수치적으로 안정한 부분공간 반복법

Numerically Stable Subspace Iteration Method

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ABSTRACT

A numerically stable technique to remove the limitation in choosing a shift in the subspace iteration method with shift is presented. A major difficulty of the subspace iteration method with shift is that because of singularity problem, a shift close to an eigenvalue can not be used, resulting in slower convergence. This study solves the above singularity problem using side conditions without sacrifice of convergence. The method is always nonsingular even if a shift is an eigenvalue itself. This is one of the significant characteristics of the proposed method. The nonsingularity is proved analytically. The convergence of the proposed method is at least equal to that of the subspace iteration method with shift, and the operation counts of above two methods are almost the same when a large number of eigenpairs are required. To show the effectiveness of the proposed method, two numerical examples are considered.

1. Introduction

Eigenvalue analysis is an important step in structural dynamic analysis when the mode superposition method is used. Many solution methods have been developed for eigenvalue analysis, and among these methods the subspace iteration method has hitherto been known to be very efficient for solving large eigenvalue problems.

The subspace iteration method was developed and named by Bathe[1]. This method combines simultaneous inverse iteration method and Rayleigh-Ritz analysis. This method has been widely used, but the following shortcomings have been identified after extensive use of the method.

(1) When the number of eigenpairs to be required is large, the convergence of the required eigenvalues can be very slow.

(2) If a large number of eigenpairs are required, the computational effort required to form and solve the subspace eigenvalue problem can be significant.

(3) When the starting iteration vectors are poorly chosen, some of the eigenvalues and corresponding eigenvectors of interest may be missed.

To overcome the above shortcomings many researchers have studied a variety of acceleration

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procedures of the subspace iteration method as follows.

Yamamoto and Ohtsubo[2] have used Chebyshev polynomials for acceleration and they have shown that improved convergence in the subspace iteration can result. Akl et al.[3] have employed over-relaxation method to accelerate the subspace iteration and they have demonstrated the effectiveness of the method. Bathe and Ramaswamy[4] have used over-relaxation and shifting techniques and they showed that the accelerated method can be applied effectively to the solution of eigenproblems in which the matrices have small or large bandwidths. Nguyen and Arora have developed the method for free vibration analysis of a large structure by partitioning it into a number of substructures to reduce the computer storage requirement. Cheu et al. have investigated the effects of selecting initial vectors on computation efficiency for subspace iteration method. Lam and Bertolini have developed selective repeated inverse iteration and multiple inverse iteration for accelerated reduction of subspace. Rajendran and Narasimhan have used another over-relaxation method. The method proposed by Bathe and Ramaswamy(1980) considers the acceleration of individual vectors using individual over-relaxation parameters, whereas the method proposed by Rajendran and Narasimhan considers the acceleration of the subspace as a whole. Qian and Dhatt have accelerated the subspace iteration by omitting some of the Rayleigh-Ritz procedure from certain iteration steps and obtaining a higher convergence rate.

Among the above accelerated techniques, a shifting technique is effectively used in the commercial FEM programs such as ADINA. Since the singularity may occur during the use of the shifting technique in the accelerated scheme such as the subspace iteration method with shift, the shift must be within a limited region to avoid the singularity.

This paper describes a technique which always guarantees the numerical stability and maintains the convergence rate of the subspace iteration method with shift even if it is an exact eigenvalue itself. The theory and concept of the proposed method are discussed briefly, and two numerical examples are presented to verify the effectiveness of the proposed method.

2. Subspace Iteration Method with Shift

The general eigenvalue problem of the structural dynamics may be written as follows.

$$KX = MX\Lambda \tag{1}$$

where K and M are the stiffness matrix and the mass matrix of the discrete or discretized system of order n, respectively, the columns of X the eigenvectors, and Λ a diagonal matrix with eigenvalues.

Applying a shift μ to eqn (1) gives

$$(K - \mu M)X = MX\Omega \tag{2}$$

where
$$\Omega = \Lambda - \mu I \tag{3}$$

and I is the unit matrix.

Suppose that the p smallest eigenvalues λ_i ($i = 1, 2, \ldots, p$) and corresponding eigenvectors x_i are required. Then the jth trial vector converges linearly to x_j at the rate of $(\lambda_j - \mu)/(\lambda_{p+1} - \mu)$. For faster convergence, q trial vectors are normally used with $q = \min\{2p, p+8\}$.

