A new method for computation of eigenvector derivatives with distinct and repeated eigenvalues in structural dynamic analysis

Zhengguang Lia, Siu-Kai Laib,c*, Baisheng Wud

^a State Key Laboratory of Automotive Simulation and Control, School of Mathematics, Jilin University, Changchun, 130012, People's Republic of China

^b Department of Civil and Environmental Engineering, The Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong, People's Republic of China

^c The Hong Kong Polytechnic University Shenzhen Research Institute, Nanshan, Shenzhen, People's Republic of China

^d School of Electro-Mechanical Engineering, Guangdong University of Technology, Guangzhou, 510006, People's Republic of China

ABSTRACT

Determining eigenvector derivatives is a challenging task due to the singularity of the coefficient matrices of the governing equations, especially for those structural dynamic systems with repeated eigenvalues. An effective strategy is proposed to construct a non-singular coefficient matrix, which can be directly used to obtain the eigenvector derivatives with distinct and repeated eigenvalues. This approach also has an advantage that only requires eigenvalues and eigenvectors of interest, without solving the particular solutions of eigenvector derivatives. The Symmetric Quasi-Minimal Residual (SQMR) method is then adopted to solve the governing equations, only the existing factored (shifted) stiffness matrix from an iterative eigensolution such as the subspace iteration method or the Lanczos algorithm is utilized. The present method can deal with both cases of simple and repeated eigenvalues in a unified manner. Three numerical examples are given to illustrate the accuracy and validity of the proposed algorithm. Highly accurate approximations to the eigenvector derivatives are obtained within a few iteration steps, making a significant reduction of the computational effort. This method can be incorporated into a coupled eigensolver/derivative software module. In particular, it is applicable for finite element models with large sparse matrices.

E-mail address: sk.lai@polyu.edu.hk (Siu-Kai Lai)

^{*}Corresponding author.

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1. Introduction

The computation of eigenvalue and eigenvector derivatives with respect to changes in structural design parameters is of wide practical importance in many fields, including structural dynamic optimization, system updating, damage detection, modification and identification [1-4]. However, determining eigenvector derivatives is still a challenging task due to the singularity of the coefficient matrices of the governing equations, especially for those structural dynamic systems with repeated eigenvalues.

To date, many methods have been developed for computing derivatives of eigenvalues and eigenvectors. The modal method was firstly derived by Fox and Kapoor [5] for the symmetric generalized eigenvalue problems. This technique requires the presence of knowledge for all eigenvectors, it is thus difficult for implementation and time-consuming for the analysis of large-scale structures. Based on the framework of this approach, Wang [6] improved the modal truncation method by using a residual static mode to approximate the contribution due to unavailable high-frequency modes. By means of the truncated modes to the eigenvector derivatives [7], the accuracy of computing the derivatives of eigenvalues and eigenvectors can be further improved. Afterwards, this approach was extended to investigate the symmetric and asymmetric systems with damping [8-10].

In an early effort, Nelson [11] proposed an efficient method to calculate the first-order derivatives of eigenvectors with distinct eigenvalues for the general real systems, by expressing the eigenvector derivatives as a particular solution and a homogeneous solution. In contrast to the modal method, the Nelson's method only requires considering both eigenvalues and eigenvectors. Friswell [12] extended the Nelson's method to find the second-order and higher-order derivatives of undamped systems. Besides, Friswell and Adhikari [13] further generalized the Nelson's method to calculate the eigenvector derivatives of symmetric and asymmetric systems. Guedria et al. [14] also applied the Nelson's method to compute the second-order derivatives of viscously damped systems.

Algebraic methods are another common approach that can be used to conduct the sensitivity analysis of mode shapes. Based on the rationale of this technique, a set of algebraic equations can be formulated using the derivatives of eigenvalue problems and the additional constraints can be determined from the derivatives of normalization. In the past, Lee and Jung [15] developed an algebraic method for the real symmetric eigenvalue problem with distinct eigenvalues. They [16] further extended the algebraic method to compute the eigenpair derivatives of symmetric systems with viscous damping. Besides, the algebraic approach was generalized for the eigensensitivities

of asymmetric viscously damped systems [17-20]. Recently, Li et al. [21] extended this type of method to calculate the first-order and second-order eigenvector derivatives of undamped and damped nonlinear systems.

Furthermore, iterative methods are often used for the sensitivity analysis of eigensystems. Rudisill and Chu [22] presented an iteration method to find the first partial derivatives of eigenvalues and eigenvectors of self-adjoint systems. Andrew [23] offered a rigorous proof for the convergence of an iterative algorithm under the conditions mentioned in [22], and some refinements were also proposed in [24, 25]. Based on the Subspace Iteration, Lanczos, Davidson and Arnoldi methods, the corresponding iterative algorithms for the analysis of eigensensitivites were established, respectively [26-30]. In addition, Alvin [31] introduced a preconditioned conjugate projected gradient (PCPG)-based technique for the analysis of eigenvalue problems. Xie [32] proposed a method that can be used to simultaneously compute the derivatives of several simple eigenvalues and the corresponding eigenvectors of unsymmetric damped systems. In the literature, some review studies [33, 34] were also presented for the computation of derivatives of the general eigensystems with distinct eigenvalues.

It is worth noting that much research efforts [5-32] are only applicable to the case of distinct eigenvalue systems. However, there are many repeated or nearly equal eigenvalues in typical structural problems caused by two or more planes of the reflective or cyclic structural symmetry, e.g., wheelsets on trains. Besides, the repeated eigenvalues are far more likely to occur in optimized structures. The calculation of the derivatives of eigenvectors with repeated eigenvalues is more difficult, because the rank of the coefficient matrices of the governing equations are lower than those of the simple eigenvalues.

Generally, there are two key issues in the computation of eigenvector derivatives for simple and repeated eigenvalues by means of the improved Nelson's method. The first problem is how to find the particular solutions to the governing equations with a singular coefficient matrix, and the second one is how to determine the eigenvector derivatives for the given particular solutions. The previously proposed methods are mainly dependent on deleting rows and columns of the singular dynamic stiffness matrix [35-37] or using the bordered matrix method [38-40] to form a non-singular coefficient matrix, which requires re-ordering the matrix and destroying its sparsity. For example, Ojalvo [35] generated insufficient equations to determine the eigenvector derivatives form the particular solutions. Mills-Curran [36] and Dailey [37] considered the information from the second-order derivatives of eigenvalue problems to calculate the eigenvector derivatives of undamped systems with repeated eigenvalues. The case in which some of the first-order derivatives of repeated eigenvalues are not distinct was also considered [39, 41,

42]. Tang et al. [43, 44] presented a method for the sensitivity analysis of repeated eigenvalues of general quadratic eigenvalue problems. Moreover, Xu and Wu [45] constructed a new normalization condition and developed an efficient method to compute the first-order derivatives of eigenvectors of symmetric viscously damped systems with distinct and repeated eigenvalues. More recently, Li et al. [46] proposed a new normalization for the left eigenvectors. Indeed, the left and right eigenvector derivatives can be computed in a parallel way for the asymmetric damped systems with distinct and repeated eigenvalues. They [47] also presented a combined normalization method to calculate the eigenvector derivatives of viscously damped systems with distinct and multiple eigenvalues.

On the other hand, Lee et al. [48] developed an algebraic method to consider the derivatives of eigensolutions of undamped eigensystems with multiple eigenvalues. Furthermore, Lee et al. [49] and Choi et al. [50] extended their algebraic method to the higher-order eigensensitivity of symmetric damped systems with repeated eigenvalues. Nevertheless, Wu et al. [40] pointed out that there exists a mistake in the derivation of the normalization of the systems with repeated eigenvalues [48].

Making use of a simultaneous iteration algorithm, Andrew and Tan [51, 52] considered the eigenpair derivatives of repeated eigenvalues and its corresponding eigenvectors. Qian [53] proposed a numerical method to compute the first-order and higher-order derivatives of multiple eigenpairs of quadratic eigenvalue problems. Application of these methods to many models, however, is occasionally confronted to convergence problems. Recently, Wu et al. [54] presented a preconditioned conjugate gradient (PCG)-based iteration method to calculate the eigenvector derivatives of real symmetric eigensystems with simple and repeated eigenvalues. Li et al. [55] proposed a method that can deal with the computation of eigenvector derivatives for middle-eigenvalue problems. Both methods in [54, 55] require other computed eigenvectors except the eigenvectors of interest.

