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Calculating Derivatives of Repeated and Nonrepeated Eigenvalues Without Explicit Use of Eigenvectors

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The analysis of inverse problems in parametric model updating often require the sensitivities of eigenvalues. The calculation of these sensitivities is mathematically related to the derivatives of the eigenvalues with respect to the model parameters. A common method to calculate these derivatives is the Nelson method, which requires the eigenvectors. The method introduced in this paper is derived from the characteristic equation of the underlying general eigenvalue problem and allows the derivatives of eigenvalues with respect to the model parameters to be calculated without explicit use of the eigenvectors. The method is extended for the case of repeated eigenvalues, which leads to restrictions on the parameterization. For repeated eigenvalues of multiplicity two, these restrictions are formulated expicitly. Applications and limitations of the method are demonstrated by examples.

Nomenclature

$A(q), B(q)$	= n-by-n matrices depending on q
$\mathbb{C}$	= set of complex numbers
$\mathcal{C}_r(\cdots)$	= rth compound matrix of the matrix $(\cdots)$
$\mathcal{I}, \mathcal{K}$	= index sets $\subseteq \{1,\ldots,m\}$
i, k	= indices $\in \{1,\ldots,n\}$
$\mathbb{N}$	= set of natural numbers
n'	= multiplicity of repeated eigenvalue
$p(q)$	= characteristic polynomial
q	= m-dimensional vector of adjustment parameters
q_r	= rth component of q
$\mathbb{R}$	= set of real numbers
r, s	= indices $\in \{1,\ldots,m\}$
$\mathbb{S}^m$	= set of m-dimensional vectors with components in $\mathbb{S}$
$\mathbb{S}^{m\times n}$	= set of m-by-n matrices with elements in $\mathbb{S}$
$\mathbb{Z}$	= set of integer numbers
δ_{ik}	= Kronecker delta
$\lambda(q)$	= eigenvalue $\in \{\lambda_1(q),\ldots,\lambda_n(q)\}$
$\lambda_i(q)$	= ith eigenvalue
$\lambda_{i,r}(q)$	= derivative of the ith eigenvalue with respect to the rth parameter
$(\cdots)^{\mathrm{ad}}$	= adjoint (adjungate) of the matrix $(\cdots)$
$(\cdots)_{(\mathcal{I},\mathcal{I})}$	= matrix resulting from selecting all rows and columns of $(\cdots)$ with indices in $\mathcal{I}$
$(\cdots)^{(i\,\vert\,k)}$	= matrix resulting from elimination of row i and column k of matrix $(\cdots)$
$(\cdots)_{,r}$	= derivative of $(\cdots)$ with respect to the rth parameter

I. Introduction

MANY engineering optimization problems, for instance optimal design or model updating, lead to a sensitivity analysis of the eigenvalue problem. In the case of nonrepeated eigenvalues, the derivatives of the eigenvalues with respect to a prechosen parameterization can be calculated analytically using Nelson's method.[1] For some parameterizations this method can be extended for the case of repeated eigenvalues.[2–6]

The purpose of this paper is to introduce an alternative method, which is based on the characteristic polynomial of the underlying eigenvalue problem. In contrast to the existing methods, the new approach presented in this paper enables the calculation of eigenvalue derivatives without using the eigenvectors. In Sec. II the method is derived for the case of nonrepeated eigenvalues. The method is extended for the case of pairs of repeated eigenvalues in Sec. III. Limitations of the method are investigated and formulated as restrictions on the parameterization. Several simulated examples are incorporated into both sections to clarify the concept.

II. Derivation of the Method for Nonrepeated Eigenvalues

Consider the general eigenvalue problem

$$(B-\lambda_i A)x_i = 0, \qquad i = 1,\ldots,n \tag{1}$$

with the $n\times n$ matrices A and B and the eigenvalues and eigenvectors λ_i, x_i, respectively, for $i=1,\ldots,n$. If $A=A(q)$, $B=B(q)$ are given functions of the parameter vector $q\in\mathbb{S}\subset\mathbb{R}^m$, then of course the eigenvectors and eigenvalues will depend on q. The investigations in this paper are restricted to the case that $A(q)$ is nonsingular and that both matrices $A(q)$ and $B(q)$ can be simultaneously diagonalized, i.e., the matrix $X(q)=[x_1(q),\ldots,x_n(q)]$ is nonsingular. These conditions cover systems with gyroscopic effects, with nonproportional damping and with rigid-body modes. Moreover the assumption is made that $A(q)$, $B(q)$, and their derivatives with respect to the parameters are continuous.

The scope of this section is to derive a method to calculate the derivatives

$$\lambda_{i,r}(q) := \frac{\partial\lambda_i(q)}{\partial q_r}, \qquad i\in\{1,\ldots,n\}, \quad r=1,\ldots,m \tag{2}$$

at parameter vector q^0. The derivation is based on the characteristic polynomial

$$\det[B(q)-\lambda(q)A(q)] = 0 \tag{3}$$

which is equivalent to

$$p(q) := \det[C(q)] = 0 \tag{4}$$

where

$$C(q) := Z(q)-\lambda(q)I_n \tag{5}$$

$$Z(q) := B(q)A^{-1}(q) \tag{6}$$

The derivative of p with respect to q_r yields

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$$\frac{\partial p(q)}{\partial q_r} = \frac{\partial \det[C(q)]}{\partial q_r} \tag{7}$$

$$= \sum_{i,k=1}^{n} \frac{\partial \det[C(q)]}{\partial [C(q)]_{ik}} \frac{\partial [C(q)]_{ik}}{\partial q_r} \tag{8}$$

$$= \sum_{i,k=1}^{n} \frac{\partial \det[C(q)]}{\partial [C(q)]_{ik}} [Z_{,r}(q) - \lambda_{,r}(q) I_n]_{ik} \tag{9}$$

$$= \sum_{i,k=1}^{n} [C^{\mathrm{ad}}(q)]_{ki} [Z_{,r}(q) - \lambda_{,r}(q) I_n]_{ik} \tag{10}$$

$$= \mathrm{tr}\{C^{\mathrm{ad}}(q)[Z_{,r}(q) - \lambda_{,r}(q) I_n]\} = 0 \tag{11}$$