If we have p initial independent vectors $x_i^{(1)}$ ($i = 1, 2, \ldots, p$) spanning p-dimensional subspace in the neighborhood of the subspace of the desired eigenvectors and the approximate eigenvectors and corresponding eigenvalues after k iterations are denoted by $x_i^{(k)}$ and $\lambda_i^{(k)}$, the subspace iteration method with the shift μ for the kth iteration may be described as follows:

Step 1. Find improved eigenvectors $\overline{X}^{(k+1)} = \begin{bmatrix} \overline{x}_1^{(k+1)}, & \overline{x}_2^{(k+1)}, & \ldots, & \overline{x}_q^{(k+1)} \end{bmatrix}$ by the simultaneous inverse iteration method;

$$(K - \mu M) \, \overline{X}^{(k+1)} = MX^{(k)} \tag{4}$$

where $\overline{X}^{(k+1)}$ and $X^{(k)}$ are the $(n \times q)$ matrices.

Step 2. Compute the projections of the matrices $(K - \mu M)$ and M onto the subspace spanned by the q vectors in $\overline{X}^{(k+1)}$;

$$\overline{K}^{(k+1)} = \overline{X}^{(k+1)^T}(K - \mu M)\, \overline{X}^{(k+1)} \tag{5}$$

$$\overline{M}^{(k+1)} = \overline{X}^{(k+1)^T} M \, \overline{X}^{(k+1)} \tag{6}$$

where $\overline{K}^{(k+1)}$ and $\overline{M}^{(k+1)}$ are the symmetric matrices.

Step 3. Solve the eigenvalue problem of reduced order q;

$$\overline{K}^{(k+1)} Q^{(k+1)} = \overline{M}^{(k+1)} Q^{(k+1)} \Omega^{(k+1)} \tag{7}$$

where $Q^{(k+1)}$ and $\Omega^{(k+1)}$ are the $(q \times q)$ matrices.

Step 4. Find an improved approximation to the eigenvectors $X^{(k+1)}$ from $\overline{X}^{(k+1)}$, the $(n \times q)$ matrix of Ritz trial vectors, and the $(q \times q)$ projected system eigenvectors $Q^{(k+1)}$:

$$X^{(k+1)} = \overline{X}^{(k+1)} Q^{(k+1)} \tag{8}$$

And the improved eigenvalues can be computed as follows.

$$\Lambda^{(k+1)} = \Omega^{(k+1)} + \mu I \tag{9}$$

Then, provided that the trial vectors in $X^{(1)}$ are not orthogonal to one of the required eigenvectors and assuming an appropriate ordering of the trial vectors, $\Lambda^{(k+1)}$ converges to Λ and $X^{(k+1)}$

converges to X as k approaches infinity. The convergence rate of the subspace iteration method with shift is

$$(\lambda_j - \mu)/(\lambda_{q+1} - \mu). \tag{10}$$

While the shifting procedure improves the convergence rate of the subspace iteration method, it needs extra operations. Therefore, shifting will only be performed when a criterion determines that the convergence will be improved sufficiently to cover the cost of the extra triangular factorization[4].

If a shift is an eigenvalue itself or very close to it, all iteration vectors immediately converge to the eigenvector corresponding to that eigenvalue. The iteration vectors can then not be orthogonalized any more and the iteration procedure becomes unstable. If the shift is very close to an eigenvalue, the last pivot element in the LDL^T factorization of the coefficient matrix usually becomes small compared with its original value and the coefficient matrix becomes close to singular. To avoid this singularity, that is, to guarantee the stability of the subspace iteration method with shift, the following condition was adopted in the subspace iteration method[4];

$$1.01\ \overline{\lambda}_{s-1} \le \mu \le 0.99\ \overline{\lambda}_s \tag{11}$$

where $\overline{\lambda}_{s-1}$ is the calculated approximation to $(s-1)$th eigenvalue and $\overline{\lambda}_s$ sth eigenvalue.

It means that a shift must be within a limited region resulting in slow convergence. Moreover, if the calculated approximation to an eigenvalue slightly differs from it, an eigenvalue may be inside of the limited region. Then, the singularity may occur although a shift is inside of the limited region. These are the significant disadvantages of the subspace iteration method with shift. The purpose of this paper is to remove the limitation in eqn (11) for choosing the value of a shift μ.

