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Technical Notes

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Improved Nelson's Method for Computing Eigenvector Derivatives with Distinct and Repeated Eigenvalues

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I. Introduction

THE computation of derivatives of eigenvalues and eigenvectors with respect to model parameters is crucial for many applications [1]. Nelson [2] proposed an approach for general real eigensystems with distinct eigenvalues where only the eigenvector of interest was required. Ojalvo [3], Mills-Curran [4], Dailey [5], and Shaw and Jayasuriya [6] developed Nelson's method for real symmetric eigensystems with repeated eigenvalues. For computation of a particular solution, the methods described in [3,5] may fail in some circumstances. Other methods have been suggested by Mills-Curran [4] and Song et al. [7], but they are difficult to implement. When a system of linear equations is solved, one hopes that the calculated solution is a close representation of the true solution. The computed solution for a system with a large condition number may be inexact due to extreme sensitivity of the solution to small changes in its coefficient matrix and right column vectors [8]. Because some diagonal elements in the coefficient matrix for particular solutions are set to units, its coefficients are not all of the same order of magnitude. So the coefficient matrix has a large condition number. In this Note, Nelson's method is first extended to the case of repeated eigenvalues for the symmetric real eigensystems and its improvements are then presented. The condition number of the coefficient matrix of the improved method is considerably reduced.

II. Extension and Improvement of Nelson's Method

Consider the following repeated eigenvalue problem for a real symmetric eigensystem:

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

$$\mathbf{X}^T\mathbf{MX} = \mathbf{I} \tag{2}$$

where $\mathbf{K}$ and $\mathbf{M}$ in $R^{n\times n}$ are the structural stiffness and mass matrices, respectively, whose elements depend continuously on the system parameters, $\mathbf{X}$ in $R^{n\times m}$ is a eigenvector matrix, $\mathbf{\Lambda} = \lambda_i\mathbf{I}$ in $R^{m\times m}$ is a diagonal matrix, and λ_i is the eigenvalue of multiplicity m. Denoting the first derivative with respect to parameter p by a prime, eigenvalue derivatives for repeated eigenvalues can be found by solving a subeigenanalysis problem [3–6]

$$\mathbf{X}^T(\mathbf{K}' - \lambda_i\mathbf{M}')\mathbf{X}\Gamma = \Gamma\mathbf{\Lambda}' \tag{3}$$

Assuming that the $\lambda_i'(i = 1, 2, \ldots, m)$ are distinct, a unique orthogonal matrix $\Gamma = [\gamma_1, \gamma_2, \ldots, \gamma_m]$ can be generated that is used to define the unique differentiable eigenvectors matrix $\mathbf{Z} = [\mathbf{z}_1, \mathbf{z}_2, \ldots, \mathbf{z}_m]$ by $\mathbf{Z} = \mathbf{X}\Gamma$. For convenience, we denote

$$\mathbf{F} \equiv \mathbf{K} - \lambda_i\mathbf{M}, \qquad \mathbf{G} \equiv (\lambda_i\mathbf{M}' - \mathbf{K}')\mathbf{Z} + \mathbf{MZ\Lambda}' \tag{4}$$

Eigenvector derivatives $\mathbf{Z}'$ satisfy

$$\mathbf{FZ}' = \mathbf{G} \tag{5}$$

From Eq. (5), $\mathbf{Z}'$ can be written as

$$\mathbf{Z}' = \mathbf{V} + \mathbf{ZC} \tag{6}$$

where $\mathbf{V}$ is a particular solution to Eq. (5) and satisfies

$$\mathbf{FV} = \mathbf{G} \tag{7}$$

Once the particular solution $\mathbf{V}$ is obtained, coefficient matrix $\mathbf{C} = [\mathbf{c}_1, \mathbf{c}_2, \ldots, \mathbf{c}_m]$ can be determined [4,5], $\mathbf{Z}'$ is then obtained.

