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REPORT DOCUMENTATION PAGE			Form Approved OMB No. 0704-0188
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1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED Final Report, 1 Oct 87 to 30 Sep 89	
4. TITLE AND SUBTITLE USE OF AN INDEFINITE INNER PRODUCT FOR COMPUTING DAMPED NATURAL MODES		5. FUNDING NUMBERS AFOSR-88-0048 61102F 2304/A3	
6. AUTHOR(S) B. N. Parlett and H. C. Chen			
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) University of California Department of Mathematics Berkeley, CA 94720 AFOSR-TR-		8. PERFORMING ORGANIZATION REPORT NUMBER 90 0734	
9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES) AFOSR/NM Building 410 Bolling AFB, DC 20332-6448		10. SPONSORING / MONITORING AGENCY REPORT NUMBER AFOSR-88-0048	
11. SUPPLEMENTARY NOTES			
12a. DISTRIBUTION / AVAILABILITY STATEMENT Approved for public release; distribution unlimited.		12b. DISTRIBUTION CODE DTIC ELECTE JUN 28 1990 S B D	
13. ABSTRACT (Maximum 200 words) A quadratic eigenvalue problem with symmetric positive definite coefficient matrices may be reduced to linear form while retaining symmetry in the new coefficients but neither of them will be positive definite. Formally the symmetric Lanczos algorithm and subspace iteration may be used to compute some eigenpairs of the linear problem. The trouble is that the basis vectors are orthogonal with respect to an indefinite inner product so there is no assurance that they will be linearly independent. Nevertheless this is an attractive way to solve the original problem and we discuss how to implement it and how it relates to the unsymmetric Lanczos procedures. We discuss complex origin shifts, reorthogonalization, and error bounds. Several methods for solving the reduced problem are mentioned but we have no fully satisfying technique. Some dangers are described and examples are given comparing our Lanczos program with a modified subspace iteration.			
14. SUBJECT TERMS		15. NUMBER OF PAGES 33	
		16. PRICE CODE	
17. SECURITY CLASSIFICATION OF REPORT UNCLASSIFIED	18. SECURITY CLASSIFICATION OF THIS PAGE UNCLASSIFIED	19. SECURITY CLASSIFICATION OF ABSTRACT UNCLASSIFIED	20. LIMITATION OF ABSTRACT SAR

USE OF AN INDEFINITE INNER PRODUCT FOR COMPUTING DAMPED NATURAL MODES

by

B. N. Parlett[†] and H. C. Chen[‡]

Abstract A quadratic eigenvalue problem with symmetric positive definite coefficient matrices may be reduced to linear form while retaining symmetry in the new coefficients but neither of them will be positive definite. Formally the symmetric Lanczos algorithm and subspace iteration may be used to compute some eigenpairs of the linear problem. The trouble is that the basis vectors are orthogonal with respect to an indefinite inner product so there is no assurance that they will be linearly independent. Nevertheless this is an attractive way to solve the original problem and we discuss how to implement it and how it relates to the unsymmetric Lanczos procedures. We discuss complex origin shifts, reorthogonalization, and error bounds. Several methods for solving the reduced problem are mentioned but we have no fully satisfying technique. Some dangers are described and examples are given comparing our Lanczos program with a modified subspace iteration.

Keywords: Linear Differential Equations, Theoretical Mathematics,
→ Lanczos Algorithm, Indefinite Inner Product, Computing

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• The authors gratefully acknowledge partial support from contract AFOSR-88-0048.

1. INTRODUCTION

In the study of Mechanics, when one analyzes how small displacements from an equilibrium state evolve in time one is led to the familiar equations of motion

$$\mathbf{M} \ddot{\mathbf{q}}(t) + \mathbf{C} \dot{\mathbf{q}}(t) + \mathbf{K} \mathbf{q}(t) = \mathbf{f}(t) \quad (1.1)$$

where $\mathbf{M}$, $\mathbf{C}$, and $\mathbf{K}$ are, respectively, the $n \times n$ mass, damping, and stiffness matrices and $\ddot{\mathbf{q}}(t)$, $\dot{\mathbf{q}}(t)$, and $\mathbf{q}(t)$ are the $n \times 1$ acceleration, velocity, and displacement vectors.

For many solid structures attached to the earth the damping coefficients are small compared with those of mass and stiffness. For structures in space damping plays a bigger role and the undamped model may not be a good approximation. To understand the response of the system to a variety of external forces $\mathbf{f}(t)$ it is still useful to know the system's dominant natural modes of vibration. This leads to the quadratic eigenvalue problem

$$(\lambda_i^2 \mathbf{M} + \lambda_i \mathbf{C} + \mathbf{K}) \mathbf{w}_i = \mathbf{0} \quad i = 1, \dots, 2n \quad (1.2)$$

In general λ_i will be complex and the associated modal shapes are given by the real and imaginary parts of $\mathbf{w}_i$. In the problems we consider $\mathbf{M}$, $\mathbf{C}$, $\mathbf{K}$ are real, symmetric, and positive definite.

Our paper has several goals. In Section 2 we make a plea for keeping symmetry explicit in the reduction to linear form even though the resulting pencil (or pair of matrices) is not definite. We are certainly not the first to make this suggestion. In Section 3 we show how to make a complex shift of origin and yet keep the eigenvalue algorithm confined to real arithmetic. This idea appears not to have been used before. Sections 4 and 5 are theoretical, showing important connections but do not contain new results. After that we describe an implementation of a Lanczos algorithm for symmetric indefinite pencils. It is designed to exploit any small bandwidth in $\mathbf{M}$, $\mathbf{C}$, $\mathbf{K}$. We describe how selective orthogonalization can be carried over from the definite case (Section 6), the numerical dangers that beset the algorithm in our case (Section 7), the solution of the reduced eigenvalue problem (Section 8), and how to compute accurate error estimates at very low cost at any step of the algorithm (Section 9). Finally, some numerical results and comparisons make up Section 10.

We mention here that certain problems need more study. (1) When $\mathbf{M}$ is singular, or nearly so, the computed Lanczos vectors can acquire large components in $\mathbf{M}$'s null space without the algorithm being able to detect that this is happening. We have a remedy but do not know how completely it cures the problem. (2) The efficient solution of the reduced eigenvalue problem is an interesting challenge. However, in the context of the whole algorithm, it is satisfactory to employ a standard, robust algorithm that does not exploit all the features of the reduced problem. A Lanczos program similar to ours has been developed independently (see [Nour-Omid & Regelbrugge, 1988]) and used effectively to solve the

equations of motion (1.1) directly without computing eigensolutions.

We follow standard notational conventions in the field of matrix computations. In particular, capital letters denote matrices, small Roman letters denote column vectors, and small Greek letters denote scalars. Also v^t denotes the transpose of v and $\bar{\alpha}$ denotes the conjugate of a complex number α . Unless the contrary is indicated $\|x\|$ denotes the Euclidean norm of x , $\|B\|$ denotes the spectral norm of B .

2. REDUCTION TO LINEAR FORM

There are several ways of rewriting (1.2) as a linear eigenvalue problem. When K and M are positive definite then 0 is not an eigenvalue and one reduction is

$$\begin{bmatrix} C & M \\ M & 0 \end{bmatrix} \begin{Bmatrix} w_i \\ \lambda_i w_i \end{Bmatrix} - \frac{1}{\lambda_i} \begin{bmatrix} -K & 0 \\ 0 & M \end{bmatrix} \begin{Bmatrix} w_i \\ \lambda_i w_i \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \end{Bmatrix} \quad (2.1)$$

Another is

$$\begin{bmatrix} -C & -M \\ M & 0 \end{bmatrix} \begin{Bmatrix} w_i \\ \lambda_i w_i \end{Bmatrix} - \frac{1}{\lambda_i} \begin{bmatrix} K & 0 \\ 0 & M \end{bmatrix} \begin{Bmatrix} w_i \\ \lambda_i w_i \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \end{Bmatrix} \quad (2.2)$$

The difference between (2.1) and (2.2) may strike the readers as frivolous. But the implications of this change go far. The reason that the distinction between (2.1) and (2.2) seems negligible is that, at the next step, when these generalized problems are reduced to standard form both (2.1) and (2.2) produce the same result since

$$\begin{bmatrix} -K & 0 \\ 0 & M \end{bmatrix}^{-1} \begin{bmatrix} C & M \\ M & 0 \end{bmatrix} = \begin{bmatrix} K & 0 \\ 0 & M \end{bmatrix}^{-1} \begin{bmatrix} -C & -M \\ M & 0 \end{bmatrix} \quad (2.3)$$

This is a nonsymmetric matrix as we would expect from the presence of complex eigenvalues.

Of course the reduction can be made by using the Cholesky factorizations

$$K = L_K L_K', \quad M = L_M L_M'$$

to produce first

$$\left(\begin{bmatrix} L_K^{-1} C L_K^{-t} & L_K^{-1} L_M \\ L_M' L_K^{-t} & 0 \end{bmatrix} - \frac{1}{\lambda_i} \begin{bmatrix} -I & 0 \\ 0 & I \end{bmatrix} \right) \begin{Bmatrix} L_K' w_i \\ \lambda_i L_M' w_i \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \end{Bmatrix} \quad (2.4)$$

and then, the standard form

$$\left(\begin{bmatrix} -L_K^{-1} C L_K^{-t} & -L_K^{-1} L_M \\ L_M' L_K^{-t} & 0 \end{bmatrix} - \frac{1}{\lambda_i} \begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix} \right) \begin{Bmatrix} L_K' w_i \\ \lambda_i L_M' w_i \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \end{Bmatrix} \quad (2.5)$$

We suggest that this reduction to standard form, either to (2.3) or (2.5), is a tactical error.

In order to explain our view the following standard terminology will be needed. A symmetric matrix is indefinite if it has eigenvalues of both signs.

