

RESEARCH ARTICLE

WILEY

Highly efficient general method for sensitivity analysis of eigenvectors with repeated eigenvalues without passing through adjacent eigenvectors

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Funding information

Ministerio de Ciencia e Innovación,
Grant/Award Number:
MTM2017-83740-P; National Research
Foundation of Korea, Grant/Award
Number: NRF-2018K1A3A1A38056941

Summary

It is well known that the sensitivity analysis of the eigenvectors corresponding to multiple eigenvalues is a difficult problem. The main difficulty is that for given multiple eigenvalues, the eigenvector derivatives can be computed for a specific eigenvector basis, the so-called *adjacent* eigenvector basis. These adjacent eigenvectors depend on individual variables, which makes the eigenvector derivative calculation elaborate and expensive from a computational perspective. This research presents a method that avoids passing through adjacent eigenvectors in the calculation of the partial derivatives of any prescribed eigenvector basis. As our method fits into the adjoint sensitivity analysis, it is efficient for computing the complete Jacobian matrix because the adjoint variables are independent of each variable. Thus our method clarifies and unifies existing theories on eigenvector sensitivity analysis. Moreover, it provides a highly efficient computational method with a significant saving of the computational cost. Additional benefits of our approach are that one does not have to solve a deficient linear system and that the method is independent of the existence of repeated eigenvalue derivatives of the multiple eigenvalues. Our method covers the case of eigenvectors associated to a single eigenvalue. Some examples are provided to validate the present approach.

KEYWORDS

eigenvector sensitivity, repeated eigenvalue, topology optimization

1 | INTRODUCTION

Eigenproblems, that is, problems regarding eigenvalues and/or eigenvectors are widely present today in differing research fields such as vibration modal analysis,¹⁻³ graph theory,⁴ cavity characterization in hyperelasticity,⁵ and image processing.⁶ In addition, whenever they constitute or form a part of the physics of optimization problems with numerous design variables, then a computationally efficient sensitivity analysis must be performed to enhance the performance. Topology optimization problems,⁷ in which a prescribed amount of a material is distributed in a design space to optimize an objective function while fulfilling some constraints, need to be particularly highlighted. Their discretized forms are finite-dimensional mathematical programming problems in which the number of design variables (called densities) is large because it typically coincides with the number of finite elements of the mesh. In such cases, the cost associated with

the computation of the derivatives may be critical sometimes. In general, computing eigenvalue derivatives with respect to either a single or vector design variable is inexpensive, whereas computing eigenvector sensitivities is an issue that is relatively much more complex and expensive. In the case of single eigenvalues, the eigenvectors are differentiable, and there are well established methods for computing the eigenvector derivatives. Comparatively, the case of eigenvectors corresponding to multiple eigenvalues is more difficult because in this scenario, there exist infinitely many eigenvectors basis (orthonormal with respect to the mass matrix) associated with the multiple eigenvalues. This adversely affects the differentiability, and even the continuity, of the eigenvectors with respect to the design variables. In this case, when a single design variable is perturbed, the multiple eigenvalues split into several single eigenvalues. Moreover, it can be shown that the eigenvector basis corresponding to the multiple eigenvalues (before perturbing the design variable) *closer* to the eigenvectors of the single eigenvalues (after perturbing the design variable) is differentiable. This particular basis is called the *adjacent basis*, and in general, and it is a very important feature, which depends on each design variable.⁸ Any other eigenvector corresponding to the multiple eigenvalues can be expressed as a linear combination of the eigenvectors of the adjacent basis, for which the partial derivatives may be computed. Moreover, the partial derivatives of the target eigenvector can be obtained as a linear combination of those of the adjacent eigenvectors.⁸ In practical cases, for example, in optimization, we are interested in computing the sensitivities of a functional depending of certain eigenvectors, which probably *follows* a prescribed reference mode shape, and with the existing methods in the literature, this can be achieved using the adjacent eigenvectors basis. From the implementation perspective, when we have to compute the partial derivatives with respect to numerous design variables, obtaining these results becomes computationally expensive and elaborate because as highlighted above, the adjacent eigenvectors depend on each design variable.

In this article, we propose a method that overcomes this difficulty. Essentially, we provide, and mathematically validate, a formula, established in Theorem 1, to compute sensitivities of general expressions depending on the eigenvectors corresponding to multiple eigenvalues without passing through the adjacent eigenvectors. These expressions are general and could be even a vector, so that our approach includes both the case of computing the derivative of a scalar function of the eigenvectors and that of vector format, as eigenvectors derivatives for instance. In fact, because our formula for sensitivity is based on an adjoint approach, we have to compute the adjoint states as a solution of a linear system, but with the very remarkable feature that this linear system is independent of each variable. Therefore, it is solved only once for computing all the partial derivatives with respect to all the design variables. All these derivatives suitably arranged conform the called hereafter Jacobian matrix. In our case, we do not have to build this matrix as it does not produce any computational advantage. An additional benefit of our method, which is present in some of the existing methods, is that such the adjoint system is well-posed, and no distinct algorithm is required for the finding solutions of a deficient system.³ This avoids the algorithm failure known to occur in certain cases, for example, when multiple eigenvalue derivatives coincide.^{9–11} This paper considers the optimization problems with multiple eigenvalues. However, it does not matter whether the eigenvalues are repeated from the very beginning due to symmetry or not, and that they may coalesce during the optimization process because our approach would continue being valid. The case of eigenvectors associated to single eigenvalues is also covered by this approach.

Topology optimization problems involving eigenmodes are, however, much more scarce in the literature. Next, some works such that either cost or constraints depends on eigenmodes are cited. A mode shape corresponding to a simple eigenvalue of a fiber laser package is designed in order to minimize the elongation of the fiber under dynamic excitation.¹² A multiobjective function is formulated in order to find optimal configurations that simultaneously satisfy (simple) eigenfrequency, eigenmode, and stiffness requirements at certain points of a vibrating structure.¹³ A similar problem is treated in Reference 14. The novelty there is to include the electromechanical coupling coefficient in the objective function so that the energy conversion is maximized for a specific mode. Eigenmodes appear in the constraints only.¹⁵ One of the objectives of that work is to determine the material distribution of a structure that maximizes the fundamental frequency and at the same time synthesizes the first two modes. Our interest in this field comes from the problem that some authors of this article treated in Reference 16. The objective in that paper was the optimal design of piezoelectric modal sensor/actuators, in which we simultaneously designed the ground structure and polarization profiles of the piezoelectric transducers (see the recent survey¹⁷). It is precisely in such cases where the computational gain of our method is much higher as we have several hundreds of variables. In this article, damping is not considered in the model, but we plan to address this issue in a future work with promising applications.

The outline of the article is the following. In Section 2, we review briefly the most commonly used techniques that are referred in the literature for computing eigenvalues and eigenvector sensitivities depending on whether the eigenvalues are single or not. The method we propose relies on these previous methods, and revisiting them is a natural approach to introduce it. In Section 3, we introduce our method and state and prove Theorem 1, which provides the formula

for computing the sensitivities of general functions depending on the eigenvectors, specially for those associated with repeated eigenvalues. And it is precisely in such cases where our method stands out above the rest as it no longer uses adjacent basis, which implies a considerable computational cost saving. Because a mode tracking procedure has to be implemented in this case, in Section 4, we introduce the approach for the optimization of costs depending on the eigenvectors with repeated eigenvalues. Section 5 illustrates our method with several examples both for the sensitivity calculation and topology optimization, confirming the significant improvement in the computational time provided by our methodology. Finally, Section 6 is devoted to conclusions. The manuscript also includes two appendices connecting our approach to previous relevant methods that were indeed our starting point in this investigation. We truly believe that these methods are clarified in the appendices and unified with our approach.

2 | REVIEW OF PREVIOUS METHODS

For the case of single (nonrepeated) eigenvalues, an eigenproblem modeling a mechanical system with n degrees of freedom may be expressed as

$$(\mathbf{K} - \lambda_j \mathbf{M})\boldsymbol{\phi}_j = \mathbf{0}, \quad j = 1, \dots, n. \quad (1)$$

Typically, $\mathbf{K}, \mathbf{M} \in \mathbb{R}^{n \times n}$ stands for the stiffness and mass matrix, respectively (in other situations they may adopt a different physical relevance), and both are real, symmetric, and positive definite. We would like to emphasize that in this study we consider neither complex nor nonsymmetric stiffness nor mass matrices. $(\lambda_j, \boldsymbol{\phi}_j)$ is a pair eigenvalue and its associated eigenvector, respectively. Hereafter, $()'$ stands for the derivative with respect to a single design variable. In this case, it is quite simple to compute the eigenvalue derivatives. Simply differentiating (1) and obviously assuming that the eigenvectors are \mathbf{M} -orthonormal implies that $\boldsymbol{\phi}_j$ is \mathbf{M} -unitary, that is,

$$\boldsymbol{\phi}_j^T \mathbf{M} \boldsymbol{\phi}_j = 1, \quad j = 1, \dots, n. \quad (2)$$

Then it is easy to obtain

$$\lambda'_k = \boldsymbol{\phi}_k^T (\mathbf{K}' - \lambda_k \mathbf{M}') \boldsymbol{\phi}_k. \quad (3)$$

However, the issue is different when we are interested in computing the eigenvector derivatives. To this purpose, by differentiating both Equations (1) and (2), we obtain the following singular linear system:

$$\begin{aligned} (\mathbf{K} - \lambda_k \mathbf{M})\boldsymbol{\phi}'_k &= -(\mathbf{K}' - \lambda_k \mathbf{M}')\boldsymbol{\phi}_k + \lambda'_k \mathbf{M} \boldsymbol{\phi}_k \\ \boldsymbol{\phi}_k^T \mathbf{M} \boldsymbol{\phi}'_k &= -\frac{1}{2} \boldsymbol{\phi}_k^T \mathbf{M}' \boldsymbol{\phi}_k. \end{aligned} \quad (4)$$