The first problem is to compute the particular solution $\mathbf{V}$ by Eq. (7). Because $\mathbf{F}$ in Eq. (4) is of rank $n - m$, it cannot be inverted. Here, we propose a rigorous approach to compute $\mathbf{V}$. Note that $\mathbf{FZ} = \mathbf{0}$ can be written as

$$[\mathbf{F}_1, \mathbf{F}_2, \ldots, \mathbf{F}_n]\begin{bmatrix} z_{11} & z_{12} & \cdots & z_{1m} \\ z_{21} & z_{22} & \cdots & z_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ z_{n1} & z_{n2} & \cdots & z_{nm} \end{bmatrix} = [\mathbf{0}] \tag{8}$$

Because $\mathbf{Z}$ is of rank m, we can select m rows from $\mathbf{Z}$ so that the determinant of matrix $\mathbf{Z}_{m,m}$ formed by these rows is nonzero. Without loss of generality, we assume that the first m rows of $\mathbf{Z}$ satisfy the requirement. Equation (8) can be rewritten as

$$[\mathbf{F}_1, \mathbf{F}_2, \ldots, \mathbf{F}_m]\mathbf{Z}_{m,m} = -[\mathbf{F}_{m+1}, \mathbf{F}_{m+2}, \ldots, \mathbf{F}_n]\begin{bmatrix} z_{(m+1)1} & z_{(m+1)2} & \cdots & z_{(m+1)m} \\ z_{(m+2)1} & z_{(m+2)2} & \cdots & z_{(m+2)m} \\ \vdots & \vdots & \ddots & \vdots \\ z_{n1} & z_{n2} & \cdots & z_{nm} \end{bmatrix} \tag{9}$$

Because $\det(\mathbf{Z}_{m,m}) \neq 0$, from Eq. (9), we derive that each of the vectors $\mathbf{F}_1, \mathbf{F}_2, \ldots, \mathbf{F}_m$ can be expressed as a linear combination of $n - m$ vectors $\mathbf{F}_{m+1}, \mathbf{F}_{m+2}, \ldots, \mathbf{F}_n$. Because the rank of $\mathbf{F}$ is $n - m$, the vectors $\mathbf{F}_{m+1}, \mathbf{F}_{m+2}, \ldots, \mathbf{F}_n$ must be linear independent. Let $\mathbf{F}^b = [\mathbf{F}_{m+1}, \mathbf{F}_{m+2}, \ldots, \mathbf{F}_n]$, then the rank of $\mathbf{F}^b$ is $n - m$. Because of the symmetry of $\mathbf{F}$, each of the first m rows of $\mathbf{F}^b$ can also be expressed as a linear combination of the remaining $n - m$ rows with rank $n - m$. Therefore, submatrix $\bar{\mathbf{F}}$ obtained by deleting the first m rows and columns from $\mathbf{F}$ is nonsingular and symmetrical. Let $\bar{\mathbf{G}}$ be the matrix achieved by eliminating the first m rows of $\mathbf{G}$. Solving the

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equation

$$\bar{\mathbf{F}}\,\bar{\mathbf{V}} = \bar{\mathbf{G}} \tag{10}$$

yields $\bar{\mathbf{V}}$. Let $\mathbf{V}^T = \begin{bmatrix} \mathbf{0}_{m,m}^T & \bar{\mathbf{V}}^T \end{bmatrix}$; the matrix $\mathbf{V}$ is a particular solution which we want. In fact, using Eqs. (3), (4), and (8) and noting we have $\mathbf{Z}^T\mathbf{G} = \mathbf{0}$, hence

$$\mathbf{Z}^T(\mathbf{F}\mathbf{V} - \mathbf{G}) = \mathbf{0} \tag{11}$$

Using Eq. (11) and partitioning $\mathbf{Z}$, $\mathbf{G}$, $\mathbf{F}$, and $\mathbf{V}$, we obtain

$$\begin{bmatrix} \mathbf{Z}_{m,m} \\ \mathbf{Z}_{n-m,m} \end{bmatrix}^T \left(\begin{bmatrix} \mathbf{F}_{m,m} & \mathbf{F}_{m,n-m} \\ \mathbf{F}_{n-m,m} & \bar{\mathbf{F}} \end{bmatrix} \begin{bmatrix} \mathbf{0}_{m,m} \\ \bar{\mathbf{V}} \end{bmatrix} - \begin{bmatrix} \mathbf{G}_{m,m} \\ \bar{\mathbf{G}} \end{bmatrix} \right) = \mathbf{0} \tag{12}$$