3. Proposed Method

3.1 Theory

Consider the simultaneous inverse iteration step in the subspace iteration method with shift;

$$(K - \mu M)\ \overline{X}^{(k+1)} = MX^{(k)} \tag{12}$$

Since if a shift is very close to an eigenvalue in eqn (12) the singularity occurs during the decomposition process, The $(k+1)$th eigenvector approximations, $\overline{X}^{(k+1)}$, can not be acquired. In this study, to solve the singularity problem the following procedures are proposed.

First, assume that a shift is close to ith eigenvalue. Then, inverse iteration step on the ith eigenvalue can be expressed as follows;

$$(K - \mu M)\ \overline{x}_i^{(k+1)} = d_{ii}^{(k+1)} M x_i^{(k)} \tag{13}$$

where the scalar $d_{ii}^{(k+1)}$ controls the length of the vector $\overline{x}_i^{(k+1)}$.

Because there are only n equations with $(n+1)$ unknowns, n components of $\overline{x}_i^{(k+1)}$ and $d_{ii}^{(k+1)}$, in eqn (13), one side condition must be introduced for the solution of eqn (13). This condition is that the current vector($x_i^{(k)}$) is orthogonal to the incremental vector($\varDelta x_i^{(k)}$) with respect to M; that is,

$$x_i^{(k)\,T} M \varDelta x_i^{(k)} = 0. \tag{14}$$

Adding the mass orthonormality relation, $x_i^{(k)\,T} M \, x_i^{(k+1)} = 1$, to the side condition, eqn (14), yields

$$x_i^{(k)\,T} M \, \overline{x}_i^{(k+1)} = 1 \tag{15}$$

where

$$\overline{x}_i^{(k+1)} = x_i^{(k)} + \varDelta x_i^{(k)}. \tag{16}$$

The inverse iteration step on the other eigenvalues make use of the existing equation, eqn (12); that is,

$$(K - \mu M) \; \overline{x}_j^{(k+1)} = M x_j^{(k)} \quad (j=1,2,\ldots,q,\, j{\neq}i) \tag{17}$$

Writing eqns (13), (15) and (17) in matrix form gives

$$\begin{bmatrix} K - \mu M & M x_i^{(k)} \\ x_i^{(k)\,T} M & 0 \end{bmatrix} \begin{bmatrix} \overline{X}^{(k+1)} \\ d_i^{(k+1)} \end{bmatrix} = \begin{bmatrix} M X^{(k)} \\ e_i \end{bmatrix} \tag{18}$$

where $x_i^{(k)\,T} M \, x_j^{(k+1)} = 0 \ (j=1,2,\ldots,q,\, j{\neq}i)$, $d_i^{(k+1)} = \langle 0,\ldots,0,(1 - d_{ii}^{(k+1)}),0,\ldots,0 \rangle$ is the row vector of order q, and $e_i = \langle 0,\ldots,0,1,0,\ldots,0 \rangle$ is the row vector of order q that all elements are zero except for ith element with unity.

Note that $\overline{X}^{(k+1)}$ from eqn (18) is used for $\overline{X}^{(k+1)}$ in eqns (5) and (6) instead of $\overline{X}^{(k+1)}$ in eqn (4). Eqn (18) is the main linear algebraic equation used in the proposed method.

The coefficient matrix of eqn (18) is of order $(n+1)$, symmetric, and nonsingular[5-6]. The nonsingularity is one of the significant advantages of the proposed method.

4. Numerical Examples

The three-dimensional framed structure used by Bathe and Wilson[1] is analyzed to verify the effectiveness of the proposed method. With the predetermined error norm of 10^6, the structure is analyzed by two methods; the subspace iteration method with shift which is not used the limited region(see eqn (11)) and the proposed method, where the error norm is computed by the following equation;

$$error \quad norm = \frac{||(K - \lambda_i^{(k)} M)x_i^{(k)}||_2}{||Kx_i^{(k)}||_2} .$$ (19)

Even if a shift is on or very close to an eigenvalue, it is shown that the proposed method can obtain the solutions without any singularity. When a shift is not close to an eigenvalue, each convergence rate for calculating the first ten eigenpairs is compared. All runs are executed in the IRIS4D-20-S17 with 10 Mips and 0.9 Mflops.

4.1 Three-dimensional framed structure

The example is the three-dimensional framed structure. Figure 1 shows the geometric configuration and material properties. The structure discretized using 100 beam elements resulting in system of dynamic eqns with a total of 468 degrees of freedom. The consistent mass matrix is used for M.

