An improved subspace iteration method with shifting

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Abstract

An efficient and stable technique to remove the limitation in choosing a shift in the subspace iteration method with shifting is presented. A major difficulty of the subspace iteration method with shifting is that, because of the singularity problem, a shift close to an eigenvalue cannot 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 shifting, and the operation counts of above two methods are almost the same for large structures. To show the effectiveness of the proposed method, two numerical examples are considered. © 1999 Elsevier Science Ltd. All rights reserved.

Keywords: Subspace iteration method; Inverse iteration; Shift; Nonsingularity; Side condition

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 [1,2]. 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 [3]:

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 is 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 procedures of the subspace iteration method as follows. Yamamoto and Ohtsubo [4] have used Chebyshev polynomials for acceleration and they have shown that improved convergence in the subspace iteration can result. Akl et al. [5, 6] have employed the over-relaxation method to accelerate the subspace iteration and they have demonstrated the effectiveness of the method. Bathe and Ramaswamy [7] 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 [8] 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. [9] have investigated the effects of selecting initial vectors on computation efficiency for subspace iteration method. Lam and Bertolini [10,11] have developed selective repeated inverse iteration and multiple inverse iteration for accelerated reduction of subspace. Rajendran and Narasimhan [12] have used another over-relaxation method. The method proposed by Bathe and Ramaswamy [7] considers the acceleration of individual eigenvectors 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 [13] 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 [14]. Since the singularity may occur during the use of the shifting technique in the accelerated scheme such as the subspace iteration method with shifting, the shift must be carefully chosen 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 shifting 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 shifting

The general eigenvalue problem of the structural dynamics may be written as follows. [15]

\[ \mathbf{K}\mathbf{x} = \mathbf{M} \mathbf{\Lambda}\mathbf{x} \]  

(1)

where \( \mathbf{K} \) and \( \mathbf{M} \) are the stiffness matrix and the mass matrix of the discrete or discretized system of order \( n \), respectively, the columns of \( \mathbf{X} \) the eigenvectors, and \( \mathbf{A} \) a diagonal matrix with eigenvalues.

Applying a shift \( \mu \) to Eq. (1) gives

\[ (\mathbf{K} - \mu \mathbf{M})\mathbf{x} = \mathbf{M} \mathbf{\Omega}\mathbf{x} \]  

(2)

where

\[ \mathbf{\Omega} = \mathbf{\Lambda} - \mu \mathbf{I} \]  

(3)

and \( \mathbf{I} \) is the unit matrix.

Suppose that the \( p \) smallest eigenvalues \( \lambda_i(1, 2, \ldots, p) \) and corresponding eigenvectors \( \mathbf{x}_i \) are required. Then the \( j \)th trial vector converges linearly to \( \mathbf{x}_j \) at the rate of \( (\lambda_j - \mu)/(\lambda_{j+1} - \mu) \). For faster convergence, \( q \) trial vectors are normally used with \( q = \min\{2p, p + 8\} \).

If we have \( p \) initial independent vectors \( \mathbf{x}_{0i}(i = 1, 2, \ldots, p) \) 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 \( \mathbf{x}^{(k)}_i \) and \( \lambda^{(k)}_i \), the subspace iteration method with the shift \( \mu \) for the \( k \)th iteration may be described as follows:

\textit{Step 1.} Find improved eigenvectors \( \overline{\mathbf{x}}^{(k+1)} = [\overline{\mathbf{x}}_1^{(k+1)}, \ldots, \overline{\mathbf{x}}_q^{(k+1)}] \) by the simultaneous inverse iteration method:

\[ (\mathbf{K} - \mu \mathbf{M})\overline{\mathbf{x}}^{(k+1)} = \mathbf{M} \mathbf{x}^{(k)} \]  

(4)

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

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

\[ \overline{\mathbf{K}}^{(k+1)} = \overline{\mathbf{x}}^{(k+1)\mathbf{T}}(\mathbf{K} - \mu \mathbf{M})\overline{\mathbf{x}}^{(k+1)} \]  