Definition 1. Let $Y \in \mathbb{R}^{n \times n}$ be symmetric but indefinite. The bilinear form defined by

$$(u, v)_Y := v' Y u$$

is called a pseudo (or indefinite or improper) inner product. It obeys all the axioms of an inner product except positivity.

Definition 2. Let $F \in \mathbb{R}^{n \times n}$, $Y \in \mathbb{R}^{n \times n}$, with Y symmetric.

F is symmetric with respect to Y , if

$$F' Y = (Y F)' = Y F,$$

or, equivalently, if

$$(u, F v)_Y = (F u, v)_Y$$

for all $u \in \mathbb{R}^n$, $v \in \mathbb{R}^n$.

In some contexts one says that F is self-adjoint in Y 's (pseudo) inner product.

The trouble with (2.2) and (2.3) is that neither of them reminds us that

$$\begin{bmatrix} -K^{-1} C & -K^{-1} M \\ I & 0 \end{bmatrix}$$

is symmetric with respect to both

$$\begin{bmatrix} C & M \\ M & 0 \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} -K & 0 \\ 0 & M \end{bmatrix}$$

Similarly the first matrix in (2.5) is symmetric with respect to

$$\begin{bmatrix} -I & 0 \\ 0 & I \end{bmatrix}$$

but not with respect to

$$\begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix}$$

We see no gain in efficiency in going all the way to (2.5) in the reduction but circumstances may change.



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In brief, (2.1) suggests the relevant symmetries but (2.2) does not. (2.1) is a special case of the problem

$$(A - \frac{1}{\lambda} B) z = 0$$

where A and B are symmetric but indefinite. A matrix pair (A, B) is sometimes called a matrix pencil. See [Gantmacher, 1959] for example. In our case we have a symmetric indefinite pencil. Excellent references for further study of these pencils see [Gohberg, Lancaster, and Rodman, 1983 and 1986].

Lemma. $B^{-1} A$ is symmetric with respect to both A and B . $A B^{-1}$ is symmetric with respect to both A^{-1} and B^{-1} .

Proof: For all u, v in $\mathbb{R}^n$,

$$(u, B^{-1} A v)_A = v^T A B^{-1} A u = (B^{-1} A u, v)_A$$

$$(u, B^{-1} A v)_B = v^T A u = (B^{-1} A u, v)_B$$

The second result can be obtained similarly. $\square$

It turns out that the Lanczos algorithm may be invoked with the operator $B^{-1} A$ using a pseudo inner product defined by A or B . The three term recurrence still holds in this more general situation. There is more on the Lanczos algorithm in Section 4.

Subspace Iteration [Bathe and Wilson, 1976] or [Rutishauser, 1970] (also called the method of Simultaneous Iterations) also extends formally to the indefinite case but the Rayleigh Ritz approximations produced at each step are no longer optimal in any meaningful sense. We have made the necessary modification to our standard SI program and use it as a simple rival to our Lanczos procedure.

In contrast to the definite case both algorithms can break down or become unstable when close to breakdown. Alarming things can happen with an indefinite (or improper) inner product: a set of *orthogonal* vectors might be linearly dependent. The geometry associated with such an improper inner product is the geometry of relativity theory.

Next we wish to point out that it is possible to work with $A B^{-1}$ instead of $B^{-1} A$ but we see no advantage to this formulation in our problem. Since $A B^{-1}$ is symmetric with respect to B^{-1} and A^{-1} we must work with these pseudo inner products. Now A^{-1} is complicated but when $B = \text{diag}(-K, M)$ then we can form the Cholesky factorization of M and K once for all. After that the computation of $B^{-1} v$ costs no more than the computation of $B v$. The need for shifts of origin (see next section) suggests the use of an operator $H^{-1} A$ and the pseudo inner product defined by A . Here H may be B or $B - \sigma A$ or $\text{Re}(B - \sigma A)$ or $\text{Im}(B - \sigma A)$.

Both forms (2.1) and (2.2) are well known. In a recent paper [Borri & Mantegazza 1977] form (2.1) is explicitly proposed when M , C , and K are all symmetric. However, no mention is made of the fact that the Rayleigh quotients used in that paper may overflow or yield $0/0$. A conventional alternative to the pseudo-symmetric form (2.1) or (2.4) is to apply the two sided Lanczos algorithm to the matrix in (2.3) or (2.5). In Section 4 we show the connection between these two approaches.

We recall that the attraction of the Lanczos algorithm is that a few of the largest eigenvalues may be found by stopping the algorithm long before the full n steps. It is usual practice to give the algorithm an operator such as $H^{-1}A$ whose largest eigenvalues are shifted reciprocals of the ones we really want. We can expect to find the p largest eigenvalues within $\max\{p+8, 2p\}$ steps. See Section 10 for examples. By reducing the $n \times n$ quadratic problem to linear form the dimension of the Lanczos vectors becomes $2n$. However the cost of implementing the Lanczos algorithm is only doubled (approximately) because the structure of the matrices A and B may be exploited. The algorithm and operation counts are given in Figure 1.

Note that we could have used the algorithm for the operator $H^{-1}A$ using the pseudo-inner product defined by H . The variation alters the subroutines supplied to the Lanczos algorithm, not the program itself. There may be advantages to the H inner product but we have not studied the matter since H may be complicated.

3. ORIGIN SHIFTS

There are applications (e.g. space structures) in which the stiffness matrix K is singular. This makes $B = \text{diag}(-K, M)$ singular too. In this situation, we need to solve a shifted problem

$$(\lambda - \sigma) A z = (B - \sigma A) z$$

where $\sigma \neq 0$ is a real shift. To preserve the block diagonal form, we note that the $B - \sigma A$ can be factored into

$$\begin{bmatrix} I & -\sigma I \\ 0 & I \end{bmatrix} \begin{bmatrix} (-K - \sigma C - \sigma^2 M) & 0 \\ 0 & M \end{bmatrix} \begin{bmatrix} I & 0 \\ -\sigma I & I \end{bmatrix} \quad (3.1)$$

We need to factor only M and the shifted stiffness matrix $K + \sigma C + \sigma^2 M$, which has the same banded structure as K in order to solve $(B - \sigma A)u = Av$ for u given v . Thus we may solve $(B - \sigma A)^{-1}Az = \frac{1}{(\lambda - \sigma)}z$ to obtain eigenvalues close to σ . This is standard practice.

In several applications the user would like to explore part of the complex plane and see how certain eigenvalues vary with changes in the matrix elements. Unfortunately, if σ is complex then $B - \sigma A$ is not

real and so $(B - \sigma A)^{-1} A$ is not a valid operator for our Lanczos algorithm.

A way out of this quandary was proposed in [Parlett and Saad, 1987]. The operator given to the Lanczos algorithm is either

$$\operatorname{Re} [(B - \sigma A)^{-1}] A \quad \text{or} \quad \operatorname{Im} [(B - \sigma A)^{-1}] A . \quad (3.2)$$

Here $\operatorname{Re} G := \frac{1}{2} (G + \bar{G})$, $\operatorname{Im} G := \frac{1}{2i^*} (G - \bar{G})$, and $\bar{G}$ is the conjugate of G . Both operators are real and have complex conjugate pairs of eigenvalues.

Let λ, z be an eigenpair of (B, A) , i.e. they satisfy $\lambda A z = B z$. By subtracting $\sigma A z$ and $\bar{\sigma} A z$ from each side and inverting one finds that

$$\operatorname{Re} [(B - \sigma A)^{-1}] A z = \frac{1}{2} \left(\frac{1}{\lambda - \sigma} + \frac{1}{\lambda - \bar{\sigma}} \right) z , \quad (3.3a)$$

$$\operatorname{Im} [(B - \sigma A)^{-1}] A z = \frac{1}{2i^*} \left(\frac{1}{\lambda - \sigma} - \frac{1}{\lambda - \bar{\sigma}} \right) z , \quad (3.3b)$$

To recover λ from the computed eigenvalues of either of these operators requires merely solving a quadratic equation for the root that is closer to σ . However λ may be recovered directly, with extra work, from the Rayleigh quotient

$$\lambda = \bar{z}^T B z / \bar{z}^T A z .$$

In order to exploit narrow bandwidth it is convenient to use complex arithmetic in (3.1) to factor $B - \sigma A$ and thus to solve, for $w \in \mathbb{C}^n$, $(B - \sigma A) w = A v$ for any given $v \in \mathbb{R}^n$. However, the subroutine returns either $\operatorname{Re} w$ or $\operatorname{Im} w$ and so there is no complex arithmetic in the Lanczos algorithm. The major computation is in factoring $K + \sigma C + \sigma^2 M$. This is done once. Note that the pseudo-inner product is defined by A and is independent of σ .

Both the real and imaginary part of $(B - \sigma A)^{-1}$ provide good enhancement of the eigenvalues close to σ . It is shown in [Parlett and Saad, 1987] that the imaginary part suppresses the unwanted eigenvalues far from σ more strongly than does the real part. More experience is needed on this aspect of the shift.

4. CONNECTION BETWEEN LANCZOS ALGORITHMS

The original formulations given by Lanczos (in [Lanczos, 1950]) considered the standard symmetric eigenvalue problem $A z = \lambda z$, i. e. $B = I$. The Lanczos vectors $\{q_k\}_{k=1}^n$ for symmetric $n \times n$ A obey the well-known 3-term recurrence relation

$$A q_k = \beta_k q_{k-1} + \alpha_k q_k + \beta_{k+1} q_{k+1} \quad k = 1, \dots, n \quad (4.1)$$

with $q_0 = 0$. The $\{q_k\}_{k=1}^n$ form an orthonormal set. The attractive feature of the Lanczos algorithm for the generalized problem $A - \lambda B$, where B is symmetric, positive definite is that, as in (4.1)

$$B^{-1} A q_k = \beta_k q_{k-1} + \alpha_k q_k + \beta_{k+1} q_{k+1}$$

The Lanczos vectors are still orthonormal but in the inner product defined by B . Usually they will not be orthogonal in the ordinary Euclidean sense.