Here $(\cdots)_{ik}$ denotes the element in row i and column k of the matrix in brackets, and $(\cdots)^{\mathrm{ad}}$ is the adjoint. (In some literature the term *adjugate* is used to avoid confusion with the Hermitian adjoint.) matrix, which consists of all principle minors of C, that is,

$$(C^{\mathrm{ad}})_{ik} := (-1)^{i+k} \det\left(C^{(i\,|\,k)}\right) \tag{12}$$

where $C^{(i\,|\,k)}$ is the matrix resulting from eliminating row i and column k of C. With reference to Eq. (6),

$$Z_{,r}(q) = \left[B_{,r}(q) - B(q) A^{-1}(q) A_{,r}(q)\right] A^{-1}(q) \tag{13}$$

For the transition from Eqs. (9) to (10), the general formula (see, for instance, Ref. 7)

$$\frac{\mathrm{d} \det(C)}{\mathrm{d} C} = \det(C) C^{-1\top} = (C^{\mathrm{ad}})^{\top} \tag{14}$$

has been used. Indeed, this formula holds for arbitrary square matrices. To clarify this point, consider the expansion of the determinant with respect to column k:

$$\det(C) = \sum_{j=1}^{n} (-1)^{j+k} (C)_{jk} \det\left[C^{(j\,|\,k)}\right] \tag{15}$$

Because the column is arbitrary, one can choose a different column for each differentiation, i.e., for fixed k the choice is

$$\frac{\partial \det(C)}{\partial (C)_{ik}} = \frac{\partial}{\partial (C)_{ik}} \left\{ \sum_{j=1}^{n} (-1)^{j+k} (C)_{jk} \det\left[C^{(j\,|\,k)}\right] \right\} \tag{16}$$

Because by definition $C^{(j\,|\,k)}$ does not depend on $(C)_{ik}$, one finds

$$\frac{\partial \det(C)}{\partial (C)_{ik}} = \sum_{j=1}^{n} (-1)^{j+k} \delta_{ij} \det\left[C^{(j\,|\,k)}\right] = (-1)^{i+k} \det\left[C^{(i\,|\,k)}\right] \tag{17}$$

where δ_{ij} is the Kronecker delta, i.e., it is one for $i = k$ and zero otherwise. In the case of nonrepeated eigenvalues at q^0, $C^{\mathrm{ad}}(q^0) \neq 0$. Hence, Eq. (11) can be solved for $\lambda_{,r}(q^0)$. Using the abbreviations

$$a_r(q) := \mathrm{tr}\left[C^{\mathrm{ad}}(q) Z_{,r}(q)\right] \tag{18}$$

$$b(q) := \mathrm{tr}[C^{\mathrm{ad}}(q)] = \sum_{i=1}^{n} \det\left[C^{(i\,|\,i)}(q)\right] \tag{19}$$

Eq. (11) reads

$$a_r(q) - \lambda_{,r}(q) b(q) = 0 \tag{20}$$

This equation enables the calculation of the eigenvalue derivatives if $b(q^0) \neq 0$, which leads to the following.

Proposition 1: If the eigenvalue problem $C = Z - \lambda I_n$ has no repeated eigenvalues and if Z is diagonalizable, then $\mathrm{tr}(C^{\mathrm{ad}}) \neq 0$ for arbitrary eigenvalue λ.

Proof: Because all eigenvalues are simple and because Z is diagonalizable, there exists a nonsingular matrix X such that

$$X^{-1} Z X = \Lambda \tag{21}$$

with the diagonal matrix $\Lambda = \{\lambda_i\}_{i=1,\ldots,n}$ of nonrepeated eigenvalues. For an arbitrary eigenvalue λ one finds

$$C = Z - \lambda I_n = X(\Lambda - \lambda I_n) X^{-1} \tag{22}$$

and thus

$$C^{\mathrm{ad}} = X(\Lambda - \lambda I)^{\mathrm{ad}} X^{-1} \tag{23}$$

A brief calculation reveals

$$\mathrm{tr}(C^{\mathrm{ad}}) = \mathrm{tr}[X(\Lambda - \lambda I)^{\mathrm{ad}} X^{-1}] \tag{24}$$

$$= \mathrm{tr}[(\Lambda - \lambda I)^{\mathrm{ad}}] \tag{25}$$

$$= \sum_{i=1}^{n} \prod_{k \neq i} (\lambda_k - \lambda) \tag{26}$$

Without loss of generality, one may assume $\lambda = \lambda_n$, yielding

$$\mathrm{tr}(C^{\mathrm{ad}}) = (\lambda_1 - \lambda_n) \cdots (\lambda_{n-1} - \lambda_n) \neq 0 \tag{27}$$

which completes the proof. □

Because $b(q^0) \neq 0$, Eq. (20) yields

$$\lambda_{,r}(q^0) = [1/b(q^0)] a_r(q^0) \tag{28}$$

Several theoretical example cases will be studied to demonstrate the capabilities of the method using the model depicted in Fig. 1 with the matrices

$$M = \begin{bmatrix} m_1 & 0 & 0 \\ 0 & m_2 & 0 \\ 0 & 0 & m_3 \end{bmatrix} \tag{29}$$

$$D = \begin{bmatrix} d_1 & 0 & 0 \\ 0 & d_2 & 0 \\ 0 & 0 & d_3 \end{bmatrix} \tag{30}$$

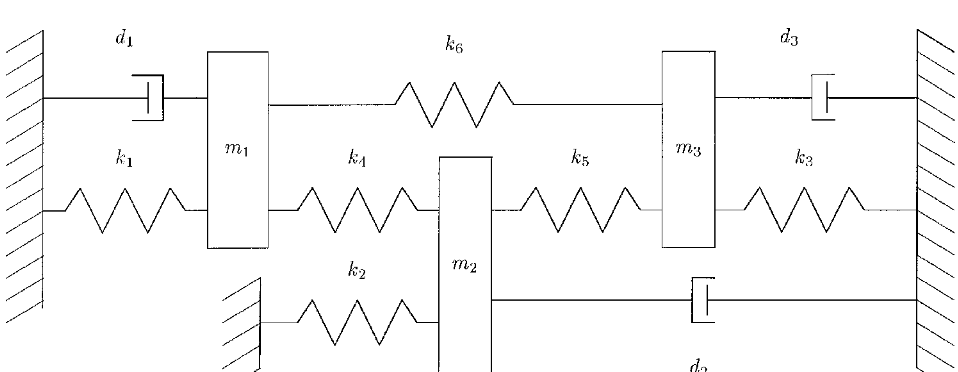

Fig. 1 Three-degree-of-freedom test model.

