains approximations to the associated eigenspaces. We write the block version of (2.1) as

$$\mathrm{M}X(t)\Lambda^2(t)+t\mathrm{C}X(t)\Lambda(t)+\mathrm{K}X(t)=0, \tag{2.2}$$

where we know solutions at $t=0$ and seek solutions at $t=1$. The idea of the subspace approximation method is to compute subspaces that contain the ranges of the Taylor

approximations to $X(t)$, and then to solve the reduced quadratic eigenvalue problems in these subspaces to obtain the approximate eigenpairs for (2.1) on the whole space.

The following notational conventions are used in our discussion:

1. The superscript (j) denotes the jth derivative with respect to t, at $t = 0$ unless t is otherwise specified. For example if $Q(t)$ is a matrix function of t then $Q^{(j)}$ is its jth derivative at $t = 0$, and $Q^{(j)}(t_0)$ is its jth derivative at $t = t_0$.
2. $\|\cdot\|$ denotes the Euclidean norm unless otherwise stated.
3. $X_j(t)$ is the jth Taylor approximation about $t = 0$ to the function $X(t)$ in (2.2).

2.1. Convergence of the block Taylor series. Suppose we know a nondefective eigenvalue λ of multiplicity p for (2.1) at $t = 0$, along with a corresponding $n \times p$ right eigenvector matrix X_0. Writing the associated eigenvalue paths as $\lambda_1(t), \ldots, \lambda_p(t)$, in (2.2), $X(t)$ is an $n \times p$ matrix function of t with $X(0) = X_0$, and $\Lambda(t)$ is a $p \times p$ matrix function of t whose eigenvalues are $\lambda_1(t), \ldots, \lambda_p(t)$. No assumptions are made here regarding the normalization of $X(t)$, since the results in this section are independent of normalization.

For nondefective λ the matrix function $X(t)$ can be taken to have a convergent Taylor series as follows. Consider a standard linearized form for (2.1), such as

$$A(t)\mathbf{z}(t) \equiv \begin{pmatrix} -t\mathrm{M}^{-1}\mathrm{C} & -\mathrm{M}^{-1}\mathrm{K} \\ \mathrm{I} & 0 \end{pmatrix} \begin{pmatrix} \lambda(t)\mathbf{x}(t) \\ \mathbf{x}(t) \end{pmatrix} = \lambda(t) \begin{pmatrix} \lambda(t)\mathbf{x}(t) \\ \mathbf{x}(t) \end{pmatrix}. \tag{2.3}$$

When λ_0 is a nondefective eigenvalue of some multiplicity p for (2.3) at $t = t_0$, the corresponding eigenspace projection $P(t)$, also called the total projection for the λ-group eigenvalues of $A(t)$, is holomorphic in a neighborhood of t_0 (see Kato, [9, Section II.1.4]). It is shown in [9, Section II.4.2] that if a projection $P(t)$ is holomorphic in some domain D containing t_0 then there is a transformation function $U(t)$ satisfying: (1) $U(t)^{-1}$ exists and both $U(t)$ and $U(t)^{-1}$ are holomorphic on D; (2) $U(t)P(t_0)U(t)^{-1} = P(t)$ on D; and (3) $U(t_0) = I$. It follows that if the p columns of Z_0 form a basis for $P(t_0)$ then the p columns of $Z(t) = U(t)Z_0$ form a holomorphic basis for $P(t)$. Now taking $Z_0 = \binom{\lambda_0 X_0}{X_0}$ and writing $Z(t) = \binom{Z_1(t)}{Z_2(t)}$, the block form of (2.3) is $A(t)Z(t) = Z(t)\Lambda(t)$, and with some manipulation, yields $\mathrm{M}Z_2(t)\Lambda^2(t) + t\mathrm{C}Z_2(t)\Lambda(t) + \mathrm{K}Z_2(t) = 0$, where $Z_2(t_0) = X_0$. Since $Z_2(t)$ is holomorphic and of full rank, taking

$$X(t) = Z_2(t)W(t) \tag{2.4}$$

for any nonsingular holomorphic $p \times p$ matrix $W(t)$ satisfying $W(t_0) = \mathrm{I}_p$ gives a holomorphic block eigenvector matrix $X(t)$. In particular if $W(t)$ is holomorphic on the whole complex plane and ρ is the convergence radius about t_0 of the Taylor series for $Z(t)$, then the convergence radius of the Taylor series for $X(t)$ about t_0 is at least ρ. (A lower bound for ρ may be computed using majorization series, described in [9, Section II.3.1]; however this is very expensive, involving explicit formation of a $2n$ matrix inverse, a $2n$ pseudoinverse, and several $2n$ matrix norms.)

Even when λ_0 is a defective eigenvalue of $A(t)$ at t_0, the total projection $P(t)$ onto the associated invariant subspace is holomorphic. Thus if $P_{\mathrm{tot}}(t)$ is the total projection for the sum of the invariant subspaces associated with p eigenvalue paths $\lambda_{i_1}(t), \lambda_{i_2}(t), \ldots, \lambda_{i_p}(t)$, then P_{tot} can be analytically continued as t goes from 0 to 1, as long as no other eigenvalue paths intersect these. $Z(t)$ can therefore also be

analytically continued, as can $X(t)$ if it is defined by (2.4), although, in this case, $X(t)$ may be rank-deficient.

2.2. A subspace approximation theorem. To specify the perturbation subspaces we first require the following definition of a generalized Krylov subspace.

DEFINITION 2.1. *For $B_1, B_2, \ldots, B_k \in \mathbf{C}^{N\times N}$, and $X \in \mathbf{C}^{N\times p}$, $0 < p \le N$, let $\mathcal{S}_j(B_1, B_2, ..., B_k, X)$, abbreviated $\mathcal{S}_j(X)$ when the B_i's are understood, denote the jth generalized Krylov subspace generated by $B_1, B_2, ..., B_k$ applied j times to X, i.e.*

$$\mathcal{S}_j(X) = \sum_{\deg(q)\le j} \{\mathrm{range}(q(B_1, B_2, ..., B_k)X)\},$$

where the sum is over all polynomials q in k variables with coefficients in $\mathbf{C}$ and degree less than or equal to j.

As an equivalent definition, let $\mathcal{S}_0(B_1, B_2, \ldots, B_k, X) = \mathrm{range}(X)$, and, for $j > 0$, if the columns of X_{j-1} form a basis for $\mathcal{S}_{j-1}(B_1, B_2, \ldots, B_k, X)$, let

$$\mathcal{S}_j(B_1, B_2, \ldots, B_k, X) = \mathrm{range}([B_1X_{j-1} \;\; B_2X_{j-1} \;\; \cdots \;\; B_kX_{j-1} \;\; X_{j-1}]).$$

THEOREM 2.2. *Let $V \in \mathbf{C}^{n\times(n-p)}$ be such that* $\mathrm{range}(V) + \mathrm{range}(X_0) = \mathbf{C}^n$, *and let F be an $n \times n$ matrix satisfying*

$$FP(\lambda_0, 0)V = V. \tag{2.5}$$

Then $\forall t$, $\forall j \ge 0$, $\mathrm{range}(X_j(t)) \subseteq \mathcal{S}_j(F\mathrm{M}, F\mathrm{C}, X_0)$.

Proof. Since $\mathcal{S}_j(X_0) \subseteq \mathcal{S}_{j+1}(X_0)$ for all $j \ge 0$, it is sufficient to show that

$$\mathrm{range}(X^{(j)}) \subseteq \mathcal{S}_j(X_0) \quad \forall j \ge 0. \tag{2.6}$$

By the definition of $\mathcal{S}_j(X_0)$, (2.6) is true for $j = 0$. We proceed by induction on j. Assume (2.6) holds for all $j < k$, where $k > 0$. Then $\mathrm{range}(X^{(i)}) \subseteq \mathcal{S}_j(X_0)$ for all i and j such that $0 \le i \le j < k$. Taking the kth derivative with respect to t of equation (2.2), setting $t = 0$, and applying F yields

$$FP(\lambda_0, 0)X^{(k)} = -\textstyle\sum_{r=0}^{k-1} \binom{k}{r} \mathrm{M}X^{(r)}(\Lambda^2)^{(k-r)} - \sum_{r=0}^{k-1} k\binom{k-1}{r} \mathrm{C}X^{(r)}\Lambda^{(k-1-r)}. \tag{2.7}$$

If the columns of Q_{k-1} form a basis for $\mathcal{S}_{k-1}(X_0)$, then $\mathrm{range}(X^{(j)}) \subseteq \mathrm{range}(Q_{k-1})$ for all $j < k$, so the range of the right-hand side of (2.7) is contained in

$$\mathrm{range}([F\mathrm{M}Q_{k-1}, F\mathrm{C}Q_{k-1}]),$$

which is in turn contained in $\mathcal{S}_k(X_0)$. Let the columns of Q_k be a basis for $\mathcal{S}_k(X_0)$, of size $n \times p_k$. Then $FP(\lambda_0, 0)X^{(k)} = Q_kT_k$ for some $p_k \times p$ matrix T_k. Writing $X^{(k)} = Q^{(k)}_{(1)} + Q^{(k)}_{(2)}$, where the columns of $Q^{(k)}_{(1)}$ are in $\mathrm{range}(X_0)$ and the columns of $Q^{(k)}_{(1)}$ are in $\mathrm{range}(V)$, and using (2.5), we have $Q^{(k)}_{(2)} = Q_kT_k$. Hence

$$\mathrm{range}(X^{(k)}) \subseteq \mathrm{range}([Q^{(k)}_{(1)} \; Q^{(k)}_{(2)}]) \subseteq \mathrm{range}([X_0 \; Q_k]) = \mathcal{S}_k(X_0).$$

Thus (2.6) holds for all $j \ge 0$, which proves the theorem. ∎

3. Subspace computations.

3.1. Applying the subspace approximation theorem. If $V = [\mathbf{v}_1 \ \ldots \ \mathbf{v}_{n-p}]$ satisfies $\mathrm{range}(V) + \mathrm{range}(X_0) = \mathbf{C}^n$, then clearly V is of full rank and $\mathrm{range}(V) \cap \mathrm{range}(X_0) = 0$. Also the $n-p$ columns of $P(\lambda_0, 0)V$ are linearly independent and therefore form a basis for $\mathrm{range}(P(\lambda_0, 0))$. Now let $\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_p$ be a basis for $\mathrm{range}(P(\lambda_0, 0))^\perp$. For any p vectors $\mathbf{w}_j \in \mathbf{C}^n$ there is an associated matrix F satisfying (2.5), specified by

$$\begin{aligned} F(P(\lambda_0, 0)\mathbf{v}_i) &= \mathbf{v}_i, \ i = 1, 2, \ldots, n-p, \\ F\mathbf{y}_j &= \mathbf{w}_j, \ j = 1, 2, \ldots, p. \end{aligned} \tag{3.1}$$

The condition

$$V \in \mathbf{C}^{n \times (n-p)}, \qquad \mathrm{range}(V) + \mathrm{range}(X_0) = \mathbf{C}^n \tag{3.2}$$

thus implies the existence of a matrix F satisfying (2.5) that is uniquely determined by $\mathbf{w}_1, \ldots, \mathbf{w}_p$. Also (3.2) alone uniquely determines $FP(\lambda_0, 0)$, since $FP(\lambda_0, 0)V = V$ and $FP(\lambda_0, 0)X_0 = 0$.

