The components and subscripts of the vector Eqs. (A34) and (A35) may be obtained by the following relationship:

i	R	V	Λ	j
1	x	V_x	h	4
2	y	V_y	a	5
3	z	V_z	b	6

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Vibration Modes of Large Structures by an Automatic Matrix-Reduction Method

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An automatic matrix reduction method is presented whereby the lower modes of structural systems with many degrees-of-freedom can be extracted by solving an eigenvalue problem of much smaller size than the actual inertia matrix. The process is effected without arbitrary lumping of masses at judiciously selected physical node-points. The method is based upon Crandall's tailoring of an eigenvalue routine created by Lanczos. The present work corrects the basic weakness in the original method, which is its numerical instability. In addition, practical suggestions for the method's implementation are made and some empirically-based conclusions are drawn concerning the relationship between the exact and reduced frequency spectrums.

Nomenclature

$[A],[B]$ = positive definite and symmetric matrices ($n \times n$)
$\{C\}$ = modal components of starting vector $\{v_1\}$
c_i = element of $\{C\}$ vector
$[I]$ = identity matrix
$[K]$ = assembled stiffness matrix ($n \times n$)
$[M]$ = assembled mass matrix ($n \times n$)
m = number of reduced degrees-of-freedom
n = number of original unreduced degrees-of-freedom
$[V]$ = transformation matrix used to effect reduction from n to m degrees-of-freedom ($n \times m$)
$\{v_i\}$ = Lanczos vectors
$\{v_i^*\}$ = see Eq. (10)
$\{\bar{v}_i\}$ = see Eq. (26)
$\{v_i^{(s)}\}$ = see Eq. (27)
$[X]$ = modal matrix for original system ($n \times n$)
$\{x\}$ = eigenvector of original system
$\{y\}$ = generalized coordinate of reduced $m \times m$ system
α_i = see Eqs. (9) and (20)
β_i = see Eqs. (13) and (18)
$\gamma_{i,j}$ = see Appendix
δ_{ij} = Kronecker delta; equals $\begin{cases} 1 \text{ for } i = j \\ 0 \text{ for } i \neq j \end{cases}$
λ = eigenvalue of unreduced system
λ_R = Rayleigh quotient and eigenvalue of reduced system
$[\lambda]$ = diagonal eigenvalue matrix of unreduced system
μ_i = see Eq. (8)
ω = natural frequency of unreduced system
$[\ ]^T$ = denotes matrix transpose
$\{\ \}^T$ = denotes vector transpose or row vector

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Introduction

STATIC, elastic stress analyses by computerized finite-element methods have evolved to a high level of sophistication and accuracy[1,2] and are now accepted as necessary tools in the analysis of extremely complex structures. The

current state-of-the-art is such that system idealizations with thousands of degrees of freedom may be systematically assembled by programing techniques based on linear matrix analysis.

At the same time, the extension of these analyses to solve structural dynamic problems for natural vibration modes, or transient responses by modal techniques, has been hampered by difficulties in accurately and efficiently handling eigenvalue problems of comparably large size. Initially, this matrix-size problem was disposed of by simple "lumping" techniques, i.e., replacing the system's mass distribution by an approximating set of discretized masses at a limited number of structural node points. This procedure was guided by intuition, the size of the problem which the computer could handle, and the desire to account for the original system's total mass in the reduced system.

Eventually, this approach was improved upon by Archer,[3] and later by Guyan,[4] and Kaufman and Hall.[5] In the works of these investigators, an attempt was made to account for the distributed nature of a system's mass through equivalent energy techniques. All of these methods are, in various ways, based upon assumed displacement functions and the judicious selection of reduced mass nodes. Hurty[6] formalized the approach of coupling together various portions of a structure (called substructures or components) to approximate the dynamic behavior of an entire structure. This approach makes use of generalized coordinates associated with only the lower modes of each structural component and displacement functions associated with motions of the connecting points. Once again, the number of modes chosen for each substructure, and the selection of special node-points to establish the substructure junctions, remained an arbitrary matter. Thus, even if we assume that the structure has been well idealized from an elastomechanics viewpoint, the accuracy which can be achieved with the current eigenvalue reduction methods would seem to depend, to a large extent, upon the skill of the analyst in mass-lumping or mode selection.