The first equation in (4) is a singular, rank- $(n - 1)$ deficient, linear system. However, a solution can be found considering second equation in (4) by using a very well-known technique, which is called Nelson's method.¹⁸ This process may be expensive depending on the number of variables involved in the problem (remember that now we are computing the derivatives of a vector). When the number of design variables, say N , is of the same order of magnitude as the number of degrees of freedom, n , in a mechanical system, as usually occurs in topology optimization problems, the algorithm becomes highly expensive because both the number and size of the linear systems to be solved are increasing precisely with N . A slightly less expensive method is the so-called algebraic method,¹⁹ which was proposed by Lee and Jung. It basically consists of re-expressing the system (4) more appropriately.

$$\begin{bmatrix} \mathbf{K} - \lambda_k \mathbf{M} & -\mathbf{M} \boldsymbol{\phi}_k \\ -\boldsymbol{\phi}_k^T \mathbf{M} & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{\phi}'_k \\ \lambda'_k \end{bmatrix} = \begin{bmatrix} -(\mathbf{K}' - \lambda_k \mathbf{M}')\boldsymbol{\phi}_k \\ \frac{1}{2} \boldsymbol{\phi}_k^T \mathbf{M}' \boldsymbol{\phi}_k \end{bmatrix}, \quad (5)$$

where now the couple, $(\boldsymbol{\phi}'_k, \lambda'_k)$, is unknown.

Contrastingly, one rarely has to compute only an eigenvector derivative. Because eigenvectors are often embedded in the physics of an underlying problem, the derivatives of a function of the eigenvectors are required instead. In line

with this and combining both the above-mentioned Nelson's method and another technique called the adjoint method,²⁰ Tcherniak proposed in Reference 21 an efficient method to compute the derivatives of scalar objective functions regarding eigenvectors of the type:

$$c = \mathbf{F}^T \boldsymbol{\phi}_k, \quad (6)$$

where \mathbf{F} is, in principle, a design-independent vector and $\boldsymbol{\phi}_k$ is a particular eigenmode or mode shape. This formulation was used in Reference 21 to maximize the magnitude of the steady-state vibrations in resonating structures for a given excitation frequency. In such cases, the sensitivity of the objective function, $\mathbf{F}^T \boldsymbol{\phi}'_k$, may be indirectly computed as

$$c' = -\mathbf{P}^T(\mathbf{K}' - \lambda_k \mathbf{M}') \boldsymbol{\phi}_k - \frac{1}{2} c \boldsymbol{\phi}_k^T \mathbf{M}' \boldsymbol{\phi}_k, \quad (7)$$

with \mathbf{P} (the so-called adjoint state) satisfying again another singular linear system,

$$\begin{aligned} (\mathbf{K} - \lambda_k \mathbf{M}) \mathbf{P} &= \mathbf{F} - c \mathbf{M} \boldsymbol{\phi}_k \\ \boldsymbol{\phi}_k^T \mathbf{M} \mathbf{P} &= 0. \end{aligned} \quad (8)$$

The above, in appearance, is similar to Equation (4), and therefore, it can be solved efficiently by using either Nelson's method or the algebraic method. Contrary to before, now the system (8) has to be solved only once regardless of the number of design variables involved.

However, the sensitivity analysis for multiple (repeated) eigenvalues is indeed much more complex owing to the mathematical fact that there exist infinite eigenvector basis of the eigenspace associated with multiple eigenvalues. Moreover, it is precisely this ambiguity that adversely affects the continuity, and therefore, causes differentiability issues. Thus, the *eigenmodes corresponding to repeated eigenvalues are not continuous, and therefore, they are nondifferentiable either*. However, differentiability can be guaranteed for a particular eigenvector basis, the so-called adjacent basis, for which explicit derivative computations can be performed. To deepen the insight into the problem itself, the reader is referred to Reference 8 and the references therein, where some of the authors have analyzed it in detail from both mathematical and numerical perspectives.

For the sake of clarity, let us consider an eigenproblem where λ is an eigenvalue of multiplicity $m = 2$

$$\mathbf{K} \boldsymbol{\Phi} = \mathbf{M} \boldsymbol{\Phi} \boldsymbol{\Lambda}, \quad (9)$$

$\boldsymbol{\Lambda} = \lambda \mathbf{I}_2 \in \mathbb{R}^{2 \times 2}$, with \mathbf{I}_2 the identity matrix, and $\boldsymbol{\Phi}$ is a matrix whose columns, $\boldsymbol{\phi}_1, \boldsymbol{\phi}_2$, are a basis of \mathbf{M} -orthonormal eigenvectors ($\boldsymbol{\Phi}^T \mathbf{M} \boldsymbol{\Phi} = \mathbf{I}_2$) associated with λ . The point is that in general $\boldsymbol{\Phi}'$ cannot be computed by the existing methods in the literature, except for a particular basis called the adjacent basis, $\mathbf{Z}_1, \mathbf{Z}_2$, which disposed by columns form the matrix, \mathbf{Z} . Both basis are related through a rotation matrix, $\boldsymbol{\Gamma}$, such as

$$\mathbf{Z} = \boldsymbol{\Phi} \boldsymbol{\Gamma}. \quad (10)$$

Imposing the condition that \mathbf{Z} is also an eigenvector basis, it is deduced that $\boldsymbol{\Gamma}$ is an orthogonal matrix (ie, $\boldsymbol{\Gamma}^T \boldsymbol{\Gamma} = \mathbf{I}_2$) and a solution of the small (2×2) eigenproblem

$$\mathbf{D} \boldsymbol{\Gamma} = \boldsymbol{\Gamma} \boldsymbol{\Lambda}', \quad \mathbf{D} = \boldsymbol{\Phi}^T (\mathbf{K}' - \lambda \mathbf{M}') \boldsymbol{\Phi}. \quad (11)$$

From the eigenproblem (11), we can also obtain $\boldsymbol{\Lambda}'$, a diagonal matrix that stores the sensitivities for the multiple eigenvalues, λ . This procedure was presented in.²² More recently in References 23 and 24, a different approach can be found, where the elements over the diagonal of $\boldsymbol{\Lambda}'$ are elegantly obtained as solutions of a small extreme-value problem. In case we order the eigenvalues as $\lambda_1 < \lambda_2$ before they coalesce, then $\lambda'_1 = \max(\text{diag}(\boldsymbol{\Lambda}'))$ and $\lambda'_2 = \min(\text{diag}(\boldsymbol{\Lambda}'))$. Notice that the small eigenvalue problem (11) has to be solved as many times as the design variables are, but this is inexpensive. An interesting point is that multiplying Equation (11) to the right by $\boldsymbol{\Gamma}^T$, we get

$$\mathbf{Z}^T (\mathbf{K}' - \lambda \mathbf{M}') \mathbf{Z} = \boldsymbol{\Lambda}', \quad (12)$$

and therefore the adjacent basis \mathbf{Z} is precisely a basis of eigenvectors of matrix $\mathbf{K}' - \lambda\mathbf{M}'$, or in other words, it is the unique \mathbf{M} -orthonormal basis such that $\mathbf{Z}^T(\mathbf{K}' - \lambda\mathbf{M}')\mathbf{Z}$ is diagonal.

However, obtaining the derivatives of the adjacent modes, that is, \mathbf{Z}' , is more complex. Before starting, we have to note that both

$$\mathbf{K}\mathbf{Z} = \mathbf{M}\mathbf{Z}\mathbf{A}, \quad (13)$$

and

$$\mathbf{Z}^T\mathbf{M}\mathbf{Z} = \mathbf{I}_2 \quad (14)$$

hold. Differentiating both Equations (13) and (14), we arrive at

$$\begin{aligned} (\mathbf{K} - \lambda\mathbf{M})\mathbf{Z}' &= -(\mathbf{K}' - \lambda\mathbf{M}')\mathbf{Z} + \mathbf{M}\mathbf{Z}\mathbf{A}' \\ \mathbf{Z}^T\mathbf{M}\mathbf{Z}' &= -\frac{1}{2}\mathbf{Z}^T\mathbf{M}'\mathbf{Z}, \end{aligned} \quad (15)$$

a system where the rank of the matrix, $(\mathbf{K} - \lambda\mathbf{M})$, is $(n - 2)$, and hence, the system, first equation in (15), is singular (indeed, rank- $(n - 2)$ deficient). It is worthy to point out that, having in mind that \mathbf{A}' is diagonal, the unique solution of the first equation in (15) is precisely the adjacent basis \mathbf{Z} . The reason is that this system is solvable if and only if the independent term $-(\mathbf{K}' - \lambda\mathbf{M}')\mathbf{Z} + \mathbf{M}\mathbf{Z}\mathbf{A}'$ is orthogonal to the subspace of solutions of the homogeneous part $((\mathbf{K} - \lambda\mathbf{M})\mathbf{Z} = \mathbf{0})$, and making the product, we get

$$\mathbf{Z}^T [-(\mathbf{K}' - \lambda\mathbf{M}')\mathbf{Z} + \mathbf{M}\mathbf{Z}\mathbf{A}'] = -\mathbf{Z}^T(\mathbf{K}' - \lambda\mathbf{M}')\mathbf{Z} + \mathbf{A}' = \mathbf{0},$$

and the adjacent basis is the only (\mathbf{M} -orthonormal) basis for which this happens since, as it was pointed out above, it is the only basis for which $\mathbf{Z}^T(\mathbf{K}' - \lambda\mathbf{M}')\mathbf{Z}$ is diagonal. Dailey's method¹ (see also Reference 9) generalizes Nelson's method to solve this singular system by combining and rearranging its terms, using both the second equation in (15) and its derivative. It is a computationally expensive method because it involves solving N linear systems of N^2 unknowns, similar to the case of single eigenvalues. It is important to mention that Dailey's method may fail under certain circumstances, and moreover, it requires a modification when multiple eigenvalue derivatives coincide.⁹⁻¹¹