To apply Theorem 2.2 we must first specify V in some way. A natural choice is to let V satisfy $\mathrm{range}(V) = \mathrm{range}(X_0)^\perp$. Let P_0^+ be the pseudoinverse of $P(\lambda_0, 0)$. Then $P_0^+ P(\lambda_0, 0)$ is the orthonormal projection into $\mathrm{null}(P)^\perp = \mathrm{range}(V)$, and if $P(\lambda_0, 0)^*\mathbf{y} = 0$ then $P_0^+\mathbf{y} = 0$. Hence the F satisfying (2.5) determined by this V and $\mathbf{w}_j = 0, \ j = 1, 2, \ldots, p$, is exactly P_0^+. (Note that in the version of the subspace theorem for the standard symmetric eigenvalue problem this choice of F gives Theorem 1.1 [16].) Now we can compute the subspaces $\mathcal{S}_j$ by solving appropriate least squares problems. The problems $\min \|P(\lambda_0, 0)\mathbf{v} - \mathbf{y}\|$ are rank-deficient, but because $\mathrm{null}(P(\lambda_0, 0)) = \mathrm{range}(X_0)$, deflation using Householder transformations can be used to obtain equivalent full rank problems. Alternatively, the least squares problems may be considered only nearly rank-deficient numerically, in which case we can choose to solve them directly by decomposing $P(\lambda_0, 0)$. This is an ill-conditioned problem, resulting in large error components in $\mathrm{range}(X_0)$ that must then be removed to gain acceptable solutions.

3.2. Computing the full perturbation subspaces. Suppose we have $X_1, X_2, \ldots, X_{j-1}$ such that

$$\mathcal{S}_{j-1} = \mathrm{range}(X_0) \oplus \mathrm{range}(X_1) \oplus \cdots \oplus \mathrm{range}(X_{j-1}).$$

Then, writing $Y_{j-1} = [X_0 \ X_1 \ \cdots \ X_{j-1}]$, $\mathcal{S}_j = \mathrm{range}([F\mathrm{M}Y_{j-1}, F\mathrm{C}Y_{j-1}, Y_{j-1}])$. Since, for $k < j-1$, the ranges of $F\mathrm{M}X_k$ and $F\mathrm{C}X_k$ are contained in $\mathrm{range}(Y_{k+1})$, which is contained in $\mathrm{range}(Y_{j-1})$, it follows that

$$\mathcal{S}_j = \mathrm{range}([F\mathrm{M}X_{j-1}, F\mathrm{C}X_{j-1}, Y_{j-1}]).$$

Setting $\mathcal{S}_{-1} = \emptyset$ and $\mathcal{S}_0 = \mathrm{range}(X_0)$, we proceed as follows to compute $\mathcal{S}_j$ for $j > 0$.

ALGORITHM 3.1. *This algorithm computes $\widehat{W}$ such that $\mathcal{S}_j = \mathcal{S}_{j-1} + \mathrm{range}(\widehat{W})$.*

0. Let X_{j-1} satisfy $\mathcal{S}_{j-1} = \mathcal{S}_{j-2} \oplus \mathrm{range}(X_{j-1})$. That is, X_{j-1} is full rank, such that the span of its columns added to $\mathcal{S}_{j-2}$ gives the space $\mathcal{S}_{j-1}$ with $\dim(\mathcal{S}_{j-1}) = \dim(\mathcal{S}_{j-2}) + \mathrm{rank}(X_{j-1})$.

1. Let the columns of W form a basis for $\mathrm{range}([\mathrm{M}X_{j-1}, \mathrm{C}X_{j-1}])$.

2. Solve the least squares problem $\min \|P(\lambda_0, 0)\hat{\mathbf{w}}_i - \mathbf{w}_i\|$ for each column of W to get $\widehat{W}$. (If solving directly, first project $\mathbf{w}_i$ into $\mathcal{S}_0^\perp$, so that the part of the solution not in the range of X_0 will be numerically significant.)

3. $\mathcal{S}_j = \mathcal{S}_{j-1} + \text{range}(\widehat{W})$, *because* $\text{range}([\widehat{W}\ X_0]) = \text{range}([FW\ X_0])$.

To add $\text{range}(\widehat{W})$ to $\mathcal{S}_{j-1}$, Modified Gram-Schmidt is used to get the orthonormal basis $[X_0\ X_1\ \cdots\ X_j]$ for $\text{range}([X_0\ X_1\ \cdots\ X_{j-1}\ \widehat{W}])$, so that

$$\mathcal{S}_j = \text{range}([X_0\ X_1\ \cdots\ X_j]) = \mathcal{S}_{j-1} \oplus \text{range}(X_j).$$

Note that this algorithm computes the generalized Krylov subspace by powers. It will be interesting, in future work, to consider computing the space using other polynomials.

3.3. Directly computing derivative subspaces. The equations leading to the proof of Theorem 2.2 suggest a way to compute the derivatives $X^{(k)}$ directly within the generalized Krylov subspace. As mentioned above, the results in Section 2.2 are independent of the normalization of $X(t)$. Now assume the normalization condition

$$X_0{}^* X(t) = \mathrm{I},\ t \in [0,1]. \tag{3.3}$$

In addition, assume we know a matrix of left eigenvectors $W_0 \in \mathbf{C}^{n\times p}$ associated with λ_0 at time $t = 0$, i.e. $W_0{}^* P(\lambda_0, 0) = 0$, such that

$$2\lambda_0 W_0{}^* \mathrm{M} X_0 \text{ is nonsingular.} \tag{3.4}$$

In some instances a value of W_0 is clear from the properties of the problem. For example when M and K are symmetric, if C is skew-symmetric then $W_0 = X_0$, and if C is symmetric then $W_0 = \overline{X}_0$, the conjugate of X_0. Condition (3.4) is guaranteed, as the following lemma shows.

LEMMA 3.2. *Let λ_0 be an eigenvalue of geometric multiplicity p for $P(\lambda, 0)$, and let X_0 and W_0 be associated full rank right and left eigenvector matrices. Then (3.4) holds if and only if λ_0 is nondefective.*

Proof. Let $P(\lambda, 0) = E(\lambda)\Gamma(\lambda)F(\lambda)$ be the Smith canonical decomposition of P (see Wilkinson [15, pp. 19–20]), so that $E(\lambda)$ and $F(\lambda)$ are nonsingular $n \times n$ matrices with determinants independent of λ, and $\Gamma(\lambda) = \text{diag}(a_j(\lambda))$, where the functions $a_j(\lambda)$ are monic polynomials in λ satisfying $a_1(\lambda) \mid a_2(\lambda) \mid \cdots \mid a_n(\lambda)$. Since λ_0 is of geometric multiplicity p,

$$\begin{aligned} a_j(\lambda_0) &\neq 0 \quad \text{for } j \leq n-p, \\ a_j(\lambda_0) &= 0 \quad \text{for } j > n-p. \end{aligned} \tag{3.5}$$

Write $f(\lambda) = W_0^* P(\lambda, 0) X_0 = (W_0 E(\lambda))\Gamma(\lambda)(F(\lambda)X_0)$, and let $\widehat{W}_0(\lambda) = E(\lambda)^* W_0$ and $\widehat{X}_0(\lambda) = F(\lambda)X_0$. $\widehat{W}_0(\lambda)$ and $\widehat{X}_0(\lambda)$ are of full rank for all values of λ, and from (3.5) and the facts

$$\widehat{W}_0(\lambda_0)^* \Gamma(\lambda_0) = 0, \quad \Gamma(\lambda_0)\widehat{X}_0(\lambda_0) = 0,$$

it follows that $\widehat{W}_0(\lambda_0)^* = [0\ w_1(\lambda_0)]$ and $\widehat{X}_0(\lambda_0) = [0\ x_1(\lambda_0)]^T$, where $w_1(\lambda_0)$ and $x_1(\lambda_0)$ are nonsingular $p \times p$ matrices. Then

$$\begin{aligned} W_0{}^*(2\lambda_0 \mathrm{M} + \mathrm{C})X_0 &= f'(\lambda_0) = \widehat{W}_0(\lambda_0)^* \Gamma'(\lambda_0)\widehat{X}_0(\lambda_0) \\ &= w_1(\lambda_0)\text{diag}(a'_{n-p+1}(\lambda_0), \ldots, a_n{}'(\lambda_0))x_1(\lambda_0). \end{aligned} \tag{3.6}$$

Condition (3.4) holds exactly when $a_j'(\lambda_0) \neq 0$ for all $j > n-p$, which is true if and only if λ_0 has algebraic multiplicity p. ∎

To get $X^{(k)}$ directly we again differentiate (2.2),

$$P(\lambda_0,0)X^{(k)} + \textstyle\sum_{r=0}^{k-1}\binom{k}{r}\mathrm{M}X^{(r)}(\Lambda^2)^{(k-r)} + \sum_{r=0}^{k-1} k\binom{k-1}{r}\mathrm{C}X^{(r)}\Lambda^{(k-1-r)} = 0, \tag{3.7}$$

and, extracting the terms in $\Lambda^{(k)}$ and using the fact that $k\binom{k-1}{j} = (k-j)\binom{k}{j}$,

$$\begin{aligned} &P(\lambda_0,0)X^{(k)} + (2\lambda_0\mathrm{M})X_0\Lambda^{(k)} \\ &\qquad = -\mathrm{M}X_0\textstyle\sum_{l=1}^{k-1}\binom{k}{l}\Lambda^{(l)}\Lambda^{(k-l)} - \mathrm{M}\sum_{j=1}^{k-1}\binom{k}{j}X^{(k-j)}(\Lambda^2)^{(j)}. \end{aligned} \tag{3.8}$$

Let V_k denote the right hand side of (3.8). Then, premultiplying (3.8) by ${W_0}^*$,

$$(2\lambda_0 W_0^*\mathrm{M}X_0)\Lambda^{(k)} = W_0^* V_k. \tag{3.9}$$

If all the values of $\Lambda^{(j)}$ and $X^{(j)}$ are known for $j < k$, we can compute V_k in a straightforward manner using its definition, so (3.9) may be solved uniquely for $\Lambda^{(k)}$. The columns of $-2\lambda_0\mathrm{M}X_0\Lambda^{(k)} + V_k$ are in the range of $P(\lambda_0,0)$. Let Z_k be any solution to

$$P(\lambda_0,0)Z_k = -2\lambda_0\mathrm{M}X_0\Lambda^{(k)} + V_k. \tag{3.10}$$

Then, for some $v_k \in \mathbf{C}^{p\times p}$, $X^{(k)} = Z_k + X_0 v_k$. By (3.3) $X_0^*Z_k + X_0^*X_0 v_k = X_0^*X^{(k)} = 0$, so $v_k = -X_0^*Z_k$ and

$$X^{(k)} = Z_k - X_0(X_0^*Z_k), \tag{3.11}$$

i.e. $X^{(k)} = (\mathrm{I} - X_0X_0^*)Z_k$, the projection of the columns of Z_k into $\mathrm{range}(X_0)^\perp$. Thus we compute $X^{(k)}$ as follows.