This paper presents a different approach to the problem of reducing the matrix size of a dynamic system which avoids the arbitrary selection of judicious node points at which to lump the system masses. The method is based upon Lanczos' algorithm[7] and the reduction was suggested by Crandall.[8] However, a necessary improvement to make the method numerically stable and practical has been developed.

Historically, Lanczos' method was first considered to be purely an n-step iteration procedure, which would transform an eigenvalue problem into one of simpler form in exactly n-steps; the solution of the simpler eigenproblem being facilitated by the fact that its matrix form was tridiagonal and that the eigenvalues could be readily extracted through a succession of approximating polynomials which eventually built up to the exact n-root characteristic polynomial. However, Crandall[8] envisioned that the procedure could be truncated to fewer ($m < n$) steps, and thus the method could be used as a basis for an approximate scheme. Unfortunately, it was soon discovered that the original method was numerically unstable[9,10] and so it fell into disfavor. Another factor adversely affecting its popularity is that, for the case when $m = n$, it yields results which are comparable to the Householder tridiagonalization scheme (which does not exhibit these instabilities), thus causing Wilkinson to write (see p. 395 of Ref. 10) "... it is difficult to think of any reason why we should use Lanczos' method in preference to Householder's."

Causey and Gregory[11] experimented with various ways of improving the accuracy of Lanczos' method and achieved some, but insufficient, success for very large systems. The iterative improvement procedure described in the present work has proven to be highly successful in a number of structural-dynamic applications.[12–14] Its effectiveness is demonstrated in this paper by a specific numerical application and comparisons with the nodal-selection method.

Problem Definition

A mathematical statement of the eigenvalue problem considered is

$$[A]\{x\} = \lambda[B]\{x\} \tag{1}$$

where $[A]$ and $[B]$ are $n \times n$ positive definite symmetric matrices. Thus, if the structural equations of free vibrations are formulated by the displacement method of finite element analysis,

$$[A] = [K],\ [B] = [M],\ \text{and}\ \lambda = \omega^2$$

Under these conditions, Eq. (1) becomes

$$[K]\{x\} = \omega^2[M]\{x\} \tag{2}$$

where $[K]$ and $[M]$ are the system's assembled stiffness and mass matrices, respectively, and the elements of $\{x\}$ are the nodal displacements of the mode with natural frequency ω.

If the force method of analysis is used, the flexibility matrix, $[K]^{-1}$, is first generated and multiplication of Eq. (2) by $1/\omega^2[M][K]^{-1}$ again yields the form given by Eq. (1), except that now

$$[A] = [M][K]^{-1}[M]$$

$$[B] = [M]$$

and

$$\lambda = 1/\omega^2$$

In either case, what is desired are accurate approximations to the lower frequencies ω and corresponding mode shapes, for large systems (large in the sense that computations for the unreduced eigenvalue problem are either beyond the capabilities of available computer facilities or prohibitively time-consuming). In addition, if the results are to be useful in dynamic response calculations by modal techniques, an accounting for higher-mode participation is also necessary.

A useful means of formulating approximate equations for freely vibrating discrete systems is via the definition of Rayleigh's quotient

$$\lambda_R = \{\bar{x}\}^T[A]\{\bar{x}\}/\{\bar{x}\}^T[B]\{\bar{x}\} \tag{3}$$

where $\{\bar{x}\}$ is an approximation to $\{x\}$. The relative accuracy of methods based upon this formulation results from the fact that the eigenvalues λ are stationary with respect to perturbations in the elements of $[A]$, $[B]$, and eigenvectors, $\{x\}$.

Thus, if a transformation for the n physical-node displacements, $\{\bar{x}\}$, into fewer ($m < n$) generalized coordinates is available, say,

$$\underset{n\times 1}{\{\bar{x}\}} = \underset{n\times m}{[V]}\ \underset{m\times 1}{\{y\}} \tag{4}$$

the corresponding Rayleigh quotient becomes

$$\lambda_R = \{y\}^T[V]^T[A][V]\{y\}/\{y\}^T[V]^T[B][V]\{y\} \tag{5}$$

Making λ_R stationary with respect to arbitrary variations in the m elements of $\{y\}$ yields the reduced eigenequation

$$[V]^T[A][V]\{y\} = \lambda_R[V]^T[B][V]\{y\} \tag{6}$$

If the reduction from the original system's n coordinates to m are viewed as imposing $n - m$ constraints upon the original system, then Rayleigh's Theorem[15] states

$$\lambda^{(j)} \leq \lambda_R{}^{(j)} \leq \lambda^{(j+n-m)} \qquad j \leq m$$

where the exact and approximate eigenvalue sets are ordered according to increasing eigenvalue-magnitude [e.g., $\lambda^{(1)} < \lambda^{(2)}$].