In general, for a nonsymmetric matrix F (we rename $B^{-1} A$ as F) there is a two-sided generalization (also given by Lanczos) in which two sets $\{p_1, \dots, p_n\}$ and $\{q_1, \dots, q_n\}$ are generated. Moreover, if $p_k^T q_k = 1$, then

$$\begin{aligned} F q_k &= \beta_k q_{k-1} + \alpha_k q_k + \gamma_{k+1} q_{k+1}, \\ F^T p_k &= \gamma_k p_{k-1} + \alpha_k p_k + \beta_{k+1} p_{k+1}, \end{aligned} \quad (4.2)$$

and the $\{p_k\}, \{q_k\}$ are biorthogonal,

$$p_i^T q_k = 0, \quad i \neq k$$

This algorithm will break down when $p_k^T q_k = 0$ with $p_k \neq 0, q_k \neq 0$. We can expect inaccuracy when $p_k^T q_k$ is very small. There is more on this point in Section 5.

For theoretical purposes it is convenient to normalize the Lanczos vectors by

$$p_k^T q_k = 1 \quad \|p_k\| = \|q_k\| \quad (4.3)$$

provided breakdown does not occur. However, in practice, it is better to keep

$$\|p_k\| = \|q_k\| = 1$$

and define

$$\omega_k = p_k^T q_k \quad (4.4)$$

If ω_k is tiny ($< 10^{-8}$ or $\epsilon^{1/2}$) then the $\{p_k\}$ and $\{q_k\}$ are nearly linearly dependent and consequently make bad bases in which to represent the solutions. The normalization (4.3) conceals any deterioration in the quality of the basis $\{q_1, \dots, q_n\}$. The normalization (4.4) makes the three term recurrence slightly more complicated. Define

$$J_n = \begin{bmatrix} \alpha_1 & \gamma_2 & & & \\ \beta_2 & \alpha_2 & \gamma_3 & & \\ & & \ddots & \ddots & \\ & & & \beta_{n-1} & \alpha_{n-1} & \gamma_n \\ & & & & \beta_n & \alpha_n \end{bmatrix} = P_n^T F Q_n,$$

$$\begin{aligned}
\Omega_n &= \text{diag}(\omega_1, \dots, \omega_n) = P_n' Q_n, \\
Q_n &= (q_1, \dots, q_n), \\
P_n &= (p_1, \dots, p_n)
\end{aligned} \tag{4.5}$$

then, in matrix form, the three term recurrence is

$$\begin{aligned}
F Q_n - Q_n \Omega_n^{-1} J_n &= 0, \\
P_n' F - J_n \Omega_n^{-1} P_n' &= 0.
\end{aligned} \tag{4.6}$$

Note that when $F = A = A'$ and $B = I$ then $P_n = Q_n$, $\Omega_n = I$, and $J_n = T_n = T_n'$.

In our pseudo-symmetric eigenvalue problem $A - \lambda B$ we face the same possibility as in (4.2) that the Lanczos process may break down and may be unstable when close to breakdown. To distinguish this algorithm from the two-sided algorithm given by (4.5) and (4.6) we label the Lanczos vectors in our algorithm as $\tilde{q}_1, \dots, \tilde{q}_n$. It is important to know when this instability occurs and so we prefer to normalize the $\tilde{q}_k$ to satisfy

$$\|\tilde{q}_k\| = 1, \quad \text{for all } k, \tag{4.7}$$

and then define

$$\tilde{\omega}_k = (\tilde{q}_k, \tilde{q}_k)_A.$$

A tiny value of $\tilde{\omega}_k$ is a sign of danger. The three term recurrence, in matrix form, is

$$\begin{aligned}
B^{-1} A \tilde{Q}_n - \tilde{Q}_n \tilde{\Omega}_n^{-1} \tilde{T}_n &= 0, \\
\tilde{T}_n &= \tilde{Q}_n' A B^{-1} A \tilde{Q}_n, \\
\tilde{\Omega}_n &= \tilde{Q}_n' A \tilde{Q}_n.
\end{aligned} \tag{4.8}$$

provided that breakdown does not occur. Note that $\tilde{T}_n$ is symmetric. Equating the k th column on each side of (4.8) yields the three term recurrence for our pseudo-symmetric formulation

$$B^{-1} A \tilde{q}_k = (\beta_k / \tilde{\omega}_{k-1}) \tilde{q}_{k-1} + (\tilde{\alpha}_k / \tilde{\omega}_k) \tilde{q}_k + (\beta_{k+1} / \tilde{\omega}_{k+1}) \tilde{q}_{k+1}, \quad k < n. \tag{4.9}$$

This equation shows the possible danger of small values among the $\{\tilde{\omega}_i\}$.

The goal of the preceding discussion was to prepare for the interesting, but natural, result that our pseudo-symmetric procedure (4.8) & (4.9) is a disguised form of the two-sided algorithm (4.6). By choosing p_1 appropriately it turns out that $p_k = A q_k$, for all k , and so there is no need to hold the p_k explicitly in memory.

Theorem. Suppose that A and B are real and symmetric. Suppose that no breakdown occurs. Let the two-sided Lanczos algorithm in (4.6) be applied with operator $B^{-1}A$ (starting with p_1 and q_1) to produce two biorthogonal sequences $\{p_k\}_{k=1}^n$, $\{q_k\}_{k=1}^n$. Let the pseudo-symmetric Lanczos procedure in (4.9) be applied with $B^{-1}A$ (starting with $\tilde{q}_1$) with pseudo-inner product defined by A to produce $\{\tilde{q}_k\}_{k=1}^n$. If $\tilde{q}_1 = q_1$ and $p_1 = A q_1 / \|A q_1\|$ then $\tilde{q}_k = q_k$ and $p_k = A q_k / \|A q_k\|$, $k = 2, \dots, n$.

Proof : We use induction and let $u \parallel v$ mean that u is a nonzero multiple of v . Put $k = 1$ in (4.9) and equate column 1 on each side of (4.6) to find

$$\tilde{q}_2 \parallel B^{-1}A \tilde{q}_1 - \tilde{q}_1 (\tilde{\alpha}_1 / \tilde{\omega}_1) ,$$

$$q_2 \parallel B^{-1}A q_1 - q_1 (\alpha_1 / \omega_1) ,$$

$$p_2 \parallel A B^{-1} p_1 - p_1 (\alpha_1 / \omega_1) .$$

By choice $\tilde{q}_1 = q_1$ and $A q_1 = p_1 \|A q_1\|$, so

$$\tilde{\omega}_1 := (\tilde{q}_1, \tilde{q}_1)_A = (q_1, q_1)_A = q_1^T p_1 \|A q_1\| = \omega_1 \|A q_1\| ,$$

$$\tilde{\alpha}_1 := (\tilde{q}_1, B^{-1}A \tilde{q}_1)_A = (q_1, B^{-1}A q_1)_A = p_1^T B^{-1}A q_1 \|A q_1\| = \alpha_1 \|A q_1\| .$$

Thus $\tilde{\alpha}_1 / \tilde{\omega}_1 = \alpha_1 / \omega_1$ and hence $\tilde{q}_2 = q_2$ and $p_2 \parallel A q_2 / \|A q_1\|$. So $p_2 = A q_2 / \|A q_2\|$.

The induction assumption is that the theorem holds for $k = j - 1$ and j . Put $k = j$ in (4.9) and equate column j on each side of (4.6) to find

$$\tilde{q}_{j+1} \parallel B^{-1}A \tilde{q}_j - \tilde{q}_j (\tilde{\alpha}_j / \tilde{\omega}_j) - \tilde{q}_{j-1} (\tilde{\beta}_j / \tilde{\omega}_{j-1}) ,$$

$$q_{j+1} \parallel B^{-1}A q_j - q_j (\alpha_j / \omega_j) - q_{j-1} (\gamma_j / \omega_{j-1}) ,$$

$$p_{j+1} \parallel A B^{-1} p_j - p_j (\alpha_j / \omega_j) - p_{j-1} (\beta_j / \omega_{j-1}) .$$

Use the induction assumption to verify that

$$\tilde{\omega}_{j-1} := (\tilde{q}_{j-1}, \tilde{q}_{j-1})_A = (q_{j-1}, q_{j-1})_A = q_{j-1}^T p_{j-1} \|A q_{j-1}\| = \omega_{j-1} \|A q_{j-1}\| ,$$

$$\tilde{\beta}_j := (\tilde{q}_{j-1}, B^{-1}A \tilde{q}_j)_A = (q_{j-1}, B^{-1}A q_j)_A = p_{j-1}^T B^{-1}A q_j \|A q_{j-1}\| = \beta_j \|A q_{j-1}\| ,$$

$$\tilde{\omega}_j := (\tilde{q}_j, \tilde{q}_j)_A = (q_j, q_j)_A = q_j^T p_j \|A q_j\| = \omega_j \|A q_j\| ,$$

$$\tilde{\alpha}_j := (\tilde{q}_j, B^{-1}A \tilde{q}_j)_A = (q_j, B^{-1}A q_j)_A = p_j^T B^{-1}A q_j \|A q_j\| = \alpha_j \|A q_j\| ,$$

$$\gamma_j := p_{j-1}^T B^{-1}A q_j = \|A q_{j-1}\| q_{j-1}^T A B^{-1}A q_j = \frac{\|A q_{j-1}\|}{\|A q_j\|} q_{j-1}^T A B^{-1} p_j = \frac{\|A q_{j-1}\|}{\|A q_j\|} \beta_j .$$

using these relations we verify that

$$\tilde{q}_{j+1} = q_{j+1} .$$

$$p_{j+1} = \|A q_{j+1}\|$$

Thus, $p_{j+1} = \|A q_{j+1}\|$ and the result holds for $k = j + 1$. By the principle of induction, if the algorithms do not break down then the theorem holds for $k = 1, 2, \dots, n$. $\square$

5. MOMENT MATRICES AND HYPERBOLIC PAIRS

The breakdown of the (generalized) form of the Lanczos algorithm may be interpreted as breakdown in the triangular factorization of a certain matrix. This connection is well known (see [Householder, 1964] or [Parlett, Taylor, and Liu, 1985]) and gives valuable insight. We review it now. Let

$$K_j = [q_1, (B^{-1}A)q_1, (B^{-1}A)^2q_1, \dots, (B^{-1}A)^{j-1}q_1].$$

This is called a Krylov matrix. When successful the Lanczos algorithm constructs a matrix

$$Q_j = [q_1, \dots, q_j]$$

of Lanczos vectors which are A -orthogonal, i.e.

$$Q_j^T A Q_j = \Omega_j = \text{diagonal}.$$

Moreover Q_j and K_j are connected by

$$K_j = Q_j L_j^T$$

where L_j is an invertible lower triangular matrix. In other words Q_j is obtained from K_j by the Gram-Schmidt process. However, Lanczos found a clever way to find q_j without actually invoking Gram-Schmidt. This result is not obvious; it expresses the fact that $B^{-1}A q_m$ is a linear combination of q_{m-1} , q_m , and q_{m+1} and from this it can be deduced that for each $m = 1, 2, \dots, j$, $(B^{-1}A)^m q_1$ is a linear combination of $q_1, q_2, \dots, q_{m+1}$ only.