ALGORITHM 3.3. *Given $\Lambda^{(0)} = \lambda_0\mathrm{I}$, $X^{(0)} = X_0$, W_0, and $\Lambda^{(1)}, \Lambda^{(2)}, \ldots, \Lambda^{(k-1)}$, $X^{(1)}, X^{(2)}, \ldots, X^{(k-1)}$, this algorithm computes $\Lambda^{(k)}$ and $X^{(k)}$.*

$X_0 = X^{(0)}$; $X_1 = X^{(k-1)}$;
$Z_\mathrm{M} = X_0\sum_{l=1}^{k-1}\binom{k}{l}\Lambda^{(l)}\Lambda^{(k-l)}$; $Z_\mathrm{C} = k\lambda_0 X_1$;
for $j = 1\colon k-1$ / compute sums on r.h.s. of (3.8) */*
$X_2 = X_1$; $X_1 = X^{(k-1-j)}$;
$L = \Lambda^{(j)}$; $L_1 = \sum_{l=0}^{j}\binom{j}{l}\Lambda^{(l)}\Lambda^{(j-l)}$; $c = \binom{k}{j}$;
$Z_\mathrm{M} = Z_\mathrm{M} + cX_2L_1$;
$Z_\mathrm{C} = Z_\mathrm{C} + (k-j)cX_1L$;
end
$V_k = -(\mathrm{M}Z_\mathrm{M} + \mathrm{C}Z_\mathrm{C})$;
$Z = 2\lambda_0\mathrm{M}X_0$; $Z = Z - X_0(X_0^*Z)$;
Solve $W_0^*Z\Lambda^{(k)} = W_0^*V_k$ for $\Lambda^{(k)}$.
Solve $P(\lambda_0,0)X = -Z\Lambda^{(k)} + V_k$ for X.
$X^{(k)} = X - X_0(X_0^*X)$;

To compute the subspace associated with s distinct nonconjugate eigenvalues we perform the above procedure for each eigenvalue independently and then combine the s computed subspaces to get the desired space. For a conjugate pair of eigenvalues it is enough to compute the subspace for one of the two, since the bases determining the two subspaces are conjugate.

3.4. Real arithmetic in subspace computations. Under certain conditions the computation of the subspaces can be arranged in a way that involves only real arithmetic, as can be seen from the following lemma, the proof of which is a straightforward case-by-case check, left to the reader.

LEMMA 3.4. *Let* M *and* K *be symmetric and let the quadratic eigenvalue problem* $(\lambda^2\mathrm{M}+\mathrm{K})\mathbf{x}=0$ *have only real eigenvectors* $\mathbf{x}$ *associated with an imaginary nondefective eigenvalue* $\lambda_0=i\omega_0\neq 0$. *Let* $\Lambda^{(k)}$ *and* $X^{(k)}$ *be as in Section 2.2 and suppose* $X_0^T\mathrm{M}X_0$ *is nonsingular. Assume* C *is a nonzero matrix. Then*

$$\begin{cases} \Lambda^{(k)}\in i\mathbf{R}^{p\times p} \text{ and } X^{(k)}\in\mathbf{R}^{n\times p}, & \text{when } k \text{ is even,}\\ \Lambda^{(k)}\in \mathbf{R}^{p\times p} \text{ and } X^{(k)}\in i\mathbf{R}^{n\times p}, & \text{when } k \text{ is odd} \end{cases}$$

Instead of looking at $\Lambda^{(k)}$ and $X^{(k)}$, let us look at the imaginary parts when the matrices are imaginary and the real parts when the matrices are real. Write

$$\Lambda^{(k)}=i^{(1-k\bmod 2)}\Omega_k,\ X^{(k)}=i^{k\bmod 2}Y_k, \tag{3.12}$$

where, by the lemma, Ω_k and Y_k are real matrices. Since the perturbation subspaces are determined by the sets $\mathrm{range}(X^{(k)})=\mathrm{range}(Y_k)$ it suffices to work with (Ω_k,Y_k) rather than $(\Lambda_k,X^{(k)})$. Substituting (3.12) into (3.8) gives

$$\begin{aligned} &i^{k\bmod 2}P(\lambda_0,0)Y_k+(2i\omega_0\mathrm{M})Y_0i^{(1-k\bmod 2)}\Omega_k=\\ &\quad -\mathrm{M}Y_0\textstyle\sum_{l=1}^{k-1}\binom{k}{l}i^{(1-l\bmod 2)+(1-(k-l)\bmod 2)}\Omega_l\Omega_{k-l}\\ &\quad -\mathrm{M}\textstyle\sum_{j=1}^{k-1}(\binom{k}{j}i^{(k-j)\bmod 2}Y_{k-j}\sum_{l=0}^{j}\binom{j}{l}i^{(1-l\bmod 2)+(1-(j-l)\bmod 2)}\Omega_l\Omega_{j-l})\\ &\quad -\mathrm{C}\textstyle\sum_{j=0}^{k-1}k\binom{k-1}{j}i^{(k-1-j)\bmod 2}Y_{k-1-j}i^{1-j\bmod 2}\Omega_j, \end{aligned} \tag{3.13}$$

which can be rewritten as

$$\begin{aligned} &P(\lambda_0,0)Y_k+(-1)^{k-1}2\omega_0\mathrm{M}Y_0\Omega_k=-\mathrm{M}Y_0\textstyle\sum_{l=1}^{k-1}\binom{k}{l}(-1)^{(k-1)(l-1)}\Omega_l\Omega_{k-l}\\ &\quad -\mathrm{M}\textstyle\sum_{j=1}^{k-1}(\binom{k}{j}Y_{k-j}\sum_{l=0}^{j}\binom{j}{l}(-1)^{(kj-1)(l(j-1)-1)}\Omega_l\Omega_{j-l}\\ &\quad -\mathrm{C}\textstyle\sum_{j=0}^{k-1}k\binom{k-1}{j}(-1)^{(k-1)(j-1)}Y_{k-1-j}\Omega_j. \end{aligned} \tag{3.14}$$

Just as in Section 3.3, we can now compute Ω_k and Y_k directly, this time using only real arithmetic.

3.5. Solving the reduced problem. If $Q\in\mathbf{C}^{n\times r}$ gives an orthonormal basis for the subspace $\mathcal{S}$, let

$$M_{\mathrm{proj}}=Q^*\mathrm{M}Q,\quad C_{\mathrm{proj}}=Q^*\mathrm{C}Q,\quad\text{and}\quad K_{\mathrm{proj}}=Q^*\mathrm{K}Q, \tag{3.15}$$

and consider the solutions $(\lambda_i,\mathbf{y}_i),\ i=1,2,\ldots,2r$, to

$$(\lambda^2M_{\mathrm{proj}}+\lambda C_{\mathrm{proj}}+K_{\mathrm{proj}})\mathbf{y}=0. \tag{3.16}$$

The approximate solutions $(\lambda_i,\mathbf{x}_i)=(\lambda_i,Q\mathbf{y}_i)$ are exactly the eigenpairs for the quadratic problem with the operators M, C, and K replaced by their projections onto $\mathcal{S}$. See Hochstenbach and van der Vorst [7] for alternative ways of getting approximate solutions from a given subspace.

The reduced quadratic problem (3.16) has complex matrices M_{proj}, C_{proj}, and K_{proj}, resulting in a complex linearized problem. These matrices can, instead, be forced to be real using the fact that, for $\mathbf{w}\in\mathbf{C}^r$, $Q\mathbf{w}=[\mathrm{real}(Q)\ \mathrm{imag}(Q)]\binom{\mathbf{w}}{i\mathbf{w}}$, which

TABLE 3.1
Flop comparison between real and complex bases.

	Flops, using Q	Flops, using [real(Q) imag(Q)]
Forming basis	done	$4nr$
Projecting	$6(2nr)(r+n)$	$4nr(2r+n)$
Solving linearized problem	$6(25)(r^3)$	$25(2r)^3$
Computing approximate eigenvectors	$6(2r)(2ns)$	$4r(2ns)$
Total	$12nr^2+12n^2r+150r^3+24nrs$	$4nr+8nr^2+4n^2r+200r^3+8nrs$

implies range(Q) $\subseteq$ range([real(Q) imag(Q)]). If Q_1 is a matrix whose columns form an orthonormal basis for [real(Q) imag(Q)], then $\mathcal{S} \subseteq$ range(Q_1). Thus using Q_1 instead of Q in (3.15) results in a reduced problem involving only real matrices, and the best eigenspace approximations in range(Q_1) are at least as good as those in $\mathcal{S}$. The corresponding linear problem is of a dimension up to twice that of the linear problem formed using Q, and the question is whether it is cheaper to find the basis Q_1, project M, C, and K onto range(Q_1), solve the resulting real linearized problem, and form the approximate eigenpairs, rather than just to work with the complex basis Q.

A simplified operation count provides an answer. Assume a real scalar operation counts as one flop and a complex one counts as six. (This is the convention used in MATLAB 5, for example.) The comparison is given in Table 3.1, showing that it is better to use Q_1 when

$$12nr^2+12n^2r+150r^3+24nrs > 4nr+8nr^2+4n^2r+200r^3+8nrs,$$

which holds exactly when the cardinality r of the complex basis satisfies

$$0 < r < \frac{n}{25}+\frac{1}{25}\sqrt{101n^2+200ns-50n}. \tag{3.17}$$

Usually we are interested in the s eigenvalues of smallest (or largest) magnitude, and the first idea might be to choose as our approximations the s smallest (or largest) λ_i and corresponding $\mathbf{x}_i$ for the projected problem. However, unless the eigenvalues are known to satisfy a minimax or interlacing property, for example in the case of overdamped systems (see e.g. Duffin [5]) or conservative gyroscopic systems (see [8, Ch. 4] and Bauchau [2]), a further check is needed to eliminate spurious values. In the next section an eigenvalue error estimate is introduced that will be used to weed out these poor approximations.

