Modified Inverse Iteration Method Using the Side Condition and The Step Length

Case I: Distinct Natural Frequencies

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(Received April 24, 1995)

An efficient numerical method which can calculate the natural frequencies and mode shapes for very large structural systems is presented. This method applies the accelerated Newton-Raphson technique to eigenproblems. If eigenvalues are not multiple, this method can calculate the natural frequencies and mode shapes without a numerical instability which may be often encountered in the inverse iteration method with shift. The efficiency of this method is verified by comparing convergence and solution time for numerical examples with those of the well-known methods such as, the subspace iteration method and the determinant search method.

1. Introduction

The analysis of a number of physical problems requires the solution of an eigenproblem. It is therefore natural that with the increased use of computational methods operating on discrete representations of physical problems, the development of efficient techniques for the calculation of eigenvalues and eigenvectors has attracted much attention. In particular, the use of finite element techniques can lead to large systems of equations, and the efficiency of an overall response analysis eigenvectors.

The determinant search method (Meirovitch, 1980; Wilkinson, 1965; Bathe, 1982; Bathe, et. al., 1973a; Bathe, et. al., 1973b) and the subspace

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iteration method (Meirovitch, 1980; Wilkinson, 1965; Bathe, 1982; Bathe, et. al., 1973a; Bathe, et. al., 1973b; Bathe, et. al., 1972; Bathe, et. al., 1980; Wilson, et. al., 1983) have been mainly used for solving eigenproblems. The determinant search method is a method which combines the polynomial iteration method, the Sturm-sequence method and the vector iteration method. This method can be efficiently used in the analysis of systems with small bandwidth, since the matrix decomposition must be executed at each step. (Bathe, et. al., 1973b) The subspace iteration method is a method which combines the simultaneous inverse iteration method and the Rayleigh-Ritz method. This method has been used mostly, but the following shortcomings have been identified after extensive use of the method. (Bathe, et. al., 1983; wilson, et. al., 1983)

1) When the inverse iteration with shift is applied to the method to increase convergence, the shift value may be close to exact eigenvalue and numerical instability may be encountered during triangularization.

2) One considering the solution of eigenvalue problem for a relatively large number of

eigenpairs, the solution time used in the subspace iteration method rises rapidly as the number of eigenpairs considered is increased. It is due to a number of factors that can be neglected when the solution of only a few eigenpairs is required.

① When p (p: the number of eigenkpairs to be required) is large, the convergence rate of the eigenvector, ϕ_p, can be close to one.

② If q (q: the number of starting iteration vectors) is increased, the number of operations per subspace iteration is increased significantly.

③ If q is increased, the convergence of the smallest eigenvalues is generally achieved in a few iterations, and the converged vectors plus ($p+1$) th to qth iteration vectors are only included in the additional iterations to provide solution stability and to accelerate the convergence of the large required eigenvalues.

Lee and Robinson (Lee, et. al., 1979) proposed an efficient solution method in order to improve numerical stability and increase convergence. To further improve the method, the accelerated Newton-Raphson technique is proposed here. (Kim, et. al., 1994) As examples for calculating eigenvalues and the corresponding mode shapes, one plane frame and one three-dimensional building frame structure are analyzed to prove the efficiency of the proposed method.

2. Method of Analysis

Consider a generalized eigenvalue problem such as,

$$K\phi_j = \lambda_j M\phi_j \quad (j=1,2,3,\cdots,n) \tag{1}$$

where K and M are the stiffness matrix and mass matrix of order n, respectively. M is assumed to be positive definite and K positive semidefinite. λ_j is the jth natural frequency squared and ϕ_j the corresponding mode shape.