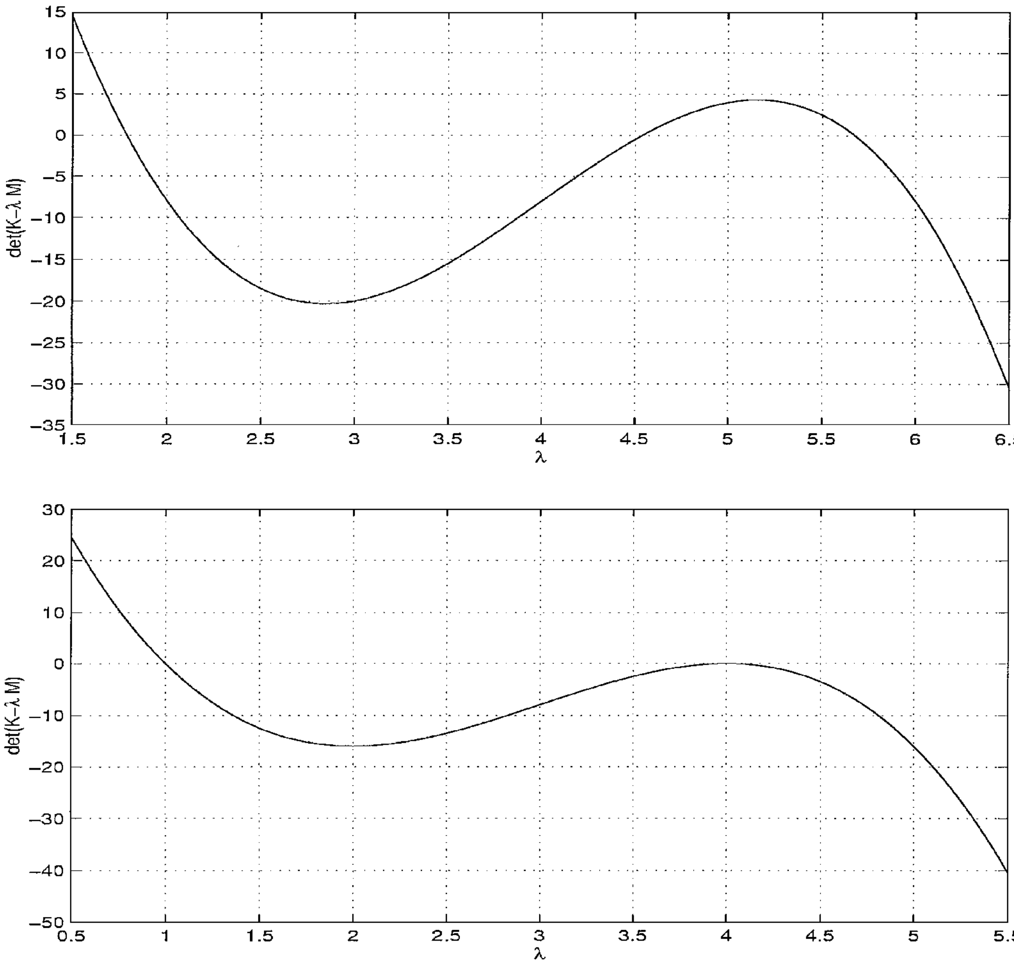

Fig. 2 Determinant of C in case of nonrepeated (top) and two repeated eigenvalues (bottom).

$$K = \begin{bmatrix} k_1 + k_4 + k_6 & -k_4 & -k_6 \\ -k_4 & k_2 + k_4 + k_5 & -k_5 \\ -k_6 & -k_5 & k_3 + k_5 + k_6 \end{bmatrix} \tag{31}$$

Remark: To apply the outlined method to large models, the computation of C^{ad} via determinants may become inefficient. In these cases the singular value decomposition $C = L\Sigma R^{\top}$, with the diagonal matrix Σ of singular values σ_i, yields (see Appendix B) $C^{\mathrm{ad}} = R\Sigma^{\mathrm{ad}}L^{\top}$, which is computationally more efficient because the ith diagonal element μ_i of the diagonal matrix Σ^{ad} is given by

$$\mu_i = \prod_{k \neq i} \sigma_k$$

.

Example 1

Consider the undamped case ($d_1 = d_2 = d_3 = 0$) with the parameterization

$$q = (m_1, m_2, m_3, k_1, k_2, k_3, k_4, k_5, k_6)^{\top} \in \mathbb{R}^9 \tag{32}$$

For the model represented by the parameter vector

$$q^0 = (1, 4, 1, 1, 8, 2, 2, 2, 1)^{\top} \tag{33}$$

the determinant of $K(q^0) - \lambda M(q^0)$ is depicted in Fig. 2 (top) for values $\lambda \in [1.5, 6.25]$. The zeroes are

$$(\lambda_1, \lambda_2, \lambda_3) = (1.785, 4.539, 5.675) \tag{34}$$

The procedure will now be demonstrated by calculating the derivative of λ_1 with respect to the parameter q_1. The matrix $C(q^0)$ is given by

$$C = \begin{bmatrix} 2.2143 & -0.5 & -1 \\ -2 & 1.2143 & -2 \\ -1 & -0.5 & 3.2143 \end{bmatrix} \tag{35}$$

which gives the adjoint

$$C^{\mathrm{ad}} = \begin{bmatrix} 2.9032 & 2.1072 & 2.2143 \\ 8.4286 & 6.1175 & 6.4286 \\ 2.2143 & 1.6072 & 1.6889 \end{bmatrix} \tag{36}$$

From Eq. (13) with $A = M$ and $B = K$, one finds for the first parameter

$$Z_{,1} = -KM^{-1}M_{,1}M^{-1} = \begin{bmatrix} -4 & 0 & 0 \\ 2 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix} \tag{37}$$

and thus from Eqs. (18) and (19)

$$a_1 = -5.1842 \tag{38}$$

$$b = 10.7096 \tag{39}$$

giving

$$\lambda_{1,1} = -5.1841/10.7096 = -0.4841 \tag{40}$$

The derivatives of all eigenvalues at q^0 with respect to (w.r.t.) the nine parameters are shown in Table 1. As expected, an increase in the mass parameters decreases the eigenvalues, and an increase in the stiffness parameters increases the eigenvalues.