(5)

\[ \overline{\mathbf{M}}^{(k+1)} = \overline{\mathbf{x}}^{(k+1)\mathbf{T}} \mathbf{M} \overline{\mathbf{x}}^{(k+1)} \]  

(6)

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

\textit{Step 3.} Solve the eigenvalue problem of reduced order \( q \):

\[ \overline{\mathbf{K}}^{(k+1)} \mathbf{Q}^{(k+1)} = \overline{\mathbf{M}}^{(k+1)} \mathbf{Q}^{(k+1)} \]  

(7)

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

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

\[ \mathbf{X}^{(k+1)} = \overline{\mathbf{x}}^{(k+1)} \mathbf{Q}^{(k+1)} \]  

(8)

And the improved eigenvalues can be computed as follows.

\[ \mathbf{A}^{(k+1)} = \mathbf{Q}^{(k+1)} + \mu \mathbf{I} \]  

(9)

Then, provided that the trial vectors in \( \mathbf{X}^{(1)} \) are not orthogonal to one of the required eigenvectors and assuming an appropriate ordering of the trial vectors, \( \mathbf{A}^{(k+1)} \) converges to \( \mathbf{A} \) and \( \mathbf{X}^{(k+1)} \) converges to \( \mathbf{X} \) as \( k \) approaches infinity. The convergence rate of the subspace iteration method with shifting is

\[ (\lambda_j - \mu)/(\lambda_{j+1} - \mu) \]  

(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 [7].
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 \( \text{LDL}^T \) 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 shifting, the following condition was adopted in the subspace iteration method [7]:

\[
1.01 \lambda_{s-1} \leq \mu \leq 0.99 \lambda_s
\]

where \( \lambda_{s-1} \) is the calculated approximation to \((s - 1)\)th eigenvalue and \( \lambda_s \) th 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 the limited region. Then, the singularity may occur even though a shift is inside of the limited region. These are the significant disadvantages of the subspace iteration method with shifting. The purpose of this paper is to remove the limitation in Eq. (11) for choosing the value of a shift \( \mu \).

### 3. Proposed method

#### 3.1. Technical background

Consider the simultaneous inverse iteration step in the subspace iteration method with shifting:

\[
(K - \mu M)X^{(k+1)} = MX^{(k)}
\]

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

First, assume that a shift is close to the \(i\)th eigenvalue. Then, the inverse iteration step on the \(i\)th eigenvalue can be expressed as follows:

\[
(K - \mu M)X_i^{(k+1)} = d_i^{(k+1)}Mx_i^{(k)}
\]

where the scalar \( d_i^{(k+1)} \) controls the length of the vector \( X_i^{(k+1)} \).

Because there are only \( n \) equations with \((n + 1)\) unknowns, \( n \) components of \( X_i^{(k+1)} \) and \( d_i^{(k+1)} \), in Eq. (13), one side condition must be introduced for the solution of Eq. (13). This condition is that the current vector \( (X_i^{(k)}) \) is orthogonal to the incremental vector \((\Delta X_i^{(k)})\) with respect to \( M \); that is,

\[
x_i^{(k)_r}M\Delta x_i^{(k)} = 0
\]

Adding the mass orthonormality relation, \( x_i^{(k)^T}Mx_i^{(k)} = 1 \), to the side condition, Eq. (14), yields

\[
x_i^{(k)}Mx_i^{(k+1)} = 1
\]

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

\[
(K - \mu M)X_j^{(k+1)} = MX_j^{(k)} \quad (j = 1 \sim q, j \neq i)
\]