In the present context the moment matrix is defined as

$$M_j = [m_{ik}] ,$$

$$m_{ik} = (q_1^T, (B^{-1}A)^{i+k-2} q_1)_A = q_1^T A (B^{-1}A)^{i+k-2} q_1.$$

A little manipulation shows that

$$M_j = K_j^T A K_j .$$

Consequently, if the Lanczos process does not breakdown,

$$M_j = L_j Q_j^T A Q_j L_j^T = L_j \Omega_j L_j^T .$$

This is the triangular factorization of M_j . We do not insist that the diagonal elements of L_j be 1.

Triangular factorization exists if all the leading principal submatrices of M_j are nonsingular (i.e. invertible). Conversely, if the last diagonal element of Ω_j is the first to vanish then the Lanczos algorithm breaks down at the end of step j .

Observe that K_j and Q_j are each $n \times j$ matrices whereas L_j is invertible. Thus K_j has full rank if and only if Q_j has full rank. It is desirable (though not essential) that Q_j have full rank.

Lemma. Let K_j , Q_j , M_j , and A be as defined above. If K_j has full rank and A is symmetric, positive definite then so is M_j and the factorization $L_j \Omega_j L_j^T$ exists with Ω_j positive definite.

Proof : For any $v \in \mathbb{R}^j$,

$$v^T M_j v = v^T K_j^T A K_j v = w^T A w > 0 ,$$

unless $w = 0$. If K_j has full rank then $w = 0$ implies $v = 0$. Hence M_j is positive definite. The leading principal submatrices of a positive definite matrix are positive definite and thus M_j permits a triangular factorization. $\square$

When A is indefinite then there exist vectors $w \neq 0$ such that $w^T A w \leq 0$ and, except in trivial cases, there will be starting vectors q_1 and j -vectors v such that the A -norm of $K_j v$ vanishes for large enough j .

Definition: v is isotropic if $v^T A v = (v, v)_A = 0$.

It is helpful to regard the occurrence of breakdown (i.e. when q_j is isotropic) not as disaster but as a reminder that A is indefinite. There is a natural way to proceed. The idea goes back to Lagrange but was put to use by D. G. Luenberger to extend the conjugate gradient algorithm [Luenberger, 1969] and by [Bunch, Kauffman, and Parlett, 1976] to stabilize triangular factorization.

By a simple rotation of coordinates the hyperbola $x^2 - y^2 = 1$ may be written as $\xi \eta = 2$. In our context the idea is to modify our generalized Lanczos algorithm as follows. If q_j is an isotropic vector then choose the value of α_{j+1} in (4.1) or (4.9) so that q_{j+1} is also isotropic. Provided that $q_j^T A q_{j+1}$ is not too small these Lanczos vectors still provide a good basis. They are no longer A -orthogonal. Nevertheless $Q_{j+1}^T A Q_{j+1}$ is block diagonal with 2×2 diagonal blocks of the form

$$\begin{bmatrix} 0 & \omega_{j,j+1} \\ \omega_{j,j+1} & 0 \end{bmatrix}$$

whenever the modification is used. We follow Luenberger [Luenberger, 1969] in calling q_j, q_{j+1} a hyperbolic pair.

In practice there is no need to wait until $q_j^T A q_j$ is negligible before switching to a hyperbolic pair for q_j and q_{j+1} . By forsaking strict A-orthogonality we gain a better conditioned basis. Similar thinking for the two sided algorithm yields the Look Ahead algorithm [Parlett, Taylor, and Liu, 1985] but the procedure is rather complicated. Our experience is limited but the only breakdowns we have encountered were produced deliberately.

6. LOSS OF ORTHOGONALITY

It is well known that the three term recurrence does not produce A-orthogonal Lanczos vectors in finite precision arithmetic. It is the convergence of the algorithm that provokes this deterioration not cancellation. There are three ways to respond to the situation.

1. Do nothing.

This technique causes Lanczos sequences to be 2 or 3 times larger than necessary. It is only of interest when the whole spectrum is wanted. The loss of orthogonality does not prevent the calculation of fully accurate eigenvalues and eigenvectors. It merely slows down the process.

2. Full reorthogonalization at each step.

Here the vector computed by the three term recurrence is explicitly orthogonalized against all preceding Lanczos vectors. This requires keeping the auxiliary vectors $\hat{p}_k (= A q_k)$ in fast memory (unless virtual memory is in use) and using them every step. However for short runs of 20 or 30 Lanczos steps the cost is not excessive.

3. Selective reorthogonalization.

Most of the benefits derived from a set of Lanczos vectors that is A-orthogonal to working accuracy are also enjoyed when the vectors are merely semi-orthogonal.

Definition. Let ϵ be the roundoff unit. Then two vectors u, v are semi-orthogonal with respect to A if

$$|u^T A v| < \sqrt{\epsilon} \|u\| \cdot \|v\| \cdot \|A\|.$$

Two techniques have been proposed for maintaining semi-orthogonality. In [Parlett and Scott, 1979] it is shown that computed vectors tend to be pulled towards converged Ritz vectors. Hence it helps to orthogonalize the current Lanczos vectors against such vectors from time to time. This remedy only addresses one mechanism that provokes orthogonality loss.

In [Simon, 1984] a recurrence was found that governs the inner products among the Lanczos vectors themselves. This recurrence permits an accurate estimate of the orthogonality loss in the current Lanczos vector to be computed at each step at a cost proportional to the number of Lanczos steps taken. It is then easy to orthogonalize the new vector against all the old ones when, and only when, necessary in order to maintain semi-orthogonality.

The recurrence extends easily to cover A-orthogonality and our algorithm incorporates this form of selective orthogonalization. As a rule of thumb selective orthogonalization has a cost about 1/3 the cost of full reorthogonalization. For large problems on some computer systems the I/O costs of reorthogonalization dominate the arithmetic costs.

A full discussion of semi-orthogonality and how to maintain it is given in [Parlett, Nour-Omid, and Liu, 1988].

7. DANGERS

The previous sections show that the symmetric quadratic eigenvalue problem

$$(\lambda^2 \mathbf{M} + \lambda \mathbf{C} + \mathbf{K}) \mathbf{u} = 0 \quad (5.1)$$

may be reduced to the simpler form

$$\left(\mathbf{T} - \frac{1}{\lambda - \sigma} \mathbf{\Omega} \right) \mathbf{u} = 0 \quad (5.2)$$

where $\mathbf{T}$ is real symmetric and tridiagonal and $\mathbf{\Omega}$ is real diagonal (or block diagonal).

Any difficulties inherent in the original problem must be inherited by the reduced problem. Important features are :

- (1) complex eigenvalues are present and are wanted.
- (2) Sometimes (depending on $\mathbf{C}$) an eigenvalues λ may be degenerate; it may belong to a nondiagonal Jordan block of $\mathbf{\Omega}^{-1} \mathbf{T}$. This can happen when λ is a double real eigenvalue (the coalescence of a conjugate pair of eigenvalues) or when both λ and $\bar{\lambda}$ are double eigenvalues.

We consider (1). Since $\mathbf{T}$ and $\mathbf{\Omega}$ are real it is desirable to postpone the use of complex arithmetic. Indeed if the HR algorithm [Bunse-Gerstner, 1981; Brebner and Grad, 1982] is used then the pair $(\mathbf{T}, \mathbf{\Omega})$ is eventually transformed into $(\tilde{\mathbf{T}}, \mathbf{\Delta})$ where

$$\mathbf{\Delta} = \text{diag}(\pm 1, \pm 1, \dots, \pm 1)$$

and $\tilde{\mathbf{T}}$ is block diagonal with 2×2 and 1×1 blocks. Each complex conjugate pairs of eigenvalues is found from a real pencil of the form

$$\begin{pmatrix} \phi & \mu \\ \mu & -\phi \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

No complex arithmetic is needed in this case but the HR algorithm is not always stable. However there are alternative techniques for finding some or all of the eigenvalues of (T, Ω) and exploiting the banded form. See Section 8.

Thus (1) is not a serious difficulty.

Now consider (2) : degenerate multiple eigenvalues. Theorem 15-2-1 in [Parlett, 1980] states that any real square matrix may be written in the form $B^{-1}A$ where A and B are real symmetric. Consequently a symmetric indefinite pair (A, B) may suffer from highly defective eigenvalues. A simple example is

$$\begin{pmatrix} 0 & 0 & 1 & \alpha \\ 0 & 1 & \alpha & 0 \\ 1 & \alpha & 0 & 0 \\ \alpha & 0 & 0 & 0 \end{pmatrix} - \lambda \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

which is a Jordan block in disguise.