Table 1 Derivatives of the eigenvalues λ using the characteristic polynomial $\det(K - \lambda M)$

Parameter	Eigenvalue derivatives at q^0		
q_r	$\partial\lambda_1/\partial q_r$	$\partial\lambda_2/\partial q_r$	$\partial\lambda_3/\partial q_r$
$r=1$	-0.4841	-2.4805	-1.0354
$r=2$	-0.2550	-0.4530	-0.0420
$r=3$	-0.2816	-0.2468	-4.4716
$r=4$	0.2711	0.5465	0.1824
$r=5$	0.1428	0.0998	0.0074
$r=6$	0.1577	0.0544	0.7879
$r=7$	0.0204	1.1133	0.1163
$r=8$	0.0004	0.3015	0.9481
$r=9$	0.0153	0.2561	1.7287

Table 2 Derivatives of the eigenvalues λ using the characteristic polynomial $\det(B - \lambda A)$

Parameter	Eigenvalue derivatives at q^0		
q_r	$\partial\lambda_1/\partial q_r$	$\partial\lambda_2/\partial q_r$	$\partial\lambda_3/\partial q_r$
$r=1$	$0.0401-0.2141j$	$0.0164-0.5841j$	$-0.0065-0.1814j$
$r=2$	$-0.0025-0.0087j$	$-0.0033-0.1065j$	$0.0058-0.0954j$
$r=3$	$-0.0015-0.9414j$	$0.0256-0.0546j$	$0.0009-0.1056j$
$r=4$	$-0.0901-0.0158j$	$-0.2743-0.0040j$	$-0.1357+0.0066j$
$r=5$	$-0.0036+0.0011j$	$-0.5+0.0022j$	$-0.0714-0.0034j$
$r=6$	$-0.3952+0.0054j$	$-0.0258-0.0117j$	$-0.0790+0.0003j$
$r=7$	$-0.0062+0.0379j$	$-0.0001+0.1288j$	$0.0063+0.1014j$
$r=8$	$0.0005+0.0015j$	$0.0014+0.0234j$	$-0.0018+0.0535j$
$r=9$	$0.0043+0.1659j$	$-0.0053+0.0122j$	$0.0010+0.0591j$
$r=10$	$-0.0068+0.0238j$	$0.0044+0.2621j$	$0.0024+0.0074j$
$r=11$	$0.0100+0.1994j$	$-0.0102+0.0704j$	$0.0001+0.0001j$
$r=12$	$-0.0127+0.3631j$	$0.0115+0.0600j$	$0.0012+0.0056j$

Example 2

Now consider the damped model with the parameterization

$$q = (m_1, m_2, m_3, d_1, d_2, d_3, k_1, k_2, k_3, k_4, k_5, k_6)^\top \in \mathbb{R}^{12} \tag{41}$$

In this case the matrices A and B are defined by

$$A(q) := \begin{pmatrix} D(q) & M(q) \\ M(q) & 0 \end{pmatrix} \tag{42}$$

$$B(q) := \begin{pmatrix} -K(q) & 0 \\ 0 & M(q) \end{pmatrix} \tag{43}$$

At parameter vector

$$q^0 = (1, 4, 1, 0.1, 0, 0.05, 1, 8, 2, 2, 2, 1)^\top \tag{44}$$

the principal eigenvalues are

$$(\lambda_1, \lambda_2, \lambda_3) = (-0.0288 + 2.3816j, -0.0287 + 2.1300j, -0.0175 + 1.3366j) \tag{45}$$

The complex derivatives of the eigenvalues with respect to the 12 model parameters are listed in Table 2. For real-valued matrices A, B Eq. (28) implies $(\lambda^*)_{,r} = (\lambda_{,r})^*$, i.e., the derivative of the conjugate eigenvalue is equal to the conjugate derivative of the eigenvalue. To verify the derivatives, the eigenvalues would have to be calculated for various parameter values. For example the eigenvalues have been calculated for damping parameters $q_4, q_6 \in [0, 0.2]$. The result is depicted in Fig. 3 for parameter q_4 (solid) and parameter q_6 (dotted). The calculated derivatives match well the slope of the tangents of the graphs at 0.1 and at 0.05, respectively. As expected from physical reasoning, the imaginary part of the eigenvalues turn out to be relatively insensitive w.r.t. the damping parameters (see right half of Fig. 3), which corresponds well to the relatively low values of the imaginary parts of the corresponding derivatives shown in rows 4 and 5 of Table 2.

In the next section the method is extended to the case of pairs of repeated eigenvalues.

III. Extension of the Method to Repeated Eigenvalues

In case of repeated eigenvalues, higher derivatives of the characteristic equation (4) have to be calculated to obtain the first derivatives of the corresponding eigenvalue. The reason is that the curve $p(\lambda)$ has a local extrema at the repeated eigenvalue. In Fig. 2 (bottom) the determinant of $K(q^0) - \lambda(q^0)M(q^0)$ is plotted for the undamped model introduced in the last section at parameter vector

$$q^0 = (1, 4, 1, 0, 8, 0, 2, 2, 1) \tag{46}$$

where two repeated eigenvalues $\lambda_2(q^0) = \lambda_3(q^0) = 4$ occur. In this case the rank of the matrix C [see Eq. (5)] is 1 because there exist two linearly independent eigenvectors associated with eigenvalue $\lambda = 4$. Hence, although $C \neq 0$, all of the principal minors of C are zero. By definition C^{ad} consists of these minors, and in the light of Eqs. (18) and (19), a_r and b are zero, too. As it will be shown later, the second derivative of the characteristic polynomial requires the derivative of C^{ad}, which is not zero because it consists of all minors of size 1 of C.