As before, a slightly less expensive approach to do the same is the extension of the aforementioned work by Lee and Jung for the case of repeated eigenvalues.²⁵ This is achieved by simply re-expressing the system (15) in terms of the new unknowns, $(\mathbf{Z}', \mathbf{A}')$, that is,

$$\begin{bmatrix} \mathbf{K} - \lambda\mathbf{M} & -\mathbf{M}\mathbf{Z} \\ -\mathbf{Z}^T\mathbf{M} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{Z}' \\ \mathbf{A}' \end{bmatrix} = \begin{bmatrix} -(\mathbf{K}' - \lambda\mathbf{M}')\mathbf{Z} \\ \frac{1}{2}\mathbf{Z}^T\mathbf{M}'\mathbf{Z} \end{bmatrix}. \quad (16)$$

The main advantage of this algebraic (or direct) method with respect to Dailey's method is that it overcomes the issue of resolution of a singular linear system, what could lead to wrong solutions, and that the computations can be performed without using the second-order derivatives of both the stiffness and mass matrices. However, the independent term of the system (16) depends on both the design variable and \mathbf{Z} (similar to the matrix). As it was mentioned above, the basis of the adjacent modes, \mathbf{Z} , changes when perturbing any of the design variables; therefore, the underlying linear system has to be updated whenever computing another derivative. If instead of the adjacent basis \mathbf{Z} in the formulation of the system (16) one uses any other \mathbf{M} -orthonormal basis Φ , then the matrix \mathbf{A}' obtained as part of the solution of (16) is not diagonal (see Appendix A).

Previous methods for computing eigenvector derivatives are direct methods, and consequently, they do not consider the possibility of simplifying the computations by the use of the adjoint method²⁰ when derivatives with respect to different variables have to be computed. This was done in the case of repeated eigenvalues for the first time by Lee in the very remarkable study in Reference 3. In that work, the following function is considered:

$$\tilde{\mathbf{G}} = \begin{bmatrix} \mathbf{Z} \\ \mathbf{A} \end{bmatrix}. \quad (17)$$

With the help of the adjoint method, $\tilde{\mathbf{G}}'$ may be indirectly computed as

$$\tilde{\mathbf{G}}' = \mathbf{U}^T(\mathbf{K}' - \lambda\mathbf{M}')\mathbf{Z} - \frac{1}{2}\mathbf{V}^T\mathbf{Z}^T\mathbf{M}'\mathbf{Z}, \quad (18)$$

where the Lagrange multipliers, \mathbf{U}, \mathbf{V} , are the unique solutions of the system,

$$\begin{bmatrix} \mathbf{K} - \lambda\mathbf{M} & -\mathbf{M}\mathbf{Z} \\ -\mathbf{Z}^T\mathbf{M} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{U} \\ \mathbf{V} \end{bmatrix} = -\mathbf{I}. \quad (19)$$

As in the algebraic method, the eigenvalues and eigenvector derivatives are computed all at once, and with the help of the adjoint method, the author highlighted that the computational cost is significantly reduced because of being independent of the number of design variables. In this respect, we do not particularly agree with that as we will show in the examples section when comparing Lee's method to ours. As far as the authors understand, in Reference 3, it is implicitly assumed that the derivatives are computed for the adjacent eigenvectors, and so, this is performed in the numerical examples. However, when one tries to compute the derivatives of another design variable, the adjacent basis has to be computed again. Otherwise, the eigenvalue derivative matrix, Λ' , becomes nondiagonal, and an appropriate rotation has to be applied to recover the derivative values (see Appendix B), evidencing that the result would be wrong.

Motivated by all the previous methods, in this work, we generalize the concepts proposed by Tcherniak²¹ and by Lee,³ and develop a highly efficient method for computing the sensitivities for general objective functions regarding eigenvectors. Starting from Lee's work, which is remarkable but also incomplete in our point of view, we explain all the details that lead us to state that Φ' , the derivatives of a fixed eigenvector basis, may be computed without computing the adjacent basis of each element. Therefore, here, we emphasize on showing a highly efficient approach to compute the sensitivities of either scalar or vector objective functions depending on the eigenvectors having repeated eigenvalues. Moreover, we present a method that naturally comprises the case of single eigenvalues as a particular one. We do not include the eigenvalue derivative calculation because it can be performed inexpensively by solving the small eigenproblem (11).

3 | A HIGHLY EFFICIENT GENERAL METHOD FOR SENSITIVITY ANALYSIS OF EIGENVECTORS

Let λ be an eigenvalue of multiplicity m and Φ a matrix whose columns $\phi_1, \phi_2, \dots, \phi_m$ are a basis of \mathbf{M} -orthonormalized eigenvectors ($\Phi^T\mathbf{M}\Phi = \mathbf{I}_m$) associated with λ . Next, we present the main result of this work, where lies the novelty of our contribution.

Theorem 1. *Let $\mathbf{G}(\Phi)$ be a vector objective function depending on a fixed \mathbf{M} -orthonormal eigenvector basis Φ associated with an eigenvalue, λ , of multiplicity m , verifying*

$$\mathbf{K}\Phi = \mathbf{M}\Phi\Lambda, \quad \Phi^T\mathbf{M}\Phi = \mathbf{I}_m, \quad \Lambda = \lambda\mathbf{I}_m \in \mathbb{R}^{m \times m}.$$

Then, the derivative of \mathbf{G} with respect to any design parameter may be directly computed as

$$\mathbf{G}' = \mathbf{P}^T(\mathbf{K}' - \lambda\mathbf{M}')\Phi - \frac{1}{2}\Delta^T\Phi^T\mathbf{M}'\Phi, \quad (20)$$

where $[\mathbf{P} \ \Delta]^T$ is the unique solution of the linear system

$$\begin{bmatrix} \mathbf{K} - \lambda\mathbf{M} & -\mathbf{M}\Phi \\ -\Phi^T\mathbf{M} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{P} \\ \Delta \end{bmatrix} = \begin{bmatrix} -\frac{\partial \mathbf{G}}{\partial \Phi} \\ \mathbf{0} \end{bmatrix}. \quad (21)$$

We would like to emphasize that the system (21) itself depends on Φ instead of the adjacent eigenvectors and that it is independent of the single variables. Moreover, it has to be solved only once regardless of the number of design variables. Indeed, our approach does not require any extra modification when multiple eigenvalue derivatives coincide, as we will show in one of the examples.

To convince ourselves of the result above mentioned and as an example, we try computing the derivatives of the adjacent eigenvectors, $\mathbf{Z} = \Phi \Gamma$, where Γ is the solution of the small ($m \times m$) eigenproblem

$$\mathbf{D}\Gamma = \Gamma\Lambda', \quad \mathbf{D} = \Phi^T(\mathbf{K}' - \lambda\mathbf{M}')\Phi, \quad (22)$$

and moreover, \mathbf{Z} verifies

$$\mathbf{K}\mathbf{Z} = \mathbf{M}\mathbf{Z}\Lambda, \quad \mathbf{Z}^T\mathbf{M}\mathbf{Z} = \mathbf{I}_m. \quad (23)$$

For this purpose, let us consider the following objective function

$$\tilde{\mathbf{G}} = \mathbf{Z}, \quad (24)$$

which indeed is differentiable, and is next modified to conveniently consider the augmented function,

$$\tilde{\mathbf{G}} = \mathbf{Z} + \mathbf{P}^T(\mathbf{K}\mathbf{Z} - \mathbf{M}\mathbf{Z}\Lambda) - \frac{1}{2}\Xi^T(\mathbf{Z}^T\mathbf{M}\mathbf{Z} - \mathbf{I}_m), \quad (25)$$

with the help of the adjoint method, where \mathbf{P} and Ξ are the vector Lagrange multipliers. Differentiating and rearranging the terms, we arrive at

$$\tilde{\mathbf{G}}' = \mathbf{P}^T(\mathbf{K}' - \lambda\mathbf{M}')\mathbf{Z} - \frac{1}{2}\Xi^T\mathbf{Z}^T\mathbf{M}'\mathbf{Z}, \quad (26)$$

being the pair (\mathbf{P}, Ξ) , the unique solution of the so-called adjoint system,

$$\begin{bmatrix} \mathbf{K} - \lambda\mathbf{M} & -\mathbf{M}\mathbf{Z} \\ -\mathbf{Z}^T\mathbf{M} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{P} \\ \Xi \end{bmatrix} = \begin{bmatrix} -\mathbf{I}_n \\ \mathbf{0}_{m \times n} \end{bmatrix}, \quad (27)$$

which is not singular, as already proved using different techniques.^{3,25}

In many practical situations prescribed previously, mode shapes are objects of interest⁸ because one needs to follow certain eigenmodes as references. If eigenvector derivatives need to be computed for any \mathbf{M} -orthonormal eigenvector basis Φ , which is related to \mathbf{Z} by Γ , it seems that any time we need to compute a derivative, the adjoint system (27) has to be solved again because the adjacent basis, \mathbf{Z} , changes when perturbing an element (or a design variable). Our approach makes us remove \mathbf{Z} from the matrix, and consequently, make the matrix only dependent on Φ . To achieve this in the top equation, we simply have to rename $\Xi = \Gamma^T\Delta$, with Δ now being the new multiplier. To do the same in the bottom equation, we use the following elementary linear algebra result.