Expanding Eq. (12) yields

$$\mathbf{Z}_{m,m}^T(\mathbf{F}_{m,n-m}\bar{\mathbf{V}} - \mathbf{G}_{m,m}) = -\mathbf{Z}_{n-m,m}^T(\bar{\mathbf{F}}\,\bar{\mathbf{V}} - \bar{\mathbf{G}}) \tag{13}$$

Using Eqs. (10) and (13) and using $\det(\mathbf{Z}_{m,m}) \neq 0$ leads to

$$\mathbf{F}_{m,n-m}\bar{\mathbf{V}} = \mathbf{G}_{m,m} \tag{14}$$

Therefore, by Eqs. (10) and (14), the $\mathbf{V}$ satisfies Eq. (7). The particular solution $\mathbf{V}$ may be obtained by solving the following system:

$$\begin{bmatrix} \mathbf{I}_{m,m} & \mathbf{0}_{m,n-m} \\ \mathbf{0}_{n-m,m} & \bar{\mathbf{F}} \end{bmatrix} \mathbf{V} - \begin{bmatrix} \mathbf{0}_{m,m} \\ \bar{\mathbf{G}} \end{bmatrix} = \mathbf{0} \tag{15}$$

Now, we extend Nelson's method to the case of repeated eigenvalues. Let $\mathbf{Z}_{m,m}$ be a submatrix composed of the l_jth ($j = 1, 2, \ldots, m$) rows of $\mathbf{Z}$ such that

$$\operatorname{abs}\left(\det \begin{bmatrix} z_{l_1 1} & z_{l_1 2} & \cdots & z_{l_1 m} \\ z_{l_2 1} & z_{l_2 2} & \cdots & z_{l_2 m} \\ \vdots & \vdots & \ddots & \vdots \\ z_{l_m 1} & z_{l_m 2} & \cdots & z_{l_m m} \end{bmatrix} \right) = \max_{k_1, k_2, \ldots, k_m} \operatorname{abs}\left(\det \begin{bmatrix} z_{k_1 1} & z_{k_1 2} & \cdots & z_{k_1 m} \\ z_{k_2 1} & z_{k_2 2} & \cdots & z_{k_2 m} \\ \vdots & \vdots & \ddots & \vdots \\ z_{k_m 1} & z_{k_m 2} & \cdots & z_{k_m m} \end{bmatrix} \right) \tag{16}$$

Then $\det(\mathbf{Z}_{m,m}) \neq 0$. Setting the l_jth ($j = 1, 2, \ldots, m$) rows and columns of $\mathbf{F}$ equal to zero, while the l_jth ($j = 1, 2, \ldots, m$) diagonal elements of $\mathbf{F}$ equal to 1, respectively, to form $\tilde{\mathbf{F}}$; and setting l_jth ($j = 1, 2, \ldots, m$) rows of $\mathbf{G}$ equal to zero to form $\tilde{\mathbf{G}}$, we may get a particular solution to Eq. (7) by solving equation

$$\tilde{\mathbf{F}}\mathbf{V} = \tilde{\mathbf{G}} \tag{17}$$

The coefficient matrix $\tilde{\mathbf{F}}$ in Eq. (17) is symmetric and nonsingular and has exactly the same bandedness as the original eigensystem.

Because elements in the coefficient matrix $\tilde{\mathbf{F}}$ in Eq. (17) are not all of the same order of magnitude, $\tilde{\mathbf{F}}$ has a large condition number. Solutions to Eq. (17) may be very sensitive to the effects of small errors in its coefficient matrix and right column vectors. To reduce the condition number, we replace the l_jth ($j = 1, 2, \ldots, m$) diagonal elements of $\tilde{\mathbf{F}}$ in Eq. (17) with the corresponding diagonal elements $k_{l_j l_j}$ of the stiffness matrix $\mathbf{K}$, and denote the newly formed matrix by $\hat{\mathbf{F}}$. Then Eq. (17) and the following system

$$\hat{\mathbf{F}}\,\hat{\mathbf{V}} = \tilde{\mathbf{G}} \tag{18}$$

have the same solution, that is, $\hat{\mathbf{V}} = \mathbf{V}$. Now the elements in the modified coefficient matrix $\hat{\mathbf{F}}$ in Eq. (18) are all of the nearly same order of magnitude, and thus $\hat{\mathbf{F}}$ has a very small condition number as compared with $\tilde{\mathbf{F}}$.