In this paper, a novel method is proposed to calculate the eigenvector derivatives of real symmetric eigensystems with distinct and repeated eigenvalues. A strategy is prescribed for constructing a non-singular coefficient matrix, which can be directly used to obtain the derivatives of eigenvectors with repeated eigenvalues, without solving the particular solutions of eigenvector derivatives. The present approach only requires considering the modes of interest, and it is very efficient to calculate the sensitivity of a few modes. Presented herein only utilizes the previously computed and factorized (shifted) stiffness matrix from the computation of associated eigenvectors. Highly accurate approximate solutions to the eigenvector derivatives can

be obtained. Besides, this technique is suitable for integrating with a coupled eigensolver/derivative software module and it can leverage the non-recurring cost of a solver.

The reminder of this paper is organized as follows. Section 2 provides a preliminary review of the theoretical background. Section 3 shows the working algorithms of the Nelson's method and its improved version. Section 4 presents a new algorithm to compute the eigenvector derivatives with distinct and repeated eigenvalues. In Section 5, a comparison study for the illustrative examples is given to verify the effectiveness of the present approach. Finally, the concluding remarks are summarized in Section 6.

2. Problem formulation

The governing eigenproblem of an undamped structural modal with n degrees of freedom (DOFs) can be expressed as

$$\mathbf{K}\mathbf{\phi}_{i} = \lambda_{i}\mathbf{M}\mathbf{\phi}_{i} \ (i = 1, 2, \dots, n) \tag{1}$$

where **K** and **M** are the $n \times n$ stiffness and mass matrices, respectively; **K** is (semi-)positive definite, **M** is positive definite; λ_i is the *i*-th eigenvalue where $\lambda_i = \omega_i^2$ is the square of the *i*-th frequency in rad/s; and φ_i is the associated eigenvector that can be normalized as follows,

$$\mathbf{\phi}_{i}^{T}\mathbf{M}\mathbf{\phi}_{j} = \delta_{ij} \tag{2}$$

where δ_{ij} $(i, j = 1, 2, \dots, n)$ is the Kronecker delta.

When the design parameter $p=p_0$, it is assumed that there exist m repeated eigenvalues λ_i (i.e., $i=s+1, s+2, \cdots, s+m$, with $s\geq 0$), that is to say, $\lambda_{s+1}=\lambda_{s+2}=\cdots=\lambda_{s+m}=\lambda_0$. The corresponding eigenvectors are denoted as $\phi_{s+1}, \phi_{s+2}, \cdots, \phi_{s+m}$. Hence, the governing equation can be re-written in the following form with $\lambda_i=\lambda_0$,

$$[\mathbf{\Phi}_m]^T \mathbf{K} [\mathbf{\Phi}_m] = \mathbf{\Lambda}_m$$

$$[\mathbf{\Phi}_m]^T \mathbf{M} [\mathbf{\Phi}_m] = \mathbf{I}_m$$

$$(3)$$

where \mathbf{I}_m is an identity matrix, $\mathbf{\Phi}_m = [\mathbf{\phi}_{s+1}, \mathbf{\phi}_{s+2}, \cdots, \mathbf{\phi}_{s+m}]$ and $\mathbf{\Lambda}_m = \mathbf{diag}(\underbrace{\lambda_0, \lambda_0, \cdots, \lambda_0}_{m})$ can

be computed by using the Lanczos algorithm or the subspace iteration method [56]. Note that the case of m = 1 corresponds to a distinct eigenvalue. To estimate the change in modal parameters

due to the perturbation of design parameters, it is required to calculate the eigenvalue and eigenvector derivatives.

3. Nelson's method and its improved version

In the case of m = 1, the calculation for the derivatives of eigenvalues and eigenvectors can be effectively solved by the Nelson's method. By differentiating Eqs. (1) and (2) yields,

$$(\mathbf{K} - \lambda_i \mathbf{M}) \mathbf{\phi}_i' = (\lambda_i' \mathbf{M} + \lambda_i \mathbf{M}' - \mathbf{K}') \mathbf{\phi}_i, \quad i = s + 1$$
(4)

$$(\mathbf{\phi}_i')^T \mathbf{M} \mathbf{\phi}_i + \mathbf{\phi}_i^T \mathbf{M}' \mathbf{\phi}_i + \mathbf{\phi}_i^T \mathbf{M} \mathbf{\phi}_i' = 0, \quad i = s + 1$$
(5)

where a prime represents the derivative with respect to the design parameter p at $p = p_0$.

Premultiplying Eq. (4) by $\mathbf{\phi}_{i}^{T}$ and exploiting Eq. (2), we have

$$\lambda_i' = \mathbf{\phi}_i^T (\mathbf{K}' - \lambda_i \mathbf{M}') \mathbf{\phi}_i, \quad i = s + 1$$
 (6)

Note that $\mathbf{K} - \lambda_i \mathbf{M} = \mathbf{K} - \lambda_0 \mathbf{M}$ is of rank n-1 and kernel $\boldsymbol{\varphi}_i$, the eigenvector derivatives $\boldsymbol{\varphi}_i'$ of Eq. (4) have the following form

$$\mathbf{\phi}_{i}' = c\mathbf{\phi}_{i} + \mathbf{v} \tag{7}$$

where \mathbf{v} is a particular solution to Eq. (4). The present approach is first to calculate some particular solutions \mathbf{v} and find the coefficients c, so that $\mathbf{\phi}'_i$ can then be solved. For convenience, we denote $\mathbf{F} = \mathbf{K} - \lambda_i \mathbf{M} = \mathbf{K} - \lambda_0 \mathbf{M}$, $\mathbf{F}' = \mathbf{K}' - \lambda_i' \mathbf{M} - \lambda_0 \mathbf{M}'$, $\mathbf{f} = -\mathbf{F}' \mathbf{\phi}_i$, a suitable particular solution \mathbf{v} can be found by the following algorithm:

- 1) Assume $\mathbf{\varphi}_i = (\varphi_{i1} \quad \varphi_{i2} \quad \cdots \quad \varphi_{in})^T$, find k such that $|\varphi_{ik}| = ||\mathbf{\varphi}_i||_{\infty}$.
- 2) Replace the k^{th} diagonal element of the \mathbf{F} with the corresponding one of the stiffness matrix \mathbf{K} , and other elements in the k^{th} row and column of the \mathbf{F} with 0, and denote the result $\overline{\mathbf{F}}$.
- 3) Replace the k^{th} element of \mathbf{f} with zero and call the result $\bar{\mathbf{f}}$.
- 4) Solve $\overline{\mathbf{F}}\mathbf{v} = \overline{\mathbf{f}}$.

Once \mathbf{v} is determined, the coefficients c can be calculated by substituting Eq. (7) into Eq. (5) as,

$$c = -\mathbf{v}^T \mathbf{M} \mathbf{\phi}_i - 0.5 \mathbf{\phi}_i^T \mathbf{M}' \mathbf{\phi}_i \tag{8}$$

The aforementioned procedure is called the Nelson's method [11], but it is only for the distinct eigenvalues. In the case of m > 1, the calculation for the derivatives of eigenvalues and eigenvectors is not straightforward. Hence, the improved Nelson's method can be used to find the eigenvalue derivatives. Let $\mathbf{X} = [\boldsymbol{\varphi}_{s+1}, \boldsymbol{\varphi}_{s+2}, \cdots, \boldsymbol{\varphi}_{s+m}]$, the eigenvalue derivatives for repeated eigenvalues λ_i ($i = s + 1, s + 2, \cdots, s + m$) can be found by solving a sub-eigenvalue problem [35-37, 41].

$$\left[\mathbf{X}^{T}(\mathbf{K}'-\lambda_{0}\mathbf{M}')\mathbf{X}-\lambda_{i}'\mathbf{I}_{m}\right]\boldsymbol{\gamma}_{i}=0,\ i=s+1,s+2,\cdots,s+m$$
(9)

where γ_i are eigenvectors of the sub-eigenvalue.