Let us assume that initial approximate solution of Eq.(1), $\lambda_j^{(0)}$ and $\phi_j^{(0)}$, are available. Denote an approximate eigenvalue and the corresponding eigenvector after k iterations by $\lambda_j^{(k)}$ and $\phi_j^{(k)}$ ($k=0,1,2,...$). Then, we have

$$r_j^{(k)} = K\phi_j^{(k)} - \lambda_j^{(k)} M\phi_j^{(k)} \tag{2}$$

where the residual vector, $r_j^{(k)}$, is not generally zero because of substitution of approximate values into Eq.(1). In order to get a solution converged to the eigenvalue and the corresponding eigenvector of the system, the residual vector should be removed. Let us apply the Newton-Raphson technique for this purpose.

$$\begin{aligned} r_j^{(k+1)} &= 0 \\ &= K\phi_j^{(k+1)} - \lambda_j^{(k+1)} M\phi_j^{(k+1)} \end{aligned} \tag{3}$$

where

$$\lambda_j^{(k+1)} = \lambda_j^{(k)} + \Delta\lambda_j^{(k)} \tag{4}$$

$$\phi_j^{(k+1)} = \phi_j^{(k)} + \Delta\phi_j^{(k)} \tag{5}$$

Substituting Eqs. (2), (4) and (5) into Eq. (3) and neglecting the higher order term, $\Delta\lambda_j^{(k)} M\Delta\phi_j^{(k)}$, we get

$$(K - \lambda_j^{(k)} M)\Delta\phi_j^{(k)} - \Delta\lambda_j^{(k)} M\phi_j^{(k)}$$
$$= -r_j^{(k)} \tag{6}$$

where $\Delta\lambda_j^{(k)}$ and $\Delta\phi_j^{(k)}$ are unknown incremental values of $\lambda_j^{(k)}$ and $\phi_j^{(k)}$.

Because there are only n equations with $n+1$ unknowns which are $\Delta\lambda_j^{(k)}$ and n components of $\Delta\phi_j^{(k)}$, a side condition must be introduced for the solution of Eq.(6). The side condition to arrive at a set of $n+1$ equations with $n+1$ unknowns is

$$(\phi_j^{(k)})^T M\Delta\phi_j^{(k)} = 0 \tag{7}$$

This is equivalent to saying that the allowable changes in the approximate eigenvector are orthogonal to the latest approximate eigenvector with respect to the mass matrix. This prevents unlimited drift in the eigenvector which is, after all, not determinded in magnitude. Error for $\phi_j^{(k+1)}$, $\theta_j^{(k+1)}$, represents the angle between $\phi_j^{(k+1)}$ and ϕ_j.

Writing Eqs.(6) and (7) in matrix form, we get

$$\begin{bmatrix} K - \lambda_j^{(k)} M & -M\phi_j^{(k)} \\ -(\phi_j^{(k)})^T M & 0 \end{bmatrix} \begin{Bmatrix} \Delta\phi_j^{(k)} \\ \Delta\lambda_j^{(k)} \end{Bmatrix}$$
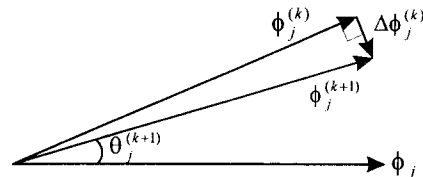$$= -\begin{Bmatrix} r_j^{(k)} \\ 0 \end{Bmatrix} \tag{8}$$

Fig. 1 The side condition (if $M=I$)

The coefficient matrix for the incremental values is of order $n+1$ and symmetric. If λ_j's are not multiple, it is nonsingular. (Lee, et. al., 1979) The case of multiple or close eigenvalues is treated in the succeeding paper.

The above algorithm using the Newton-Raphson technique, despite of its rapid convergence, is not efficient, since a new coefficient matrix has to be formed and refactorized in each iteration step. The complete elimination procedure in each iteration may be avoided by using the modified Newton-Raphson technique in Eq. (8).

$$\begin{bmatrix} K - \lambda_j^{(0)} M & -M\phi_j^{(k)} \\ -(\phi_j^{(k)})^T M & 0 \end{bmatrix} \begin{Bmatrix} \Delta\phi_j^{(k)} \\ \Delta\lambda_j^{(k)} \end{Bmatrix}$$
$$= -\begin{Bmatrix} r_j^{(k)} \\ 0 \end{Bmatrix} \qquad (9)$$

The coefficient matrix in Eq. (9) using the modified Newton-Raphson technique can be written as (Lee, et. al., 1979)

$$k_j^{(k+1)} = h^2 k_j^{(k)} \qquad (10)$$
$$\theta_j^{(k+1)} = h\theta_j^{(k)} \qquad (11)$$

where $k_j^{(k)} = \left| \dfrac{\lambda_j - \lambda_j^{(k)}}{\lambda_j} \right|$, and $h = \max\limits_{\substack{i \\ i \neq j}} \left| \dfrac{\lambda_j - \lambda_j^{(0)}}{\lambda_i - \lambda_i^{(0)}} \right|$.