Thus, all the λ_R are contained between $\lambda^{(1)}$ and $\lambda^{(n)}$ and the approximations become exact for $m = n$, i.e.,

$$\lambda_R{}^{(j)} = \lambda^{(j)} \qquad n = m$$

The essence of the reduction scheme lies in the definition of the transformation matrix $[V]$. For example, it is well known that a $[V]$ matrix made up of exact modal vectors would yield diagonal, reduced $(m \times m)$ matrices for $[V]^T[A][V]$ and $[V]^T[B][V]$ in Eq. (6). In the present work, Lanczos' algorithm is used to build up the $[V]$ matrix, vector by vector, $\{v_i\}$, i.e.,

$$\underset{n\times m}{[V]} = [v_1 \mid v_2 \mid \ldots \mid v_m] \tag{7}$$

such that the reduced matrices, $[V]^T[B][V]$ and $[V]^T[A][V]$, are diagonal and tridiagonal, respectively, and the eigenvalues of the reduced system accurately approximate the higher end of the eigenspectrum of $[B]^{-1}[A]$.

Lanczos-Crandall Computational Procedure

Following Crandall's[8] development of Lanczos' method, for systems in the form of Eq. (1), the $\{v_i\}$ are generated in the following manner: set $i = 1$ and select an n-element vector $\{v_1\}$,

1) compute

$$\mu_i = \{v_i\}^T[B]\{v_i\} \tag{8}$$

2) compute

$$\alpha_i = (1/\mu_i)\{v_i\}^T[A]\{v_i\} \tag{9}$$

3) compute

$$\{v_{i+1}{}^*\} = [B]^{-1}[A]\{v_i\} \tag{10}$$

4) set

$$\{v_2\} = \{v_2{}^*\} - \alpha_1\{v_1\} \tag{11}$$

5) for $i = 2,3, \ldots, (m-1) \leq (n-1)$ compute

$$\{v_{i+1}\} = \{v_{i+1}{}^*\} - \alpha_i\{v_i\} - \beta_{i-1}\{v_{i-1}\} \tag{12}$$

where

$$\beta_{i-1} = (1/\mu_{i-1})\{v_{i-1}\}^T[A]\{v_i\} \tag{13}$$

and the μ's, α's, and $\{v^*\}$'s are given by Eqs. (8–10).

Experimentation with the algorithm outlined in Eqs. (8–13) revealed that numerical precision problems rapidly overpowered the computational accuracy. Thus, effective measures for correcting the difficulties are offered in the following section. However, before elaborating upon these, several theoretical conclusions of practical significance are noted here and in the Appendix.

It is easily seen that the construction of every $\{v\}$ involves a Schmidt orthogonalization of each new vector with the two previous vectors only. However, it can also be shown (see Appendix), theoretically at least, that all the $\{v\}$'s are mutually orthogonal with respect to the weighting matrix $[B]$, i.e.,

$$\{v_i\}^T[B]\{v_j\} = \mu_i\delta_{ij} \qquad i,j \leq m \tag{14}$$

where δ_{ij} is the Kronecker delta.

Besides the restriction that m be no greater than n, $\{v_1\}$ must also satisfy the requirement that it contain at least m components of the original system's eigenvectors (as defined by the usual eigenvector expansion form of a vector). The significance of this consideration with regard to the numerical generation of appropriate vectors is discussed in the following subsections. Referring to Eq. (12), it is noted that the leading term in the creation of each $\{v_i\}$ is identical to the generation of each vector by the power method.[10] Since the power method yields the eigenvalues in descending order (highest one first) and the lower modes are of greatest interest, it is generally desirable to let $[A] = [M][K]^{-1}[M]$, $[B] = [M]$ and $\lambda = 1/\omega^2$; we could also set $[A] = [L]^{-1}[M][L^t]^{-1}$, $[B] = [I]$ and $\lambda = 1/\omega^2$, where $[L]$ is the lower triangular decomposition of $[K]$.