For the case of a distinct eigenvalue, that is, $m = 1$, the row-column index l_1 is chosen to correspond to the largest magnitude element in the eigenvector $\mathbf{X}$.

III. Numerical Example

The validity of the proposed method will be demonstrated by a numerical example. Consider the cantilever beam finite element model with square section [5]. The system has a twice repeated eigenvalue: 1.8414. The eigenvector matrix where the derivative can be defined is

$$\mathbf{Z} = \begin{bmatrix} +6.9074e-2 & 0 \\ 0 & +6.9074e-2 \\ 0 & +4.7541e-2 \\ -4.7541e-2 & 0 \\ +2.3452e-2 & 0 \\ 0 & +2.3452e-2 \\ 0 & +4.0168e-2 \\ -4.0168e-2 & 0 \end{bmatrix}$$

For the 2-repeated eigenvalues, the condition numbers of $\tilde{\mathbf{F}}$ and $\hat{\mathbf{F}}$ are 2.5159×10^4 and 14.9305, respectively. Therefore, the condition number of $\tilde{\mathbf{F}}$ is remarkably reduced. In the computation of derivatives, using Eq. (16), we have $l_1 = 1$, $l_2 = 2$. The right-hand side vector $\tilde{\mathbf{G}}$ in Eq. (17) and the vector $\tilde{\mathbf{G}}_p$, a small perturbation of $\tilde{\mathbf{G}}$, are as follows:

$$\tilde{\mathbf{G}} = \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ -3.0702 & 0 \\ +22.168 & 0 \\ 0 & 0 \\ 0 & 0 \\ -18.077 & 0 \end{bmatrix}, \qquad \tilde{\mathbf{G}}_p = \begin{bmatrix} 0 & +0.0100 \\ +0.0100 & 0 \\ 0 & 0 \\ -3.0702 & 0 \\ +22.168 & 0 \\ 0 & 0 \\ 0 & 0 \\ -18.077 & 0 \end{bmatrix}$$

The exact eigenvector derivative $\mathbf{Z}'$ is obtained by solving Eqs. (17) or (18) and the approximate solutions $\tilde{\mathbf{Z}}'_p$ and $\hat{\mathbf{Z}}'_p$ computed by solving Eqs. (17) and (18) with $\tilde{\mathbf{G}}_p$ instead of $\tilde{\mathbf{G}}$, respectively, are listed as follows:

$$\mathbf{Z}' = \begin{bmatrix} -2.0519e-3 & 0 \\ 0 & 0 \\ 0 & 0 \\ +5.1086e-3 & 0 \\ +1.2002e-3 & 0 \\ 0 & 0 \\ 0 & 0 \\ -1.9990e-3 & 0 \end{bmatrix}$$

$$\tilde{\mathbf{Z}}'_p = \begin{bmatrix} -2.0519e-3 & -1.4949e-1 \\ +2.0440e-3 & 0 \\ -5.4759e-3 & 0 \\ +5.1086e-3 & +1.0977e-1 \\ +1.2002e-3 & -5.4150e-2 \\ -2.7012e-3 & 0 \\ -4.6266e-3 & 0 \\ -1.9990e-3 & +9.2748e-2 \end{bmatrix}$$

$$\hat{\mathbf{Z}}'_p = \begin{bmatrix} -2.0519e-3 & -1.2458e-5 \\ +1.7033e-7 & 0 \\ -4.5632e-7 & 0 \\ +5.1086e-3 & +9.1478e-6 \\ +1.2002e-3 & -4.5125e-6 \\ -2.2510e-7 & 0 \\ -3.8555e-7 & 0 \\ -1.9990e-3 & +7.7290e-6 \end{bmatrix}$$

These results illustrate the effectiveness of the proposed method.

VI. Conclusions

An improved Nelson's method has been presented for computing eigenvector derivatives with distinct and repeated eigenvalues for the symmetric real eigensystems. The Nelson's method for distinct eigenvalues has first been extended to the case of repeated eigenvalues and its improvements have then been proposed. The improvement preserves the symmetry of the coefficient matrix and has exactly the same bandedness as the original eigensystem. Particularly, the condition number of a coefficient matrix for a particular solution has remarkably been reduced. Numerical examples have demonstrated the validity of the proposed method.

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