Lemma 1. Let $\mathbf{A}, \mathbf{B} \in \mathbb{R}^{m \times m}$, with $|\mathbf{A}| \neq 0$. Then $\mathbf{A}\mathbf{B} = \mathbf{0}$ implies $\mathbf{B} = \mathbf{0}$.

Proof. It is elementary that considering $\mathbf{A} = [\mathbf{a}_1 | \mathbf{a}_2 | \dots | \mathbf{a}_m]$ as a matrix whose columns, \mathbf{a}_i , are vectors that are linearly independent, a particular row of matrix $\mathbf{A}\mathbf{B}$ is given by a linear combination of \mathbf{a}_i . Moreover, it will become a zero vector if such a row of \mathbf{B} is identically null. ■

Recalling the adjoint system (27), the bottom equation leads to

$$\mathbf{Z}^T\mathbf{M}\mathbf{P} = \mathbf{0} \quad \Rightarrow \quad \Gamma^T\Phi^T\mathbf{M}\mathbf{P} = \mathbf{0}, \quad (28)$$

and now using Lemma 1, we can conclude that

$$\Phi^T\mathbf{M}\mathbf{P} = \mathbf{0}, \quad (29)$$

as Γ^T is a nonsingular matrix. Thus, in summary

$$\tilde{\mathbf{G}}' = \mathbf{P}^T(\mathbf{K}' - \lambda\mathbf{M}')\mathbf{Z} - \frac{1}{2}\Delta^T\Gamma\mathbf{Z}^T\mathbf{M}'\mathbf{Z}, \quad (30)$$

being the pair $(\mathbf{P}, \mathbf{\Delta})$ solution of the new adjoint system,

$$\begin{bmatrix} \mathbf{K} - \lambda \mathbf{M} & -\mathbf{M}\mathbf{\Phi} \\ -\mathbf{\Phi}^T \mathbf{M} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{P} \\ \mathbf{\Delta} \end{bmatrix} = \begin{bmatrix} -\mathbf{I}_n \\ \mathbf{0}_{m \times n} \end{bmatrix}. \quad (31)$$

The above matrix has to be solved only once because it depends on the initial basis, $\mathbf{\Phi}$, only. Using (10) in Equation (30), we obtain

$$\tilde{\mathbf{G}}' = \left(\mathbf{P}^T (\mathbf{K}' - \lambda \mathbf{M}') \mathbf{\Phi} - \frac{1}{2} \mathbf{\Delta}^T \mathbf{\Phi}^T \mathbf{M}' \mathbf{\Phi} \right) \mathbf{\Gamma}. \quad (32)$$

Defining the new objective function, $\mathbf{G} = \mathbf{\Phi}$, the latter implies that

$$\mathbf{G}' = \mathbf{P}^T (\mathbf{K}' - \lambda \mathbf{M}') \mathbf{\Phi} - \frac{1}{2} \mathbf{\Delta}^T \mathbf{\Phi}^T \mathbf{M}' \mathbf{\Phi}, \quad (33)$$

with $(\mathbf{P}, \mathbf{\Delta})$ being the solution of the system (31). We would like to emphasize that this fact represents a real substantial computational advantage for the sensitivity analysis, as we will show in the examples section. Thus, the derivative, \mathbf{G}' , may be computed without the need of computing \mathbf{Z} or \mathbf{Z}' , and moreover, $\mathbf{Z}' = \mathbf{\Phi}' \mathbf{\Gamma}$. This mathematical fact may also be proved in the algebraic method (see Appendix A) and Lee's method (see Appendix B), and it has not been reported before in the literature, as far as the authors' knowledge.

The vector format used for the above objective function allows us to compute all at once the eigenvector derivatives from the desired design variables. But of course, we may extend now our method to consider scalar objective functions that linear depend on the eigenvectors as

$$g = \mathbf{F}_1^T \boldsymbol{\phi}_1 + \mathbf{F}_2^T \boldsymbol{\phi}_2 + \dots + \mathbf{F}_m^T \boldsymbol{\phi}_m, \quad (34)$$

or equivalently as

$$g = \text{trace}(\mathbf{G}), \quad \mathbf{G} = \mathbf{F}^T \mathbf{\Phi} \in \mathbb{R}^{m \times m}, \quad (35)$$

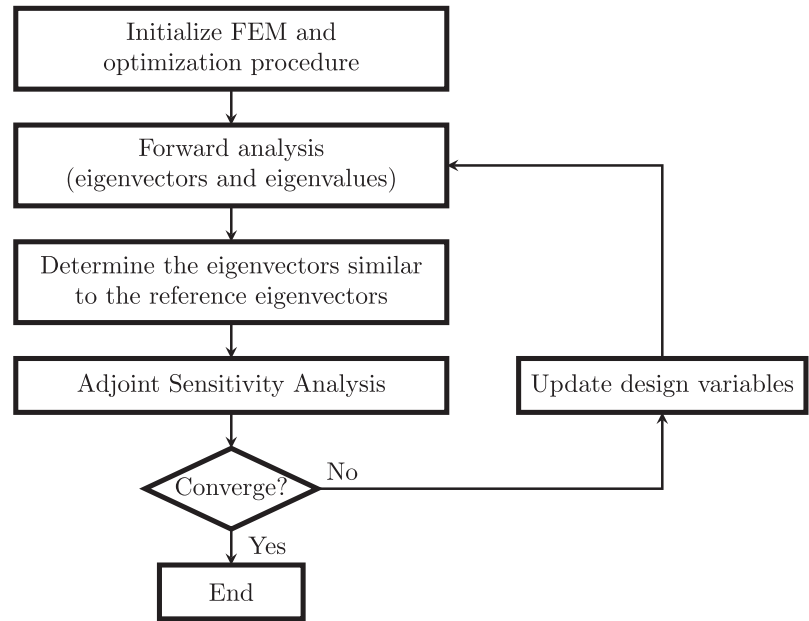
with \mathbf{F} a matrix whose columns $\mathbf{F}_1, \mathbf{F}_2, \dots, \mathbf{F}_m$ are independent design vectors that store some information related to the physics of the problem. The way to proceed would be the same, but \mathbf{I}_n in the system (30) would be replaced with \mathbf{F} . We could also extend this to scalar quadratic functions on eigenmodes measuring some types of energy.

Finally, we would like to point out that our method is also valid in the case of eigenvectors corresponding to simple eigenvalues. In such a case, the matrix $\mathbf{\Phi}$ becomes a column vector and the old multiplier $\mathbf{\Delta}$ associated to the \mathbf{M} -orthonormal condition is now a scalar.

4 | IMPLEMENTATION IN OPTIMIZATION: MODE TRACKING

When a functional involved in an optimization problem, either the cost or a constraint, depends on a mode shape it must be very clear on which specific mode shape is such a dependence, since mode shapes change and mode switching (change of order of eigenvalues in the spectrum) may happen during the optimization process when updating variables. In addition, this fact clearly becomes more important in problems where multiple eigenvalues occur. Therefore cost and constraints must clearly depend on selected mode shapes, and the idea is to select the closest eigenmodes to given vectors. Without this feature, the above adjoint sensitivity analysis cannot be successfully incorporated into the optimization algorithm as we run the risk of wrongly computing derivatives. This issue has been extensively analyzed.⁸ There, a method motivating the *modal assurance criterion* for selecting the eigenvectors was proposed and implemented.²⁶ In this article, we propose a slightly more direct method, wherein at every optimization iteration, a small optimization problem with rotation angle as the optimization variable should be solved to determine the angle that rotates the computed eigenvectors to the reference ones.

FIGURE 1 The flowchart of the optimization procedure



We restrict ourselves in the following analysis to an eigenvalue multiplicity of 2, but our method could be easily generalized to any larger multiplicity. Using

$$\Phi^{ref} = [\phi_1^{ref} \ \phi_2^{ref}],$$

for the reference modal shapes and

$$\tilde{\Phi} = [\tilde{\phi}_1 \ \tilde{\phi}_2],$$

as the eigenvectors provided by our numerical simulation package, we search for the right rotation angles as the solution to the optimization problem:

$$\min_{\theta} (\min(f_1, f_2)), \quad (36)$$

with

$$\begin{aligned} f_1(\theta) &= |\Phi^{ref} - \tilde{\Phi} \Gamma| \\ f_2(\theta) &= |\Phi^{ref} - \tilde{\Phi}^{switch} \Gamma|, \quad \tilde{\Phi}^{switch} = [\tilde{\phi}_2 \ \tilde{\phi}_1], \end{aligned} \quad (37)$$

and

$$\Gamma = \begin{bmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{bmatrix}.$$

Now, denoting θ^* as the optimal solution of (36), the desired eigenmodes are obtained from Φ as

$$\Phi = \begin{cases} \tilde{\Phi} \Gamma, & \text{if } f_1(\theta^*) \leq f_2(\theta^*) \\ \tilde{\Phi}^{switch} \Gamma, & \text{if } f_1(\theta^*) > f_2(\theta^*) \end{cases}, \quad (38)$$

where the optimum angle of the optimization problem in Equation (37) is denoted by θ^* . The above optimization formulation is for two repeated eigenmodes. If there are three repeated eigenmodes, the Euler rotation angles should be determined. Subsequently, the optimization framework in Figure 1 can be implemented.

