A preconditioned conjugate projected gradient method for computing eigenvector derivatives with repeated eigenvalues

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Abstract: A preconditioned conjugate projected gradient (PCPG) method is given to solve the repeated eigenvector derivatives with respect to design parameters in finite element models. The factored stiffness matrix is used as a preconditioner, the new method can provide the approximate solutions to repeated eigenvector derivatives. This method can be used as an eigenvector sensitivities solver which can be coupled as an eigensolver/derivative software. Moreover, the new method can be used for industrial-size models. Finally, a numerical example is provided to illustrate the superior efficiency of the present method.

1. Introduction
Eigenvector derivatives of eigenvalues is fast developed in recent years. Because of their important applications in topology optimization, structure vibration, damage detection, finite element modification, and so on [1-3]. The eigen-pair derivatives can be used to estimate the change in the modal parameters, and the stiffness and mass matrices could be given the perturbations about the modal parameters. Recently, many works have been accomplished to improve the accuracy and efficiency of the finite element systems [4, 5].

Nelson [1] given a famous method in 1976, which is called Nelson’s method today, Nelson’s method is a direct method. Then Friswell and Adhikari [2] extended Nelson's method, which is used to solve the complex systems. Alvin [3] given a preconditioned conjugate projected gradient (PCPG) method to solve the control equations, then obtain the eigenvector derivatives of undamped system. However, those methods [1-3] could not be used for computing the eigenvector derivatives with repeated eigenvalues.

Ojalvo [4], Mills-Curran [5] and Shaw and Jayasuriya [6] developed Nelson's method, for undamped systems, the eigenvector derivatives with repeated eigenvalues are obtained. Dailey [7] given a new numerical method to deal with the repeated eigenvector derivatives. Wu [8] given an improved Nelson method, the new modified method is combined [4-6] and improved the accuracy of the repeated eigenvector derivatives. Furthermore, Wu [9] given a preconditioned conjugate gradient (PCG) method, which is very effective for the problems of both distinct and repeated eigenvector derivatives.

Since early works, the direct methods and numerical methods of eigenvector derivatives have been developed for the undamped/damped vibration systems. However, compared with the distinct eigenvalue case, the calculation methods of the repeat eigenvalue case are relatively deficient. In this
paper, we intend to modify the PCPG method to compute the eigenvector derivative problem with repeated eigenvalues.

The paper is organized as follows. In Section 2, the problem and formulas are provided. Section 3 shows a PCPG method, which is used to compute the repeated eigenvector derivatives, a careful projection is added in the right hand of control equation. In Section 4, the results are illustrated by a numerical example. Finally, concluding remarks are given in Section 5.

2. Problem and formulas

The problem of dynamics can be given as:

\[
\begin{align*}
K\phi_i &= \lambda_i M\phi_i \\
\phi_j^T M\phi_j &= \delta_{ij} \quad i,j = 1,2,\ldots,n
\end{align*}
\]

(1)

where \( K \) and \( M \) are the stiffness and mass matrices, \( \lambda_i \) is the \( i \)th eigenvalue. \( \phi_i \) is the associated eigenvector, \( \delta_{ij} \) is the Kronecker delta.

Another form of Eq. (1) can be given as:

\[
\begin{align*}
[\Phi_i, \Psi_h]^T K[\Phi_i, \Psi_h] &= \Lambda_i \\
[\Phi_i, \Psi_h]^T M[\Phi_i, \Psi_h] &= I
\end{align*}
\]

(2)

where \( \Phi_i = [\phi_1, \phi_2, \ldots, \phi_i] \), \( \Psi_h = [\phi_{i+1}, \phi_{i+2}, \ldots, \phi_n] \), \( \Lambda_i = \begin{bmatrix} \lambda_i & 0 \\ 0 & \Lambda_h \end{bmatrix} \), \( \Lambda_i = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_i) \), \( \Lambda_h = \text{diag}(\lambda_{i+1}, \lambda_{i+2}, \ldots, \lambda_n) \). \( \Lambda_i \) and \( \Phi_i \) are the computed lower eigenvalues and associated eigenvectors; \( \Lambda_h \) and \( \Psi_h \) are the un-computed higher eigenvalues and associated eigenvectors, respectively.