4. First order error and stopping criterion.

4.1. Error in eigenvalues. For any given matrices $\widetilde{\mathrm{M}}$, $\widetilde{\mathrm{C}}$, and $\widetilde{\mathrm{K}}$, with $\widetilde{\mathrm{M}}$ nonsingular, suppose the pair $(\mu, \mathbf{y})$ is an approximation to an eigenpair $(\lambda_i, \mathbf{x}_i)$ for

$$(\lambda^2\widetilde{\mathrm{M}}+\lambda\widetilde{\mathrm{C}}+\widetilde{\mathrm{K}})\mathbf{x}=0, \tag{4.1}$$

with λ_i a simple eigenvalue and μ not equal to any eigenvalue of (4.1), and suppose we know the associated residual $\mathbf{r} = (\mu^2\widetilde{\mathrm{M}} + \mu\widetilde{\mathrm{C}} + \widetilde{\mathrm{K}})\mathbf{y}$. Consider the problem

$$(\lambda(\epsilon)^2\widetilde{\mathrm{M}} + \lambda(\epsilon)\widetilde{\mathrm{C}} + \widetilde{\mathrm{K}} - (1 - \epsilon\tfrac{\|\mathbf{y}\|}{\|\mathbf{r}\|})\tfrac{\mathbf{r}\mathbf{u}^T}{\mathbf{u}^T\mathbf{y}}))\mathbf{x}(\epsilon) = 0, \tag{4.2}$$

where $\mathbf{u}$ is any vector such that $\mathbf{u}^T\mathbf{y} \neq 0$. It is straightforward to check that $(\mu, \mathbf{y})$ is a solution to (4.2) at $\epsilon = 0$. Since μ is not an eigenvalue of (4.1), $\mathbf{z} = \mathbf{y}$ is the unique solution to $(\mu^2\widetilde{\mathrm{M}} + \mu\widetilde{\mathrm{C}} + \widetilde{\mathrm{K}})\mathbf{z} = \mathbf{r}$, and any nonzero vector $\hat{\mathbf{y}}$ satisfying

$$(\mu^2\widetilde{\mathrm{M}} + \mu\widetilde{\mathrm{C}} + \widetilde{\mathrm{K}})\hat{\mathbf{y}} - \mathbf{r}(\tfrac{\mathbf{u}^T\hat{\mathbf{y}}}{\mathbf{u}^T\mathbf{y}}) = 0$$

must be a multiple of $\mathbf{y}$. Thus μ is a simple eigenvalue, so for all sufficiently small ϵ the solution $(\lambda(\epsilon), \mathbf{x}(\epsilon))$ with $\mathbf{x}(\epsilon)^*\mathbf{x}_0 = 1$ exists, and we can write the Taylor series

$$\begin{array}{c} \lambda(\epsilon) = \mu + \epsilon\dot{\lambda}(0) + \epsilon^2\frac{\ddot{\lambda}(0)}{2} + \cdots \\ \mathbf{x}(\epsilon) = \frac{\mathbf{y}}{\|\mathbf{y}\|} + \epsilon\dot{\mathbf{x}}(0) + \epsilon^2\frac{\ddot{\mathbf{x}}(0)}{2} + \cdots \end{array}. \tag{4.3}$$

Substituting (4.3) into (4.2), and using the fact that the coefficient of the first power of ϵ (and in fact that of each power of ϵ) on the left-hand side of (4.2) is zero,

$$(2\mu\dot{\lambda}(0)\widetilde{\mathrm{M}} + \dot{\lambda}(0)\widetilde{\mathrm{C}} + \tfrac{\|\mathbf{y}\|}{\|\mathbf{r}\|}\tfrac{\mathbf{r}\mathbf{u}^T}{\mathbf{u}^T\mathbf{y}})\tfrac{\mathbf{y}}{\|\mathbf{y}\|} + (\mu^2\widetilde{\mathrm{M}} + \mu\widetilde{\mathrm{C}} + \widetilde{\mathrm{K}} - \tfrac{\mathbf{r}\mathbf{u}^T}{\mathbf{u}^T\mathbf{y}})\dot{\mathbf{x}}(0) = 0,$$

and

$$\dot{\lambda}(0)(2\mu\widetilde{\mathrm{M}} + \widetilde{\mathrm{C}})\tfrac{\mathbf{y}}{\|\mathbf{y}\|} + \tfrac{\mathbf{r}}{\|\mathbf{r}\|} + (\mu^2\widetilde{\mathrm{M}} + \mu\widetilde{\mathrm{C}} + \widetilde{\mathrm{K}})\dot{\mathbf{x}}(0) - \mathbf{r}(\tfrac{\mathbf{u}^T\dot{\mathbf{x}}(0)}{\mathbf{u}^T\mathbf{y}}) = 0. \tag{4.4}$$

Setting

$$\mathbf{u} = (\mu^2\widetilde{\mathrm{M}} + \mu\widetilde{\mathrm{C}} + \widetilde{\mathrm{K}})^T\mathbf{w} \tag{4.5}$$

for any $\mathbf{w}$ satisfying

$$\mathbf{w}^T\mathbf{r} \neq 0, \tag{4.6}$$

and premultiplying (4.4) by $\mathbf{w}^T$ gives $\dot{\lambda}(0)\mathbf{w}^T(2\mu\widetilde{\mathrm{M}} + \widetilde{\mathrm{C}})\frac{\mathbf{y}}{\|\mathbf{y}\|} + \frac{\mathbf{w}^T\mathbf{r}}{\|\mathbf{r}\|} = 0$; thus

$$\dot{\lambda}(0) = -\tfrac{\|\mathbf{y}\|}{\|\mathbf{r}\|}(\tfrac{\mathbf{w}^T\mathbf{r}}{\mathbf{w}^T(2\mu\widetilde{\mathrm{M}}+\widetilde{\mathrm{C}})\mathbf{y}}),$$

and

$$\lambda(\epsilon) - \mu = -\epsilon - \tfrac{\|\mathbf{y}\|}{\|\mathbf{r}\|}(\tfrac{\mathbf{w}^T\mathbf{r}}{\mathbf{w}^T(2\mu\widetilde{\mathrm{M}}+\widetilde{\mathrm{C}})\mathbf{y}}) + O(\epsilon^2) \quad \text{as } \epsilon \to 0. \tag{4.7}$$

Next observe that at $\epsilon = \frac{\|\mathbf{r}\|}{\|\mathbf{y}\|}$, λ_i is by assumption a simple eigenvalue of (4.2), so if $\frac{\|\mathbf{r}\|}{\|\mathbf{y}\|}$ is small enough we have

$$|\lambda_i - \mu| = \tfrac{|\mathbf{w}^T\mathbf{r}|}{|\mathbf{w}^T(2\mu\widetilde{\mathrm{M}}+\widetilde{\mathrm{C}})\mathbf{y}|} + O\left((\tfrac{\|\mathbf{r}\|}{\|\mathbf{y}\|})^2\right) \quad \text{as } \tfrac{\|\mathbf{r}\|}{\|\mathbf{y}\|} \to 0. \tag{4.8}$$

Then a reasonable criterion for a solution pair $(\mu, \mathbf{y})$ to be acceptable is

$$\max\left(\tfrac{|\mathbf{w}^T\mathbf{r}|}{|\mathbf{y}^T(2\mu\widetilde{\mathrm{M}}+\widetilde{\mathrm{C}})\mathbf{y}|}, (\tfrac{\|\mathbf{r}\|}{\|\mathbf{y}\|})^2\right) < \mu\,\mathrm{tol} \tag{4.9}$$

for some tolerance tol, i.e., the relative error in the eigenvalue is on the order of tol. A good choice of $\mathbf{w}$ is clearly $\mathbf{w} = \bar{\mathbf{r}}$, since this $\mathbf{w}$ fails to satisfy (4.6) only when $\mathbf{r} = 0$, in which case the approximate solution is of course acceptable. Then (4.9) becomes

$$\frac{\|\mathbf{r}\|^2}{\min(|\mathbf{r}^*(2\mu\widetilde{\mathrm{M}} + \widetilde{\mathrm{C}})\mathbf{y}|,\ \|\mathbf{y}\|^2)} < \mu\,\mathrm{tol}. \tag{4.10}$$

Now suppose we want approximations of the form $\mathbf{y}_i = W\mathbf{z}_i$, with $W \in \mathbf{C}^{n\times r}$ of full rank and $\mathbf{z}_i$ satisfying $(\mu_i^2\widetilde{\mathrm{M}}_{\mathrm{proj}} + \mu_i\widetilde{\mathrm{C}}_{\mathrm{proj}} + \widetilde{\mathrm{K}}_{\mathrm{proj}})\mathbf{z}_i = 0$, where $\widetilde{\mathrm{M}}_{\mathrm{proj}} = W^*\widetilde{\mathrm{M}}W$, $\widetilde{\mathrm{C}}_{\mathrm{proj}} = W^*\widetilde{\mathrm{C}}W$, and $\widetilde{\mathrm{K}}_{\mathrm{proj}} = W^*\widetilde{\mathrm{K}}W$. In other words suppose we are interested in pairs $(\mu_i, \mathbf{z}_i)$ resulting from solving a reduced quadratic eigenvalue problem as in Section 3.5. Using (3.17), the following is an algorithm to solve the reduced quadratic eigenvalue problem and to select approximate solutions.

ALGORITHM 4.1. *Given a full rank matrix $W \in \mathbf{C}^{n\times r}$, this algorithm computes approximations to the $s < 2r$ eigenvalues of (4.1) smallest in magnitude, along with corresponding eigenvector approximations.*

1. *If r satisfies condition (3.17), compute a real orthonormal basis W_1 for* range([real(W) imag(W)]), *and set $W = W_1$.*
2. *Form $\widetilde{\mathrm{M}}_{\mathrm{proj}} = W^*\widetilde{\mathrm{M}}W$, $\widetilde{\mathrm{C}}_{\mathrm{proj}} = W^*\widetilde{\mathrm{C}}W$, and $\widetilde{\mathrm{K}}_{\mathrm{proj}} = W^*\widetilde{\mathrm{K}}W$.*
3. *Linearize and use methods for small, dense matrices to compute the eigenvalues $\mu_1, \mu_2, \ldots, \mu_{2r}$ and corresponding eigenvectors $\mathbf{z}_1, \mathbf{z}_2, \ldots, \mathbf{z}_{2r}$ of*

$$(\mu^2\widetilde{\mathrm{M}}_{\mathrm{proj}} + \mu\widetilde{\mathrm{C}}_{\mathrm{proj}} + \widetilde{\mathrm{K}}_{\mathrm{proj}})\mathbf{z} = 0.$$

4. *For $i = 1, 2, \ldots, 2r$, compute $\mathbf{y}_i = W\mathbf{z}_i$.*
5. *Use criterion (4.10) to select the approximate eigenpairs $(\mu_{i_j}, \mathbf{y}_{i_j})$, $j = 1, 2, \ldots, s$ with the smallest values of* $\mathrm{relerrs}_i \equiv \frac{1}{|\mu_i|}\frac{\|\mathbf{r}_i\|^2}{\min(|\mathbf{r}_i^*(2\mu\widetilde{\mathrm{M}}+\widetilde{\mathrm{C}})\mathbf{y}_i|,\ \|\mathbf{y}\|^2)}$.