$\theta_j^{(k)}$ represents the angle between $\phi_j^{(k)}$ and ϕ_j, that is, an error in $\phi_j^{(k)}$. As shown in Eqs. (10) and (11), the convergence rate of eigenvalue, $k_j^{(k)}$, is quadratic in h and that of eigenvector, $\theta_j^{(k)}$, linear in h.
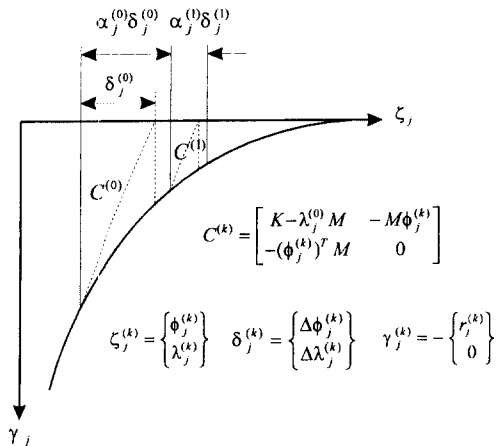

Fig. 2   The accelerated Newton-Raphson technique

Once the submatrix $K - \lambda_j^{(0)} M$ is decomposed into the LDL^T (L: lower triangular matrix, D: diagonal matrix), a small number of operations are required for the solution of Eq. (9) in the succeeding iterations, since the vector $M\phi_j^{(k)}$ in the coefficient matrix is only changed in each iteration. However, due to negligence of the small nonlinear term $(\lambda_j^{(k+1)} - \lambda_j^{(0)}) M\Delta\phi_j^{(k)}$, the convergence is lower. Thus, the number of iterations for a solution is increased. The above scheme has been presented by Lee and robinson. (Lee, et. al., 1979)

To further improve the eigenvector, the accelerated scheme is proposed here, (Kim, et. al., 1994) that is,

$$\phi_j^{(k+1)} = \phi_j^{(k)} + \alpha_j^{(k)} \Delta\phi_j^{(k)} \qquad (12)$$

$\alpha_j^{(k)}$ is a value to minimize the norm of the residual vector. It can be evaluated by using the least square technique as follows;

$$\frac{\partial}{\partial \alpha_j^{(k)}} \{ (r_j^{(k+1)})^T r_j^{(k+1)} \} = 0 \qquad (13)$$

$$\alpha_j^{(k)} = -\frac{(\Delta\phi_j^{(k)})^T (K - \lambda_j^{(k+1)} M)(K - \lambda_j^{(k+1)} M) \phi_j^{(k)}}{(\Delta\phi_j^{(k)})^T (K - \lambda_j^{(k+1)} M)(K - \lambda_j^{(k+1)} M) \Delta\phi_j^{(k)}}$$
$$(14)$$

Note that $\lambda_j^{(k+1)}$ and $\Delta\phi_j^{(k)}$ have been obtained by Eq. (9).

If the order of the system is n, and the bandwidths of the stiffness matrix and mass matrix are m_a and m_b, the number of operations for evaluating $\alpha_j^{(k)}$ in the first iteration step is $2nm_a + 2nm_b + 7n + 1$. This is large compared to $5nm_a + 2nm_b + 6n$ which is required in each iteration step in Eq. (9). However, only the number of $7n + 1$ operations is required to evaluate $\alpha_j^{(k)}$ after the 2nd iteration, which is negligible, because we use computational results in the previous step. Thus, solution time of the proposed method is decreased by improving convergence.