In the general case of a repeated eigenvalue λ of multiplicity n', the rank of C is $n - n'$ if there exist n' linearly independent eigenvectors for the repeated eigenvalue. Hence for all $k < n'$ all minors of size $n - k$ are zero. Because the kth derivative of the characteristic polynomial consists of all minors of size $n - k$, all derivatives up to order $n' - 1$ are trivially fulfilled; each term is identically zero. To obtain an equation for the derivatives of a repeated eigenvalue of multiplicity n', the n'th derivative of the characteristic equation has to be calculated. The resulting equation is of type

$$a\lambda_{,r_1}\cdots\lambda_{,r_{n'}} + a_{r_1}\lambda_{,r_2}\cdots\lambda_{,r_{n'}} + \cdots + a_{r_1\cdots r_{n'-1}}\lambda_{,r_{n'}} + a_{r_1\cdots r_{n'}} = 0 \tag{47}$$

where the indices $r_1, \ldots, r_{n'}$ run independently from 1 to m. This equation is of degree n' in the unknown derivatives and in general is difficult to solve. To clarify the concept, the extension of method is restricted to the case $n' = 2$, which is most common and covers important applications in dynamics.

Suppose $\lambda(q^0)$ has multiplicity 2; then $C^{\mathrm{ad}}(q^0) = 0$, and hence

$$\left.\frac{\partial^2 p(q)}{\partial q_r \partial q_s}\right|_{q=q^0} = \operatorname{tr}\left[C^{\mathrm{ad}}_{,s}(q^0)C_{,r}(q^0)\right] \tag{48}$$

$$= \operatorname{tr}\left\{C^{\mathrm{ad}}_{,s}(q^0)\left[Z_{,r}(q^0) - \lambda_{,r}(q^0)I_n\right]\right\} = 0 \tag{49}$$

To calculate the derivative of C^{ad} with respect to parameter q_s, one finds with reference to Eqs. (12) and (17)

$$\frac{\partial[C^{\mathrm{ad}}(q)]_{ik}}{\partial q_s} = (-1)^{i+k}\sum_{j,l=1}^{n-1}\frac{\partial\det\left[C^{(k|i)}(q)\right]}{\partial\left[C^{(k|i)}(q)\right]_{jl}}\frac{\partial\left[C^{(k|i)}(q)\right]_{jl}}{\partial q_s} \tag{50}$$

$$= (-1)^{i+k}\sum_{j,l=1}^{n-1}\left\{\left[C^{(k|i)}(q)\right]^{\mathrm{ad}}\right\}_{lj} \times\left\{[Z_{,s}(q)]^{(k|i)} - \lambda_{,s}(q)(I_n)^{(k|i)}\right\}_{jl} \tag{51}$$

$$= (-1)^{i+k}\operatorname{tr}\left(\left[C^{(k|i)}(q)\right]^{\mathrm{ad}} \times\left\{[Z_{,s}(q)]^{(k|i)} - \lambda_{,s}(q)(I_n)^{(k|i)}\right\}\right) \tag{52}$$

Defining the matrices $D_s(q)$ and $E(q)$ element-wise by

$$[D_s(q)]_{ik} := (-1)^{i+k}\operatorname{tr}\left\{\left[C^{(k|i)}(q)\right]^{\mathrm{ad}}[Z_{,s}(q)]^{(k|i)}\right\} \tag{53}$$

$$[E(q)]_{ik} := (-1)^{i+k}\operatorname{tr}\left\{\left[C^{(k|i)}(q)\right]^{\mathrm{ad}}(I_n)^{(k|i)}\right\} \tag{54}$$

Eq. (49) now reads

$$\left.\frac{\partial^2 p(q)}{\partial q_r \partial q_s}\right|_{q=q^0} = \operatorname{tr}\left\{\left[D_s(q^0) - \lambda_{,s}(q^0)E(q^0)\right]\left[Z_{,r}(q^0) - \lambda_{,r}(q^0)I_n\right]\right\} = 0 \tag{55}$$

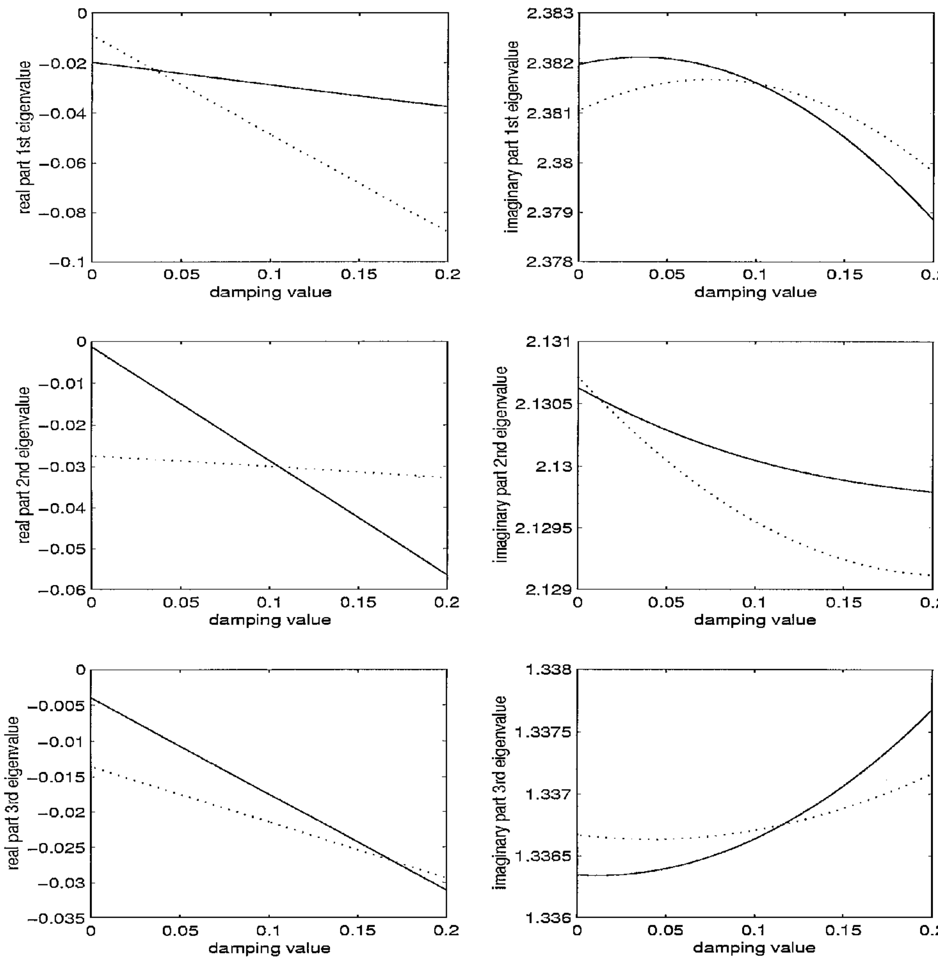

Fig. 3 Eigenvalues as functions of the damping parameters (——, first, and ...., second).