We supposed that \( \lambda_{i+1} = \lambda_{i+2} = \cdots = \lambda_{i+m} = \lambda_0 \) where \( s > 0, s < l \), \( \lambda_0 \) is the \( m \) \((1 < m \leq l << n)\) repeated eigenvalues. Let \( X = [\phi_{i+1}, \phi_{i+2}, \ldots, \phi_{i+m}] \), we have

\[
\begin{align*}
KX &= MX\Lambda_m \\
X^T MX &= I_m
\end{align*}
\]

(3)

The sub-eigenproblem is shown as follows:

\[
[X^T (K' - \lambda_0 M') X - \lambda_0^2 I_m] y_i = 0, \quad i = s + 1, s + 2, \ldots, s + m
\]

(4)

an orthogonal matrix \( \Gamma = [\gamma_{s+1}, \gamma_{s+2}, \ldots, \gamma_{s+m}] \) is obtained by Eq.(4), let \( Z = [z_{s+1}, z_{s+2}, \ldots, z_{s+m}] \), where \( Z = X\Gamma \).

The eigenvector derivatives equation can be given as:

\[
(K - \lambda_0 M)z_i' = f_i, \quad i = s + 1, s + 2, \ldots, s + m
\]

(5)

where \( f_i = -(K' - \lambda M' - \lambda_0 M)z_i \).

The eigenvector derivative \( z_i' \) can be given as:

\[
z_i' = v_i + Zc_i = v_i + \sum_{k=s+1}^{s+m} c_{ik} z_k, \quad i = s + 1, s + 2, \ldots, s + m
\]

(6)
where $\mathbf{v}_i$ is a particular solution, so we have $\mathbf{(K}_i^\lambda \mathbf{M})\mathbf{v}_i = \mathbf{f}_i, i = s + 1, s + 2, \cdots, s + m$.

The coefficient matrix in Eq. (6) is $\mathbf{c}_i = \mathbf{[c_{(s+1)i}, c_{(s+2)i}, \cdots, c_{(s+m)i}]}^T$, which is given as follows:

$$c_{ii} = -\mathbf{z}_i \mathbf{z}_i^T (\frac{1}{2} \mathbf{M}' \mathbf{z}_i + \mathbf{M} \mathbf{v}_i),$$

$$i = s + 1, s + 2, \cdots, s + m$$

and

$$c_{kl} = \frac{\mathbf{z}_l^T (\mathbf{K}_i^\lambda - 2\lambda' \mathbf{M}' - \lambda_0 \mathbf{M}^\lambda) \mathbf{z}_k + 2\mathbf{z}_i^T \mathbf{F}\mathbf{v}_k}{2(\lambda_0' - \lambda'_k)},$$

$$i \neq k, i, k = s + 1, s + 2, \cdots, s + m$$

### 3. PCPG method

How to obtain the particular solution $\mathbf{v}_i$ is the key problem. Here $\mathbf{v}_i$ can be shown as the mode expansion form:

$$\mathbf{v}_i = \sum_{j=1}^{l} d_i(j)\varphi_j + \bar{v}_i$$

where

$$d_i(j) = \frac{\varphi_j^T \mathbf{f}_i}{\lambda_j - \lambda_i}, j \neq i, i = s + 1, s + 2, \cdots, s + m$$

So, the unknown part $\mathbf{v}_i$ can be given as:

$$\mathbf{(K}_i^\lambda \mathbf{M})\bar{v}_i = \mathbf{f}_i - \sum_{j=1}^{l} \varphi_j^T \mathbf{f}_i \mathbf{M} \varphi_j$$