In this paper, it is assumed that λ_i' ($i=s+1,s+2,\cdots,s+m$) are all distinct. The method mentioned in Ref. [36] will break down if any of the derivatives λ_i' can be repeated. A few of methods that discuss this situation are described in [38, 39, 41]. A unique $m \times m$ orthogonal matrix $\mathbf{\Gamma} = [\boldsymbol{\gamma}_{s+1}, \boldsymbol{\gamma}_{s+2}, \cdots, \boldsymbol{\gamma}_{s+m}]$ can then be generated, which can be used to define a unique and differentiable eigenvector matrix $\mathbf{Z} = [\mathbf{z}_{s+1}, \mathbf{z}_{s+2}, \cdots, \mathbf{z}_{s+m}]$ for the repeated eigenvalues by $\mathbf{Z} = \mathbf{X}\mathbf{\Gamma}$. Let $\mathbf{F}_i' = \mathbf{K}' - \lambda_i' \mathbf{M} - \lambda_0 \mathbf{M}'$, $\mathbf{f}_i = -\mathbf{F}_i' \mathbf{z}_i$, the eigenvector derivatives \mathbf{z}_i' satisfy the following

$$\mathbf{F}\mathbf{z}_{i}' = \mathbf{f}_{i}, \qquad i = s + 1, s + 2, \dots, s + m \tag{10}$$

where **F** is matrix of rank n-m, and its null space is spanned by **Z**. \mathbf{z}'_i can be written as

$$\mathbf{z}_{i}' = \mathbf{v}_{i} + \mathbf{Z}\mathbf{c}_{i} = \mathbf{v}_{i} + \sum_{k=s+1}^{s+m} c_{ki}\mathbf{z}_{k}, \qquad i = s+1, s+2, \dots, s+m$$
(11)

in which \mathbf{v}_i is a particular solution to Eq. (10) and satisfies

$$\mathbf{F}\mathbf{v}_{i} = \mathbf{f}_{i}, \qquad i = s + 1, s + 2, \dots, s + m. \tag{12}$$

Once the particular solution \mathbf{v}_i is determined, the coefficients c_{ki} can be calculated by [36, 37]

$$c_{ii} = -\mathbf{z}_i^T \left(\frac{1}{2}\mathbf{M}'\mathbf{z}_i + \mathbf{M}\mathbf{v}_i\right), \qquad i = s+1, s+2, \dots, s+m$$
(13a)

$$c_{ki} = \frac{\mathbf{z}_{k}^{T}(\mathbf{K''} - 2\lambda_{i}'\mathbf{M'} - \lambda_{i}\mathbf{M''})\mathbf{z}_{i} + 2\mathbf{z}_{k}^{T}\mathbf{F}_{i}'\mathbf{v}_{i}}{2(\lambda_{i}' - \lambda_{k}')}, \quad i \neq k, \quad i, k = s + 1, s + 2, \dots, s + m$$
(13b)

The eigenvector derivatives \mathbf{z}'_i can then be determined using Eq. (11).

The improved Nelson's method mainly focuses on the solutions of \mathbf{v}_i , it can be obtained by the following algorithm [57]:

1) Let $\mathbf{Z}_{m,m}$ be a sub-matrix composed of the l_j th $(j=1,2,\cdots,m)$ rows of $\mathbf{Z}=\mathbf{X}\boldsymbol{\Gamma}$, such that

$$\mathbf{abs} \left(\det \begin{bmatrix} z_{l_{1}(s+1)} & z_{l_{1}(s+2)} & \cdots & z_{l_{1}(s+m)} \\ z_{l_{2}(s+1)} & z_{l_{2}(s+2)} & \cdots & z_{l_{2}(s+m)} \\ \vdots & \vdots & \ddots & \vdots \\ z_{l_{m}(s+1)} & z_{l_{m}(s+2)} & \cdots & z_{l_{m}(s+m)} \end{bmatrix} \right) = \max_{k_{1},k_{2},\cdots k_{m}} \mathbf{abs} \left(\det \begin{bmatrix} z_{k_{1}(s+1)} & z_{k_{1}(s+2)} & \cdots & z_{k_{1}(s+m)} \\ z_{k_{2}(s+1)} & z_{k_{2}(s+2)} & \cdots & z_{k_{2}(s+m)} \\ \vdots & \vdots & \ddots & \vdots \\ z_{k_{m}(s+1)} & z_{k_{m}(s+2)} & \cdots & z_{k_{m}(s+m)} \end{bmatrix} \right)$$
(14)

- 2) Set the l_j^{th} $(j=1,2,\cdots,m)$ rows and columns of \mathbf{F} to zero, and the l_j^{th} $(j=1,2,\cdots,m)$ diagonal element of \mathbf{F} is equal to the l_j^{th} $(j=1,2,\cdots,m)$ diagonal element of stiffness matrix \mathbf{K} to form $\overline{\mathbf{F}}$.
- 3) Set the l_j th $(j=1,2,\cdots,m)$ rows of \mathbf{f}_i $(i=s+1,s+2,\cdots,s+m)$ to zero to form $\overline{\mathbf{f}}_i$ $(i=s+1,s+2,\cdots,s+m)$.
- 4) Solve $\overline{\mathbf{F}}\mathbf{v}_i = \overline{\mathbf{f}}_i (i = s + 1, s + 2, \dots, s + m)$.

Using the Nelson's method and its improved version, the eigenvector derivatives are divided into a homogeneous solution and a particular solution and the calculation requires the eigenvalues and eigenvectors of interest only. The Nelson's method and its improved version are exact methods without considering the rounding error. However, these methods involve a great computational effort if many eigenvector derivatives are concerned for large-scale structural problems due to the matrix decomposition (e.g., using LDL^T decomposition) in particular solutions. To quantify the method, some tools for measuring the algebraic operations are needed. One way to quantify this is with the notion of a flop [56], which is a floating point operation. A dot product of length l involves 2l flops, a LDL^T decomposition of $n \times n$ nonsingular symmetric matrix needs $b^2n + 4bn$ flops, where b is the semi-bandwidth of the coefficient matrix. Note that the improved Nelson's method requires a LDL^T decomposition, forward substitutions, backward substitutions and calculation of $\bar{\mathbf{f}}_i$ in the algorithm to obtain the particular solution for each eigenvector derivative. The calculation of the particular solutions takes $(b^2n + 8bn + n) + (12bn + 8n)$, and the calculation of the coefficients c_{ki} requires (24m - 16)bn + (22m - 14)n. Therefore, using the improved Nelson's method to determine the

eigenvector derivatives with m repeated eigenvalues requires $b^2n + 24m^2bn + (22m - 5)mn + 4bn$ flops. Since the semi-bandwidth b is roughly equal to \sqrt{n} [58], and repeated eigenvalues m is much smaller than n, the improved Nelson's method requires about $n^2 + (24m^2 + 4)n^{3/2}$.

We will present an efficient method for the computation of \mathbf{z}'_i in Section 4, by constructing a non-singular coefficient matrix and prescribing a pre-conditional SQMR strategy. Based on the present approach, highly accurate approximations to the eigenvector derivatives can be obtained.

4. Newly Proposed Method for Eigensensitivity Analysis

Since the coefficient matrix \mathbf{F} in Eqs. (4) and (10) is singular in nature, it cannot be inverted. Here, we propose an alternative approach to construct a non-singular matrix, so that the eigenvector derivative can be determined.

In the case of m = 1, we fist calculate the distinct eigenvalue derivatives λ_i' by Eq.(6), and then remove the singularity of \mathbf{F} using Eq.(5). Note that $(\boldsymbol{\varphi}_i')^T \mathbf{M} \boldsymbol{\varphi}_i = \boldsymbol{\varphi}_i^T \mathbf{M} \boldsymbol{\varphi}_i'$ is a 1×1 matrix, we can obtain the following form,

$$\mathbf{\phi}_{i}^{T}\mathbf{M}\mathbf{\phi}_{i}^{\prime} = -0.5\mathbf{\phi}_{i}^{T}\mathbf{M}^{\prime}\mathbf{\phi}_{i} \tag{15}$$

Multiplying Eq. (15) by $\mathbf{M}\mathbf{\phi}_i$ and adding to Eq. (4), we obtain

$$(\mathbf{F} + \mathbf{M}\mathbf{\phi}_i \mathbf{\phi}_i^T \mathbf{M})\mathbf{\phi}_i' = (\mathbf{F}' - 0.5\mathbf{M}\mathbf{\phi}_i \mathbf{\phi}_i^T \mathbf{M}')\mathbf{\phi}_i$$
(16)

Denote $(\mathbf{F} + \mathbf{M}\boldsymbol{\varphi}_i \boldsymbol{\varphi}_i^T \mathbf{M}) = \mathbf{G}$, once the matrix \mathbf{G} is a non-singular, the eigenvector derivatives can then be determined by Eq.(16). We will prove that \mathbf{G} is a non-singular symmetrical matrix in the following.