In Steps 4 and 5 of Algorithm 4.1 the computation is done only once for each complex conjugate pair. Note that if W is orthogonal, $\|\mathbf{y}_i\| = \|\mathbf{z}_i\|$.

4.2. Error in eigenvectors. If instead of (4.5) we set

$$\mathbf{u} = \bar{\mathbf{y}} \tag{4.11}$$

and define $\mathbf{v} = (\mu^2\widetilde{\mathrm{M}} + \mu\widetilde{\mathrm{C}} + \widetilde{\mathrm{K}})^{-1}(2\mu\widetilde{\mathrm{M}} + \widetilde{\mathrm{C}})\mathbf{y}$, we can show the following.

LEMMA 4.2. *If $\angle(\mathbf{y}, \mathbf{v}) \neq 0$, then $\angle(\mathbf{y}, \mathbf{x}_i) = \angle(\mathbf{y}, \mathbf{v}) + O\left((\frac{\|\mathbf{r}\|}{\|\mathbf{y}\|})^2\right)$ as $\frac{\|\mathbf{r}\|}{\|\mathbf{y}\|} \to 0$.*

For the proof of the lemma two other results are needed.

PROPOSITION 4.3. $\|\dot{\mathbf{x}}(0)\|^2 = (\frac{\|\mathbf{y}\|}{\|\mathbf{r}\|})^2\frac{1}{\left|\left(\frac{\mathbf{y}}{\|\mathbf{y}\|}\right)^*\mathbf{v}\right|^2}\ (\|\mathbf{v}\|^2 - |(\frac{\mathbf{y}}{\|\mathbf{y}\|})^*\mathbf{v}|^2)$.

Proof. Applying $(\mu^2\widetilde{\mathrm{M}} + \mu\widetilde{\mathrm{C}} + \widetilde{\mathrm{K}})^{-1}$ to (4.4),

$$\dot{\mathbf{x}}(0) = -\dot{\lambda}(0)\tfrac{\mathbf{v}}{\|\mathbf{y}\|} + (\tfrac{1}{\|\mathbf{r}\|} - \tfrac{\mathbf{u}^T\dot{\mathbf{x}}(0)}{\mathbf{u}^T\mathbf{y}})\mathbf{y},$$

and since $\mathbf{y}^*\dot{\mathbf{x}}(0) = 0$, it follows that $0 = -\dot{\lambda}(0)\frac{\mathbf{y}^*\mathbf{v}}{\|\mathbf{y}\|} + (\frac{1}{\|\mathbf{r}\|} - \frac{\mathbf{u}^T\dot{\mathbf{x}}(0)}{\mathbf{u}^T\mathbf{y}})\|\mathbf{y}\|^2$, so

$$\dot{\mathbf{x}}(0) = -\dot{\lambda}(0)\tfrac{\mathbf{v}}{\|\mathbf{y}\|} + \tfrac{\dot{\lambda}(0)\mathbf{y}^*\mathbf{v}}{\|\mathbf{y}\|^3}\mathbf{y}.$$

Now let $\mathbf{z}$ be a nonzero vector satisfying

$$\mathbf{z}^*(\mu^2\widetilde{\mathrm{M}} + \mu\widetilde{\mathrm{C}} + \widetilde{\mathrm{K}} - \tfrac{\mathbf{r}\mathbf{u}^T}{\mathbf{u}^T\mathbf{y}}) = 0.$$

Then $\mathbf{z}^*(\mu^2\widetilde{\mathrm{M}} + \mu\widetilde{\mathrm{C}} + \widetilde{\mathrm{K}}) = (\frac{\mathbf{z}^*\mathbf{r}}{\mathbf{u}^T\mathbf{y}})\mathbf{u}^T$, so $\mathbf{z}^* = \alpha\mathbf{u}^T(\mu^2\widetilde{\mathrm{M}} + \mu\widetilde{\mathrm{C}} + \widetilde{\mathrm{K}})^{-1}$ for some α. Applying $\mathbf{z}^*$ to (4.4) yields

$$\dot\lambda(0)\mathbf{z}^*(2\mu\widetilde{\mathrm{M}} + \widetilde{\mathrm{C}})\tfrac{\mathbf{y}}{\|\mathbf{y}\|} + \tfrac{\mathbf{z}^*\mathbf{r}}{\|\mathbf{r}\|} = 0,$$

$$\dot\lambda(0) = -\tfrac{\|\mathbf{y}\|}{\|\mathbf{r}\|}\tfrac{\mathbf{z}^*\mathbf{r}}{\mathbf{z}^*(2\mu\widetilde{\mathrm{M}}+\widetilde{\mathrm{C}})\mathbf{y}} = -\tfrac{\|\mathbf{y}\|}{\|\mathbf{r}\|}\tfrac{\mathbf{u}^T\mathbf{y}}{\mathbf{u}^T\mathbf{v}}.$$

Hence

$$\begin{aligned}\dot{\mathbf{x}}(0) &= -\tfrac{\|\mathbf{y}\|}{\|\mathbf{r}\|}\tfrac{\mathbf{u}^T\mathbf{y}}{\mathbf{u}^T\mathbf{v}}\left(-\tfrac{\mathbf{v}}{\|\mathbf{y}\|} + \tfrac{\mathbf{y}^*\mathbf{v}}{\|\mathbf{y}\|^3}\mathbf{y}\right)\\ &= -\tfrac{1}{\|\mathbf{r}\|}\tfrac{\mathbf{u}^T\mathbf{y}}{\mathbf{u}^T\mathbf{v}}\left(-\mathbf{v} + \left[(\tfrac{\mathbf{y}}{\|\mathbf{y}\|})^*\mathbf{v}\right]\tfrac{\mathbf{y}}{\|\mathbf{y}\|}\right).\end{aligned}$$

Using (4.11),

$$\begin{aligned}\|\dot{\mathbf{x}}(0)\|^2 &= |\tfrac{1}{\|\mathbf{r}\|}\tfrac{\mathbf{u}^T\mathbf{y}}{\mathbf{u}^T\mathbf{v}}|^2 \left\|-\mathbf{v} + [(\tfrac{\mathbf{y}}{\|\mathbf{y}\|})^*\mathbf{v}]\tfrac{\mathbf{y}}{\|\mathbf{y}\|}\right\|^2\\ &= (\tfrac{\|\mathbf{y}\|}{\|\mathbf{r}\|})^2\ |\tfrac{\|\mathbf{y}\|}{\mathbf{y}^*\mathbf{v}}|^2\left(\|\mathbf{v}\|^2 - \tfrac{(\mathbf{v}^*\mathbf{y})(\mathbf{y}^*\mathbf{v})}{\|\mathbf{y}\|^2} - \tfrac{(\mathbf{y}^*\mathbf{v})(\mathbf{v}^*\mathbf{y})}{\|\mathbf{y}\|^2} + \tfrac{|\mathbf{y}^*\mathbf{v}|^2}{\|\mathbf{y}\|^2}\right)\\ &= (\tfrac{\|\mathbf{y}\|}{\|\mathbf{r}\|})^2\tfrac{1}{|(\frac{\mathbf{y}}{\|\mathbf{y}\|})^*\mathbf{v}|^2}\ \left(\|\mathbf{v}\|^2 - |(\tfrac{\mathbf{y}}{\|\mathbf{y}\|})^*\mathbf{v}|^2\right). \qquad \square\end{aligned}$$

PROPOSITION 4.4. *If* $\dot{\mathbf{x}}(0) \neq 0$,

$$\angle(\mathbf{x}(\epsilon), \mathbf{y}) = \cos^{-1}\tfrac{1}{\sqrt{1+\epsilon^2\|\dot{\mathbf{x}}(0)\|^2}} + O(\epsilon^2)\ \textit{as}\ \epsilon \to 0.$$

Proof. The proof is elementary calculus using the Taylor expansion of $f(w) = \cos^{-1}(w^{-1/2})$ in the appropriate interval.

Proof of Lemma 4.2 $\angle(\mathbf{y}, \mathbf{v}) \neq 0$ exactly when $|(\frac{\mathbf{y}}{\|\mathbf{y}\|})^*\mathbf{v}| \neq \|\mathbf{v}\|$, so, from Proposition 4.3,

$$\|\dot{\mathbf{x}}(0)\|^2 = (\tfrac{\|\mathbf{y}\|}{\|\mathbf{r}\|})^2\tfrac{1}{|(\frac{\mathbf{y}}{\|\mathbf{y}\|})^*\mathbf{v}|^2}\left(\|\mathbf{v}\|^2 - |(\tfrac{\mathbf{y}}{\|\mathbf{y}\|})^*\mathbf{v}|^2\right) \neq 0,$$

and applying Proposition 4.4 at $\epsilon = \frac{\|\mathbf{r}\|}{\|\mathbf{y}\|}$ we have

$$\begin{aligned}\angle(\mathbf{x}_i, \mathbf{y}) &= \cos^{-1}\frac{1}{\sqrt{1+\frac{1}{\left|(\frac{\mathbf{y}}{\|\mathbf{y}\|})^*\mathbf{v}\right|^2}(\|\mathbf{v}\|^2 - \left|(\frac{\mathbf{y}}{\|\mathbf{y}\|})^*\mathbf{v}\right|^2)}} + O\left((\tfrac{\|\mathbf{r}\|}{\|\mathbf{y}\|})^2\right)\ \text{as}\ \tfrac{\|\mathbf{r}\|}{\|\mathbf{y}\|} \to 0\\ &= \cos^{-1}\tfrac{\left|(\frac{\mathbf{y}}{\|\mathbf{y}\|})^*\mathbf{v}\right|}{\|\mathbf{v}\|} + O\left((\tfrac{\|\mathbf{r}\|}{\|\mathbf{y}\|})^2\right)\ \text{as}\ \tfrac{\|\mathbf{r}\|}{\|\mathbf{y}\|} \to 0\\ &= \angle(\mathbf{y}, \mathbf{v}) + O\left((\tfrac{\|\mathbf{r}\|}{\|\mathbf{y}\|})^2\right)\ \text{as}\ \tfrac{\|\mathbf{r}\|}{\|\mathbf{y}\|} \to 0. \qquad \square\end{aligned}$$

Computing $\mathbf{v}$ to examine this eigenvector error estimate at each step would be expensive; instead it is useful to calculate the estimate at the end of the computation to look at the final quality of the computed eigenvectors.