If T has some off diagonal elements that vanish then the reduced eigenvalue problem splits up into smaller pieces. Each piece consists of a T with all its β_i values nonzero.

Lemma: If no off diagonal entry β_i of T vanishes then to each eigenvalue of $T - (\lambda - \sigma)^{-1} \Omega$ there corresponds exactly one eigendirection.

Proof: The minor of the (i, j) entry is $(\beta_1 \beta_2 \cdots \beta_{j-1}) \neq 0$ for all λ and so the rank never drops below $j-1$.

□

However it is still possible to have eigenvalues of high multiplicity.

This result is to be expected. Whatever the geometric multiplicity of an eigenvalue of $A - \lambda B$ the Lanczos algorithm can only "see" the projection of the starting vector q_1 onto the invariant subspace associated with the eigenvalue. Thus, in exact arithmetic, it is possible for $T - \lambda \Omega$ to have generalized eigenvectors with lower grades than the true multiplicity of the associated eigenvalues. It is exactly the same in the truly symmetric case. The Lanczos algorithm cannot "see" geometric multiplicities.

Unfortunately it is the presence of degenerate eigenvalues that causes breakdown of the HR algorithm.

Example of a multiple eigenvalue :

$$\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} - \lambda \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

has 0 as a double eigenvalue with eigenvector $(1, -1)^t$ and any vector other than the eigenvector is a generalized eigenvector of grade 2. There is no simpler symmetric representation of such an eigenvalue.

We are studying the effect of multiple eigenvalues on the performance of the Lanczos algorithm.

There is another difficulty more insidious than the first two.

(3) Undetected growth of Lanczos vectors in certain directions. The following example was given by Dr. T. Ericsson [private communication]

Example :

$$A = \text{diag}(1, -1, x, x, \dots, x),$$

$$B = \text{diag}(-1, 1, x, x, \dots, x),$$

$$q_1 = (\sigma, \sigma, x, x, \dots, x)^t.$$

Then $(q_1, q_1)_A$ is independent of σ and consequently both T and Ω will be independent of σ . The trouble is that

$$z = (1, 1, 0, \dots, 0)^t$$

is an eigenvector of $B^{-1}A$ with eigenvalue 1 and $(z, z)_A = (z, z)_B = 0$. Arbitrarily large multiples of z could be present in the Lanczos vectors (on account of q_1) and the Lanczos algorithm would be blind to them. This possibility of undetectable growth in certain directions is a generalization of the phenomenon reported in [Nour-Omid, Parlett, Ericsson, & Jensen, 1987] where the direction was in the null space of A . Here it is the isotropic eigenvectors that are invisible.

It remains to be seen whether the practice of keeping all Lanczos vectors with Euclidean length 1 will alleviate the problem or merely drive the Lanczos vectors into the space spanned by undetectable eigenvectors.

8. HOW TO SOLVE $T - \lambda \Omega$

(1) Use EISPACK on $\Omega_j^{-1} T_j$. (Subroutines HQR1 or HQR2)

The tridiagonal form will be expanded to Hessenberg form by the QR algorithm. Thus no advantage is taken of the compact tridiagonal form. The arithmetic effort is approximately $8j^3$ to find all the eigenvalues at step j .

(2) The HR algorithm [Bunse-Gerstner, 1981; Brebner and Grad, 1982].

Let $\delta_i^2 = |\omega_i|$, $i = 1, \dots, j$, and $\Delta = \text{diag}(\delta_1, \dots, \delta_j)$. The pencil (T, Ω) is equivalent to $(\Delta^{-1} T \Delta^{-1}, \tilde{\Omega})$ where $\tilde{\Omega}_{ii} = \omega_i / |\omega_i|$, $i = 1, \dots, j$. The HR algorithm is a generalization of the symmetric tridiagonal QR algorithm. However hyperbolic rotations of the form

$$\begin{bmatrix} \cosh \theta & \sinh \theta \\ \sinh \theta & \cosh \theta \end{bmatrix} \quad \text{or} \quad \begin{bmatrix} \sec \theta & \tan \theta \\ \tan \theta & \sec \theta \end{bmatrix}$$

are used in place of plane rotations whenever the associated diagonal elements of $\tilde{\Omega}$ have opposite signs. Complex shifts may be used without evoking complex arithmetic in the same way as they are used in the unsymmetric QR algorithm.

The only weakness is that the HR algorithm can break down for certain shift values and can also be unstable when the shift is close to breakdown. In addition it will find all the eigenvalues at each step. This is overkill. When the algorithm succeeds it needs approximately $10j^2$ arithmetic operations for a $j \times j$ pair (T, Ω) .

(3) The LR algorithm applied to $\Omega_j^{-1} T_j$.

This is closely related to the HR algorithm. It is efficient, finds all the eigenvalues and can break down.

(4) ANALYZEJ

This application of Laguerre's algorithm was developed for use with the two-sided Lanczos algorithm. A data structure consisting of some eigenvalues of the pencil (T_{j-1}, Ω_{j-1}) together with their error estimates is updated to produce some eigenvalues of (T_j, Ω_j) and their error estimate. These estimates are measures of how close the eigenvalue is to an eigenvalue of the original pair $(A, B - \sigma A)$.

To update one eigenvalue a sequence of Laguerre iterates is computed starting with an old one. The calculation of the Laguerre iterate takes full advantage of the tridiagonal form but complex arithmetic is used. The program is still under development. The difficulty is to detect and find new large eigenvalues that are not close to any at the previous Lanczos step. One remedy is simply to find all eigenvalues of (T_j, Ω_j) at each step.

9 ERROR BOUNDS

Let

$$(T_j - \theta \Omega_j) s = 0, \quad (9.1)$$

with $\|s\| = 1$, define a typical eigenpair (θ, s) of the reduced problem. Let F be the operator given to the Lanczos algorithm and let F be symmetric with respect to A . After j steps, in exact arithmetic,

$$F Q_j - Q_j \Omega_j^{-1} T_j = q_{j+1} (\beta_{j+1} / \omega_{j+1}) e_j^t \quad (9.2)$$

The 'Ritz vectors' corresponding to θ in (9.1) is defined by

$$y := Q_j s. \quad (9.3)$$

To obtain an error bound for the approximate eigenpair (θ, y) one postmultiplies (9.2) by s and uses (9.1) to obtain

$$F y - y \theta = q_{j+1} (\beta_{j+1} / \omega_{j+1}) s(j) \quad (9.4)$$

and

$$\|F y - y \theta\| = (\beta_{j+1} / \omega_{j+1}) |s(j)| \quad (9.5)$$

since $\|q_{j+1}\| = 1$. Unfortunately, it is not possible to evaluate $\|y\|$ without computing y . Note that $y^t A y = s^t \Omega_j s$ but this quantity might be 0 or negative in general.

When A is positive definite then it defines a proper norm on $\mathbb{R}^n$ via

$$\|v\|_A = (v^t A v)^{1/2}$$

In that case $\|q_i\|_A = \sqrt{\omega_i}$, $i = 1, \dots, j$, and

$$\begin{aligned} \|F y - y \theta\|_A &= (\beta_{j+1} / \sqrt{\omega_{j+1}}) |s(j)|, \\ \|y\|_A &= (s^t \Omega_j s)^{1/2}. \end{aligned} \quad (9.6)$$

The following error bound extends well known results for symmetric matrices. Consequently (9.6) yields error bounds without the need for computing with vectors in $\mathbb{R}^n$.

Theorem A. If F is symmetric with respect to a symmetric positive definite A then, for any $y \in \mathbb{R}^n \setminus 0$ and $\theta \in \mathbb{R}$, there is an eigenvalue λ of F satisfying

$$|\lambda - \theta| \leq \|F y - y \theta\|_A / \|y\|_A.$$

Proof :

$$\begin{aligned} \|y\|_A &= \|(F - \theta)^{-1} (F - \theta) y\|_A \leq \\ &\|(F - \theta)^{-1}\|_A \|F y - y \theta\|_A = \|F y - y \theta\|_A / \min_{\lambda} |\lambda - \theta| \end{aligned} \quad \square$$

This result depends strongly on the existence of a full set of A -orthogonal eigenvectors for F and is not valid, or necessary meaningful, when A is indefinite. Thus we cannot use (9.6) just as it is.

For indefinite A we may invoke the results presented in [Kahan, Parlett, and Jiang, 1982] and adapt them to our problem. Two residual norms are required. Let

$$u := F y - y \theta \quad , \quad \bar{v} := \bar{x}^T F - \theta \bar{x}^T \quad , \quad (9.7)$$

where $\bar{y}^T x \neq 0$, $\|y\| = \|x\| = 1$. Now we are obliged to work in $\mathbb{C}^n$ rather than $\mathbb{R}^n$.

Theorem B. With the notation given above $(\theta, y, \bar{x}^T)$ is an eigentriple of $F - E$ for some E satisfying

$$\|E\| \leq \max\{\|u\|, \|\bar{v}\|\} \quad .$$

Note that $\|\bar{v}\| = \|v\|$. In other words, if $\|u\|$ and $\|v\|$ are both tiny then $(\theta, y, \bar{x}^T)$ are an eigentriple for an operator almost indistinguishable from the given one.