Improved Computational Procedure

Selection of a Starting Vector

An exact modal expansion of the initial guess vector is given by

$$\{v_1\} = [X]\{C\} \tag{15}$$

where $[X]$ is the $n \times n$ matrix whose columns are the system eigenvectors. Substituting Eq. (15) into the relation for $\{v_2\}$ [Eq. (11)], we find that

$$\{v_2\} = [B]^{-1}[A][X]\{C\} - \alpha_1[X]\{C\} \tag{16}$$

which by Eq. (1) yields

$$\{v_2\} = [X](\lceil\lambda\rfloor - \alpha_1[I])\{C\} \tag{17}$$

where $\lceil\lambda\rfloor$ is the diagonal matrix of system eigenvalues and $[I]$ is the $n \times n$ identity matrix. Thus, if any element, c_i, of $\{C\}$ is zero, the corresponding eigenvector, $\{x^{(i)}\}$, will make no contribution to $\{v_2\}$ either. Furthermore, a continuation of this generation process for the remaining $\{v\}$'s reveals that $\{x^{(i)}\}$ will contribute to none of the $\{v_i\}$ if $c_i = 0$.

It is, therefore, evident that progressively poorer eigenvector approximations will be generated in the Lanczos scheme as the number of eigenvector components which are absent from the initial guess vector increases.

Finally, since the $\{v_i\}$ are mutually orthogonal, the initial vector $\{v_1\}$ must contain at least m eigenvectors $(m \leq n)$; otherwise the $[V]$ construction process will eventually degenerate to the point where a zero column appears, i.e.,

$$\{v_j\} = \{0\}, \qquad j \leq m$$

and the remaining vectors cannot be generated.

It should also be noted that this premature vanishing of the $\{v\}$-vectors will occur, no matter what choice is made for $\{v_1\}$, if the system contains repeated eigenvalues. In this case, a maximum of $n - p$ vectors can be generated by Eqs. (8–13), where p is the number of multiplicities[10].

If for either of the aforementioned reasons, a null $\{v\}$-vector is encountered, it is always possible to continue the process by choosing, for the current vector, any vector which is orthogonal to the preceding ones.

From the preceding discussion, it is evident that a desirable $\{v_1\}$ is one for which $c_i \neq 0$, for all $i \leq n$ in Eq. (15). However, since there is generally no a priori knowledge of the modal matrix, $[X]$, $\{v_1\}$ should be selected in such a way as to make it as "irregular," with regard to the system eigenvectors, as possible so that it is then more likely to contain a mixture of all the mode shapes. Empirically speaking, it has been found that this is best achieved through the use of a random number generator routine to obtain each of the elements of $\{v_1\}$. Furthermore, the resulting eigenproblem, Eq. (6), appears relatively insensitive to the various starting vectors which are generated in this manner.

Numerical Scaling and Tridiagonalization of the Reduced System

Repeated multiplication of the $\{v_i\}$ by $[B]^{-1}[A]$[See Eq. (10)] leads to unnecessary magnification or contraction (depending upon whether the largest eigenvalue is greater

or less than unity, respectively) of the vectors, which can easily lead to computational difficulties. Therefore, a numerical scaling procedure which avoids these problems, and which leads to a simple form for the reduced eigenequation, is presented: Set $i = 1$; select $\{\bar{v}_1\}$ as per the previous subsection,

1) compute

$$\beta^2_{i-1} = \{\bar{v}_i\}^T[B]\{\bar{v}_i\} \tag{18}$$

2) set

$$\{v_i\} = \{\bar{v}_i\}/\beta_{i-1} \tag{19}$$

3) compute

$$\alpha_i = \{v_i\}^T[A]\{v_i\} \tag{20}$$

4) compute

$$\{\bar{v}_2\} = [B]^{-1}[A]\{v_1\} - \alpha_1\{v_1\}$$

5) for $i = 2,3,\ldots,(m-1) \leq (n-1)$, compute

$$\{\bar{v}_{i+1}\} = [B]^{-1}[A]\{v_i\} - \alpha_i\{v_i\} - \beta_{i-1}\{v_{i-1}\} \tag{21}$$

where the α's, β's, and $\{v\}$'s are given by Eqs. (18–20).