which leads to

$$a(q^0)\lambda_{,s}(q^0)\lambda_{,r}(q^0) + \lambda_{,s}(q^0)b_r(q^0) + c_s(q^0)\lambda_{,r}(q^0) + g_{sr}(q^0) = 0 \tag{56}$$

with the definitions

$$a(q^0) := \mathrm{tr}[E(q^0)] = \sum_{i=1}^{n} \mathrm{tr}\{[C^{(i|i)}(q^0)]^{\mathrm{ad}}\} \tag{57}$$

$$b_r(q^0) := -\mathrm{tr}[E(q^0)Z_{,r}(q^0)] \tag{58}$$

$$c_s(q^0) := -\mathrm{tr}[D_s(q^0)] \tag{59}$$

$$g_{sr}(q^0) := \mathrm{tr}[D_s(q^0)Z_{,r}(q^0)] \tag{60}$$

Equation (56) is equivalent to

$$axx^\top + xb^\top + cx^\top + G = 0 \tag{61}$$

where the rth component of the vectors x, b, and c are $\lambda_{,r}$, b_r, and c_r, respectively, and the element in row r and column s the matrix G is g_{rs}. Before discussing the solution of Eq. (61), it will be shown that G is symmetric and that $b = c$. In the light of Eq. (48), the symmetry of G and the equality of b and c are equivalent with the arbitrariness of the order of differentiation $r \leftrightarrow s$. Hence it is sufficient to prove the following proposition.

Proposition 2: Let $C = C(q)$ be an arbitrary square matrix possessing continuous derivatives w.r.t the m parameters $q \in \mathbb{R}^m$, and let $(\cdots)_{,r}$ denote the derivative w.r.t. the rth parameter, then

$$\mathrm{tr}[(C^{\mathrm{ad}})_{,r}C_{,s}] = \mathrm{tr}[(C^{\mathrm{ad}})_{,s}C_{,r}] \tag{62}$$

Proof: Differentiating $C^{\mathrm{ad}}C = \det(C)I$ w.r.t. the rth parameter yields

$$(C^{\mathrm{ad}})_{,r}C + C^{\mathrm{ad}}C_{,r} = \det(C)_{,r}I \tag{63}$$

Multiplying this equation by C^{ad} and reordering leads to

$$\det(C)(C^{\mathrm{ad}})_{,r} = \det(C)_{,r}C^{\mathrm{ad}} - C^{\mathrm{ad}}C_{,r}C^{\mathrm{ad}} \tag{64}$$

from which one finds

$$\det(C)\,\mathrm{tr}[(C^{\mathrm{ad}})_{,r}C_{,s}] = \det(C)_{,r}\mathrm{tr}(C^{\mathrm{ad}}C_{,s}) - \mathrm{tr}(C^{\mathrm{ad}}C_{,r}C^{\mathrm{ad}}C_{,s}) \tag{65}$$

This expression is invariant w.r.t. the interchange of r and s if and only if

$$\det(C)_{,r}\,\mathrm{tr}(C^{\mathrm{ad}}C_{,s}) = \det(C)_{,s}\,\mathrm{tr}(C^{\mathrm{ad}}C_{,r}) \tag{66}$$

which is indeed the case because

$$\det(C)_{,r} = \mathrm{tr}(C^{\mathrm{ad}}C_{,r}) \tag{67}$$

□

Proposition 2 is, of course, equivalent to the fact that the order of differentiation is arbitrary if the first derivatives are continuous. Now Eq. (61) reads

$$axx^\top + xb^\top + bx^\top + G = 0 \tag{68}$$

with $G = G^\top$. To calculate the derivatives x from Eq. (68), one has to show the following:

1) $a \neq 0$.

2) Equation (68) is consistent.

The first point requires the following proposition.

Proposition 3: If $Z(q^0)$ is diagonalizable and possesses repeated eigenvalues of multiplicity $n' = 2$, then $a(q^0) \neq 0$.

The proof of Proposition 3 can be found in Appendix A. The second point depends on the parameterization of the matrices $A(q)$ and $B(q)$. As was reported in Ref. 6, the derivatives of repeated eigenvalues do not exist for every parameterization because in general $\partial\lambda(q)/\partial q^\top$ is not continuous at q^0 (see, for instance, Ref. 5). An example for this case is presented later in this paper. The question of a permissible parameterization here is related to the consistency of Eq. (11). Because $a \neq 0$, Eq. (68) can be rewritten as

$$(x + b/a)(x + b/a)^\top = \underbrace{(bb^\top/a - G)/a}_{=:H} \tag{69}$$

In this case the question of the existence of a solution leads to the following.

Theorem 1: The derivative of the repeated eigenvalue of multiplicity 2 with respect to the m parameters q exists if H, as defined in Eq. (69), has a decomposition

$$H = \sigma u u^\top, \qquad \sigma \in \mathbb{C}, \quad u \in \mathbb{C}^m \tag{70}$$

If Theorem 1 holds, the two solutions of Eq. (69) are

$$x = -b/a \pm \sqrt{\sigma} u \tag{71}$$

In case $\sigma = 0$ both derivatives are identical.

Before some examples are presented, the issue of a permissible parameterization is addressed. In practical applications the problem is to select a subset from a given set of parameters such that the derivatives of a repeated eigenvalue with respect to all parameters of that subset exist. Each parameter subset having that property is called *permissible*. The problem is to formulate a criterion of permissibility. For the extended Nelson method (see Ref. 6) such a criterion has been formulated. For the characteristic equation-based method presented in this paper, a criterion can be formulated by a modification of Theorem 1.

Theorem 2: Let H be as defined by Eq. (69) for an arbitrary set $\mathcal{S}_\mathcal{K}$ of m parameters with indices $\mathcal{K} := \{1, \ldots, m\}$. Each subset $\mathcal{P}_\mathcal{I}$ of parameters, represented by the subset $\mathcal{I} \subset \mathcal{K}$ of indices, is permissible if Theorem 1 holds for $(H)_{(\mathcal{I},\mathcal{I})}$, which denotes that matrix resulting from selecting all columns and rows of H with indices in $\mathcal{I}$.