In the case of m>1, we calculate the distinct eigenvalue derivatives λ_i' and the differentiable eigenvectors $\mathbf{Z} = [\mathbf{z}_{s+1}, \mathbf{z}_{s+2}, \cdots, \mathbf{z}_{s+m}]$ by Eq.(9). Differentiating Eq.(10) yields

$$\mathbf{F}_{i}'\mathbf{z}_{i}' = -0.5\mathbf{F}\mathbf{z}_{i}'' - 0.5(\mathbf{K}'' - \lambda_{i}''\mathbf{M} - 2\lambda_{i}'\mathbf{M}' - \lambda_{i}\mathbf{M}'')\mathbf{z}_{i} \qquad i = s + 1, s + 2, \dots, s + m$$

$$(17)$$

Premultiplying Eq. (17) by \mathbf{z}_{j}^{T} $(j = s + 1, s + 2, \dots, s + m, j \neq i)$ and exploiting Eq. (2), we have

$$\mathbf{z}_{j}^{T}\mathbf{F}_{i}'\mathbf{z}_{i}' = -0.5\mathbf{z}_{j}^{T}\mathbf{F}_{i}''\mathbf{z}_{i} \qquad i, j = s + 1, s + 2, \dots, s + m, j \neq i$$
(18)

where $\mathbf{F}_{i}'' = (\mathbf{K}'' - 2\lambda_{i}'\mathbf{M}' - \lambda_{i}\mathbf{M}'')$. By differentiating the normalization $\mathbf{z}_{i}^{T}\mathbf{M}\mathbf{z}_{i} = 1$, we obtain

$$\mathbf{z}_{i}^{T}\mathbf{M}\mathbf{z}_{i}^{\prime} = -0.5\mathbf{z}_{i}^{T}\mathbf{M}^{\prime}\mathbf{z}_{i} \tag{19}$$

Premultiplying Eq. (18) by $\mathbf{F}_{i}^{\prime}\mathbf{z}_{j}$ and Eq. (19) by $\mathbf{M}\mathbf{z}_{i}$ and combining the results to Eq. (10), we arrive at

$$\left(\mathbf{F} + \mathbf{L}_{i} \mathbf{L}_{i}^{T} + \sum_{j=s+1, j \neq i}^{s+m} \mathbf{L}_{j} \mathbf{L}_{j}^{T}\right) \mathbf{z}_{i}^{\prime} = \mathbf{f}_{i} - 0.5 \left(\mathbf{L}_{i} \mathbf{z}_{i}^{T} \mathbf{M}^{\prime} \mathbf{z}_{i} + \sum_{j=s+1, j \neq i}^{s+m} \mathbf{L}_{j} \mathbf{z}_{j}^{T} \mathbf{F}_{i}^{\prime\prime} \mathbf{z}_{i}\right), \quad i = s+1, s+2, \dots, s+m$$
(20)

where

$$\mathbf{L}_{i} = \mathbf{M}\mathbf{z}_{i}, \quad i = s+1, s+2, \cdots, s+m \tag{21a}$$

$$\mathbf{L}_{j} = \mathbf{F}_{i}^{\prime} \mathbf{z}_{j} = (\mathbf{K}^{\prime} - \lambda_{i}^{\prime} \mathbf{M} - \lambda_{0} \mathbf{M}^{\prime}) \mathbf{z}_{j}, \quad j = s + 1, s + 2, \dots, s + m, j \neq i$$
(21b)

Denote
$$\left(\mathbf{F} + \mathbf{L}_i \mathbf{L}_i^T + \sum_{j=s+1, j \neq i}^{s+m} \mathbf{L}_j \mathbf{L}_j^T\right) = \mathbf{G}_i \quad (i = s+1, s+2, \dots, s+m), \text{ where } \mathbf{G} = \mathbf{G}_i \text{ for } m = 1.$$

Next, we will show that the coefficient matrix G_i is a non-singular matrix. Denote

$$\mathbf{Z}_{i} = [\mathbf{z}_{s+1}, \mathbf{z}_{s+2}, \dots, \mathbf{z}_{i-1}, \mathbf{z}_{i+1}, \dots, \mathbf{z}_{s+m}], (i = s+1, s+2, \dots, s+m)$$
(22)

and the eigenmatrix is

$$\mathbf{\Phi} = \left[\mathbf{\phi}_{1}, \mathbf{\phi}_{2}, \cdots, \mathbf{\phi}_{s}, \mathbf{z}_{s+1}, \mathbf{z}_{s+2}, \cdots, \mathbf{z}_{s+m}, \mathbf{\phi}_{s+m+1}, \cdots, \mathbf{\phi}_{n}\right]$$
(23)

we obtain

$$\mathbf{\Phi}^{T}\mathbf{G}_{i}\mathbf{\Phi} = \mathbf{\Phi}^{T}\left(\mathbf{K} - \lambda_{i}\mathbf{M} + \mathbf{M}\mathbf{z}_{i}\mathbf{z}_{i}^{T}\mathbf{M} + \mathbf{F}_{i}'\mathbf{Z}_{i}\mathbf{Z}_{i}^{T}\mathbf{F}_{i}'\right)\mathbf{\Phi}$$
(24)

Without loss of generality, we assume i = s + 1 and denote that $\mathbf{\Phi} = [\mathbf{\Phi}_l, \mathbf{Z}_i, \mathbf{\Phi}_h]$, $\mathbf{\Phi}_l = [\mathbf{\phi}_1, \mathbf{\phi}_2, \dots, \mathbf{\phi}_s, \mathbf{z}_{s+1}]$, and $\mathbf{\Phi}_h = [\mathbf{\phi}_{s+m+1}, \dots, \mathbf{\phi}_n]$. Using Eqs. (1), (2) and (3), $\mathbf{\Phi}^T \mathbf{G}_i \mathbf{\Phi}$ can be split into

$$\mathbf{\Phi}^{T}\mathbf{G}_{i}\mathbf{\Phi} = \begin{bmatrix} \mathbf{\Phi}_{l}^{T} \\ \mathbf{Z}_{i}^{T} \\ \mathbf{\Phi}_{h}^{T} \end{bmatrix} (\mathbf{K} - \lambda_{i}\mathbf{M} + \mathbf{M}\mathbf{z}_{i}\mathbf{z}_{i}^{T}\mathbf{M}) [\mathbf{\Phi}_{l}, \mathbf{Z}_{i}, \mathbf{\Phi}_{h}] + \begin{bmatrix} \mathbf{\Phi}_{l}^{T} \\ \mathbf{Z}_{i}^{T} \\ \mathbf{\Phi}_{h}^{T} \end{bmatrix} \mathbf{F}_{i}^{\prime}\mathbf{Z}_{i}\mathbf{Z}_{i}^{T}\mathbf{F}_{i}^{\prime} [\mathbf{\Phi}_{l}, \mathbf{Z}_{i}, \mathbf{\Phi}_{h}]$$

$$[\mathbf{\Lambda}_{l} \quad 0 \quad 0] [\mathbf{\Phi}_{l}^{T}]$$
(25)

$$= \begin{bmatrix} \mathbf{\Lambda}_{l} & 0 & 0 \\ 0 & \mathbf{0}_{m-1,m-1} & 0 \\ 0 & 0 & \mathbf{\Lambda}_{h} \end{bmatrix} + \begin{bmatrix} \mathbf{\Phi}_{l}^{T} \\ \mathbf{Z}_{i}^{T} \\ \mathbf{\Phi}_{h}^{T} \end{bmatrix} \mathbf{F}_{i}^{\prime} \mathbf{Z}_{i} \mathbf{Z}_{i}^{T} \mathbf{F}_{i}^{\prime} [\mathbf{\Phi}_{l}, \mathbf{Z}_{i}, \mathbf{\Phi}_{h}]$$

where $\Lambda_l = diag(\lambda_1 - \lambda_0, \lambda_2 - \lambda_0, \dots, \lambda_s - \lambda_0, 1)$, $\Lambda_h = diag(\lambda_{s+m+1} - \lambda_0, \lambda_{s+m+2} - \lambda_0, \dots, \lambda_n - \lambda_0)$, and $\mathbf{0}_{m-1,m-1}$ is a $(m-1)\times(m-1)$ zero matrix. Following Eq. (9), we have

$$\mathbf{Z}_{i}^{T}\mathbf{F}_{i}^{\prime}\mathbf{Z}_{i} = diag(\lambda_{s+2}^{\prime} - \lambda_{i}^{\prime}, \lambda_{s+3}^{\prime} - \lambda_{i}^{\prime}, \dots, \lambda_{s+m}^{\prime} - \lambda_{i}^{\prime}) \equiv \mathbf{D}$$
(26)