A typical element of the $m \times m$ matrix $[V]^T[A][V]$, appearing in the reduced eigenproblem [given by Eq. (6)], is $\{v_i\}^T[A]\{v_j\}$. This can be conveniently expressed in terms of the α's and β's, via Eq. (21), as shown below,

$$\{v_i\}^T[A]\{v_j\} = \{v_i\}^T[B]([B]^{-1}[A]\{v_j\}) = \{v_i\}^T[B](\bar{v}_{j+1} + \alpha_j\{v_j\} + \beta_{j-1}\{v_{j-1}\}) \tag{22}$$

Applying the orthogonality condition Eq. (14) to the right side, and noting that Eqs. (18) and (19) make $\mu_i = 1$, yields

$$\{v_i\}^T[A]\{v_j\} = (\beta_j\delta_{i,j+1} + \alpha_j\delta_{i,j} + \beta_{j-1}\delta_{i,j-1}) \tag{23}$$

Thus, Eq. (6) assumes the form

$$[V]^T[A][V]\{y\} = \lambda_R\{y\} \tag{24}$$

where $[V]^T[A][V]$ is tridiagonal and symmetric,

$$[V]^T[A][V] = \begin{bmatrix} \alpha_1 & & & & \\ \beta_1 & \alpha_2 & & \text{Symmetric} & \\ 0 & \beta_2 & \alpha_3 & & \\ & & & & \\ 0 & & 0 & \beta_m & \alpha_m \end{bmatrix} \tag{25}$$

and Eq. (24) is readily solvable by any number of standard eigensolution methods.[10]

Orthogonality Corrections

Although the vectors $\{v_i\}$, as generated by Eqs. (8–13), form a theoretically orthogonal set, experience[11] has shown that the corresponding numerical results degrade rapidly as the computations proceed such that the later $\{v_i\}$'s are far-removed from orthogonality to the earlier ones. This is caused by the repeated multiplications, to generate new $\{v\}$'s, by $[B]^{-1}[A]$ which tends to amplify the contributions of the $\{v_i\}$ eigenvector components in proportion to the associated eigenvalues. Thus, because of unavoidable computational roundoff or truncations, drifting of the later $\{v\}$'s results such that solution of the corresponding reduced system, Eq. (6), yields a false "bunching" of eigenvalues at the higher end. To correct this problem, Gregory[9] experimented with the use of higher-precision computer operations, but found only a marginal improvement in the final results.

Later, Lanczos, himself, suggested a reorthogonalization correction procedure of the form

$$\{v_i\} = \{\bar{v}_i\} - \sum_{j=1}^{i-1} \frac{\{v_{i-j}\}^T[B]\{\bar{v}_i\}}{\mu_{i-j}}\{v_{i-j}\} \tag{26}$$

where $\{\bar{v}_i\}$ is the value of $\{v_i\}$ as computed by Eq. (12). While this improves matters substantially, it still does not eliminate the precision problem adequately. However, the present authors have found that the introduction of an iterative reorthogonalization loop, as outlined below, can make the $\{v_i\}$ as orthogonal as necessary for extremely large original systems, i.e.,

1) compute

$$\{\bar{v}_i^{(s+1)}\} = \{\bar{v}_i^{(s)}\} - \sum_{j=1}^{i-1}\{v_{i-j}\}^T[B]\{\bar{v}_i^{(s)}\}\{v_{i-j}\} \tag{27}$$

$$s = 1,2,\ldots;\ i = 2,3,\ldots,m$$

2) test all coefficients of $\{v_{i-j}\}$ until

$$\{v_{i-j}\}^T[B]\{\bar{v}_i^{(s)}\} < \epsilon \tag{28}$$

(where ϵ is some arbitrarily small specified tolerance)

3) after Eq. (28) is satisfied, set

$$\{\bar{v}_i^{(s+1)}\} = \{\bar{v}_i\} \tag{29}$$

Steps 1–3, given by Eqs. (27–29), should be performed immediately after Eq. (21). In this way, the mutual orthogonality of the $\{v\}$'s can be preserved to the very high level of accuracy required for systems which originally are very large.

Numerical Results and Conclusions

For illustrative purposes, the present method was employed to reduce a structural assemblage of bar, beam, and plate elements with 44 nodal-mass degrees-of-freedom to a system with 30 dynamic degrees-of-freedom. For comparison purposes, the frequencies were also computed by the reduction method of Ref. 5. The numerical results for these solutions are presented in Table 1, along with the exact 44 frequencies of the unreduced system.