Elevation   Plan

Column in Front Building : $A = 0.2787\,m^2$, $I = 8.631 \times 10^{-3}\,m^4$
Column in Front Building : $A = 0.3716\,m^2$, $I = 10.787 \times 10^{-3}\,m^4$
All Beams into x-Direction : $A = 0.6096\,m^2$, $I = 6.473 \times 10^{-3}\,m^4$
All Beams into y-Direction : $A = 0.2787\,m^2$, $I = 8.631 \times 10^{-3}\,m^4$

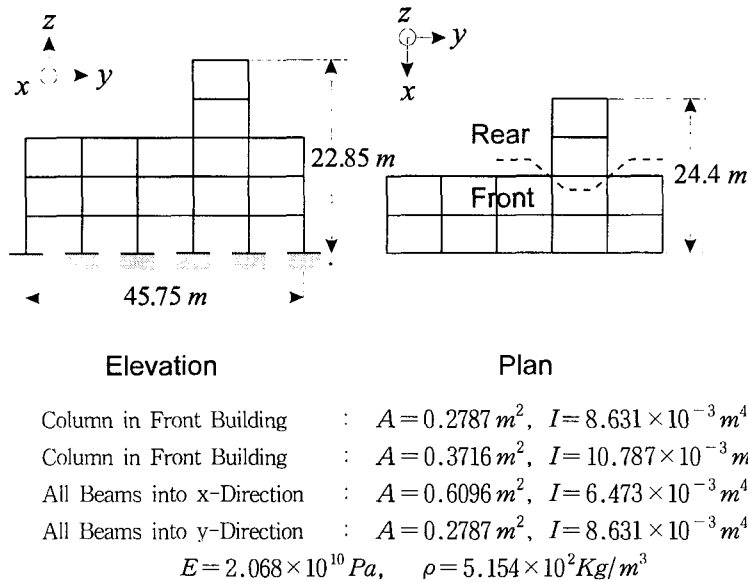$$E = 2.068 \times 10^{10}\,Pa, \quad \rho = 5.154 \times 10^2\,Kg/m^3$$

Figure 1. Three-dimensional framed structure

Some results are shown in Table 1 and in Figures 2 to 7. The solution time for two methods are summarized in Table 1. When a shift is on 1.01 λ_5, the subspace iteration method with shift and the proposed method obtain the required ten eigenpairs. However, when the shift is on λ_5, the subspace iteration method with shift does not calculate the solutions while the proposed method finds the solutions. It shows that the iteration procedure for the proposed method can converge without any singularity even if the shift is the same exactly to an eigenvalue.

For each solution method, the convergence of each eigenpair is depicted in Figures 2 to 7. Figures 2 to 4 show that when the shift is on 1.01 λ_5 the convergence of the proposed method is nearly equal to

that of the subspace iteration method with shift. Figures 5 to 7 show that when the shift is the same exactly to the fifth eigenvalue the proposed method converges well without any singularity while the subspace iteration method with shift can not converge due to the singularity. As the above results, the proposed method can choose a more aggressive shift than the subspace iteration method with shift.

Table 1. Solution time for the lowest ten eigenvalues of the 3-dim. framed structure

	Analysis methods	Solution time, sec (ratio)
Shift = 1.01 λ_5	Subspace iteration method with shift	485.36 (1.00)
	Proposed method	492.16 (1.01)
Shift = λ_5	Subspace iteration method with shift	No solution
	Proposed method	491.70
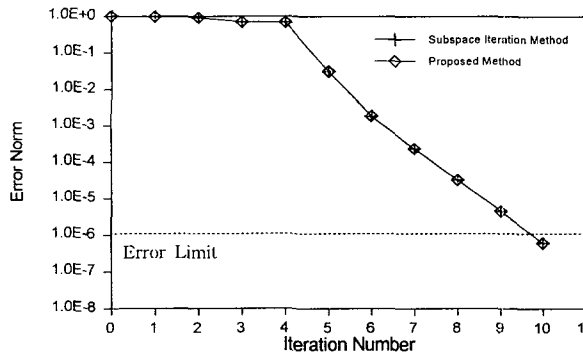
Figure 2. Error norm versus iteration number of the first eigenpair of the three-dimensional framed structure in case of shift = 1.01 λ_5.
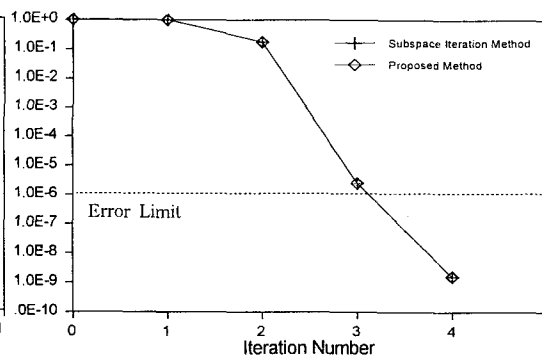