$$\mathbf{\Phi}^{T}\mathbf{G}_{i}\mathbf{\Phi} = \begin{bmatrix} \mathbf{\Lambda}_{l} & 0 & 0 \\ 0 & \mathbf{0}_{m-1,m-1} & 0 \\ 0 & 0 & \mathbf{\Lambda}_{h} \end{bmatrix} + \begin{bmatrix} \mathbf{\Phi}_{l}^{T}\mathbf{F}_{i}'\mathbf{Z}_{i}\mathbf{Z}_{i}^{T}\mathbf{F}_{i}'\mathbf{\Phi}_{l} & \mathbf{\Phi}_{l}^{T}\mathbf{F}_{i}'\mathbf{Z}_{i}\mathbf{D} & \mathbf{\Phi}_{l}^{T}\mathbf{F}_{i}'\mathbf{Z}_{i}\mathbf{Z}_{i}^{T}\mathbf{F}_{i}'\mathbf{\Phi}_{h} \\ \mathbf{D}\mathbf{Z}_{i}^{T}\mathbf{F}_{i}'\mathbf{\Phi}_{l} & \mathbf{D}^{2} & \mathbf{D}\mathbf{Z}_{i}^{T}\mathbf{F}_{i}'\mathbf{\Phi}_{h} \\ \mathbf{\Phi}_{h}^{T}\mathbf{F}_{i}'\mathbf{Z}_{i}\mathbf{Z}_{i}^{T}\mathbf{F}_{i}'\mathbf{\Phi}_{l} & \mathbf{\Phi}_{h}^{T}\mathbf{F}_{i}'\mathbf{Z}_{i}\mathbf{D} & \mathbf{\Phi}_{h}^{T}\mathbf{F}_{i}'\mathbf{Z}_{i}\mathbf{Z}_{i}^{T}\mathbf{F}_{i}'\mathbf{\Phi}_{h} \end{bmatrix}$$

$$(27)$$

$$= \begin{bmatrix} \mathbf{\Phi}_{l}^{T} \mathbf{F}_{i}^{\prime} \mathbf{Z}_{i} \mathbf{Z}_{i}^{T} \mathbf{F}_{i}^{\prime} \mathbf{\Phi}_{l} + \mathbf{\Lambda}_{l} & \mathbf{\Phi}_{l}^{T} \mathbf{F}_{i}^{\prime} \mathbf{Z}_{i} \mathbf{D} & \mathbf{\Phi}_{l}^{T} \mathbf{F}_{i}^{\prime} \mathbf{Z}_{i} \mathbf{Z}_{i}^{T} \mathbf{F}_{i}^{\prime} \mathbf{\Phi}_{h} \\ \mathbf{D} \mathbf{Z}_{i}^{T} \mathbf{F}_{i}^{\prime} \mathbf{\Phi}_{l} & \mathbf{D}^{2} & \mathbf{D} \mathbf{Z}_{i}^{T} \mathbf{F}_{i}^{\prime} \mathbf{\Phi}_{h} \\ \mathbf{\Phi}_{h}^{T} \mathbf{F}_{i}^{\prime} \mathbf{Z}_{i} \mathbf{Z}_{i}^{T} \mathbf{F}_{i}^{\prime} \mathbf{\Phi}_{l} & \mathbf{\Phi}_{h}^{T} \mathbf{F}_{i}^{\prime} \mathbf{Z}_{i} \mathbf{D} & \mathbf{\Phi}_{h}^{T} \mathbf{F}_{i}^{\prime} \mathbf{Z}_{i} \mathbf{Z}_{i}^{T} \mathbf{F}_{i}^{\prime} \mathbf{\Phi}_{h} + \mathbf{\Lambda}_{h} \end{bmatrix}$$

where **D** is non-singular, because λ'_i $(i = s + 1, s + 2, \dots, s + m)$ is distinct.

Introducing the following equations with the unknowns X_1 , X_2 and X_3 , we have

$$\begin{bmatrix} \mathbf{\Phi}_{l}^{T} \mathbf{F}_{i}^{\prime} \mathbf{Z}_{i} \mathbf{Z}_{i}^{T} \mathbf{F}_{i}^{\prime} \mathbf{\Phi}_{l} + \mathbf{\Lambda}_{l} & \mathbf{\Phi}_{l}^{T} \mathbf{F}_{i}^{\prime} \mathbf{Z}_{i} \mathbf{D} & \mathbf{\Phi}_{l}^{T} \mathbf{F}_{i}^{\prime} \mathbf{Z}_{i} \mathbf{Z}_{i}^{T} \mathbf{F}_{i}^{\prime} \mathbf{\Phi}_{h} \\ \mathbf{D} \mathbf{Z}_{i}^{T} \mathbf{F}_{i}^{\prime} \mathbf{\Phi}_{l} & \mathbf{D}^{2} & \mathbf{D} \mathbf{Z}_{i}^{T} \mathbf{F}_{i}^{\prime} \mathbf{\Phi}_{h} \\ \mathbf{\Phi}_{h}^{T} \mathbf{F}_{i}^{\prime} \mathbf{Z}_{i} \mathbf{Z}_{i}^{T} \mathbf{F}_{i}^{\prime} \mathbf{\Phi}_{l} & \mathbf{\Phi}_{h}^{T} \mathbf{F}_{i}^{\prime} \mathbf{Z}_{i} \mathbf{D} & \mathbf{\Phi}_{h}^{T} \mathbf{F}_{i}^{\prime} \mathbf{Z}_{i} \mathbf{Z}_{i}^{T} \mathbf{F}_{i}^{\prime} \mathbf{\Phi}_{h} + \mathbf{\Lambda}_{h} \end{bmatrix} \begin{bmatrix} \mathbf{X}_{1} \\ \mathbf{X}_{2} \\ \mathbf{X}_{3} \end{bmatrix} = \mathbf{0}$$

$$(28)$$

Multiplying Eq. (28) by the non-singular matrix $\begin{bmatrix} \mathbf{I}_{l} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{D}^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{I}_{h} \end{bmatrix}$, we get

$$\begin{bmatrix} \mathbf{\Phi}_{l}^{T} \mathbf{F}_{i}^{\prime} \mathbf{Z}_{i} \mathbf{Z}_{i}^{T} \mathbf{F}_{i}^{\prime} \mathbf{\Phi}_{l} + \mathbf{\Lambda}_{l} & \mathbf{\Phi}_{l}^{T} \mathbf{F}_{i}^{\prime} \mathbf{Z}_{i} \mathbf{D} & \mathbf{\Phi}_{l}^{T} \mathbf{F}_{i}^{\prime} \mathbf{Z}_{i} \mathbf{Z}_{i}^{T} \mathbf{F}_{i}^{\prime} \mathbf{\Phi}_{h} \\ \mathbf{Z}_{i}^{T} \mathbf{F}_{i}^{\prime} \mathbf{\Phi}_{l} & \mathbf{D} & \mathbf{Z}_{i}^{T} \mathbf{F}_{i}^{\prime} \mathbf{\Phi}_{h} \\ \mathbf{\Phi}_{h}^{T} \mathbf{F}_{i}^{\prime} \mathbf{Z}_{i} \mathbf{Z}_{i}^{T} \mathbf{F}_{i}^{\prime} \mathbf{\Phi}_{l} & \mathbf{\Phi}_{h}^{T} \mathbf{F}_{i}^{\prime} \mathbf{Z}_{i} \mathbf{D} & \mathbf{\Phi}_{h}^{T} \mathbf{F}_{i}^{\prime} \mathbf{Z}_{i} \mathbf{Z}_{i}^{T} \mathbf{F}_{i}^{\prime} \mathbf{\Phi}_{h} + \mathbf{\Lambda}_{h} \end{bmatrix} \begin{bmatrix} \mathbf{X}_{1} \\ \mathbf{X}_{2} \\ \mathbf{X}_{3} \end{bmatrix} = \mathbf{0}$$
(29)

where \mathbf{I}_l is an identity matrix with the order equal to $\mathbf{\Lambda}_l$, while \mathbf{I}_h is an identity matrix with the order equal to $\mathbf{\Lambda}_h$.