In our case, if $F = B^{-1} A$ then $F^T = A B^{-1}$ and we have from (9.4),

$$B^{-1} A y - y \theta = q_{j+1} (\beta_{j+1} / \omega_{j+1}) s(j) \quad .$$

The second residual is obtained easily by premultiplying by A .

$$(A B^{-1}) (A y) - (A y) \theta = A q_{j+1} (\beta_{j+1} / \omega_{j+1}) s(j) \quad .$$

Let

$$\beta(j) = (\beta_{j+1} / \omega_{j+1}) |s(j)| \quad . \quad (9.8)$$

Then $(\theta, y, A y)$ is an eigentriple of $F - E$ for some E satisfying

$$\|E\| \leq \beta(j) \max\left\{ \frac{1}{\|y\|}, \frac{\|A q_{j+1}\|}{\|A y\|} \right\} \quad . \quad (9.9)$$

When the computation has proceeded enough that $|\beta(j)|$ is very small then first order perturbation theory may be invoked to obtain an accurate error estimate for θ by regarding F as a change to $F - E$. If λ is the eigenvalue of F closest to θ we have, in general,

$$|\lambda - \theta| = \frac{\|y\| \cdot \|x\|}{|\bar{y}^T x|} \cdot \frac{|\bar{y}^T E x|}{\|y\| \cdot \|x\|} + O(\|E\|^2) \quad , \quad (9.10)$$

The first term on the left is independent of E and is the condition number of θ as an eigenvalue of $F - E$:

$$\text{cond}(\theta) = \|y\| \cdot \|x\| / |\bar{y}^T x| \quad . \quad (9.11)$$

We now adapt these results to our problem. Note that

$$\|y\| = |\bar{s}^T Q_j^T Q_j s| \leq j |\bar{s}^T s| = j \quad .$$

and

$$\|\bar{y}^T A y\| = |\bar{s}^T Q_j^T A Q_j s| \leq |\bar{s}^T \Omega_j s| \quad .$$

Now we can obtain an error bound. As $\|E\| \rightarrow 0$, using (9.9)

$$\begin{aligned}
 |\lambda - \theta| &\leq \text{cond}(\theta) \cdot \|E\| + O(\|E\|^2) , \\
 &\leq \frac{\|y\| \cdot \|A y\|}{|\bar{y}^T A y|} \beta(j) \max \left\{ \frac{1}{\|y\|}, \frac{\|A q_{j+1}\|}{\|A y\|} \right\} + O(\|E\|^2) , \\
 &\leq \frac{\beta(j)}{|\bar{s}^T \Omega_j s|} \max(\|A y\|, \|A q_{j+1}\| \cdot \|y\|) + O(\|E\|^2) , \\
 &\leq \frac{\beta(j) \sqrt{j}}{|\bar{s}^T \Omega_j s|} \|A\| + O(\|E\|^2) .
 \end{aligned} \tag{9.12}$$

The attraction of the last inequality is that the dominant term can be calculated at step j , without recourse to n -vectors, provided that $\|A\|$ is provided along with the subroutine that multiplies vectors by A . It is useful to compare (9.12) with (9.6) and Theorem A.

We use $\beta(j) / |\bar{s}^T \Omega_j s|$ as a provisional error estimate. When the required number of Ritz values θ have passed this test then, and not before, the Ritz vector y may be computed. At that point the more precise factor

$$\max(\|A y\|, \|A q_{j+1}\| \cdot \|y\|)$$

may be computed at the cost of forming $A y$.

At the end of a Lanczos run a multiple of $A q_{j+1}$ is available and its Euclidean norm can be computed at the cost one dot product. No extra call on A is necessary for that term.

10. NUMERICAL EXAMPLES

In this section, we use several Test Problems to assess the performance of the proposed algorithm to extract the eigenpairs of damped dynamic systems. The mass, damping, and stiffness matrices of discretized systems are computed using the FEAP, a Finite Element Analysis Program, [Zienkiewicz 1977, Chapter 24]. The results reported herein are obtained using a VAX Station II/GPX computer system using the Ultrix 1.2 operating system and the f77 Fortran compiler. To show the savings resulting from the use of selective orthogonalization (SRO), we have added a full re-orthogonalization (FRO) option to our program and present the comparisons in Table 1.

Test problem 1 : The structure is modeled as a cantilever beam with a lumped translational viscous-damper attached at the tip. The beam is modeled using the elementary beam theory where the geometrical configuration and physical properties are shown in Figure 2. The consistent mass is used to define M . The damping matrix C has only one nonzero element representing the magnitude c of the

lumped damper. The cantilever beam is divided into 20 equal elements and has 40 degrees of freedom. The order of the associated (A, B) is 80.

We use the Lanczos algorithm with the FRO scheme to solve this problem. Figure 3 summarizes the results of 8 experiments. Here, we call a Ritz pair *good* if the pseudo length of its associated residual vector is less than 10^{-8} . This criterion ensures that a good Ritz pair approximates the wanted eigenpair to high accuracy. From the results in Figure 3, we see that the first few eigenpairs can be extracted at a fairly low cost compared to the other eigenpairs. This is because the re-orthogonalization cost is greater at later steps in the Lanczos algorithm.

In this problem, we have run the algorithm to compute all eigenvalues in order to test the robustness of the computer program developed. However we emphasize that the algorithm is intended only for partial solution of a large eigenproblem. After the 80 steps, we see that the pseudo length of the 81th Lanczos vector is 0.9×10^{-15} , which is at the round-off level, implying that the computed Lanczos vectors have spanned the whole solution space as they should in exact arithmetic. This desirable result will ensure that all the Ritz pairs obtained from the solution of the reduced tri-diagonal system are good and hence are accurate eigenpairs of the system.

Test Problem 2 : The system consists of two beams connected by a hinge with a rotational viscous-damper. The geometrical configuration and physical properties of the system are shown in Figure 4. The consistent mass matrix is used for M . The damping matrix C has only four nonzero elements, which are due to the lumped rotational damper. The system is divided into 40 equal elements and has 83 degrees of freedom. The associated (A, B) is of order 166. The system is unrestrained and has rigid body modes, so we apply a shift to the (A, B) to compute the eigenpairs of this unrestrained system. The Lanczos algorithm with FRO scheme is used to solve this problem. Figure 5 summarizes the results of 9 experiments. Similar conclusions as in the first test problem can be inferred from Figure 5. The pseudo length of the 167th Lanczos vector is 0.1×10^{-14} , which again exhibits the robustness of the computer program developed.

In general, the starting vector for the Lanczos algorithm may be chosen arbitrarily. However, if the starting vector is orthogonal to any of the eigenvectors of (A, B) , all the Lanczos vectors will also be orthogonal to these eigenvectors. In practice, round-off errors eventually will introduce components along these eigenvectors; however, round-off enters slowly and the convergence to these eigenvectors is deferred. Therefore, we need to avoid the possibility of the starting vector being orthogonal to the wanted eigenvectors of the system. Since the structural system in this test problem is symmetric, there are anti-symmetric modes as well as symmetric modes. If a symmetric starting vector is used, such as $(1, 1, \dots, 1)$, all the Lanczos vectors will be symmetric. Accordingly, all the anti-symmetric modes of

the structure will be suppressed by this biased starting vector. To obtain all the required lower modes, we must avoid choosing either a symmetric or an anti-symmetric starting vector. This is a strong reason for using a random vector to start.

Test Problem 3 : This problem is a three dimensional space truss system. There are 44 nodes and the 4 end nodes are fully restrained, as shown in Figure 6. Thus, there are 120 degrees of freedom and the associated (A, B) is of order 240. All truss bars have the same density and Young's modulus but different damping, as shown in Figure 6, resulting in a nonproportionally damped system. We use the Lanczos algorithm with the FRO scheme to generate 60 Lanczos vectors. We also use the Lanczos algorithm with the proposed SRO scheme to generate 60 Lanczos vectors. The results from the two schemes are compared in Table 1. The SRO scheme is shown to be adequate to compute the desired solution.

Test Problem 4 : This problem is a larger three dimensional space truss system. There are 300 nodes and the 4 end nodes are fully restrained, as shown in Figure 7. A typical cell is the same as the typical cell in the test problem 3. There are 888 degrees of freedom and the order of the associated (A, B) is 1776. We use the Lanczos algorithm with the FRO scheme to generate 80 Lanczos vectors. We also use the Lanczos algorithm with the SRO scheme to generate 80 Lanczos vectors. The results from the two schemes are also compared in Table 1.

From Table 1, we see that the 60 Ritz pairs obtained provide 28 good eigenpairs for test problem 3 and the 80 Ritz pairs obtained provide 40 good eigenpairs for test problem 4 for both FRO and SRO cases. That is, approximately two Lanczos vectors, on the average, are required to capture a new eigenvector for these two large problems. This implies that the Krylov subspace generated by $B^{-1}A$ and a random vector is very effective in approximating the least dominant eigenvectors of the damped dynamic systems considered.

By maintaining semi-orthogonality between the Lanczos vectors with the SRO scheme, the resulting Ritz values are as accurate as those obtained with the FRO scheme, as shown in Table 1. But a great part of the re-orthogonalization steps can be eliminated by using the SRO scheme instead of the FRO scheme. That is, we can eliminate partial re-orthogonalization effort without sacrificing accuracy of the final solution when solving $\lambda A z = B z$ with the SRO scheme. This is in agreement with the case of solving $\omega^2 M w = K w$ by a standard Lanczos algorithm with the SRO scheme.

To assess the efficiency of the Lanczos algorithm, the lower mode solutions of the above four test problems are also computed using a subspace iteration algorithm. The subspace iteration algorithm reported in [Chen and Taylor, 1986] is used for this purpose. The subspace dimension is determined by $\min\{2n, n+8\}$, where n is the number of wanted eigenpairs. Table 2 compares the cost of the Lanczos

Table 1 Results of Test Problems 3 and 4

item problem	Test Problem 3		Test Problem 4	
	FRO	SRO	FRO	SRO
number of Lanczos vectors generated	60	60	80	80
number of re-orthogonalizations	1770	602	3159	1246
CPU time spent on generating Lanczos vectors	40.3	32.6	536.6	473.5
CPU time spent on solving reduced eigenproblem	50.8	51.7	100.9	101.2
total CPU time spent on solving the whole problem	113.9	106.7	893.2	830.9
number of good Ritz pairs obtained	28	28	40	40

algorithm with the cost of the subspace iteration algorithm. It is apparent that the Lanczos algorithm is considerably more efficient than the subspace iteration algorithm for the examples considered. However more sophisticated versions of subspace iteration might perform somewhat better than ours but not enough to alter the striking contrasts in Table 2.