Some of the eigenvalues and corresponding eigenvectors of interest may be missed when the initial approximations are not suitable. In order to check whether this occurs, the Sturm-sequence property (Bathe, 1982) may be applied. A computed eigenvalue can be checked using the above property with negligible extra computation, since the decomposition of the matrix (K
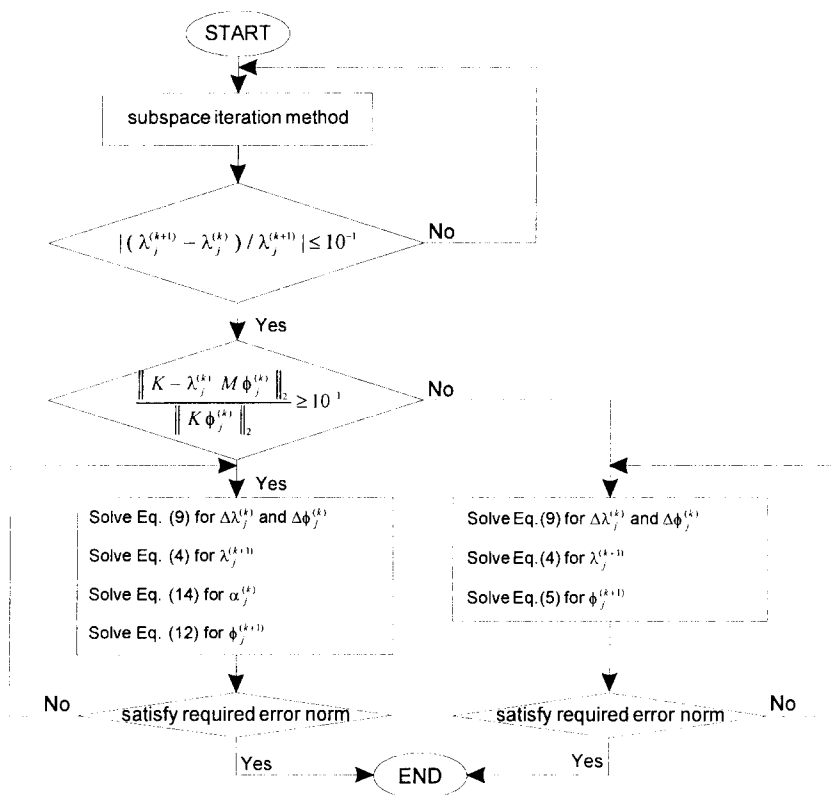
START

subspace iteration method

$|(\lambda_j^{(k+1)} - \lambda_j^{(k)})/\lambda_j^{(k+1)}| \le 10^{-1}$ No

Yes

$\dfrac{\|K - \lambda_j^{(k)} M \phi_j^{(k)}\|_2}{\|K \phi_j^{(k)}\|_2} \ge 10^{-1}$ No

Yes

Solve Eq. (9) for $\Delta\lambda_j^{(k)}$ and $\Delta\phi_j^{(k)}$

Solve Eq. (4) for $\lambda_j^{(k+1)}$

Solve Eq. (14) for $\alpha_j^{(k)}$

Solve Eq. (12) for $\phi_j^{(k+1)}$

Solve Eq. (9) for $\Delta\lambda_j^{(k)}$ and $\Delta\phi_j^{(k)}$

Solve Eq. (4) for $\lambda_j^{(k+1)}$

Solve Eq. (5) for $\phi_j^{(k+1)}$

No   satisfy required error norm   satisfy required error norm   No

Yes   END   Yes

Fig. 3   Algorithm for the proposed method

$-\lambda_j^{(0)} M)$ has already been carried out during the procedure for the solution of Eq. (9). If some of the eigenvalues of interest are detected to be missing, the solutions can be found by the proposed method.

3. Numerical Examples

The plane frame and the three-dimensional building from which K. J. Bathe used (Bathe, et. al., 1972) are analyzed to verify the efficiency of the proposed method. When the predetermined error norm is 1.E-09, the structures are analyzed by three different methods; the subspace iteration method, the determinant search method and the proposed method, where the error norm (Bathe, et. al., 1982) is computed by

$$\text{error norm} = \frac{\|(K - \lambda_j^{(k)} M) \phi_j^{(k)}\|_2}{\|K \phi_j^{(k)}\|_2} \quad (15)$$

Each convergence rate and solution time (CPU

time) used to calculate 15 eigenpairs are compared. Intermediate results with relative error of 1. E-01 in the subspace iteration method are used as initial values of the proposed method. The relative error (Bathe, et. al., 1982) in the subspace iteration method is computed as follows

$$\text{relative error} = \left|\frac{\lambda_j^{(k+1)} - \lambda_j^{(k)}}{\lambda_j^{(k+1)}}\right| \quad (16)$$