The judicious elimination procedure, used in conjunction with the method of Ref. 5, was based upon retaining those thirty degrees-of-freedom associated with the largest diagonal elements of the flexibility matrix. This seemed logical since the elements of the diagonal mass matrix were all equal, and the lower system frequencies were of greatest interest.

With reference to the numerical results of Table 1, the first 15 frequencies of the complete system ($n = 44$), truncated to $m = 30$ via the method of Ref. 5, are accurate to within $\frac{1}{4}\%$ (except for the 12th which is off by a few percent), whereas the present method yields 22 frequencies within the same tolerance.

It should also be noted that the frequencies are more uniformly distributed for the present method. This may be seen with the aid of Fig. 1, which shows the exact eigenvalues beyond the 15th plotted successively as points, and the eigenvalues of both reduction methods plotted by horizontal lines. Note that the remaining frequencies, calculated by the present method, tend to reflect the centroids of various groupings of exact frequencies. However, the higher frequencies, by the method of Ref. 5, appear much more random with respect to the exact system frequency spectrum, which is probably due to the somewhat arbitrary selection of the reduced degrees of freedom. The present method was used to obtain the modal response results of a 292 degree-of-freedom structural dynamic idealization of a ship's deckhouse, subject to a blast loading.[12] The results, which were based upon a reduction to 100 degrees of freedom, compared favorably with those obtained experimentally. Based upon these

Table 1 Comparison of exact (unreduced-system) and approximate (reduced-system) frequencies

Mode number	44 exact frequencies (Jacobi's method), cps	30 reduced-system frequencies		Mode number	44 exact frequencies (Jacobi's method), cps	30 reduced-system frequencies	
		Present method, cps	Kaufman-Hall method (Ref. 5), cps			Present method, cps	Kaufman-Hall method (Ref. 5), cps
1	2.233	2.233	2.233	23	79.44		82.45
2	5.558	5.558	5.558	24	83.59		83.57
3	7.035	7.035	7.035	25	89.97	89.22	
4	8.468	8.468	8.468	26	99.62		
5	9.730	9.730	9.730	27	102.9	101.9	102.8
6	11.73	11.73	11.73	28	106.7		104.1
7	14.17	14.17	14.17	29	112.3	109.7	
8	19.06	19.06	19.06	30	127.0		
9	21.43	21.43	21.68	31	130.1	130.5	
10	21.95	21.95	22.07	32	147.0		
11	26.91	26.91	26.95	33	162.1		161.2
12	28.90	28.90	30.81	34	162.3		
13	37.00	37.00	37.22	35	169.0	166.4	166.9
14	39.00	39.00	39.16	36	192.1		
15	44.87	44.87	44.97	37	202.3		
16	48.71	48.71		38	206.1		205.9
17	52.09	52.09		39	209.9	209.5	209.2
18	58.21	58.21	58.02	40	213.0		210.0
19	64.21	64.21	63.81	41	218.2		
20	65.98	65.98		42	232.1	248.6	230.9
21	72.18	72.19	67.21	43	251.8		
22	79.30	79.47	77.37	44	353.1	352.3	352.9