To clarify the procedure for calculating the derivatives of a repeated eigenvalue of multiplicity $n' = 2$, a flowchart of the algorithm is shown schematically in Fig. 4. For the complete set of all m parameters, the matrix H is calculated, and its rank is checked using the singular value decomposition. If the rank of H is larger than one, all permissible parameters subsets are evaluated by checking the rank of the matrices resulting from choosing $m' < m$ columns and rows of H. Starting with all parameter subsets of cardinality $m' = 2$, one has to calculate the ranks of $m(m-1)/2$ matrices of size 2 by 2.

Example 3

The undamped model introduced in the last section with the parameterization

$$q = (m_1, m_2, m_3, k_1, k_2, k_3, k_4, k_5, k_6)^\top \in \mathbb{R}^9 \tag{72}$$

has eigenvalues $\lambda_1 = 1$, $\lambda_2(q^0) = \lambda_3(q^0) = 4$ at parameter vector

$$q^0 = (1, 4, 1, 0, 8, 0, 2, 2, 1) \tag{73}$$

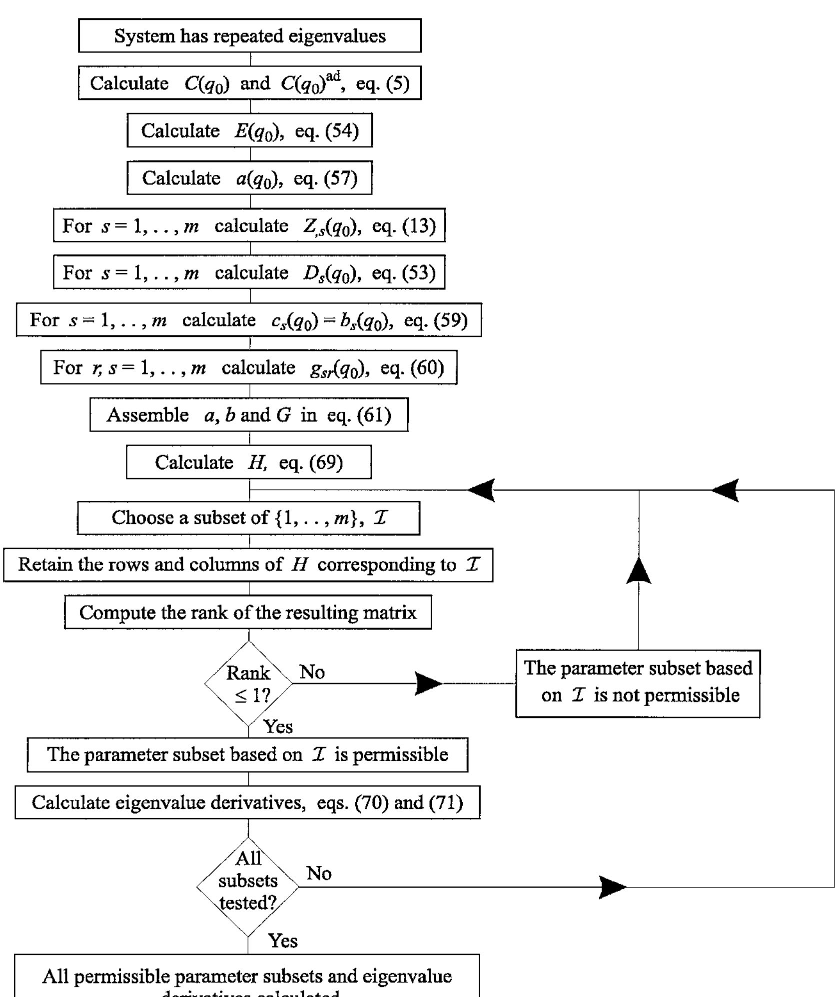

Fig. 4 Flowchart of the algorithm to calculate the derivatives of a repeated eigenvalue of multiplicity $n' = 2$.

The procedure to calculate the derivatives of the repeated eigenvalue with respect to the $m = 9$ parameters leads to $a = -24$ and

$$b = (-32, -8, -32, 8, 2, 8, 14, 14, 24)^\top \tag{74}$$

$$G = (1/1296)\begin{bmatrix} -57{,}600 & -13{,}536 & -54{,}144 & 14{,}400 & 3384 & 13{,}536 & 24{,}984 & 23{,}256 & 42{,}336 \\ -13{,}536 & -3600 & -13{,}536 & 3384 & 900 & 3384 & 6084 & 6084 & 9936 \\ -54{,}144 & -13{,}536 & -57{,}600 & 13{,}536 & 3384 & 14{,}400 & 23{,}256 & 24{,}984 & 42{,}336 \\ 14{,}400 & 3384 & 13{,}536 & -3600 & -846 & -3384 & -6246 & -5814 & -10{,}584 \\ 3384 & 900 & 3384 & -846 & -225 & -846 & -1521 & -1521 & -2484 \\ 13{,}536 & 3384 & 14{,}400 & -3384 & -846 & -3600 & -5814 & -6246 & -10{,}584 \\ 24{,}984 & 6084 & 23{,}256 & -6246 & -1521 & -5814 & -11{,}025 & -10{,}161 & -18{,}036 \\ 23{,}256 & 6084 & 24{,}984 & -5814 & -1521 & -6246 & -10{,}161 & -11{,}025 & -18{,}036 \\ 42{,}336 & 9936 & 42{,}336 & -10{,}584 & -2484 & -10{,}584 & -18{,}036 & -18{,}036 & -32{,}400 \end{bmatrix} \tag{75}$$

which enables the computation of H defined by the right-hand side of Eq. (69). From the singular values $\sigma_1 = 3.5$, $\sigma_2 = 2.076$, $\sigma_i \leq 10^{-16}$, $i = 3, \ldots, 9$, of H, one finds rank$[H] = 2$, which means, with reference to Theorem 1, that the derivatives to all nine parameters do not exist. To find out all permissible subsets $\mathcal{I} \subset \mathcal{K} := \{1, \ldots, 9\}$, Theorem 2 has been applied. For all $m(m-1)/2 = 36$ subsets $\mathcal{I}$ of cardinality 2, the singular values of $(H)_{(\mathcal{I},\mathcal{I})}$ have been calculated to evaluate their ranks. For instance, the subset $\mathcal{I} = \{1, 4\}$ leads to