### Table 1

<table>
<thead>
<tr>
<th>Operation count for subspace iteration method with shifting</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Operation</strong></td>
</tr>
<tr>
<td>Multiplication</td>
</tr>
<tr>
<td>Factorization</td>
</tr>
<tr>
<td>Multiplication</td>
</tr>
<tr>
<td>Solve for ( X_i^{(k+1)} )</td>
</tr>
<tr>
<td>Multiplication</td>
</tr>
<tr>
<td>Multiplication</td>
</tr>
<tr>
<td>Solve for ( Z_i^{(k+1)} ) and ( \Omega_i^{(k+1)} )</td>
</tr>
<tr>
<td>Multiplication</td>
</tr>
<tr>
<td>Subtotal</td>
</tr>
<tr>
<td>Multiplication</td>
</tr>
<tr>
<td>Factorization</td>
</tr>
<tr>
<td>Total</td>
</tr>
</tbody>
</table>
Writing Eqs. (13), (15) and (17) in matrix form gives

\[
\begin{bmatrix}
K - \mu M & Mx_i^{(k)} \\
x_i^{(k)^T} M & 0
\end{bmatrix}
\begin{bmatrix}
\tilde{x}^{(k+1)} \\
d_i^{(k+1)}
\end{bmatrix}
= \begin{bmatrix}
MX_i^{(k)} \\
x_i^{(k)^T} M
\end{bmatrix}
\]  

(18)

where \(x_i^{(k)^T} M \tilde{x}^{(k+1)} = 1\) for \(j = 1, q, j \neq i\), \(d_i^{(k+1)} = (0, \ldots, 0, 0, 1 - d_i^{(k+1)}, 0, \ldots, 0)\) is the row vector of order \(q\) and \(c_i = (0, \ldots, 0, 1, 0, \ldots, 0)\) is the row vector of order \(q\) that all elements are zero except for \(i\)th element with unity.

Note that \(\tilde{x}^{(k+1)}\) from Eq. (18) is used for \(\tilde{x}^{(k+1)}\) in Eqs. (5) and (6) instead of \(\tilde{x}^{(k+1)}\) in Eq. (4). Eq. (18) is the main linear algebraic equation used in the proposed method.

The coefficient matrix of Eq. (18) is of order \((n + 1)\), symmetric and nonsingular. The nonsingularity is one of the significant advantages of the proposed method and will be shown in the next section.

3.2. Proof of the nonsingularity of the coefficient matrix \([16–18]\)

The most remarkable characteristic of the proposed method is that nonsingularity is always guaranteed. Let the coefficient matrix of Eq. (18) be denoted by \(C\), that is

\[
C = \begin{bmatrix}
K - \mu M & Mx_i^{(k)} \\
x_i^{(k)^T} M & 0
\end{bmatrix}
\]  

(19)

If \(C\) is nonsingular when the shift \(\mu\) becomes an exact eigenvalue, then it will be also nonsingular for a nonclose shift. The resulting \(C^*\) will be

\[
C^* = \begin{bmatrix}
K - \mu M & Mx_i \\
x_i^T M & 0
\end{bmatrix}
\]  

(20)

Nonsingularity of the proposed method is, therefore, proved by introducing the new eigenvalue problem of the resulting matrix such as

\[
C^* Y = M^* Y D
\]  

(21)

where \(D\) and \(Y\) are the eigenvalue and the associated eigenvector matrices of the new eigenvalue problem, respectively, and

\[
M^* = \begin{bmatrix}
M & 0 \\
0 & 1
\end{bmatrix}
\]  

(22)
The eigenpairs of the eigenvalue problem (21), \( y_j \) and \( g_j \) for \( j = 1, 2, \ldots, n + 1 \), are as follows:

- **Eigenvector**

\[
y_j = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_{n+1} \end{bmatrix}
\]  

(23)

and

\[
D = \text{diag}(\gamma_1, \gamma_2, \ldots, \gamma_{n+1})
\]  

(24)

The eigenpairs of the eigenvalue problem (21), \( y_j \) and \( g_j \) for \( j = 1, 2, \ldots, n + 1 \), are as follows:

- **Eigenvector**

\[
y_j = \frac{1}{\sqrt{2}} \begin{bmatrix} x_1 \\ 1 \\ \vdots \\ x_k \end{bmatrix}, \quad \frac{1}{\sqrt{2}} \begin{bmatrix} x_1 \\ -1 \\ \vdots \\ x_k \end{bmatrix}, \quad \begin{bmatrix} x_k \\ 0 \end{bmatrix}, \\
\]

\( k = 1, 2, \ldots, n, k \neq i \)

- **Eigenvalue**

\[
g_j = -1, \quad (\lambda_k - \lambda_i) \quad k = 1, 2, \ldots, n, k \neq i
\]

Considering the determinant of Eq. (21), the relationship can be obtained as follows:

\[
\det[C^*] = \det[M^*] \det[D]
\]

\[
= - \det[M] \prod_{k=1}^{n} (\lambda_k - \lambda_i)
\]  

(25)

The determinant of \( C^* \) is not zero because of \( \det[M] \neq 0 \) by definition. The nonsingularity of the coefficient matrix in Eq. (18) is shown. That is, the numerical stability of the proposed method is proved analytically. The proposed method, therefore, makes up for the disadvantage that the subspace iteration method with shifting has the limitations; no limited regions are needed in the proposed method.

### 3.3. Operation count and summary of algorithm

Consider the number of central processor operations in order to obtain an estimate of the cost required for solving an eigenvalue problem. The actual cost must include, of course, the cost of the peripheral processor time. This time is, however, not considered in this investigation since it depends on the system and the programming technique.

#### Table 4

<table>
<thead>
<tr>
<th>Analysis methods</th>
<th>Solution time, s (ratio)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Shift = 1.01 ( \lambda_3 )</td>
<td></td>
</tr>
<tr>
<td>Subspace iteration method with shifting</td>
<td>201.85 (1.00)</td>
</tr>
<tr>
<td>Proposed method</td>
<td>204.78 (1.01)</td>
</tr>
<tr>
<td>Shift = ( \lambda_3 )</td>
<td></td>
</tr>
<tr>
<td>Subspace iteration method with shifting</td>
<td>No solution</td>
</tr>
<tr>
<td>Proposed method</td>
<td>204.35</td>
</tr>
</tbody>
</table>

### Fig. 1. Plane framed structure. \( A = 0.2787 \text{ m}^2 \), \( I = 8.631 \times 10^{-3} \text{ m}^4 \), \( E = 2.068 \times 10^{10} \text{ Pa} \), \( \rho = 5.154 \times 10^2 \text{ kg/m}^3 \).

- **Y**: \( [y_1 \ y_2 \ \cdots \ y_{n+1}] \)

### Fig. 2. Error norm versus iteration number of the first eigenpair of the plane framed structure in case of shift = 1.01\( \lambda_3 \).

### Fig. 3. Error norm versus iteration number of the third eigenpair of the plane framed structure in case of shift = 1.01\( \lambda_3 \).
Let one operation equal one multiplication which is nearly always followed by an addition. Assume that the half-bandwidths of $K$ and $M$ are $m_K$ and $m_M$, respectively. The steps for the subspace iteration method with shifting with the operations are summarized in Table 1, and for the proposed method in Table 2.

The number of operations of the subspace iteration method with shifting is

$$T_s = qn(2m_K + 4m_M + 2q + 4) + n(m_K^2 + 3m_K + 2m_M + 2),$$

and that for the proposed method is

$$T_p = qn(2m_K + 4m_M + 2q + 5) + n(m_K^2 + 3m_K + 2m_M + 2).$$

The proposed method needs more operations per each iteration step, $qn + n(m_K + 1)$, than the subspace iteration method with shifting. While the number of operations for the $LDL^T$ factorization step is proportional to $m_K^2$, the difference of the number of operations between two methods is proportional to $m_K$, which is negligible. Therefore, the larger the bandwidths of the stiffness matrix are, the smaller the ratio of the difference between the operation count to the system degree of freedom. This means that the number of operations for the aforementioned two methods, the subspace iteration method with shifting and the proposed method, is almost the same for large structures.