Sequentially, premultiplying Eq. (29) by the non-singular matrices $\begin{bmatrix} \mathbf{I}_{l} & -\mathbf{\Phi}_{l}^{T}\mathbf{F}_{l}^{\prime}\mathbf{Z}_{l} & \mathbf{0} \\ \mathbf{0} & \mathbf{I}_{m-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{I}_{h} \end{bmatrix}$

and
$$\begin{bmatrix} \mathbf{I}_{l} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{I}_{m-1} & \mathbf{0} \\ \mathbf{0} & -\mathbf{\Phi}_{h}^{T} \mathbf{F}_{i}^{\prime} \mathbf{Z}_{i} & \mathbf{I}_{h} \end{bmatrix}$$
, the resulting equation becomes

$$\begin{bmatrix} \mathbf{\Lambda}_{l} & 0 & 0 \\ \mathbf{Z}_{i}^{T} \mathbf{F}_{i}^{\prime} \mathbf{\Phi}_{l} & \mathbf{D} & \mathbf{Z}_{i}^{T} \mathbf{F}_{i}^{\prime} \mathbf{\Phi}_{h} \\ 0 & 0 & \mathbf{\Lambda}_{h} \end{bmatrix} \begin{bmatrix} \mathbf{X}_{1} \\ \mathbf{X}_{2} \\ \mathbf{X}_{3} \end{bmatrix} = \mathbf{0}$$
(30)

in which I_{m-1} is an $(m-1)\times(m-1)$ identity matrix. Referring to the above equation, we can easily get

$$X_1 = 0, X_2 = 0, X_3 = 0$$
 (31)

The matrix $\mathbf{\Phi}^T \mathbf{G}_i \mathbf{\Phi}$ is thus proved to be non-singular, and the coefficient matrix in Eq. (20) is non-singular and symmetric indefinite.

Computing the eigenvector derivatives by Eq. (20) only requires the interested eigenvectors, we can determine the eigenvector sensitivity directly and accurately. However, the form and decomposition of the coefficient matrix \mathbf{G}_i require a lot of full-in operations, it is a time-consuming procedure. The SQMR algorithm [59] is the standard conjugate gradient-type Krylov subspace methods for solving symmetric indefinite linear systems. Unlike other conjugate gradient-type methods, the SQMR algorithm can be combined with arbitrary symmetric preconditioners. Reference [60] pointed out that a good preconditioner must satisfy two requirements, namely (a) the preconditioned system should be solved easily and is convergent rapidly; and (b) the preconditioner should be constructed readily. The present choice is motivated by the potential availability of the factorization $\mathbf{K} - \mu \mathbf{M}$ from the computation of eigenvalues and eigenvectors via iterative methods such as the Lanczos algorithm or the subspace iteration method, where μ is shifting. As a result, an iterative method based on the SQMR algorithm with a preconditioner $\mathbf{K} - \mu \mathbf{M}$ is established. In this paper, we only consider the left preconditioner, the implementation of the SQMR algorithm for solving Eq. (20) is described below.

Algorithm 1

1:Choose $\mathbf{u}_0 \in \mathfrak{R}^N$

2:Compute
$$\mathbf{b} = \mathbf{f}_i - 0.5 \left(\mathbf{L}_i \mathbf{z}_i^T \mathbf{M}' \mathbf{z}_i + \sum_{j=s+1, j \neq i}^{s+m} \mathbf{L}_j \mathbf{z}_j^T \mathbf{F}_i'' \mathbf{z}_i \right)$$

3:Set
$$\mathbf{r}_0 = \mathbf{b} - \mathbf{G}_i \mathbf{u}_0$$

$$4: Solve(\mathbf{K} - \mu \mathbf{M})\mathbf{t} = \mathbf{r}_0$$

5:Set
$$\tau_0 = \|\mathbf{t}\|_2$$
, $\mathbf{q}_0 = \mathbf{t}$, $v_0 = 0$, $\mathbf{d}_0 = \mathbf{0}$, and $\rho_0 = \mathbf{r}_0^T \mathbf{q}_0$

6: For
$$n = 1, 2, \dots, do$$

$$7: \mathbf{t} = \mathbf{G}_i \mathbf{q}_{n-1}$$

8:
$$\sigma_{n-1} = \mathbf{q}_{n-1}^T \mathbf{t}$$
, if $\sigma_{n-1} = 0$, then stop.

9:
$$\alpha_{n-1} = \frac{\rho_{n-1}}{\sigma_{n-1}}, \mathbf{r}_n = \mathbf{r}_{n-1} - \alpha_{n-1} \mathbf{t}$$

10: Solve
$$(\mathbf{K} - \mu \mathbf{M})\mathbf{t} = \mathbf{r}_n$$

11:
$$v_n = \frac{\|\mathbf{t}\|_2}{\tau_{n-1}}, \quad c_n = \frac{1}{\sqrt{1 + v_n^2}}, \quad \tau_n = \tau_{n-1} v_n c_n$$

12:
$$\mathbf{d}_n = c_n^2 v_n^2 \mathbf{d}_{n-1} + c_n^2 \alpha_{n-1} \mathbf{q}_{n-1}$$

13:
$$\mathbf{u}_n = \mathbf{u}_{n-1} + \mathbf{d}_n$$

14:If \mathbf{u}_n has converged, then stop.

15:If $\rho_{n-1} = 0$, then stop.

16:
$$\rho_n = \mathbf{r}_n^T \mathbf{t}$$
, $\beta_n = \frac{\rho_n}{\rho_{n-1}}$, $\mathbf{q}_n = \mathbf{t} + \beta_n \mathbf{q}_{n-1}$

17:End for.

Note that the shifted stiffness matrix is given in the factorized form $\mathbf{K} - \mu \mathbf{M} = \mathbf{L} \mathbf{D} \mathbf{L}^T$ from the computation of partial eigensolutions. The solution to the system in the form of $(\mathbf{K} - \mu \mathbf{M})\mathbf{t} = \mathbf{r}_n$ involves only the computation of forward and backward substitutions. The matrix \mathbf{G}_i does not require to be formed directly, $\mathbf{G}_i \mathbf{q}_{n-1} = \left(\mathbf{F} + \mathbf{L}_i \mathbf{L}_i^T + \sum_{j=s+1, j\neq i}^{s+m} \mathbf{L}_j \mathbf{L}_j^T\right) \mathbf{q}_{n-1}$ can

be obtained using the matrix-vector multiplication.

The following computation procedures are performed for obtaining the derivatives of eigenvectors. Note that all implicitly defined matrix-matrix products in the following algorithm are simplified to the matrix-vector products in the implementation.

- 1. If m = 1, then solve the eigenvalue derivatives for the eigenvalues λ_i by using Eq.(6). Else, solve a sub-eigenanalysis problem $\left[\mathbf{X}^T(\mathbf{K}' \lambda_0 \mathbf{M}')\mathbf{X} \lambda_i'\mathbf{I}_m\right]\boldsymbol{\gamma}_i = 0, \ i = s+1, s+2, \cdots, s+m$ to yield the eigenvalue derivatives for the repeated eigenvalues λ_0 and the differentiable eigenvectors \mathbf{z}_i .
- 2. Compute $\mathbf{f}_i = -\mathbf{F}_i'\mathbf{z}_i$, $i = s + 1, s + 2, \dots, s + m$.
- 3. Apply "Algorithm 1" mentioned above to obtain $\mathbf{z}'_i = \mathbf{u}_n$, $i = s + 1, s + 2, \dots, s + m$.

For the computation of derivatives of all eigenvectors, we need to solve a set of linear systems with the same coefficient matrix $\mathbf{K} - \mu \mathbf{M}$ only. The (shifted) stiffness matrix can be factored using the iterative eigensolution such as the Lanczos algorithm or the subspace iteration method, no other matrix factorization is required. The present method involves about (12m+32)bn+14mn+25n flops before the cycle, and 12bn+3mn+21n flops in each cycle. Suppose the eigenvector derivatives obtained by performing average k iterations for one eigenvector, the semi-bandwidth b is roughly equal to \sqrt{n} [58], and the repeated eigenvalues m is much smaller than n, the new method requires about $(12m^2+32m+12km)n^{3/2}$ flops. Figure 1 shows a comparison of computational efforts between the present method and the improved Nelson's method, which indicates the efficiency of the proposed method.

The relative error of the eigenvector derivatives is defined as follows:

$$e_r = \frac{\left\|\mathbf{z}_a' - \mathbf{z}_d'\right\|_2}{\left\|\mathbf{z}_d'\right\|_2} \tag{32}$$

where \mathbf{z}'_a and \mathbf{z}'_d denote the eigenvector derivatives obtained by using the present method and the improved Nelson's method, respectively. The advantage of the present method over the direct one is highlighted by the computational effort. The performance of the present method will be discussed in the subsequent section.

5. Numerical Examples and Results

In this section, three examples are given to illustrate the efficiency of the proposed method. The Harwell-Boeing (HB) compressed storage format for the matrices is used. The related computations are based on the Intel(R) Math Kernel Library (MKL) 11.2. The given examples are computed by a PC with Intel Xeon-E5-2620 CPU with 2.0 GHz and 24 GB RAM. The compiler is Intel(R) Visual Fortran Compiler XE 15.0.