5. A hybrid method. Because the perturbation subspaces are constructed to contain the ranges of the Taylor series for the eigenspaces, the subspace approximations discussed above yield, within their convergence radius, eigenpair approximations that converge at least as well as the corresponding Taylor series, in other words at least linearly. To accelerate this convergence we would like to switch, at an appropriate stage, to a generalization of the quadratically convergent Rayleigh quotient iteration.

5.1. Block Rayleigh quotient iteration. Suppose the vectors $X = [\mathbf{x}_1\ \mathbf{x}_2\ \cdots\ \mathbf{x}_s]$ form a basis for a space spanned by approximate right eigenvectors of the problem (4.1), and define a block Rayleigh quotient of (4.1) for X to be any $s \times s$ matrix Λ satisfying

$$X^*\widetilde{\mathrm{M}}X\Lambda^2 + X^*\widetilde{\mathrm{C}}X\Lambda + X^*\widetilde{\mathrm{K}}X = 0.$$

A block generalization of Lancaster's Rayleigh Quotient Iteration [10] can be described as follows.

ALGORITHM 5.1. *(Block RQI 1) This algorithm performs general block Rayleigh quotient iterations, starting with any X_1, to compute approximate eigenpairs for (4.1).*
For $l = 1, 2, 3, \ldots$
0. Given range(X_l)*, an approximate span of right eigenvectors for (4.1).*
1. Find Λ_l (not unique) such that $(X_l^*\widetilde{\mathrm{M}}X_l)\Lambda_l^2 + (X_l^*\widetilde{\mathrm{C}}X_l)\Lambda_l + (X_l^*\widetilde{\mathrm{K}}X_l) = 0$.
2. Solve $\widetilde{\mathrm{M}}Y_{l+1}\Lambda_l^2 + \widetilde{\mathrm{C}}Y_{l+1}\Lambda_l + \widetilde{\mathrm{K}}Y_{l+1} = X_l$ for Y_{l+1}.
3. Let W be a basis for range(Y_{l+1})*, and apply Algorithm 4.1 to solve the reduced problem and get approximate solutions $(\lambda_i, W\mathbf{x}_i)$, $i = 1, 2, \ldots, s$.*
4. Set $X_{l+1} = W[\mathbf{x}_1\ \mathbf{x}_2\ \cdots \mathbf{x}_s]$.

It is straightforward to check that Λ is a block Rayleigh quotient of (4.1) for X if it is of the form $\Lambda = Y\Omega Y^{-1}$, where $\Omega = \mathrm{diag}(\omega_i)$ is a matrix of eigenvalues and $Y = [\mathbf{y}_1\ \mathbf{y}_2\ \cdots\ \mathbf{y}_s]$ is a full rank matrix of eigenvectors for the reduced quadratic eigenvalue problem, i.e.

$$(\omega_i^2 X^*\widetilde{\mathrm{M}}X + \omega_i X^*\widetilde{\mathrm{C}}X + X^*\widetilde{\mathrm{K}}X)\mathbf{y}_i = 0, \quad i = 1, 2, \ldots, s. \tag{5.1}$$

Now suppose the approximate pairs $(\lambda_i, \mathbf{x}_i)$, $i = 1, 2, \ldots, s$, have been obtained by choosing any s of the $2r$ approximate solutions resulting from solving a reduced problem of size r as in Section 3.5. Then the problem (5.1) has solutions $(\lambda_i, \mathbf{e}_i)$, $i = 1, 2, \ldots, s$, where $\mathbf{e}_i \in \mathbf{C}^s$ is the ith standard basis vector, so the matrix $\Lambda = \mathrm{diag}(\lambda_i) = \mathrm{I}_s\,\mathrm{diag}(\lambda_i)\,\mathrm{I}_s$ is a block Rayleigh quotient of (4.1) for X. With this Rayleigh quotient, Algorithm 5.1 becomes the following.

ALGORITHM 5.2. *(Block RQI 2) This algorithm performs block Rayleigh quotient iterations to compute approximate eigenpairs for (4.1), starting only with eigenpairs obtained by solving a reduced quadratic problem.*
For $l = 1, 2, 3, \ldots$
0. Given $(\lambda_i, \mathbf{x}_i)$, $i = 1, 2, \ldots, s$, a set of approximate eigenpairs for (4.1) obtained by solving a reduced problem as in Section 3.5.
1. Solve $\lambda_i{}^2\widetilde{\mathrm{M}}\mathbf{y}_{l+1,i} + \lambda_i\widetilde{\mathrm{C}}\mathbf{y}_{l+1,i} + \widetilde{\mathrm{K}}\mathbf{y}_{l+1,i} = \mathbf{x}_{l,i}$, $i = 1, 2, \ldots, s$, for the columns of Y_{l+1}.

2. Let W be a basis for $\mathrm{range}(Y_{l+1})$*, and apply Algorithm 4.1 to solve the reduced problem and get approximate solutions* $(\lambda_i, W\mathbf{x}_i)$*,* $i = 1, 2, \ldots, s$*.*

3. Set $X_{l+1} = W[\mathbf{x}_1\ \mathbf{x}_2\ \cdots \mathbf{x}_s]$*.*

The subspace approximation method switches to this RQI when the largest relative change in consecutive eigenvalue iterates remains less than some tolerance, i.e. when the eigenvalues have in a sense "nearly" converged.

5.2. Hybrid algorithm. Now we have discussed all the individual parts of the hybrid method and are ready to summarize the whole algorithm.

ALGORITHM 5.3. *Given nondefective eigenvalues* $\lambda_1, \lambda_2, \ldots, \lambda_l$ *of multiplicities* $n_1, n_2, \ldots n_l$*, and associated eigenvector matrices* $X_{(1)} \in \mathbf{C}^{n\times n_1}, X_{(2)} \in \mathbf{C}^{n\times n_2}, \ldots, X_{(l)} \in \mathbf{C}^{n\times n_l}$*, for (2.1) at* $t = 0$*, along with tolerances* tol_1 *(default* 10^{-3}*) and* tol*, this algorithm computes the corresponding values at* $t = 1$*.*

0. Initialize: $\mathrm{relchange} = 2tol_1 \cdot \mathrm{ones}(p, 1)$*;* $j = 0$*;* $W_0 = [\,]$*;* $\mathrm{convgct} = 0$*;*
If we know the left eigenvector matrix, $\mathrm{anyleftvec} = 1$*, else* $\mathrm{anyleftvec} = 0$*.*

1. While $\max(\mathrm{relerrs}) > tol$ *and* $\mathrm{convgct} < 2$*,*
$j = j + 1$*;*
For $i = 1{:}\,l$*, /* compute new vectors, columns of* $X_{(i)}^{(j)}$*, to add to space */*
If $\mathrm{anyleftvec} = 1$*, compute* $X_{(i)}^{(j)}$ *using Algorithm 3.3, else compute* $X_{(i)}^{(j)}$ *using Algorithm 3.1.*
Use Modified Gram-Schmidt to compute basis W_j *for*
$\mathcal{S}_j = \overset{j}{\underset{m=0}{+}} (\overset{l}{\underset{i=1}{+}} \mathrm{range}(X_{(i)}^{(m)})) = (\overset{l}{\underset{i=1}{+}} \mathrm{range}(X_{(i)}^{(j)})) + \mathrm{range}(W_{j-1})$.
Solve reduced prob. in $\mathcal{S}_j$*; compute new* relerrs *and approx.* $(\lambda_i, \mathbf{x}_i)$ *using Alg. 4.1.*
If $j > 1$ *set* relchange *to rel. changes in computed eigenvalues from previous step.*
If $\max(\mathrm{relchange}) \le tol_1$*,* $\mathrm{convgct} = \mathrm{convgct} + 1$*; else* $\mathrm{convgct} = 0$*.*

2. While $\max(\mathrm{relerrs}) > tol$*,*
Apply Block RQI Algorithm 5.2, beginning with $X = [\mathbf{x}_1\ \mathbf{x}_2\ \cdots\ \mathbf{x}_p]$*.*

6. Complexity. The subspace approximation method spends over 95% of its time performing five tasks: computing the right-hand side V_k of (3.8) in the direct subspace computation; solving the least squares problems in the subspace computation or the linear systems in the block Rayleigh quotient iteration; applying Modified Gram-Schmidt to compute bases; solving the reduced (projected) quadratic eigenvalue problems; and computing the error estimates.

For a crude analysis of these costs, assume that the maximum relative error estimate decreases by a factor ρ at each step. (Because the convergence is at least linear, such a value eventually exists.) If e_0 is the original maximum relative error estimate, the number of steps needed for convergence with tolerance tol is the smallest integer m greater than or equal to $\log_\rho \frac{e_0}{tol}$. Starting with p eigenpairs, the following are computed: pm values of V_k, requiring a total of at most $6pm$ matrix-vector products and $(m+1)^2$ matrix-matrix products of size $p \times p$; pm least square solutions (or ill-conditioned linear system solutions); orthonormalization of $2p(m+1)$ n-vectors; solutions of $m+1$ projected problems, with real bases of dimension $2p, 4p, \ldots, 2p(m+1)$, requiring work as shown in Table 3.1; and $2p(m+1)$ error estimates each requiring 6 matrix-vector products and 3 inner-products.

TABLE 6.1
Work performed by the subspace approximation method

Task	Flops
Computing V_k	$6(6pm(4nq) + (m+1)^2p^3)$
Linear solves (direct)	$6(pm)(4nq + 2nq^2)$
Modified Gram-Schmidt	$n(2p(m+1))^2$
Solving reduced problems	$\sum_{j=1}^{m+1}(8np^2j^2 + 4n^2jp + 200(jp)^3 + 8npj)$
Relative error estimates	$6(2p(m+1))(24nq + 6n)$
Total	$O(6q^2pnm + \frac{2}{3}p^2nm^3 + pn^2m^2 + 25p^3m^4)$

If $P(\lambda, t)$ is banded, let q denote the maximum of the upper and lower bandwidths of all the matrices in $P(\lambda, t)$. When the linear systems are solved directly, the method performs work at most on the order of that shown in Table 6.1, and in fact with the switch to the locally faster-converging block RQI the total amount of work done should be even less. For general sparse matrices a similar analysis can be performed using the applicable flop counts for matrix-vector multiplications and the solution of linear systems or least squares problems.

7. Numerical examples.

7.1. A truss problem. Consider a long and slender truss structure shown in Figure 7.1. This example is designed to measure the effectiveness of the numerical algorithms for problems with proportional and nonproportional damping.