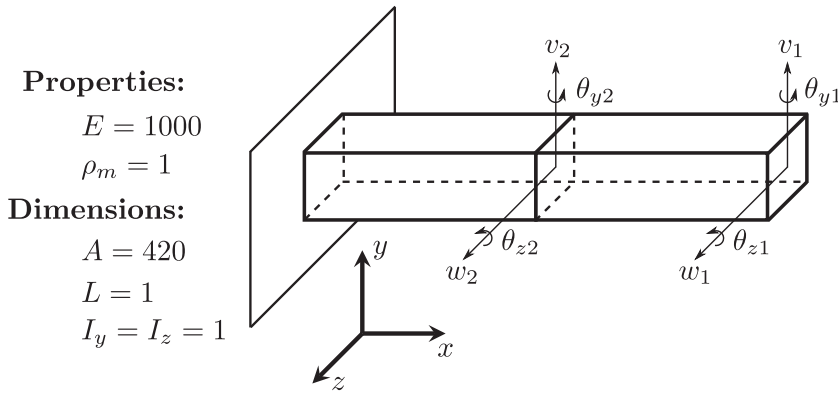


FIGURE 2 Two-element cantilever beam with multiple eigenvalues

5 | NUMERICAL EXAMPLES

This section is devoted to showing some numerical examples that corroborate our method. The two first ones are focused on the sensitivity analysis in different structure types, and the last one considers the application of a topology optimization problem.

5.1 | Two-element cantilever beam with multiple eigenvalues

For the first example, a two-element cantilever beam with multiple eigenvalues is considered, as shown in Figure 2. This is a reference example in the computation of sensitivities of eigenvectors with repeated eigenvalues.^{1,3} The design variable is the z-axis area moment of the second element with the material properties shown in Figure 2.

Without loss of generality, both the global stiffness and mass matrices with clamped boundary conditions are given by

$$K = \frac{E}{L} \begin{bmatrix} \frac{24I_z}{L^2} & 0 & 0 & 0 & -\frac{12I_z}{L^2} & 0 & 0 & \frac{6I_z}{L} \\ & \frac{24I_y}{L^2} & 0 & 0 & 0 & -\frac{12I_y}{L^2} & -\frac{6I_y}{L} & 0 \\ & & 8I_y & 0 & 0 & \frac{6I_y}{L} & 2I_y & 0 \\ & & & 8I_z & -\frac{6I_z}{L} & 0 & 0 & 2I_z \\ & & & & \frac{12I_z}{L^2} & 0 & 0 & -\frac{6I_z}{L} \\ & & sym & & & \frac{12I_y}{L^2} & \frac{6I_y}{L} & 0 \\ & & & & & & 4I_y & 0 \\ & & & & & & & 4I_z \end{bmatrix} \quad (39)$$

$$M = \frac{\rho AL}{420} \begin{bmatrix} 312 & 0 & 0 & 0 & 54 & 0 & 0 & -13L \\ & 312 & 0 & 0 & 0 & 54 & 13L & 0 \\ & & 8L^2 & 0 & 0 & -13L & -3L^2 & 0 \\ & & & 8L^2 & 13L & 0 & 0 & -3L^2 \\ & & & & 156 & 0 & 0 & -22L \\ & & sym & & & 156 & 22L & 0 \\ & & & & & & 4L^2 & 0 \\ & & & & & & & 4L^2 \end{bmatrix}. \quad (40)$$

The displacement vector for the first and second elements is

$$\mathbf{q} = [v_1, z_1, \theta_{y1}, \theta_{z1}, v_2, z_2, \theta_{y2}, \theta_{z2}]^T. \quad (41)$$

Taking the z-axis area moment of the first element as the design variable, $b = I_z$, the differentiation of the above matrices is as follows:

$$\frac{dK}{db} = \frac{E}{L} \begin{bmatrix} \frac{12}{L^2} & 0 & 0 & \frac{6}{L} & -\frac{12}{L^2} & 0 & 0 & \frac{6}{L} \\ & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ & & 0 & 0 & 0 & 0 & 0 & 0 \\ & & & 4 & -\frac{6}{L} & 0 & 0 & 2 \\ & & & & \frac{12}{L^2} & 0 & 0 & -\frac{6}{L} \\ & & sym & & & 0 & 0 & 0 \\ & & & & & & 0 & 0 \\ & & & & & & & 4 \end{bmatrix}, \quad \frac{dM}{db} = 0. \quad (42)$$

In our computation environment (64bit OS, the “eigs” command with “sm” option in Matlab 2018a), the eigenvectors and eigenvalues obtained are the following

$$\Phi = [\phi_1 \ \phi_2] = \begin{bmatrix} -0.0026 & 0.0233 \\ 0.0233 & 0.0026 \\ -0.0399 & -0.0044 \\ -0.0044 & 0.0399 \\ -0.0075 & 0.0687 \\ 0.0687 & 0.0075 \\ -0.0473 & -0.0052 \\ -0.0052 & 0.0473 \end{bmatrix}, \quad (43)$$

and $\lambda_1 = \lambda_2 = 1.8414$. Notice that the eigenvectors (43) are different from the adjacent vectors reported,^{1,3} but the rotation of $\theta = 83.7^\circ$ converts them into the adjacent vectors \mathbf{Z} found in References 1 and 3, that is,

$$\mathcal{Z} = \Phi \times \begin{bmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{bmatrix} = \begin{bmatrix} 0 & -0.0234 \\ -0.0234 & 0 \\ 0.0401 & 0 \\ 0 & -0.0401 \\ 0 & -0.0690 \\ -0.0690 & 0 \\ 0.0475 & 0 \\ 0 & -0.0475 \end{bmatrix}. \quad (44)$$

The adjacent eigenvector sensitivities computed by our method coincide with the ones in References 1 and 3, and they are

$$\mathcal{Z}' = \left[\frac{\partial \mathcal{Z}_1}{\partial b} \ \frac{\partial \mathcal{Z}_2}{\partial b} \right] = \begin{bmatrix} 0 & -0.0012 \\ 0 & 0 \\ 0 & 0 \\ 0 & -0.0019 \\ 0 & 0.0020 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0.0051 \end{bmatrix}, \quad (45)$$

$d\mathcal{Z}_2/db$	R (%)
-0.0012	100.00
-0.0000	100.00
0.0000	100.00
-0.0020	100.00
0.0021	100.00
-0.0000	100.00
0.0000	100.00
0.0051	100.00

TABLE 1 Design sensitivity coefficients of \mathbf{Z}_2 and their comparison with the central finite difference method

$d\phi_1/db$	$d\phi_2/db$	$\Delta\phi_1/\Delta b$	$\Delta\phi_2/\Delta b$	R_1 (%)	R_2 (%)
-0.0001	0.0012	-0.0001	0.0012	100.0000	100.0066
-0.0000	0.0000	0.0000	-0.0000	100.0000	100.0000
0.0000	-0.0000	-0.0000	0.0000	100.0000	100.0000
-0.0002	0.0020	-0.0002	0.0020	100.0000	100.0068
0.0002	-0.0020	0.0002	-0.0020	100.9435	100.0000
-0.0000	0.0000	0.0000	-0.0000	100.0000	100.0000
0.0000	-0.0000	-0.0000	0.0000	100.0000	100.0000
0.0006	-0.0051	0.0006	-0.0051	100.2605	100.0000

TABLE 2 Design sensitivity coefficients of Φ and their comparison with the central finite difference method

and the sensitivities of the eigenvalues, computed by Equation (11), are given by

$$\Lambda' = \begin{bmatrix} 0 & 0 \\ 0 & 0.0918 \end{bmatrix}. \quad (46)$$

Note that the off-diagonal values of Λ' are zero. The above sensitivity analysis implies that a perturbation in the design variable changes one of the eigenvalues associated with \mathbf{Z} . To show the accuracy of the computed sensitivity of the adjacent vectors with respect to the design variable, b , it is common to compute the ratio, R , of the values predicted by the design sensitivity analysis and those by the central finite difference method (approximated sensitivity values). In this work, we use the following formula:

$$R = \frac{(\mathcal{Z}(b + \Delta b) - \mathcal{Z}(b - \Delta b))/(2\Delta b)}{d\mathcal{Z}/db} \times 100(\%), \quad \Delta b = 10^{-4}. \quad (47)$$

It was considered that adjacent vectors should be employed to compute the sensitivity of the eigenvectors. However, as we stated in the previous section, this is actually not correct. Table 1 compares the sensitivity values obtained with our method and the numerical values computed with the central difference method. As illustrated, the ratios are almost 100%, showing that the sensitivities are accurately computed. Indeed, if we take now the first two columns of Table 2, Φ' , and we multiply them by

$$\Gamma = \begin{bmatrix} -0.9940 & 0.1090 \\ -0.1090 & -0.9940 \end{bmatrix} = \begin{bmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{bmatrix}, \quad \theta = 83.7^\circ, \quad (48)$$

then we recover $\mathbf{Z}' = \Phi' \Gamma$, that is, the same sensitivities as Equation (45) shows.

Currently, the results of our present approach match with those of both Dailey's and Lee's method, but our method neither requires the second-order derivative terms of both the stiffness and mass matrices nor needs computing the adjacent basis.