Example 5.1 A square plate structure with four clamped edges is considered. The length of each side is 12m. In order to reinforce the plate, two horizontal and two vertical ribs with a 0.1m \times 0.3m rectangular cross-section are added to the plate, as shown in Fig. 2. The modulus of elasticity for the plate structure is $E = 2 \times 10^{11} \, \text{Pa}$, the Poisson's ratio is v = 0.3 and the plate thickness is 0.1m. A finite element model, consisted of 2,138,454 DOFs, is constructed to simulate the dynamic behaviour of the square plate structure. The height of the horizontal ribs p is chosen as a design parameter and its initial value is $p_0 = 0.3 \, \text{m}$.

In this example, the lowest 15 natural frequencies and its associated eigenvectors are solved by using the subspace iteration method with shifting. They are used to calculate the eigenvector derivatives. The computed frequencies and the shift are listed in Tables 1 and 2, respectively.

To compute the eigenvector derivatives, a relative error tolerance $\|\mathbf{r}_n\|_2/\|\mathbf{r}_0\|_2 = 10^{-8}$ is used in this example. For comparison, the exact solutions of the eigenvector derivatives using the improved Nelson's method in [57] are calculated. The CPU computational time of the present method and the improved Nelson's method for the eigenvector derivatives is presented in Table 3. The CPU computational time of the present method is considerably reduced by about 77% with respect to the improved Nelson's method. Besides, the relative errors of the eigenvector derivatives obtained by the present method and the improved Nelson's method are shown in Table 4. It is found that, the maximum relative error is 0.128% at 51.67Hz, the corresponding mode shape is shown in Fig. 3. Besides, comparisons of the contour maps for the eigenvector derivatives of translational and rotational DOFs are shown in Figs. 4 and Fig. 5, respectively. The results of both methods are very close to each other.

Example 5.2 A clamped pipe structure with a square section is shown in Fig. 6. The thickness of this pipe is 0.001m. The modulus of elasticity of the structure is $E = 2 \times 10^{11}$ Pa and the Poisson's ratio is v = 0.3. A finite element model with 48,000 DOFs is built up to simulate the dynamic behaviour of the cantilevered structure. The thickness p of the purple side (top side) of the structure is selected as a design parameter and its initial value is $p_0 = 0.001$ m.

For this example, the lowest 16 natural frequencies and its associated eigenvectors are solved

by using the subspace iteration method with shifting, and they are used to calculate the eigenvector derivatives. The computed frequencies and the shift are listed in Tables 5 and 6, respectively.

The computational performance of the present method and the improved Nelson's Method for the eigenvector derivatives is shown in Table 7. By comparing both methods, the computational time of the present approach is significantly reduced by about 67%. Moreover, the relative errors of the eigenvector derivatives obtained by the present method and the improved Nelson's method are presented in Table 8. It is observed that, the maximum relative error is 0.00796% at 2.42Hz, the corresponding mode shape is shown in Fig. 7. Comparisons of the contour maps for the eigenvector derivatives of translational and rotational DOFs is presented in Figs. 8 and Fig. 9, respectively. It is found that the results of both methods are also very close to each other for this example.

Example 5.3 An assembled car door structure [55] is shown in Fig. 10. The modulus of elasticity is $E = 2 \times 10^{11} \, \text{Pa}$, the Poisson's ratio is v = 0.3 and the mass density is $\rho = 7980 \, \text{kg/m}^3$ for all these parts. A finite element model is established to simulate the car door structure shown in Fig.10b. The model has 31,919 shell elements and 192,732 DOFs. The thickness of the inner door is chosen as a design parameter and its initial value is 0.9 mm.

For this example, what we interested are the eigenvector derivatives with frequencies near 35 Hz, 40 Hz, 45 Hz, 50 Hz and 55 Hz. The frequencies and its associated eigenvectors are calculated with the help of the Lanczos method with the shifted frequencies 35 Hz, 40 Hz, 45 Hz, 50 Hz and 55 Hz, and they are used for calculation of the interesting eigenvector derivatives. The computed frequencies are shown in Table 9. In this example, only several frequencies are considered. Without using other modal information at this time as an auxiliary, the computational complexity will be effectively reduced.

The computational performance of the present method and the improved Nelson's Method for the eigenvector derivatives is shown in Table 10. By comparing both methods, the computational time of the present method is significantly reduced by about 72%. Moreover, the relative errors of the eigenvector derivatives obtained by the present method and the improved Nelson's method are presented in Table 11, which illustrates the accuracy of the former is satisfactory.

6. Conclusions

In summary, a new method is presented for the computation of eigenvector derivatives with distinct or repeated eigenvalues for the real symmetric eigensystems. A strategy is proposed for the formulation of a non-singular coefficient matrix that can be directly used to obtain the eigenvector derivatives with distinct and repeated eigenvalues. The existing factored (shifted) stiffness matrix from an iterative eigensolution such as the Lanczos algorithm or the subspace iteration method can be adopted as a preconditioner, such that we can achieve highly accurate approximations to the eigenvector derivatives. The present method can deal with both cases of simple and repeated eigenvalues in a unified manner, and it is particularly suitable for large sparse matrices that arise in industrial-sized finite element models. This approach can also be integrated into a coupled eigensolver/derivative software module and it can leverage the non-recurring cost of a solver. Based on the present study, the computational effort of the proposed approach can be considerably reduced with respect to the existing method. Further extensions of the present technique to the problem of damped and asymmetric systems will be considered.

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Captions of Figures

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- Fig. 2. A square plate structure.
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- **Fig. 4.** Comparison of the eigenvector derivatives of translational DOFs of the square plate structure at 51.67Hz (a) Present method and (b) Improved Nelson's method.
- **Fig. 5.** Comparison of the eigenvector derivatives of rotational DOFs of the square plate structure at 51.67Hz (a) Present method and (b) Improved Nelson's method.
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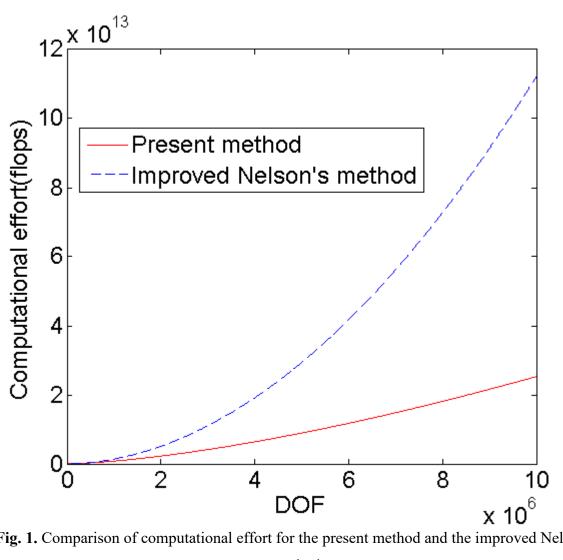


Fig. 1. Comparison of computational effort for the present method and the improved Nelson's method

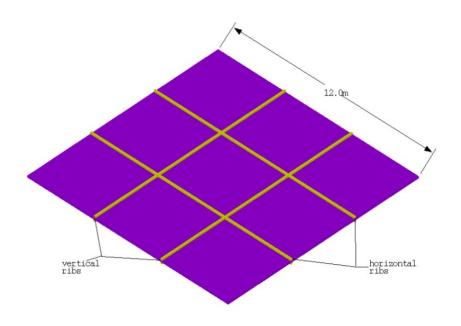


Fig. 2. A square plate structure.

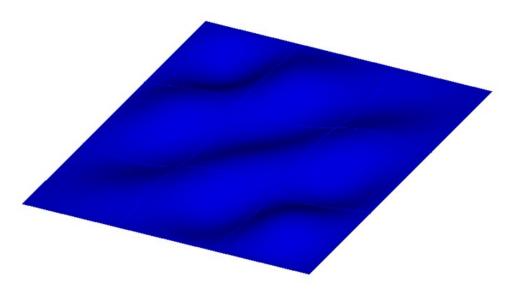


Fig. 3. Mode shape of the square plate structure with 51.67 Hz.

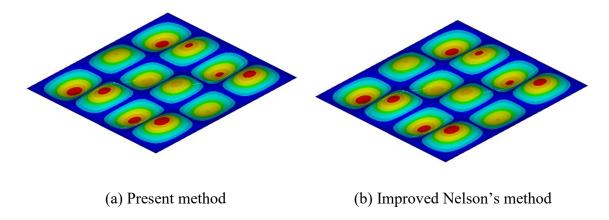


Fig. 4. Comparison of the eigenvector derivatives of translational DOFs of the square plate structure at 51.67 Hz (a) Present method and (b) Improved Nelson's method.