$\alpha_j^{(k)}$ is applied to the eigenpair whose error norm is over 1.E-01. All runs are executed in the IRIS4D-20-S17 with 10 Mips and 0.9 Mflops.
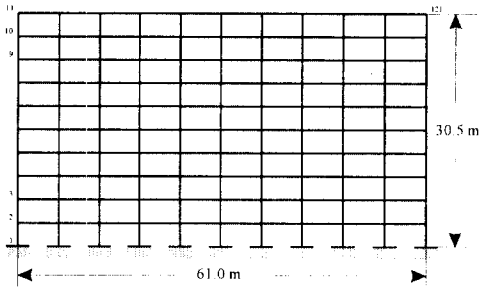
3.1 Plane frame structure

The plane frame structure which has 10 stories and 10 bays shown in Fig. 4 consists of 210 beam elements, 121 nodes and 330 degrees-of-freedom. The mean half-bandwidth of both the stiffness matrix and mass matrix is 30. $\alpha_j^{(k)}$ is applied to the 13th, the 14th and the 15th eigenpair with error norm exceeding 1.E-01.

Solution times for three methods are summarized in Table 1. If we let the solution time for the proposed method be 1, it takes 2.7 times for the subspace iteration method, 2.3 times for the determinant search method. For each solution method, the convergence of eigenpairs to which $\alpha_j^{(k)}$ is applied is depicted in Fig. 5 to Fig. 7. According to them, it is obvious that the convergence of the proposed method is superior to that of the subspace iteration and of the determinant search method. The absolute values of $\alpha_j^{(k)}$ calculated in the above numerical example range from 0.85 to 1.5.

3.2　Three dimensional building frame

Three dimensional building frame shown in Fig. 8 consists of 191 beam elements, 100 nodes and 468 degrees-of-freedom. The mean half-bandwidth of both the stiffness matrix and mass matrix is 91. $\alpha_j^{(k)}$ is applied to the 12th, the 14th and the 15th eigenpair with error norm exceeding 1.E-01.

$A = 0.2787 \ m^2 \qquad I = 8.631 \times 10^{-3} \ m^4$

$E = 2.068 \times 10^{10} \ Pa \qquad \rho = 5.154 \times 10^2 \ kg/m^3$
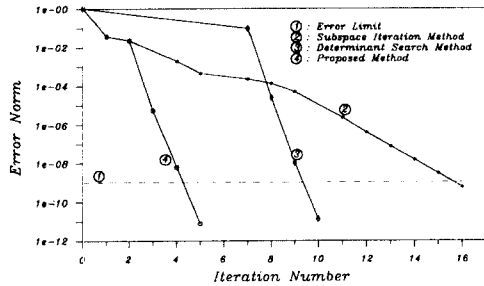
Fig. 4　Plane frame structures

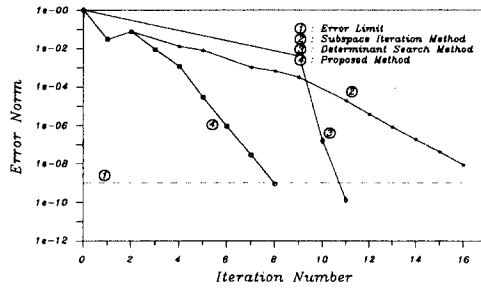**Fig. 6**　Convergence of the 14th eigenpair
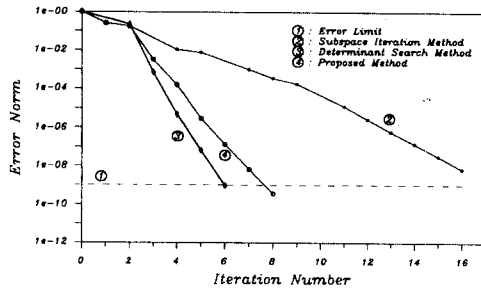