Breakdown occurs when $\omega_j = 0$ for some j . The algorithm provides a bad basis if there are any ω_j as small as $\sqrt{\epsilon} = 10^{-8}$. In Figure 8 we plot the $\text{sign}(\omega_j) * \log \frac{1}{|\omega_j|}$ against j . The result is typical for our examples. Quite quickly $|\omega_j|$ drops to 10^{-3} but seems to stay at that level without deteriorating for 120 steps. We have no explanation of this phenomenon.

Acknowledgement The authors would like to thank Professor R. L. ylor (Department of Civil Engineering), Zhishun Liu (Mathematics Department), and Dr. Bahram No mid (Lockheed Palo Alto Research Labs) for valuable discussions.

Table 2 Results from different algorithms

Test Problem	Lanczos algorithm		subspace iteration algorithm	
	No. of good Ritz pairs	CPU time (second)	No. of good Ritz pairs	CPU time (second)
1	8	8.5	8	40.2
2	20	41.7	16	214.6
3	28	113.9	24	1012.9
4	40	893.2	40	20992.8

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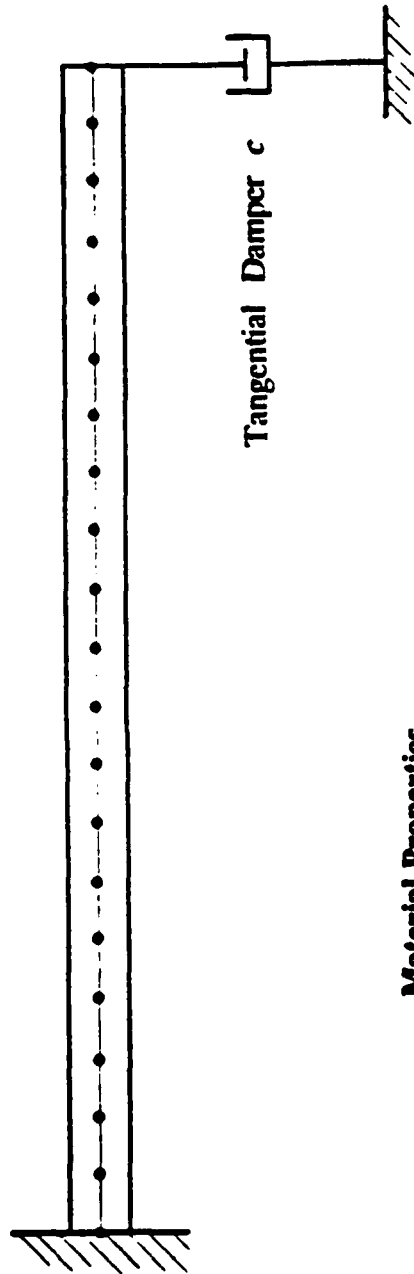
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Figure 1 Outline of Lanczos inner loop with operator $H^{-1}A$

Step 1 :	Operation Count
pick a starting vector r (default is random) $p = A r$ solve $H q = p$ $\beta_1 = q^T q ^{1/2}$ $q \leftarrow q / \beta_1$ $p = A q$ $\omega_1 = (q^T p)$ solve $H r = p$ $\alpha_1 = (r^T p)$ $r \leftarrow r - q (\alpha_1 / \omega_1)$ $oldp = A r$ $\beta_2 = r^T r ^{1/2}$ $\omega_2 = (r^T oldp) / r^T r$ store q as q_1	$2\mu(M) + \mu(C)$ $v(K)$ $2n$ $2n$ $2\mu(M) + \mu(C)$ $v(K)$ $2n$ $2n$ $2\mu(M) + \mu(C)$ $2n$
Loop : For $j = 2, 3, \dots$	Operation Count
$oldq \leftarrow q$ $oldp \leftarrow p$ $q = r / \beta_j$ $p \leftarrow p / \beta_j$ solve $H r = p$ ($r^T oldp$ should equal β_j) $r \leftarrow r - oldq (\beta_j / \omega_{j-1})$ $\alpha_i \leftarrow r^T p$ $r \leftarrow r - q (\alpha_j / \omega_j)$ $oldp = A r$ $\beta_{j+1} = r^T r ^{1/2}$ $\omega_{j+1} = (r^T oldp) / r^T r$ (repeat to maintain local orthogonality) store q as q_j	$2n$ $2n$ $v(K)$ $2n$ $2n$ $2n$ $2\mu(M) + \mu(C)$ $2n$



Material Properties

modulus	1000
length	5
density	1
inertia	1
area	1

Figure 2 Test Problem 1

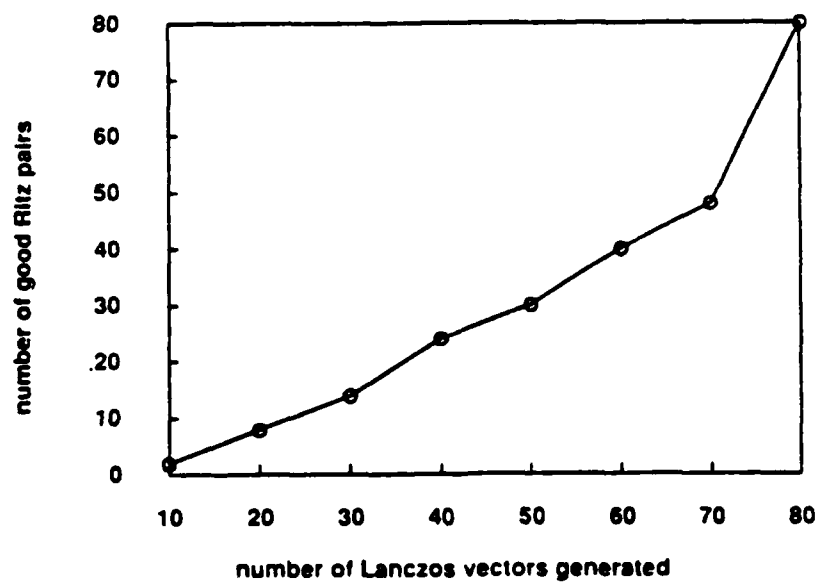
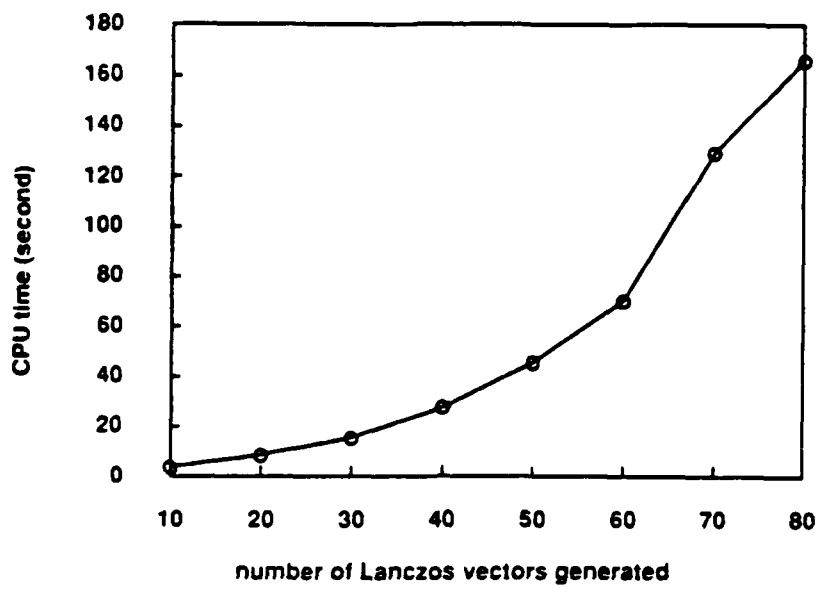
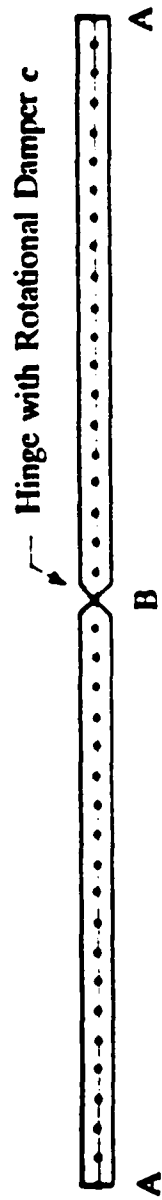