Figure 3. Error norm versus iteration number of the fifth eigenpair of the three-dimensional framed structure in case of shift = 1.01 λ_5.
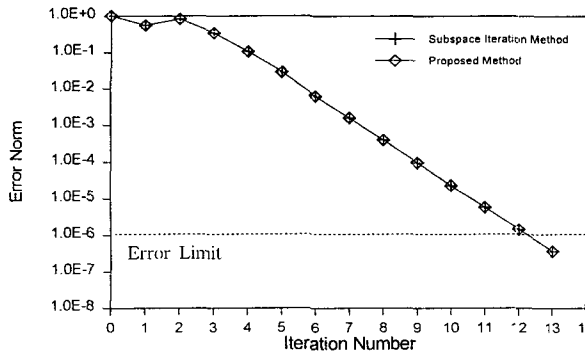

Figure 4. Error norm versus iteration number of the tenth eigenpair of the three-dimensional framed structure in case of shift = 1.01 λ_5.
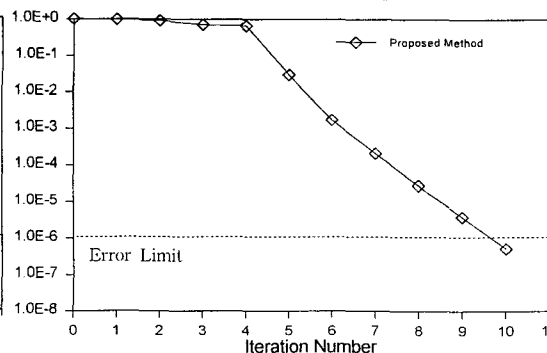

Figure 5. Error norm versus iteration number of the first eigenpair of the three-dimensional framed structure in case of shift = λ_5.
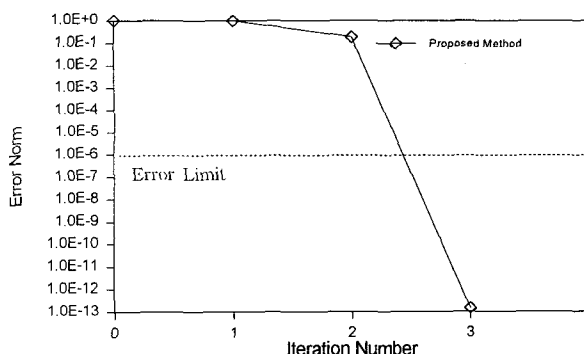
Figure 6. Error norm versus iteration number of the fifth eigenpair of the three-dimensional framed structure in case of shift = λ_5.
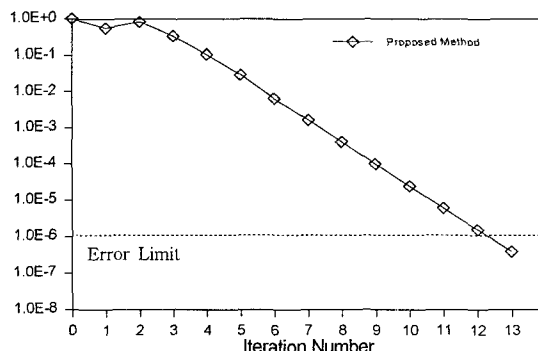
Figure 7. Error norm versus iteration number of the tenth eigenpair of the three-dimensional framed structure in case of shift = λ_5.

5. Conclusions

This paper proposes a numerically stable acceleration technique using side conditions for the improvement of the subspace iteration method with shift. The characteristics of the proposed method identified by the analytical and the numerical results from numerical examples are summarized as follows:

(1) The nonsingularity of the proposed method is always guaranteed, which is proved analytically; even if the shift is an eigenvalue itself, the proposed method can obtain the solutions without any singularity.

(2) The convergence rate of the proposed method is at least equal to that of the subspace iteration method with shift, and the operation counts of the proposed method and the subspace iteration method with shift are almost the same when the number of eigenpairs to be required is large.

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