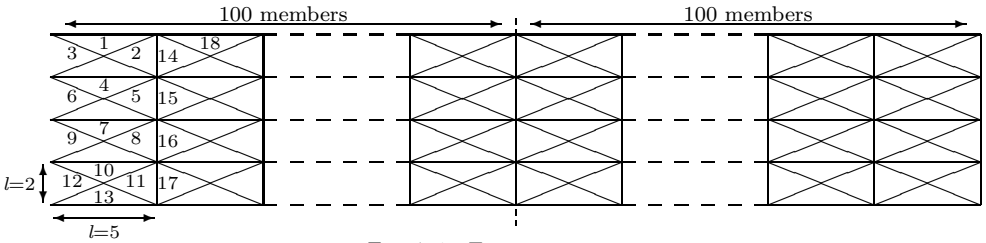

FIG. 7.1. *Truss structure.*

The element stiffness and mass matrices are given as

$$K_e = \frac{AE}{l}\begin{pmatrix} 1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \qquad \text{and} \qquad M_e = \frac{\rho Al}{6}\begin{pmatrix} 2 & 0 & 1 & 0 \\ 0 & 2 & 0 & 1 \\ 1 & 0 & 2 & 0 \\ 0 & 1 & 0 & 2 \end{pmatrix}.$$

For each member let the cross sectional area A be 1.0 and assume the other constants have the values $E = 10^7$ and $\rho = 1.0$. Values of the length l are given in the figure. The assembled matrices K and M are symmetric positive definite, of order 2000. The members are numbered as shown, so that K has a bandwidth of 13 and M has a bandwidth of 12. Assume the eight smallest eigenpairs $(\mu_1, \mathbf{x}_1), \ldots, (\mu_8, \mathbf{x}_8)$ for the generalized eigenvalue problem $\mathrm{K}\mathbf{x} = \mu\mathrm{M}\mathbf{x}$ have been computed, i.e. assume the undamped problem has been solved.

7.1.1. Proportional damping. The first example is of simple proportional damping, with 5% damping in the first eight modes and zero damping in all the others. The damping matrix is then $\mathrm{C}_{\mathrm{prop}} = \mathrm{M}(\sum_{j=1}^{8} 2(.05)\omega_j \phi_j \phi_j^T)\mathrm{M}$, where $\omega_j = \sqrt{\mu_j}$ and $\phi_j = (\mathbf{x}_j^T \mathrm{M} \mathbf{x}_j)^{-1/2} \mathbf{x}_j$ for $j = 1, \ldots 8$. This is a symmetric, positive semi-definite matrix of rank 8, which is dense but easy to apply as an operator. Taking the undamped problem $(\lambda^2 \mathrm{M} + \mathrm{K})\mathbf{x} = 0$ as the original, unperturbed problem, to which solutions are known, we use the subspace approximation method to solve the damped problem $(\lambda^2 \mathrm{M} + \lambda \mathrm{C}_{\mathrm{prop}} + \mathrm{K})\mathbf{x} = 0$ for the sixteen eigenvalues of least magnitude. As shown in Section 3.4, the subspace computation involves only real arithmetic.

The true eigenvalues of the damped equation are simply the roots of the quadratic polynomials $\lambda^2 + 0.1\lambda\sqrt{\mu_j} + \mu_j$ and, as expected, the subspace approximation method computes these values in the first step, using the first subspace, since the original eigenspaces and final eigenspaces are the same. The acceptance tolerance is taken to be 10^{-5}. The first eight pairs of paths are nearly linear and all other eigenvalue paths are constant; there is no risk of path crossing. Table 7.1 shows a comparison with vector RQI started from the same original values, and with **eigs**, the MATLAB implementation of ARPACK [12], applied to the second linearization of (1.2) with N = I. All three methods converged to the correct solutions, but the subspace approximation method is clearly appropriate for this problem, and one sees that the method's performance is orders of magnitude better than that of the other two methods.

TABLE 7.1
Comparison of methods for proportionally damped truss problem.

	Subsp.Approx.	RQI	**eigs**
CPU time (seconds)	0.35	25.4	57
max *relerrs* (estimate)	6.56×10^{-6}	8.47×10^{-6}	9.92×10^{-6}
max *rel.err.* (actual)	1.52×10^{-8}	1.97×10^{-8}	1.36×10^{-8}

7.1.2. Nonproportional damping. In the second example, half the structure has 1% damping and the other half has 2% damping (to the right and left, resp., of the dotted vertical center line in Figure 7.1). The resulting damping matrix $\mathrm{C}_{\mathrm{npr}}$,

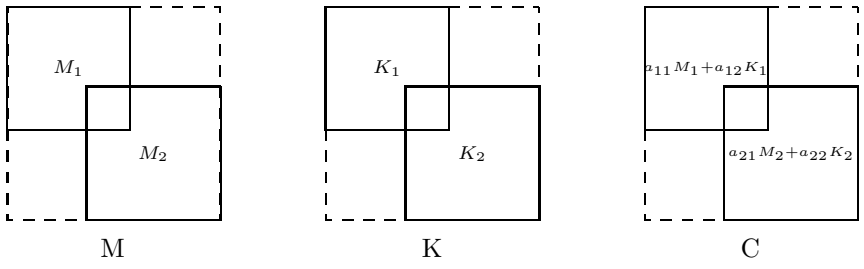

FIG. 7.2. *Block form of nonproportional damping matrix.*

assembled as indicated in Figure 7.2, is composed of two overlapping submatrices along the diagonal, each of which is a different linear combination of the corresponding submatrices of M and K associated with the two different damping percentages. The values a_{ij} used in the linear combinations are given by $\binom{a_{i1}}{a_{i2}} = \frac{2\xi_i}{\omega_1+\omega_2}\binom{\omega_1\omega_2}{1}$, where $\xi_1 = 0.01$, $\xi_2 = 0.02$, and $\omega_1 = \sqrt{\mu_1}$ and $\omega_2 = \sqrt{\mu_2}$ are the two smallest natural frequencies for the undamped problem. Because of the elements in common between the 1% and 2% damping, $\mathrm{C}_{\mathrm{npr}}$ is not itself a combination of M and K of the form

$\sum_{j=0}^{p} \alpha_j \mathrm{M}(\mathrm{M}^{-1}\mathrm{K})^j$, so this is nonproportional damping (see e.g. Clough and Penzien [3, Ch.12]) and cannot be solved using the traditional modal superposition.

The results of applying the subspace approximation method to compute the first 16 eigenvalues of the damped problem are summarized in Table 7.2, again compared with RQI and **eigs**. The acceptance tolerance is taken to be 10^{-6}. In this problem, iterative solution via QMR with MATLAB's default parameters is used both in the subspace approximation and in the vector RQI. Linearization ((1.2), first equation) is used in **eigs**, with the choice N = K and with the default parameters because no advantage was found in making other choices. One sees that the relative accuracy of the computed eigenvalues is about the same for all three methods, as is the order of the error angles in the computed eigenvectors. Figure 7.3 shows the eigenvalue paths (left graph) and convergence of the subspace approximation method (right graph) The paths are less linear than those for the proportional damping problem, but they are smooth and well separated from other eigenvalue paths, showing that the problem is very suitable for subspace approximation. Note that faster convergence could have been achieved by switching to the block RQI early, after step 2, yielding a time savings of 8.6%. However, further work is needed to automate the "tweaking" of the hybrid method.

TABLE 7.2
Comparison of methods for nonproportionally damped truss problem.

	Subsp.Approx.	RQI	**eigs**
CPU time (sec.)	1.85	6.58	11.31
maximum *relerrs*	8.75×10^{-7}	9.80×10^{-7}	7.25×10^{-7}
max. $\angle$ error (rad.)	8.02×10^{-8}	8.82×10^{-8}	8.30×10^{-8}

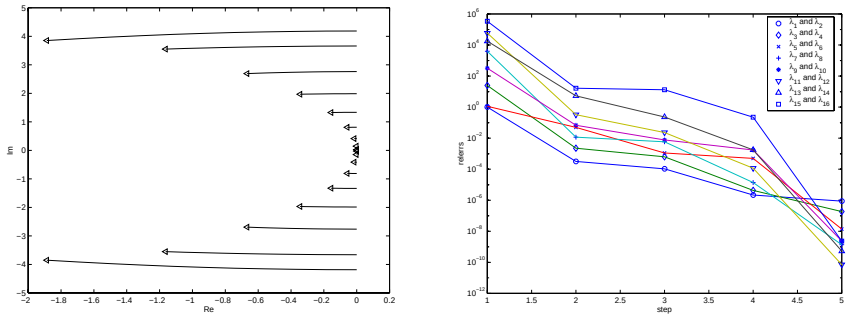

FIG. 7.3. *Eigenvalue paths and convergence of subsp. approx. method for nonprop. problem.*

7.2. Humboldt Bay Middle Channel Bridge Example. This example illustrates the possible application of the subspace approximation method in the analysis of a bridge structure including soil properties. The following is a description of the Middle Channel Bridge, from Conte et al. [4].

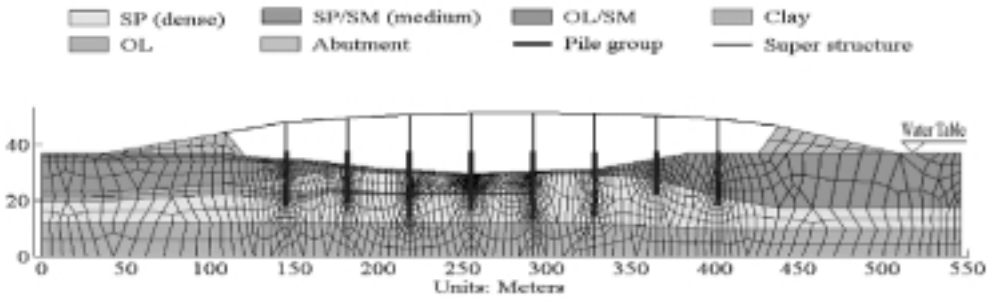

FIG. 7.4. *Finite element model of Middle Channel Bridge*

> The Humboldt Bay Middle Channel Bridge, near Eureka in northern California, ... is a 330 meters long, 9-span composite structure .... It is supported on eight pile groups, each of which consists of 5 to 16 prestressed concrete piles, in soils vulnerable to liquefaction (under extreme earthquake shaking conditions). The river channel has an average slope from the banks to the center of about 7% (4 degrees). The foundation soil is composed of mainly dense fine-to-medium sand (SP/SM), organic silt (OL), and/or stiff clay layers. In addition, thin layers of loose sand and soft clay (OL/SM) are located near the ground surface. ... A two-dimensional nonlinear model of the Middle Channel Bridge, including the superstructure, piers, and supporting piles was developed ... as shown in [Figure 7.4].