5.2 | Four-edge clamped plate working in-plane

The next example considers a four-edge clamped plate to ensure repeated frequencies. This example was first studied.⁸ The plate is modeled using square finite elements, whose elemental stiffness and mass matrices are

$$\mathbf{K}_e = \frac{Et}{8(1-\nu)} \begin{bmatrix} 4 & 1 & -2 & -1 & -2 & -1 & 0 & 1 \\ & 4 & 1 & 0 & -1 & -2 & -1 & -2 \\ & & 4 & -1 & 0 & -1 & -2 & 1 \\ & & & 4 & 1 & -2 & 1 & -2 \\ & & & & 4 & 1 & -2 & -1 \\ & & & & & 4 & 1 & 0 \\ & & & & & & 4 & -1 \\ & & & & & & & 4 \end{bmatrix} +$$

$$\frac{Etv}{24(1-\nu^2)} \begin{bmatrix} 4 & 3 & -2 & 3 & 2 & -3 & 4 & -9 \\ & -4 & -9 & 4 & -3 & 2 & 9 & -2 \\ & & -4 & -3 & 4 & 9 & 2 & 3 \\ & & & -4 & -9 & -2 & 3 & 2 \\ & & & & -4 & 3 & -2 & 9 \\ & & & & & -4 & -9 & 4 \\ & & & & & & -4 & -3 \\ & & & & & & & -4 \end{bmatrix},$$

and

$$\mathbf{M}_e = \frac{\rho_m t L^2}{36} \begin{bmatrix} 4 & 0 & 2 & 0 & 1 & 0 & 2 & 0 \\ & 4 & 0 & 2 & 0 & 1 & 0 & 2 \\ & & 4 & 0 & 2 & 0 & 1 & 0 \\ & & & 4 & 0 & 2 & 0 & 1 \\ & & & & 4 & 0 & 2 & 0 \\ & & & & & 4 & 0 & 2 \\ & & & & & & 4 & 0 \\ & & & & & & & 4 \end{bmatrix},$$

where E and ν are Young's modulus and Poisson's ratio of the material, t and L are the thickness and length of the plate, and ρ_m is the material density. ρ_e which is the design variable in each element, which physically represents the structural density. Both the global stiffness and mass matrices are constructed by assembling the elemental matrices in the following way:

$$\mathbf{K} = \sum_{e=1}^n \rho_e^p \mathbf{K}_e, \quad \mathbf{M} = \sum_{e=1}^n \rho_e \mathbf{M}_e, \quad (49)$$

where the solid isotropic material with penalization (SIMP) method²⁷ with penalization factor $p = 3$ is used to interpolate the stiffness matrix. Figure 3 shows the first two eigenvectors, which correspond to the same eigenvalue (the first one). Next, we discuss the results obtained for the different mesh sizes.

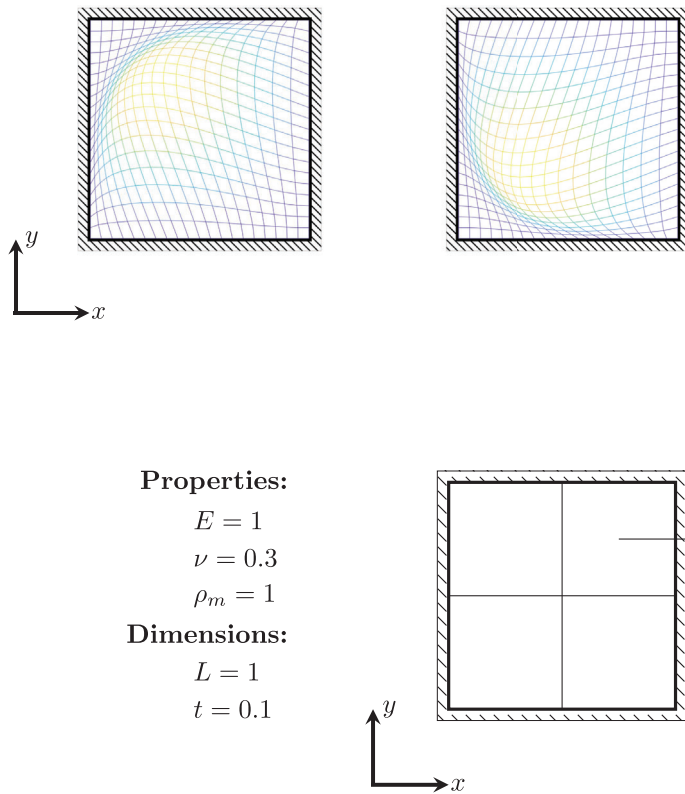


FIGURE 3 The first two eigenvectors of Example 5.2
 [Colour figure can be viewed at wileyonlinelibrary.com]

$$\left\{ \begin{array}{l} Z'_{\text{Dailey's approach}} = \begin{bmatrix} 0.8385 & 0.8385 \\ 0.8385 & -0.8385 \end{bmatrix} \\ Z'_{\text{Lee's method}} = \begin{bmatrix} 0.8385 & 0.8385 \\ 0.8385 & -0.8385 \end{bmatrix} \\ Z'_{\text{Present method}} = \begin{bmatrix} 0.8385 & 0.8385 \\ 0.8385 & -0.8385 \end{bmatrix} \end{array} \right.$$

FIGURE 4 Plate discretized with four finite elements

Case 2 × 2: As the plate is divided into four finite elements, as represented in Figure 4, the unknowns correspond to the eigenvectors values at the central node only. We have computed the derivatives of the adjacent eigenvectors with respect to the four design variables, showing very similar results for all the elements. Therefore, only the results for a particular element are shown. As expected, the same results are obtained with our method, Lee's and Dailey's method.

Case 3 × 3: This case is particularly interesting from a computational perspective. The derivatives of certain eigenvector basis are computed in the usual way, giving again same results using the three methods, except for the finite element place at the middle of the plate. And this is due to the following peculiarity: the derivative values of eigenvalues in that element coincide. This means that Dailey's method is not able to compute the derivatives of the adjacent eigenvectors since matrix \mathbf{F} is not unique (remember that such a matrix is computed from a small eigenproblem with repeated eigenvalues). Instead, Friswell's method has to be used in order to compute properly the derivatives for this element. However, both our method and Lee's method compute the derivatives correctly in any element and more specifically at the element in the middle without an extra effort (see Figure 5) and those coincide with the ones obtained by a finite difference scheme method. In this element, we opted for showing Φ' rather than \mathbf{Z}' as matrix \mathbf{F} is not unique.

Case 4 × 4: Unlike the previous case, eigenvalues derivatives are different in any element, then we expect to get the same eigenvectors derivatives with the three methods and numerically as well. In fact, derivatives values coincide for all elements in green, but they show some discrepancies for all elements in red, see Figure 6. Judging from the numerical results, we just consider that Dailey's approach is not working properly in these examples and those small differences are due to computational errors of the method itself. Curiously, a similar behaviour is observed for the cases 5 × 5, 6 × 6, and so on, that is, Dailey's approach fails in some elements, whereas our method coincides with Lee's method in any element and both are in agreement with numerical derivatives.

As Figure 7 clearly shows (notice that semilog scale is used in time), our method saves a lot of computational time compared with the other two. And the reason is quite simple: our approach lets us compute eigenvector derivatives for the case of multiple eigenvalues in a very straightforward way, and not element by element by using the (usual) auxiliary adjacent eigenvector basis. For several variables and judging from Figure 7, Lee's method is still more expensive than Dailey's as the system of the former has m rows and m columns more, being m the multiplicity of the repeated eigenvalue. And the only gain with respect to Dailey's approach is the fact that it has not to compute second-order derivatives of both

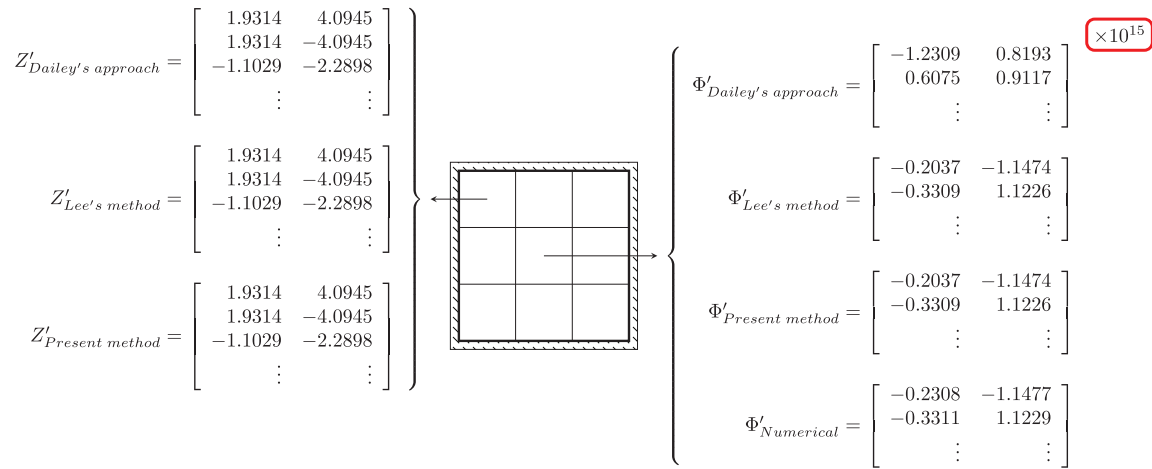


FIGURE 5 Plate discretized with 9 finite elements [Colour figure can be viewed at wileyonlinelibrary.com]

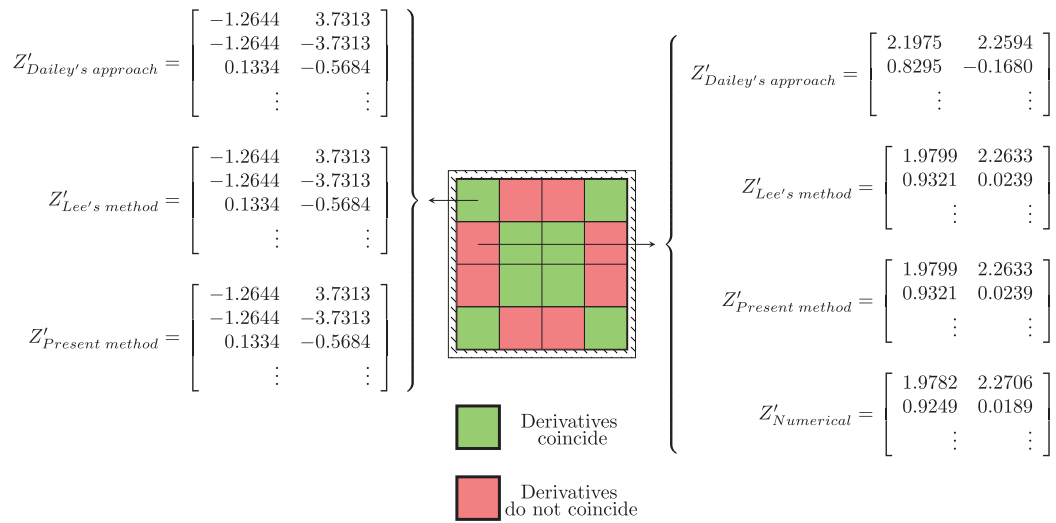


FIGURE 6 Plate discretized with 16 finite elements

stiffness and mass matrices. So, in summary, our method undoubtedly presents an important computational advantage with respect to the other two methods as the number of elements increases.