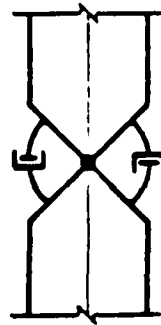
Figure 3 Results of Test Problem 1



Material Properties

beam	1	2
modulus	1000	1000
length	20	20
density	1	1
inertia	1	1
area	1	1

$$M = c \dot{\Delta\theta}$$



Detail for Rotational Damper

Figure 4 Test Problem 2

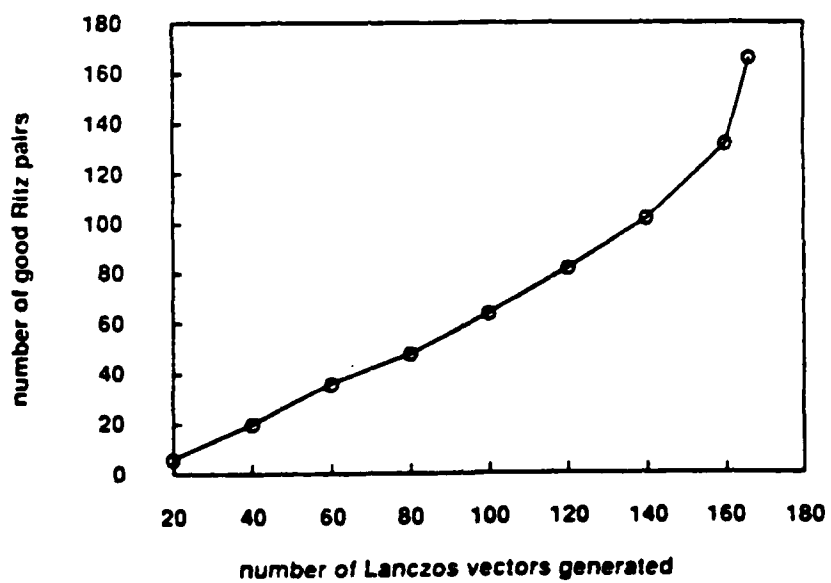
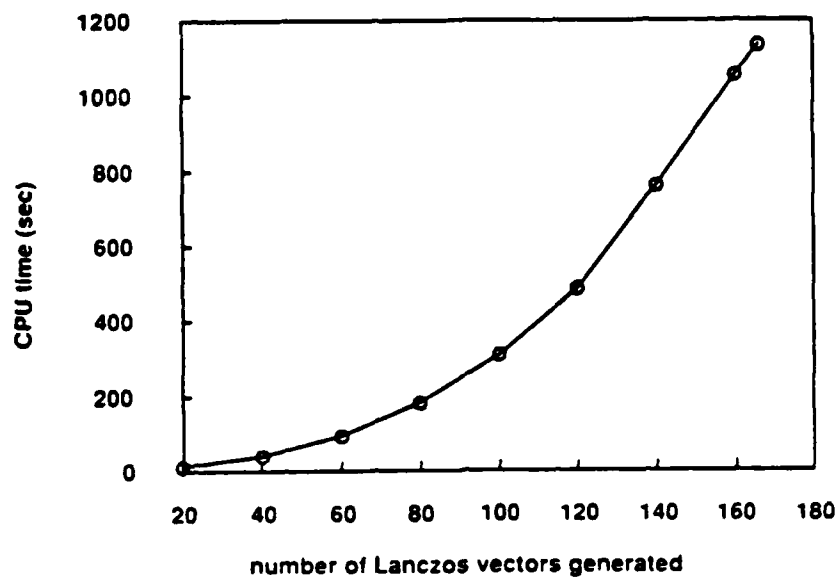
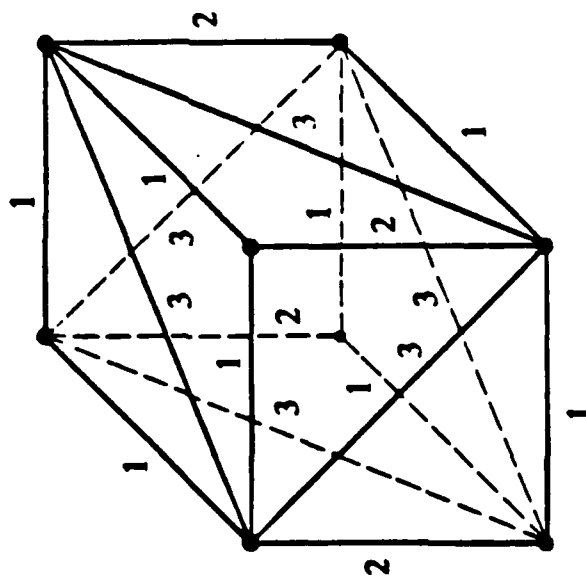
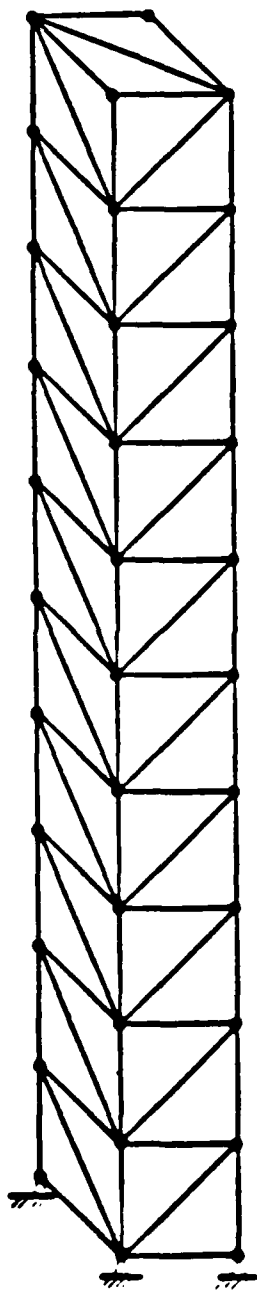


Figure 5 Results of Test Problem 2



Typical Cell

Material Properties

member	1	2	3
modulus	1	1	1
density	1	1	1
inertia	1	1	1
area	1	1	1
damping	0.5	1.0	2.0

Figure 6 Test Problem 3

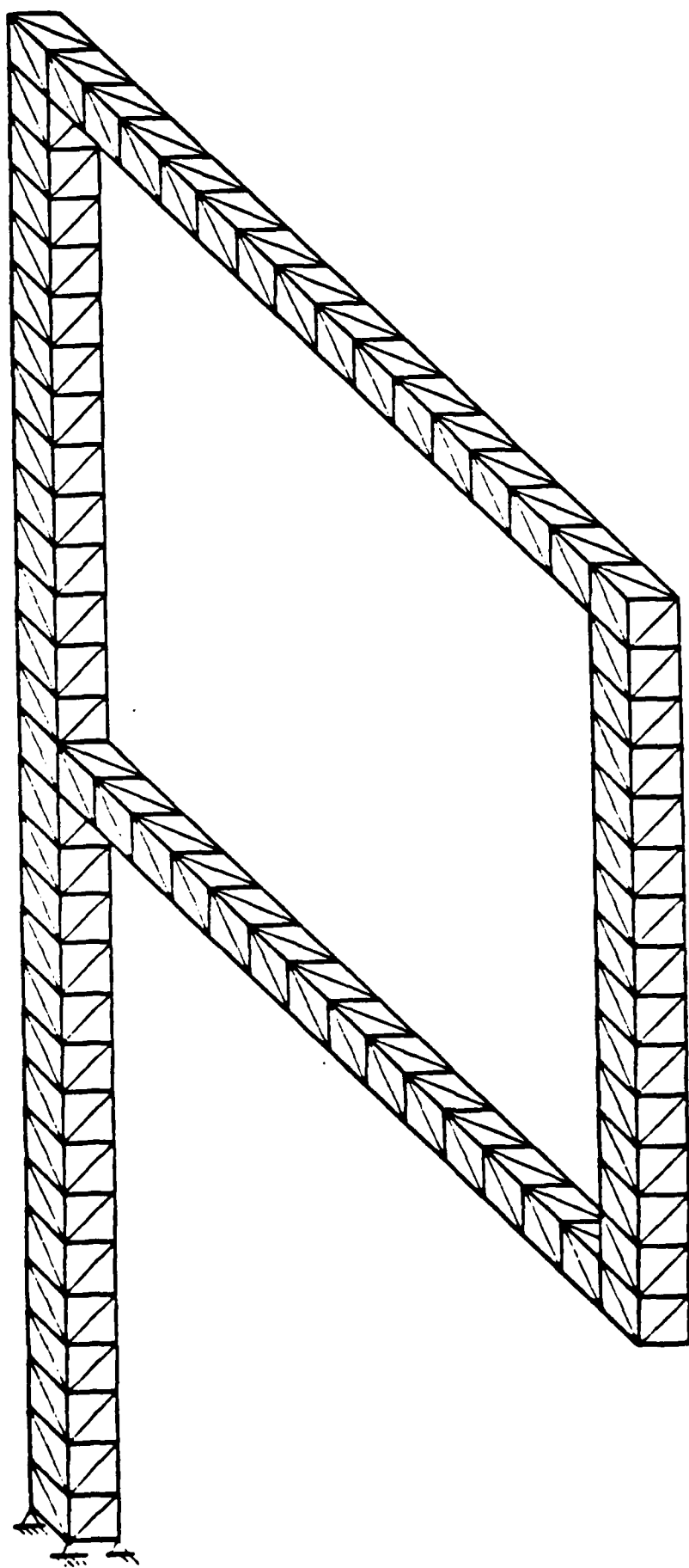


Figure 7 Test Problem 4

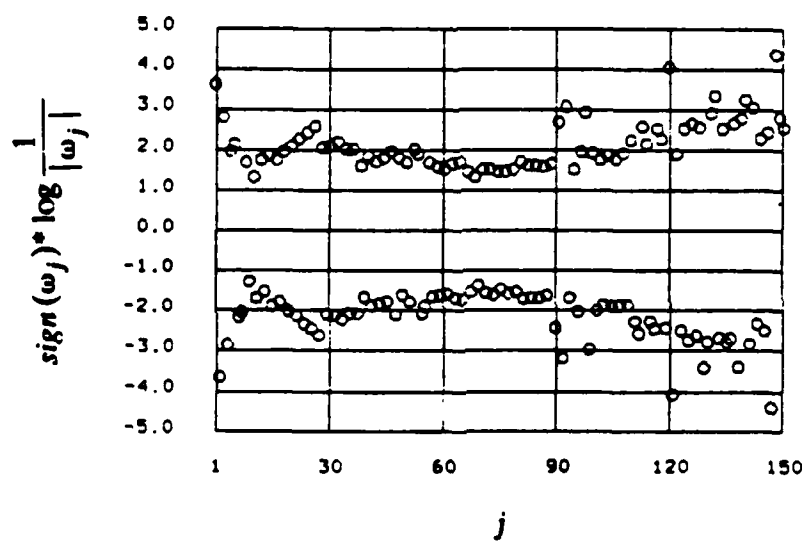


Figure 8 $\text{sign}(\omega_j) * \log \frac{1}{|\omega_j|}$ versus j