Fig. 7　Convergence of the 15th eigenpair

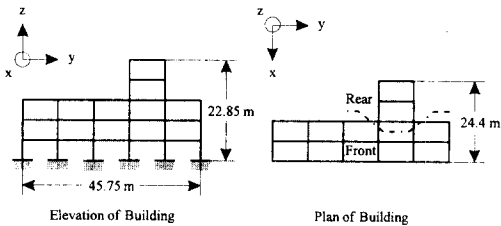**Fig. 5**　Convergence of the 13th eigenpair

Table 1　Solution time (CPU time, sec) of plane frame

Methods	Solution Time (ratio)
Proposed Method	58.1 (1.00)
Subspace Iteration Method	155.4 (2.7)
Determinant Search Method	133.5 (2.3)

Elevation of Building　　　　Plan of Building

Column in Front Building : $A = 0.2787 \ m^2$, $I = 8.631 \times 10^{-3} \ m^4$
Column in Rear Building : $A = 0.3716 \ m^2$, $I = 10.789 \times 10^{-3} \ m^4$
All Beams into x - Direction : $A = 0.6096 \ m^2$, $I = 6.473 \times 10^{-3} \ m^4$
All Beams into y - Direction : $A = 0.2787 \ m^2$, $I = 8.631 \times 10^{-3} \ m^4$
$E = 2.068 \times 10^{10} \ Pa$, $\rho = 5.154 \times 10^2 \ kg/m^3$

Fig. 8　Three dimensional building frame

Solution times for three methods are summarized in Table 2. If we let the solution time for the proposed method be 1, it takes 3.3 times for the

Table 2 Solution Time (CPU time, sec) of three dimensional building Frame

Methods	Solution Time (ratio)
Proposed Method	27.4 (1.00)
Subspace Iteration Method	723.9 (3.3)
Determinant Search Method	1111.4 (5.1)
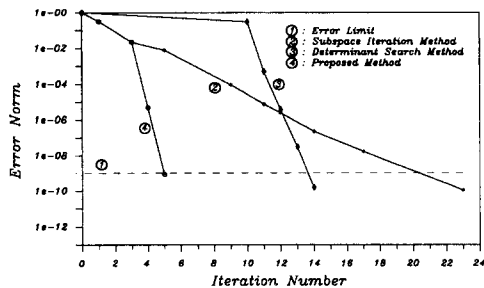
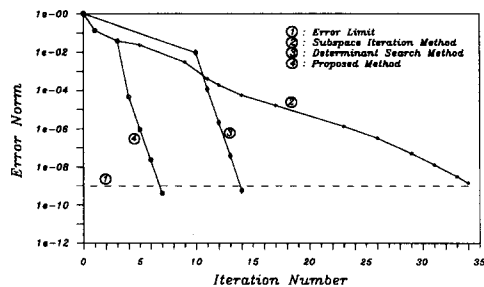**Fig. 9** Convergence of the 12th eigenpair
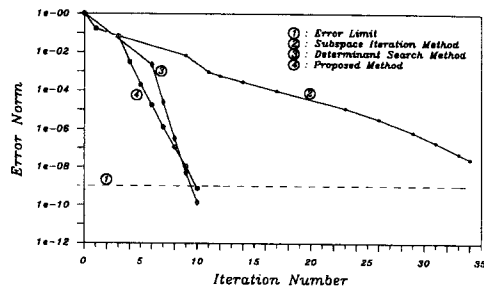

Fig. 10 Convergence of the 14th eigenpair

Fig. 11 Convergence of the 15th eigenpair

subspace iteration method, 5.1 times for the determinant search method. For each solution method, the convergence of eigenpairs to which $\alpha_j^{(k)}$ is applied is presented in Fig. 9 to Fig. 11. We can see that the convergence of the proposed method is superior to that of the subspace iteration and of determinant search method. The absolute value of $\alpha_j^{(k)}$ calculated in the above numerical example has the value of 0.85 to 1.02.

4. Conclusions

This paper proposes an efficient solution method using the accelerated Newton-Raphson technique for eigenproblems. As shown in numerical examples of Sec. 3, characterstics of the proposed method are identified as follows;

① Since each eigenpair is obtained independently, an eigenpair is not affected by the eigenpairs previously calculated.

② Even a shift near an exacet eigenvalue occurs, numerical instability problems are not encountered during traingularization.

③ Demerits of the general methods, such as much solution time and slow convergence, can be removed by using the proposed method.

5. Acknowledgement

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