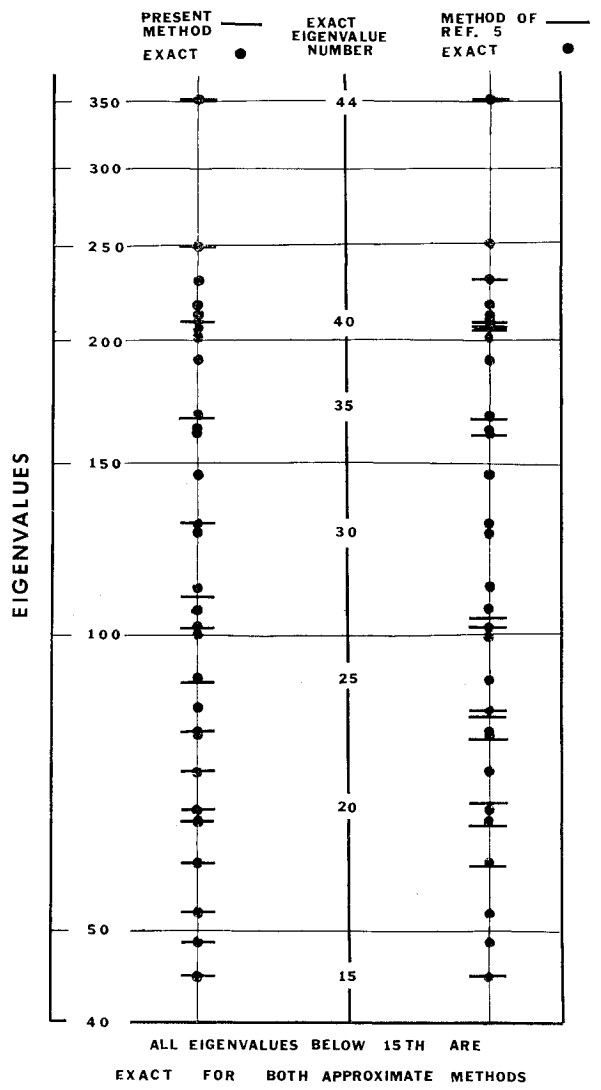

Fig. 1 Comparison of exact and approximate eigenvalues for sample problem.

and other numerical applications,[13,14] the following conclusions can be drawn. A first grouping of more than $m/2$ lower frequencies of the reduced system agrees very closely with the corresponding number of exact (unreduced) frequencies. The remaining reduced frequencies are spread across the remaining exact spectrum, with the last one representing a lower bound on the highest exact frequency of the unreduced system. The present reduction method yields good results and is much more automatic than the methods of Refs. 3–6, since it does not require an arbitrary lumping of masses to reduce the matrix size of the original eigenvalue problem.

The last conclusion is based upon the fact that the reduction methods in the cited references require the arbitrary selection of specific nodes above and beyond those necessary for determination of the elastostatic influence coefficient matrix. The newly proposed procedure, however, does not involve any such selection, since the entire reduction becomes automatic once a starting vector is selected. Furthermore, if the starting vector is chosen in the manner proposed. even this degree of arbitrariness is removed.

Appendix

To establish the theoretical mutual orthogonality of all the Lanczos vectors, with respect to weighting matrix $[B]$, consider the generation of a typical new vector $\{v_i\}$ by Eqs. (8–13) with the assumption that all $i - 3$ additional vectors are necessary to insure the mutual orthogonality of the $\{v\}$'s, i.e.,

$$\{v_i\} = [B]^{-1}[A]\{v_{i-1}\} - \alpha_{i-1}\{v_{i-1}\} - \beta_{i-2}\{v_{i-2}\} - \gamma_{i,i-3}\{v_{i-3}\} - \gamma_{i,i-4}\{v_{i-4}\} - \ldots - \gamma_{i,1}\{v_1\} \quad \text{(A1)}$$

The α,β,γ coefficients are chosen to ensure that

$$[V]^T[B][V] = \lceil \mu \rfloor \quad \text{(A2)}$$

where $\lceil \mu \rfloor$ is a diagonal matrix.

Transposing all of the terms on the right side of Eq. (A1) except the first, and converting to matrix form, yields

$$[V][H] = [B]^{-1}[A][V] \quad \text{(A3)}$$

where $[H]$ is an upper Hessenberg matrix of the form

$$[H] = \begin{bmatrix} \alpha_1 & \beta_1 & \gamma_{4,1} & \cdots & \cdots & \gamma_{n+1,1} \\ 1 & \alpha_2 & \beta_2 & \gamma_{5,2} & & \vdots \\ & 1 & \alpha_3 & \ddots & \ddots & \vdots \\ & & \ddots & \ddots & \ddots & \gamma_{n+1,n-2} \\ & 0 & & \ddots & \ddots & \beta_{n-1} \\ & & & & 1 & \alpha_n \end{bmatrix}$$

Premultiplication of Eq. (A3) by $[V]^T[B]$, and application of Eq. (A2), yields

$$\lceil \mu \rfloor [H] = [V]^T[A][V]$$

Since $[V]^T[A][V]$ is symmetric and $\lceil \mu \rfloor$ is diagonal, $[H]$ must be tridiagonal and so Eqs. (8–13) are sufficient to guarantee Eq. (A2).

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