5.3 | A topology optimization example: A reinforcement problem

To show the validity and effectiveness of the present adjoint sensitivity analysis in topology optimization, the following problem is considered: the reinforcement problem of a clamped plate that minimizes the sound power radiated from the structure into a surrounding acoustic medium subject to a volume constraint is considered. Without going into details,²⁸ such optimization problem may be formulated as follows

$$\begin{aligned} \min_{\rho \in [0,1]} : \quad & \Pi = \phi_2^T S_n \phi_2 + \phi_3^T S_n \phi_3 \\ \text{s.t.} : \quad & \mathbf{K}(\rho) \Phi = \mathbf{M}(\rho) \Phi \Lambda, \quad \Phi = [\phi_2 \ \phi_3], \quad \Lambda = \begin{bmatrix} \lambda_2 & 0 \\ 0 & \lambda_3 \end{bmatrix} \\ & V(\rho) \leq V^* \end{aligned} \quad (50)$$

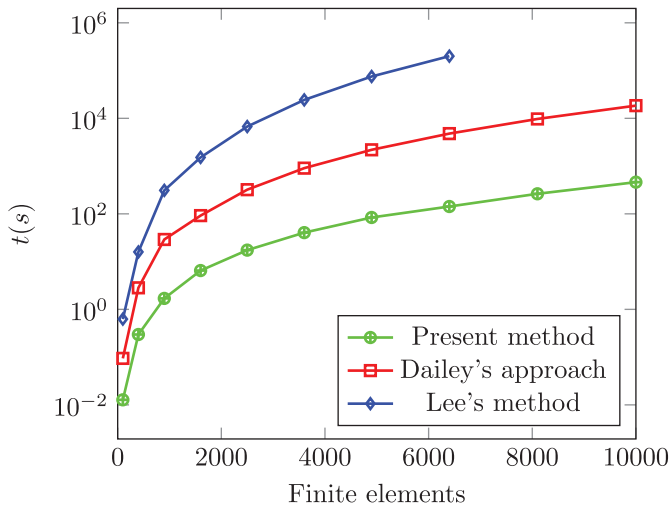


FIGURE 7 Computation time in the three methods vs number of elements [Colour figure can be viewed at wileyonlinelibrary.com]

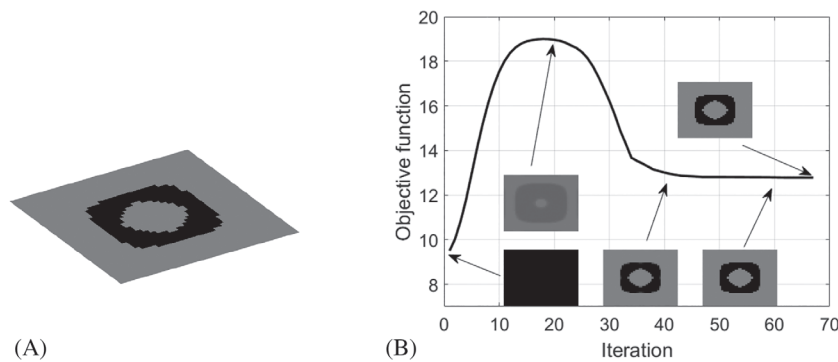


FIGURE 8 An optimization result with the second and the third eigenmodes ($V^* = 20\%$). A, An optimal layout and, B, the optimization history

More specifically, the above optimization problem aims to determine the reinforcement design for a plate vibrating initially at $\lambda_2 = \lambda_3 = 4.6769$ for a maximum volume fraction of $V^* = 20\%$. As the eigenvalues are dependent on the design variables, their values change during the optimization process. Even their orders may dramatically change. In this example, to prevent this issue, the reinforcement problem is considered.

The method of moving asymptotes (MMA) is used²⁹ as optimizer. Regarding the computational time, Dailey's approach requires 22.7 seconds per iteration, whereas ours needs 2.7 seconds only. This gap becomes larger as the number of elements increases, as shown in the previous example. As this kind of problems typically requires hundreds of iterations for convergence, the computational saving is multiplied by this factor. As a matter of curiosity, Figure 8A shows the optimized reinforcement (or $\rho = 1$), in the form of a ring-type structure, and Figure 8B shows the normalized objective function and iteration history.

6 | CONCLUSIONS

In this article, a highly efficient method for computing the derivatives of general functionals, which could eventually be of vector format, depending on eigenvectors is developed. Our method includes the cases of both eigenvectors with and without repeated eigenvalues, but the emphasis is on the remarkably more difficult case of multiple eigenvalues. Our method overcomes the main difficulties of the sensitivity analysis of eigenvectors with repeated eigenvalues, providing a simple, direct, and highly efficient procedure from a computational perspective. Next, we highlight the main points of the work:

1. The derivative formula in Equation (20) established in Theorem 1 for computing the derivatives of a general cost depending on a prescribed modal basis associated with multiple eigenvalues does not require computation of the adjacent basis. As the adjacent eigenvectors vary with respect to single variables, we would like to emphasize the

significant computational saving of this formula when computing the elements of the Jacobian matrix with respect to a variables vector. This eventually may have numerous components of the same order of magnitude as the stiffness and mass matrices dimensions.

2. Because we are using an adjoint sensitivity method, the system (21) does not depend on single variables and is in agreement with the previous observation, that is, the computation of the elements of the Jacobian matrix with respect to a variable vector it has to be solved only once.
3. In this method, no singular linear system has to be solved. This is a very interesting fact as we have mentioned above that Dailey's method fails in certain cases. Furthermore, no second-order derivative computations of both the stiffness and mass matrices are required. In addition, our method works well when multiple eigenvalue derivatives coincide. This has been pointed out in Section 5.2.
4. Figure 7 shows reduction in computational time in different examples of several orders of magnitude when using our method and compare with Lee's method. This fact lets us conduct topology optimization problems of hundreds of variables that involve eigenvectors of repeated eigenvalues significantly faster than previous techniques doing the same.

ACKNOWLEDGEMENTS

A major part of this work was performed while Gil Ho Yoon was performing research at the Department of Mathematics, ETSII (UCLM), during the months of September 2018 and February 2019. The work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT)(NRF-2018K1A3A1A38056941) (Korea) and Agencia Estatal de Investigacion, Ministerio de Ciencia e Innovacion, and FEDER (EU) through grant MTM2017-83740-P (Spain).

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SUPPORTING INFORMATION

Additional supporting information may be found online in the Supporting Information section at the end of this article.

How to cite this article: Yoon GH, Donoso A, Carlos Bellido J, Ruiz D. Highly efficient general method for sensitivity analysis of eigenvectors with repeated eigenvalues without passing through adjacent eigenvectors. *Int J Numer Methods Eng*. 2020;121:4473-4492. <https://doi.org/10.1002/nme.6442>

APPENDIX A. PROOF THAT THE ALGEBRAIC METHOD DOES NOT REQUIRE COMPUTING ADJACENT EIGENVECTORS FOR THE CASE OF MULTIPLE EIGENVALUES

We recall here the algebraic method for the case of multiple eigenvalues, which may be expressed as

$$\begin{bmatrix} \mathbf{K} - \lambda \mathbf{M} & -\mathbf{M}\mathbf{Z} \\ -\mathbf{Z}^T \mathbf{M} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{Z}' \\ \Lambda' \end{bmatrix} = \begin{bmatrix} -(\mathbf{K}' - \lambda \mathbf{M}')\mathbf{Z} \\ \frac{1}{2}\mathbf{Z}^T \mathbf{M}' \mathbf{Z} \end{bmatrix}, \quad (\text{A1})$$

or equivalently as

$$\begin{aligned} (\mathbf{K} - \lambda \mathbf{M})\mathbf{Z}' - \mathbf{M}\mathbf{Z}\Lambda' &= -(\mathbf{K}' - \lambda \mathbf{M}')\mathbf{Z} \\ -\mathbf{Z}^T \mathbf{M}\mathbf{Z}' &= \frac{1}{2}\mathbf{Z}^T \mathbf{M}' \mathbf{Z}. \end{aligned} \quad (\text{A2})$$

Next, we perform the following: First, \mathbf{Z} is replaced with $\Phi \Gamma$ in both equations, that is,

$$\begin{aligned} (\mathbf{K} - \lambda \mathbf{M})\mathbf{Z}' - \mathbf{M}\Phi \Gamma \Lambda' &= -(\mathbf{K}' - \lambda \mathbf{M}')\Phi \Gamma \\ -\Gamma^T \Phi^T \mathbf{M}\mathbf{Z}' &= \frac{1}{2}\Gamma^T \Phi^T \mathbf{M}' \Phi \Gamma. \end{aligned} \quad (\text{A3})$$

Second, the right-hand side is multiplied by Γ^T , recalling that $\Gamma \Gamma^T = \mathbf{I}_m$, finally arriving at

$$\begin{aligned} (\mathbf{K} - \lambda \mathbf{M})\mathbf{Z}' \Gamma^T - \mathbf{M}\Phi \Gamma \Lambda' \Gamma^T &= -(\mathbf{K}' - \lambda \mathbf{M}')\Phi \\ -\Gamma^T \Phi^T \mathbf{M}\mathbf{Z}' \Gamma^T &= \frac{1}{2}\Gamma^T \Phi^T \mathbf{M}' \Phi. \end{aligned} \quad (\text{A4})$$

Considering $\mathbf{Z}'\mathbf{I}^T$ and $\mathbf{I}\mathbf{A}'\mathbf{I}^T$ as the new unknowns and requiring that \mathbf{I}^T is a common factor in the bottom Equation (A4), we rewrite both equations in a matrix format as follows:

$$\begin{bmatrix} \mathbf{K} - \lambda\mathbf{M} & -\mathbf{M}\Phi \\ -\Phi^T\mathbf{M} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{Z}'\mathbf{I}^T \\ \mathbf{I}\mathbf{A}'\mathbf{I}^T \end{bmatrix} = \begin{bmatrix} -(\mathbf{K}' - \lambda\mathbf{M}')\Phi \\ \frac{1}{2}\Phi^T\mathbf{M}'\Phi \end{bmatrix}. \quad (\text{A5})$$

If we compare both systems, that is, Equations (A1) and (A5), then the unknown vector $\mathbf{Z}'\mathbf{I}^T$ has to be Φ' .