For example, consider the large structure of which the orders of the stiffness and mass matrices, i.e. $n$, are 100,000, respectively, and the mean half-bandwidths of those matrices, i.e. $m_K$ and $m_M$, are 1000, respectively. The 50 eigenvalues and corresponding eigenvectors are required and the number of the iteration vectors, $q$, is 58. If the number of operations required for solutions of the subspace iteration method with shifting, $T_s$, and that of the proposed method, $T_p$, are 100, respectively, the number of operations of the proposed method and the subspace iteration method with shifting are almost the same as shown in Table 3.

### 4. Numerical examples

The plane framed structure and the three-dimensional framed structure used by Bathe and Wilson [2] are analyzed to verify the effectiveness of the proposed method. With the predetermined error norm of $10^{-6}$, the structures are analyzed by two methods; the
subspace iteration method with shifting which is not used the limited region (see Eq. (11)) and the proposed method, where the error norm is computed by the following equation:

\[
\text{error norm} = \frac{\| (K - \lambda^E_i M) x^E_i \|_2}{\| x^E_i \|_2}
\]

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 10 eigenpairs is compared. All runs are executed in the IRIS4D-20-S17 with 10 Mips and 0.9 MFlops.

### 4.1. Plane framed structure

The first example is a plane framed structure. The geometric configuration and the material properties are shown in Fig. 1. The structure was discretized using 210 beam elements resulting in system of dynamic equations with a total of 330 degrees of freedom. The consistent mass matrix is used for \( M \).

Some results are shown in Table 4 and in Figs. 2–7. The solution time for two methods are summarized in Table 4. When a shift is on 1.01 \( \lambda_3 \), the subspace iteration method with shifting and the proposed method calculate the required 10 eigenpairs. However, when the shift is on \( \lambda_3 \), the subspace iteration method with shifting does not find the solutions, while the proposed method obtains 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, as analytically proved in the article 3.2. This is one of the significant advantages of the proposed method.

For each solution method, the convergence of each eigenpair is depicted in Figs. 2–7. Figs. 2–4 show that when the shift is on 1.01 \( \lambda_3 \), the convergence of the proposed method is nearly equal to that of the accelerated subspace iteration method.
Figs. 5–7 show that when the shift is exactly the same to the third eigenvalue the proposed method converges very well, while the subspace iteration method with shifting cannot converge due to the singularity. As the above results, the proposed method can choose a more exact shift than the subspace iteration method with shifting, thus the proposed method may be the more computationally efficient.

4.2. Three-dimensional framed structure

The second example is the three-dimensional framed structure. Fig. 8 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 $M$.

Some results are shown in Table 5 and in Figs 9–14. The solution time for two methods are summarized in Table 5; when the a shift is on $1.01\lambda_5$, the subspace iteration method with shifting and the proposed method obtain the required 10 eigenpairs. However, when the shift is on $\lambda_5$, the subspace iteration method with shifting 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, as analytically proved in Section 3.2.

For each solution method, the convergence of each eigenpair is depicted in Figs. 9–14. Figs. 9–11 show that when the shift is on $1.01\lambda_5$ the convergence of the proposed method is nearly equal to that of the subspace iteration method with shifting. Figs. 12–14 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 shifting cannot converge due to the singularity. As the above results, the proposed method can choose a more aggressive shift than the subspace iteration method with shifting.
5. Conclusions

This paper proposes a stable acceleration technique using side conditions for the improvement of the subspace iteration method with shifting. 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 shifting, and the operation counts of the proposed method and the subspace iteration method with shifting are almost the same for large structures.

3. The proposed method can choose a more aggressive shift than the subspace iteration method with shifting, thus the proposed method may be more computationally efficient.

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