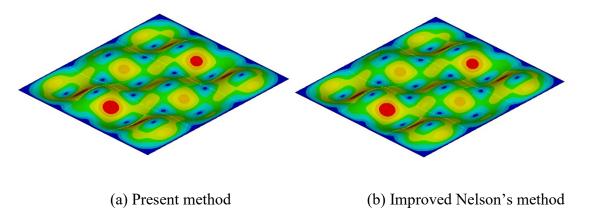


Fig. 5. Comparison of the eigenvector derivatives of rotational DOFs of the square plate structure at 51.67 Hz (a) Present method and (b) Improved Nelson's method.

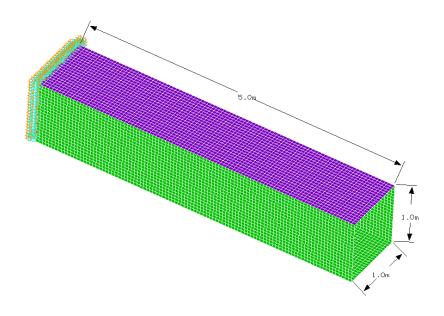


Fig. 6. A clamped pipe structure.

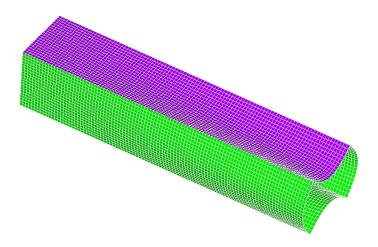


Fig. 7. Mode shape of the clamped pipe structure with 2.42 Hz.

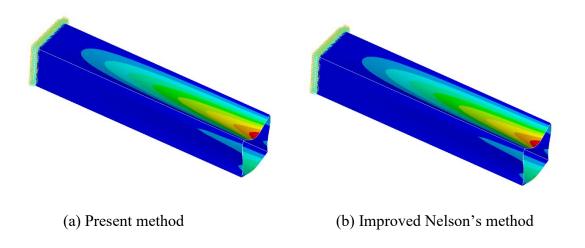


Fig. 8. Comparison of the eigenvector derivatives of translational DOFs of the clamped pipe structure at 2.42 Hz (a) Present method and (b) Improved Nelson's method

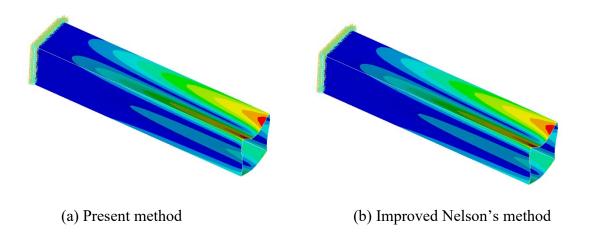


Fig. 9. Comparison of the eigenvector derivatives of rotational DOFs of the clamped pipe structure at 2.42 Hz (a) Present method and (b) Improved Nelson's method.



(a) Assembly of car door

(b) FE model of car door



(c) Car inner door

Fig.10. A car door structure [55].

Table 1
Computed frequencies of the square plate structure (Hz).

Mode number	1	2	3	4	5	6	7	8
Frequency (Hz)	6.99	14.19	14.19	20.79	26.20	26.54	31.77	31.77
Mode number	9	10	11	12	13	14	15	
Frequency (Hz)	38.43	41.12	41.12	45.39	48.06	51.67	51.67	

Table 2
Computed shift of the square plate structure (Hz).

Shifting number	1	2	3	4	5	6	7	8
Shift (Hz)	0	10.032	22.462	29.076	33.982	42.339	47.708	48.061

Table 3Comparison of the CPU run-time(s) in Example 1.

Mode	Emaguamay	Frequency's	Improved Nelson's	Draggart mother d (a)
Number	Frequency	derivative	method (s)[57]	Present method (s)
1	6.99	4.8832	138.14	19.41
2	14.19	1.7060	144.12	22.39
3	14.19	18.1621	144.12	22.39
4	20.79	14.5930	140.04	40.13
5	26.20	17.5855	140.22	35.45
6	26.54	18.0030	140.42	41.18
7	31.77	1.3562	145.89	22.55
8		33.78407	143.07	22.33
9	38.43	3.0680	139.44	45.61
10	41.12	-1.59472	145.13	27.52
11	71.12	48.1823	143.13	21.32
12	45.39	16.0998	133.64	37.73
13	48.06	35.1431	138.50	19.44
14	51.67	4.2609	141.33	46.80
15		14.0353	171.33	70.00
		Total Time	1546.87	358.21

Table 4Relative errors of the eigenvector derivatives in Example 1.

Frequency (Hz)	6.99	14.19	14.19	20.79	26.20	26.54	31.77	31.77
Used shift (Hz)	0.00	10.03	10.03	10.03	22.46	22.46	29.08	29.08
$e_r(\%)$	1.65E-6	2.22E-2	1.94E-4	1.21E-4	3.48E-6	3.51E-6	4.38E-4	1.13E-1
								_
Frequency (Hz)	38.43	41.12	41.12	45.39	48.06	51.67	51.67	
Used shift (Hz)	33.98	33.98	33.98	42.34	47.70	48.06	48.06	
$e_{r}(\%)$	1.06E-4	1.22E-1	2.27E-2	1.28E-5	5.26E-6	1.28E-1	5.25E-3	

Table 5
Computed frequencies of the clamped pipe structure (Hz).

Mode number	1	2	3	4	5	6	7	8
Frequency (Hz)	2.42	2.63	3.03	3.62	3.78	3.78	3.94	3.94
Mode number	9	10	11	12	13	14	15	16
Frequency (Hz)	4.25	4.25	4.41	4.74	4.74	5.38	5.41	5.41

Table 6
Computed shift of the clamped pipe structure (Hz).

Shifting number	1	2	3	4	5	
Shift (Hz)	0	2.14	2.67	3.01	3.35	
Shifting number	6	7	8	9	10	
Shift (Hz)	3.83	3.97	4.44	4.63	5.20	

Table 7 Comparison of the CPU run-time (s) in Example 2.

Mode	E	Frequency's	Improved Nelson's	Duana 41 - 1 (-)
Number	Frequency	derivative	method (s) [57]	Present method (s)
1	2.42	606.02	1.85	0.31
2	2.63	657.18	1.82	0.27
3	3.03	757.33	1.85	0.22
4	3.62	905.58	1.83	0.41
5	3.78	753.01	1.95	1.14
6	3.70 -	1130.57	1.93	1.14
7	3.94	859.25	1.97	0.80
8	3.94 -	1109.69	1.97	0.80
9	4.25	1062.96	**	**
10	- T.23 -	1063.00		
11	4.41	1101.34	1.85	0.75
12	4.74	999.80	1.97	0.77
13		1370.16	1.97	0.77
14	5.38	1344.76	1.86	0.60
15	5.41	927.74	1.97	0.99
16	. <i>J</i> .T1 -	1778.93	1.77	0.77
		Total Time	18.92	6.26

^{**} Because λ'_i is repeated, the calculation is ignored in this study.

Table 8Relative errors of the eigenvector derivatives in Example 2.

Frequency (Hz)	2.42	2.63	3.03	3.62	3.78	3.78	3.94	3.94
Used shift (Hz)	0	2.14	3.01	3.35	3.35	3.35	3.83	3.83
$e_r(\%)$	7.96E-3	7.62E-3	2.16E-4	3.67E-3	2.17E-4	3.88E-5	4.48E-4	1.00E-4
Frequency (Hz)	4.25	4.25	4.41	4.74	4.74	5.38	5.41	5.41
Used shift (Hz)	**	**	3.97	4.63	4.63	5.20	5.20	5.20
$e_r(\%)$	**	**	9.66E-5	8.15E-4	2.54E-5	3.28E-4	6.72E-6	1.64E-3

Table 9
Computed frequencies of the car door structure (Hz).

Interested	35	40	45	50	55
Frequency (Hz)	33	40	43	30	55
Actual	34.92	39.19	45.22	51.31	56.65
Frequency (Hz)	34.92	39.19	43.22	31.31	30.03

Table 10
Comparison of the CPU run-time(s) in Example 3.

Frequency	Frequency's derivative	Improved Nelson's method (s) [57]	Present method (s)
34.92	296.9478	4.58	1.17
39.19	103.8682	4.62	1.33
45.22	380.9213	4.62	1.13
51.31	672.3358	4.54	1.38
56.65	839.4070	4.56	1.38
	Total Time	22.92	6.39

Table 11Relative errors of the eigenvector derivatives in Example 3.

Frequency(Hz)	34.92	39.19	45.22	51.31	56.65
$e_r(\%)$	3.24E-3	3.37E-2	3.36E-2	4.76E-1	1.60E-1