The example here is not intended to accurately model the various soil properties, since each soil type could have its own frequency dependent damping properties. Nevertheless, for illustrative purposes, the following realistic damping values are tested: 2% damping on the bridge structure and first 2%, then 7% damping on the soil (denoted here, respectively, as C_2 (a proportional damping matrix) and C_7 (a nonproportional damping matrix)). The properties of the 5164×5164 symmetric matrices M, C, and K are given in Table 7.3.

TABLE 7.3
Mass, stiffness, and damping matrices for the bridge problem.

matrix	bandedness	sparsity	max(eig)	min(eig)
M	diagonal	5038 nonzero elts.	1.31×10^3	0
K	bandwidth 5102	0.3% nonzero	4.94×10^{11}	9.95×10^2
C_2	bandwidth 5102	0.3% nonzero	1.12×10^9	2.26×10^0
C_7	bandwidth 5102	0.3% nonzero	1.12×10^9	7.93×10^0

Since M is singular, with 126 zero diagonal elements, and K is positive definite, to guarantee continuous eigenvalue paths we may swap the roles of M and K and instead solve for the largest eigenvalues μ for the problems

$$(\mu^2 \widehat{\mathrm{K}} + \widehat{\mathrm{M}})\mathbf{x} = 0 \text{ (undamped)} , \tag{7.1}$$

$$(\mu^2 \widehat{\mathrm{K}} + \mu \widehat{\mathrm{C}} + \widehat{\mathrm{M}})\mathbf{x} = 0 \quad \text{(damped)} . \tag{7.2}$$

The desired eigenvalues are then the reciprocals $\lambda = \frac{1}{\mu}$, and the eigenvectors are unaffected by the interchange. This interchange is not needed for the subspace approximation method, since we are interested only in the smallest (finite) eigenvalue

paths. However, when the corresponding linearized problem ((1.2), second eqn.) is solved for comparison purposes, the interchange is necessary in order to have a symmetric positive definite matrix on the right-hand side of the linearized eigenvalue problem, $\mathcal{A}\mathbf{x} = \lambda\mathcal{B}\mathbf{x}$.

We begin by using the MATLAB **eigs** function to compute the first 20 eigenpairs of the undamped problem. Taking these as the unperturbed solutions, the subspace approximation method is then applied to solve the damped problems, with the MATLAB 'slash' operator to solve the least squares problems. The CPU times for these results are shown in Table 7.4. Solving the undamped problem using **eigs** and then solving the problem with damping matrix C_7 using the subspace approximation method takes 44 seconds of CPU time, and even when an intermediate problem with damping matrix C_2 is computed, the total time required is 64 seconds, 40% of the time required by **eigs** to solve the linearized problem. (When started with the undamped problem, the subspace computation involves only real arithmetic, so less work is performed in that case.) If the undamped problem has been solved previously and its solutions are already available, using the subspace approximation method to compute the solutions with damping matrix C_7 requires 25% of the time required by **eigs** to solve the same problem.

TABLE 7.4
CPU times for bridge example.

problem	method	CPU time (sec.)
undamped	**eigs**	4.7
damping: C_2	Subsp.Approx. starting from $C = 0$	0.9
damping: C_7	Subsp.Approx. starting from C_2	58
damping: C_7	Subsp.Approx. starting from $C = 0$	38
damping: C_7	**eigs**, using linearization (1.2), second eqn.	159

7.3. Path crossing example. Unlike the previous examples, the problem in this section displays changes in eigenvalue order as well as some switching from complex to real values along the eigenvalue paths.

In this example, M and K are given as BCSSTM12 and BCSSTK12 from the Harwell-Boeing collection. These matrices have order 1473, and the matrix C is taken to be the block combination of M and K such that if $M_1 = M(1{:}\,600, 1{:}\,600)$ and $M_2 = M(540{:}\,1473, 540{:}\,1473)$, and if K_1, K_2 are defined in the same way from K, then

$$c_{ij} = \begin{cases} a_{11}m_{ij} + a_{12}k_{ij}, & \text{when } i < 540 \text{ or } j < 540 \\ (a_{11} + a_{21})m_{ij} + (a_{12} + a_{22})k_{ij}, & \text{when } 540 \le i, j \le 600 \\ a_{21}m_{ij} + a_{22}k_{ij}, & \text{when } i > 600 \text{ or } j > 600 \end{cases},$$

where $\binom{a_{i1}}{a_{i2}} = \frac{2\xi_i}{\omega_1+\omega_2}\binom{\omega_1\omega_2}{1}$, with $\xi_1 = 0.05$, $\xi_2 = 0.10$, and ω_1 and ω_2 as the first and tenth natural frequencies for the undamped problem. Now $\|M\| = 1.34 \times 10^1$, $\|C\| = 6.68 \times 10^5$, and $\|K\| = 6.56 \times 10^8$. The eigenvalue paths are shown in Figure 7.5. Path crossing and order changes can be observed. The subspace approximation method correctly computes, with tolerance 10^{-5}, the first 20 perturbed eigenvalues

and vectors starting with the first 10 complex conjugate pairs of eigenvalues and corresponding eigenvectors. The vector RQI method, started with the same values and using the same convergence tolerance, computes only the values numbered 4, 5, 6, 7, 12, 13, 14, 15, 17, and 18 (ordered by magnitude). **Eigs** computes all 20 values, and takes only 77 seconds of CPU time versus 92 using the subspace approximation method. However the solutions from **eigs** are much less accurate, as can be seen in Table 7.5, and decreasing the *tol* parameter of **eigs** by a factor of 10^5 causes negligible improvement in the errors while increasing the computation time to 124 seconds.

TABLE 7.5
Results for size 1473 example.

	Subsp.Approx	**eigs**
maximum relerrs	2.5×10^{-7}	1.1×10^{-3}
maximum $\angle$ error est. (rad.)	3.7×10^{-6}	1.7×10^{-3}
CPU time	92	77

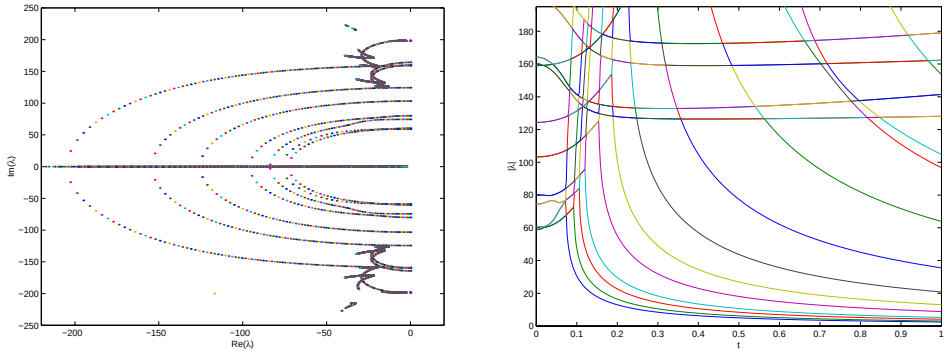

FIG. 7.5. *Eigenvalue paths and moduli of eigenvalues for size 1473 example.*

8. Summary and future directions. In this paper we developed a method for computing a few eigenvalues and eigenvectors of a quadratic eigenvalue problem assuming that solutions to the corresponding generalized (undamped) eigenvalue problem are known. The Taylor series for the block eigenvector matrix $X(t)$ was shown to converge, and the range of the kth Taylor polynomial was shown to be contained in the kth generalized Krylov subspace $\mathcal{S}_k(F\mathrm{M}, F\Delta\mathrm{C}, X_0)$, where F is a matrix such that $FP(\lambda_0, 0)$ fixes a space complementary to the range of the original block eigenvector matrix X_0.

We discussed how to compute the generalized Krylov subspaces by solving a sequence of least squares problems, and also how to directly compute the derivative subspaces range($[X_0\ X^{(1)}\ \cdots\ X^{(k)}]$) assuming that certain additional assumptions hold. Computing reduced problems in these subspaces was described. Using a first order error analysis a reasonable acceptance criterion was developed. After generalizing Lancaster's Rayleigh quotient iteration to a block algorithm, we assembled a hybrid method starting with the linearly converging subspace approximations and switching to the faster converging RQI as a finishing procedure. From several numerical experiments it is clear that solving the quadratic eigenvalue problem as a perturbed quadratic eigenvalue problem using the subspace approximation method

has some advantages both in speed and in accuracy over solving the problem from scratch using a standard linearization approach.

The theory in this paper extends to more general perturbed quadratic eigenvalue problems and to other polynomial eigenvalue problems [8]. Suppose that $(\lambda^N(t)\widehat{\mathrm{A}}_N(t) + \lambda^{N-1}(t)\widehat{\mathrm{A}}_{N-1}(t) + \cdots + \lambda(t)\widehat{\mathrm{A}}_1(t) + \widehat{\mathrm{A}}_0(t))\mathbf{x}(t) = 0$ and that $FP(\lambda_0, 0)$ fixes a space complementary to range(X_0). Then range$(\widehat{X}^{(j)}) \subseteq \mathcal{S}_j(F\mathrm{A}_1, \ldots, F\mathrm{A}_N, F\Delta\mathrm{A}_0, F\Delta\mathrm{A}_1, \ldots, F\Delta\mathrm{A}_N, X_0)$ for $j = 0, 1, 2, \ldots$. Future study of such extensions should prove fruitful.

Another important direction for future work is towards the reduction of the subspace dimension. Suppose a dense standard or generalized eigenvalue problem of size up to N is considered small and a problem of size greater than N is considered large. Then we should ensure that the reduced problems our method requires to be solved remain "small." The derivative subspaces grow linearly, while the generalized Krylov subspaces $\mathcal{S}_j$ can grow exponentially with j; either way a mechanism is needed for stopping the growth when the subspace reaches size $N/2$.

Three possible approaches are: (1) Switching early to block RQI. (2) Restarting with a subspace of dimension s spanned by the approximate eigenvectors based on the fact that the approximate eigenpairs $\{(\mu_i, \mathbf{y}_i)\}$ are exact solutions to the problems $(\lambda^2\widehat{\mathrm{M}}(1) + \lambda\widehat{\mathrm{C}}(1) + \widehat{\mathrm{K}}(1) - \frac{\mathbf{r}_i\mathbf{u}_i^T}{\mathbf{u}_i^T\mathbf{y}_i})\mathbf{x} = 0$, where $\mathbf{u}_i^T\mathbf{y}_i \neq 0$, $i = 1, 2, \ldots, s$. (3) Cutting the timestep and using a homotopy continuation method.

In summary, there are several interesting avenues to pursue in continuing this work on the subspace approximation method for perturbed, quadratic, and polynomial eigenvalue problems.

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