### The PCPG algorithm is given as follows:

#### PCPG Algorithm

$k = 0$

$\mathbf{w}_0 = 0$

$$\bar{r}_0 = \mathbf{f}_i - \sum_{j=s+1}^{l} \varphi_j^T \mathbf{f}_i \mathbf{M} \varphi_j$$

while ($\|\bar{r}_k\|_2 \geq \varepsilon\|\bar{r}_0\|_2$)

Solve $\mathbf{K}\bar{y}_k = (\mathbf{I} - \mathbf{M} \Phi \Phi^T)\bar{r}_k$

$$\mathbf{y}_k = (\mathbf{I} - \mathbf{\Phi} \Phi^T \mathbf{M})\bar{y}_k$$

$k = k + 1$

if $k = 1$

$q_1 = y_0$

else
\[
\begin{aligned}
\beta_k &= \frac{\mathbf{r}_{k-1}^T \mathbf{y}_{k-1}}{\mathbf{r}_{k-2}^T \mathbf{y}_{k-2}} \\
\mathbf{q}_k &= \mathbf{y}_{k-1} + \beta_k \mathbf{q}_{k-1}
\end{aligned}
\]

end if

\[\alpha_k = \frac{\mathbf{r}_{k-1}^T \mathbf{y}_{k-1}}{\mathbf{q}_k^T (\mathbf{K} - \lambda_0 \mathbf{M}) \mathbf{q}_k}\]

\[\mathbf{w}_k = \mathbf{w}_{k-1} + \alpha_k \mathbf{q}_k\]

\[\mathbf{r}_k = \mathbf{r}_{k-1} - \alpha_k (\mathbf{K} - \lambda_0 \mathbf{M}) \mathbf{q}_k\]

end

\[\mathbf{v}_k = \mathbf{w}_k\]

Here \(\varepsilon\) is the error tolerance, in this paper, we choose \(\varepsilon = 10^{-6}\). The PCPG algorithm with relative residual error at iteration \(k\) can be given as:

\[e_k = \frac{\|\mathbf{r}_k\|}{\|\mathbf{r}_0\|}\quad (12)\]

Since Alvin [3] first given a PCPG method to deal with eigenvector derivatives with distinct eigenvalues. While we introduce the PCPG algorithm for solving the repeated eigenvector derivatives problems.

4. Numerical example

In this section, an example is shown to explain the high performance of the PCPG method. The Intel Visual Fortran XE 2015 with Math Kernel Library 11.2 is used in this paper, the Harwell-Boeing (HB) sparse matrix format is used. The computational program of the example is completed on the platform: Intel 15-3450, quad-core CPU with 3.10GHz, 8GB RAM.

Example: A square plate structure is shown in Figure 1. The four edges of the square plate are clamped. The length of the square plate is 10 m, the thickness of the plate is 0.1m. Two ribs are added
to its midlines, and the cross-section is 0.1m×0.3m. The Poisson's ratio is \( v = 0.3 \) and the modulus of elasticity for structure is \( E = 2\times10^{11} \) Pa. The model has 58806 DOFs. The design parameter is chosen as the height \( p \) and its initial value is \( P_0 = 0.3m \).

The preconditioner is \( K \). We are interested in the four pair modes with repeated eigenvalues. By using the PCPG method, the relative residual errors for computing \( \mathbf{v}_i \) are shown in Figure 2. And the relative residual error \( e_k \) is decreased markedly. While the CPU run-times of PCPG method are given in Table 1. We can see that, the computing times of the PCPG method are very short.

![Figure 2. The convergence of the relative residual errors.](image)

| Mode | CPU run-times (s) |
|------|-------------------|
| 2,3  | 0.5420            |
| 7,8  | 0.6220            |
| 9,10 | 0.8740            |
| 14,15| 1.007             |

5. Conclusions
In this paper, we extended the Alvin’s method, and a PCPG method is used to find the eigenvector derivatives with repeated eigenvalues. The projections of the method are given in the right hand of the control equations. Now, the PCPG method is used as a computer solver for computing the eigenvector derivatives. Finally, the PCPG method can be used for the large finite element system with eigenvector derivative problems.

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