APPENDIX B. COMMENT ON LEE'S METHOD

Similar conclusions can be obtained from Lee's method.³ Let us recall here the vector objective function that was used in Lee's work, that is,

$$\tilde{\mathbf{G}} = \begin{bmatrix} \mathbf{Z} \\ \mathbf{A} \end{bmatrix} \in \mathbb{R}^{(n+m) \times m}. \quad (\text{B1})$$

With the help of the adjoint method, the augmented function can be defined as follows:

$$\mathbf{L} = \tilde{\mathbf{G}} + \mathbf{U}^T(\mathbf{K}\mathbf{Z} - \mathbf{M}\mathbf{Z}\mathbf{A}) - \frac{1}{2}\mathbf{V}^T(\mathbf{Z}^T\mathbf{M}\mathbf{Z} - \mathbf{I}_m). \quad (\text{B2})$$

By differentiating the augmented function, the following equations can be obtained:

$$\begin{aligned} \mathbf{L}' = \tilde{\mathbf{G}}' &= \frac{\partial \tilde{\mathbf{G}}}{\partial \mathbf{Z}}\mathbf{Z}' + \frac{\partial \tilde{\mathbf{G}}}{\partial \mathbf{A}}\mathbf{A}' + \mathbf{U}^T(\mathbf{K}' - \lambda\mathbf{M}')\mathbf{Z} \\ &\quad - \mathbf{U}^T\mathbf{M}\mathbf{Z}\mathbf{A}' + \mathbf{U}^T(\mathbf{K} - \lambda\mathbf{M})\mathbf{Z}' - \frac{1}{2}\mathbf{V}^T\mathbf{Z}^T\mathbf{M}'\mathbf{Z} - \mathbf{V}^T\mathbf{Z}^T\mathbf{M}\mathbf{Z}'. \end{aligned} \quad (\text{B3})$$

Requiring the implicit derivatives to vanish leads to

$$\begin{aligned} \frac{\partial \tilde{\mathbf{G}}}{\partial \mathbf{Z}} + \mathbf{U}^T(\mathbf{K} - \lambda\mathbf{M}) - \mathbf{V}^T\mathbf{Z}^T\mathbf{M} &= \mathbf{0} \\ \frac{\partial \tilde{\mathbf{G}}}{\partial \mathbf{A}} - \mathbf{U}^T\mathbf{M}\mathbf{Z} &= \mathbf{0}. \end{aligned} \quad (\text{B4})$$

Therefore, \mathbf{G}' may be indirectly computed as

$$\tilde{\mathbf{G}}' = \mathbf{U}^T(\mathbf{K}' - \lambda\mathbf{M}')\mathbf{Z} - \frac{1}{2}\mathbf{V}^T\mathbf{Z}^T\mathbf{M}'\mathbf{Z}, \quad (\text{B5})$$

or more clearly as

$$\tilde{\mathbf{G}}' = \begin{bmatrix} \mathbf{Z}' \\ \mathbf{A}' \end{bmatrix} = \begin{bmatrix} \mathbf{U}_1^T(\mathbf{K}' - \lambda\mathbf{M}')\mathbf{Z} - \frac{1}{2}\mathbf{V}_1^T\mathbf{Z}^T\mathbf{M}'\mathbf{Z} \\ \mathbf{U}_2^T(\mathbf{K}' - \lambda\mathbf{M}')\mathbf{Z} - \frac{1}{2}\mathbf{V}_2^T\mathbf{Z}^T\mathbf{M}'\mathbf{Z} \end{bmatrix}. \quad (\text{B6})$$

where $\mathbf{U} = [\mathbf{U}_1 \ \mathbf{U}_2]$ and $\mathbf{V} = [\mathbf{V}_1 \ \mathbf{V}_2]$ are the unique solutions of the linear system:

$$\begin{bmatrix} \mathbf{K} - \lambda\mathbf{M} & -\mathbf{M}\mathbf{Z} \\ -\mathbf{Z}^T\mathbf{M} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{U}_1 & \mathbf{U}_2 \\ \mathbf{V}_1 & \mathbf{V}_2 \end{bmatrix} = -\mathbf{I}_{(n+m) \times (n+m)}. \quad (\text{B7})$$

We can conveniently decouple the following two systems:

$$\begin{bmatrix} \mathbf{K} - \lambda\mathbf{M} & -\mathbf{M}\mathbf{Z} \\ -\mathbf{Z}^T\mathbf{M} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{U}_1 \\ \mathbf{V}_1 \end{bmatrix} = \begin{bmatrix} -\mathbf{I}_n \\ \mathbf{0}_{m \times n} \end{bmatrix}, \quad (\text{B8})$$

and

$$\begin{bmatrix} \mathbf{K} - \lambda \mathbf{M} & -\mathbf{M}\mathbf{Z} \\ -\mathbf{Z}^T \mathbf{M} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{U}_2 \\ \mathbf{V}_2 \end{bmatrix} = \begin{bmatrix} \mathbf{0}_{n \times m} \\ -\mathbf{I}_m \end{bmatrix}. \quad (\text{B9})$$

Again, replacing \mathbf{Z} with $\Phi \Gamma$ and using Lemma 1 in both these systems, we arrive at

$$\begin{bmatrix} \mathbf{K} - \lambda \mathbf{M} & -\mathbf{M}\Phi \\ -\Phi^T \mathbf{M} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{U}_1 \\ \tilde{\mathbf{V}}_1 \end{bmatrix} = \begin{bmatrix} -\mathbf{I}_n \\ \mathbf{0}_{m \times n} \end{bmatrix}, \quad (\text{B10})$$

where $\tilde{\mathbf{V}}_1 = \Gamma \mathbf{V}_1$ and

$$\begin{bmatrix} \mathbf{K} - \lambda \mathbf{M} & -\mathbf{M}\Phi \\ -\Phi^T \mathbf{M} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \tilde{\mathbf{U}}_2 \\ \tilde{\mathbf{V}}_2 \end{bmatrix} = \begin{bmatrix} \mathbf{0}_{n \times m} \\ -\mathbf{I}_m \end{bmatrix}, \quad (\text{B11})$$

with $\tilde{\mathbf{U}}_2 = \mathbf{U}_2 \Gamma^T$ and $\tilde{\mathbf{V}}_2 = \Gamma \mathbf{V}_2 \Gamma^T$, which can be combined as

$$\begin{bmatrix} \mathbf{K} - \lambda \mathbf{M} & -\mathbf{M}\Phi \\ -\Phi^T \mathbf{M} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{U}_1 & \tilde{\mathbf{U}}_2 \\ \tilde{\mathbf{V}}_1 & \tilde{\mathbf{V}}_2 \end{bmatrix} = -\mathbf{I}_{(n+m) \times (n+m)}. \quad (\text{B12})$$

Now, we may write Equation (B6) as

$$\tilde{\mathbf{G}}' = \begin{bmatrix} \mathbf{Z}' \\ \Lambda' \end{bmatrix} = \begin{bmatrix} \left(\mathbf{U}_1^T (\mathbf{K}' - \lambda \mathbf{M}') \Phi - \frac{1}{2} \tilde{\mathbf{V}}_1^T \Phi^T \mathbf{M}' \Phi \right) \Gamma \\ \Gamma^T \left(\tilde{\mathbf{U}}_2^T (\mathbf{K}' - \lambda \mathbf{M}') \Phi - \frac{1}{2} \tilde{\mathbf{V}}_2^T \Phi^T \mathbf{M}' \Phi \right) \Gamma \end{bmatrix}. \quad (\text{B13})$$

Thus,

$$\mathbf{G}' = \begin{bmatrix} \Phi' \\ \Gamma \Lambda' \Gamma^T \end{bmatrix} = \begin{bmatrix} \left(\mathbf{U}_1^T (\mathbf{K}' - \lambda \mathbf{M}') \Phi - \frac{1}{2} \tilde{\mathbf{V}}_1^T \Phi^T \mathbf{M}' \Phi \right) \\ \left(\tilde{\mathbf{U}}_2^T (\mathbf{K}' - \lambda \mathbf{M}') \Phi - \frac{1}{2} \tilde{\mathbf{V}}_2^T \Phi^T \mathbf{M}' \Phi \right) \end{bmatrix}, \quad (\text{B14})$$

where

$$\mathbf{G} = \begin{bmatrix} \Phi \\ \Gamma \Lambda \Gamma^T \end{bmatrix}, \quad (\text{B15})$$

as it is implicitly assumed in Lee's method. Moreover, this proves that the matrix $\Gamma \Lambda' \Gamma^T$ is not diagonal.