$$(H)_{(\mathcal{I},\mathcal{I})} = \frac{1}{9}\begin{pmatrix} 16 & -4 \\ -4 & 1 \end{pmatrix} = (4, -1)^\top(4, -1)/9 \tag{76}$$

which obviously has rank one. Selecting elements 1 and 4 of vector b, Eq. (69) corresponds to

$$\left[x - \tfrac{1}{24}(-32, 8)^\top\right]\left[x - \tfrac{1}{24}(-32, 8)^\top\right]^\top = (4, -1)^\top(4, -1)/9 \tag{77}$$

with the two solutions [see Eq. (71)]

$$x^\top \in \{(-8, 2)/3, (0, 0)\} \tag{78}$$

The evaluation of ranks of all $\binom{9}{3} = 9!/(3!6!) = 84$ matrices $(H)_{(\mathcal{I},\mathcal{I})}$ corresponding to all subsets $\mathcal{I}$ with cardinality 3 reveals that there exists only one permissible subset $\mathcal{I} = \{2, 5, 9\}$. Moreover, none of the 124 subsets with cardinality 4 is permissible.

All of the results are summarized in Table 3. There are five sets of two parameters and one set of three parameters that are permissible. The corresponding derivatives are shown in columns 3 and 4 of Table 3. The results of the last two rows correspond to those found by Prells and Friswell.[6] They reported that the number of permissible parameters can only exceed the multiplicity n' of the repeated eigenvalue if the corresponding matrix derivatives are linearly dependent. The result shown in the last row of Table 3 corresponds to the derivative with respect parameters associated with m_2, k_2, and k_6. From the definition of the matrices [see Eqs. (29) and (31)], one finds that the matrix derivative associated with m_2 is indeed the same as that associated with k_2. The derivatives w.r.t. each single parameter are listed in Table 4. To verify these results, the corresponding graphs of $\lambda_2(q_r)$ (solid) and of $\lambda_3(q_r)$ (dotted) are depicted in Fig. 5. Although the derivative w.r.t. each single parameter (see Table 4) exists, the derivatives w.r.t. more than one parameter do not exist in general because they are not continuous at q^0. For example, the surfaces $\lambda_2(q_3, q_9)$ and $\lambda_3(q_3, q_9)$ are plotted in Fig. 6 over the square $(q_3, q_9) \in [0.95, 1.05]^2$. To clarify the situation, the same two surfaces are shown in Fig. 7 with a different viewing angle. At the point $(q_3, q_9) = (1, 1)$ the surfaces meet at a corner, which corresponds to the only common point $\lambda_2 = \lambda_3 = 4$. Hence the derivatives are not continuous at that point. The situation is different for a permissible set of parameters as shown, for example, in Fig. 8 for parameters $(q_3, q_6) \in [0.95, 1.05] \times [-0.05, 0.05]$. The surfaces $\lambda_2(q_3, q_6)$ and $\lambda_3(q_3, q_6)$ represent two intersecting planes. At the point $(q_3, q_6) = (1, 0)$ the derivative is continuous.

Table 3 Permissible subsets of cardinality >1 of the undamped model and the corresponding derivatives of the repeated eigenvalues

Set number	$\mathcal{I}$	$\lambda_{2,\mathcal{I}}$	$\lambda_{3,\mathcal{I}}$
1	{1, 4}	(0, 0)	(−8/3, 2/3)
2	{2, 5}	(0, 0)	(−2/3, 1/6)
3	{2, 9}	(0, 2)	(−2/3, 0)
4	{3, 6}	(0, 0)	(−8/3, 2/3)
5	{5, 9}	(0, 2)	(1/6, 0)
6	{2, 5, 9}	(0, 0, 2)	(−2/3, 1/6, 0)

Example 4

Keeping parameters $(q_1, q_3, q_4, q_6, q_7, q_9) = (1, 1, 0, 0, 2, 1)$ constant and defining two new parameters by

$$q_1 \leftarrow -1.41q_2 + 0.35q_5 + 0.5q_9 \tag{79}$$

$$q_2 \leftarrow -0.37q_2 - 1.49q_5 \tag{80}$$

gives an example with equal derivatives at $q^0 = -(2.34, 13.4)^\top$. With reference to Eq. (68), one finds $a = -24$, $b = (24, 0)^\top$, and

$$G = -\begin{pmatrix} 24 & 0 \\ 0 & 0 \end{pmatrix}$$

Hence $H = 0$, and the derivatives $x = -(1, 0)^\top$ are the same for both repeated eigenvalues.

Example 5

Consider the damped model at parameter values

$$q^0 = (1, 4, 1, 0.1, 0.4, 0.1, 0, 8, 0, 2, 2, 1)^\top \tag{81}$$

which has two repeated complex eigenvalues

$$(\lambda_1, \lambda_2, \lambda_3) = (-0.05 + 0.9987j, \; -0.05 + 1.9994j, -0.05 + 1.9994j) \tag{82}$$

With reference to Eqs. (57) and (58), one finds $a = 95.94$ and $b_1 = b_3 = 1.599 + 31.95j$, $b_2 = -0.3997 + 7.9875j$, $b_4 = b_5 = b_6 = b_7 = b_8 = b_9 = 15.99 - 0.3999j$, $b_{10} = b_{11} = 51.9675 - 1.2996j$, and $b_{12} = 47.97 - 1.1996j$. The rank of the matrix H is 4. The evaluation of permissible parameter subsets leads to seven subsets of cardinality 2:

$$\{1, 4\}, \{1, 7\}, \{2, 5\}, \{2, 8\}, \{3, 6\}, \{3, 9\}, \{5, 8\} \tag{83}$$

and to three subsets of cardinality 3:

Table 4 Permissible singleton sets of the undamped model and the corresponding derivatives of the repeated eigenvalues

	r								
Eigenvalue	1	2	3	4	5	6	7	8	9
$\lambda_{2,r}$	0	0	0	0	0	0	0	0	2
$\lambda_{2,r}$	−8/3	−2/3	−8/3	2/3	1/6	2/3	7/6	7/6	0

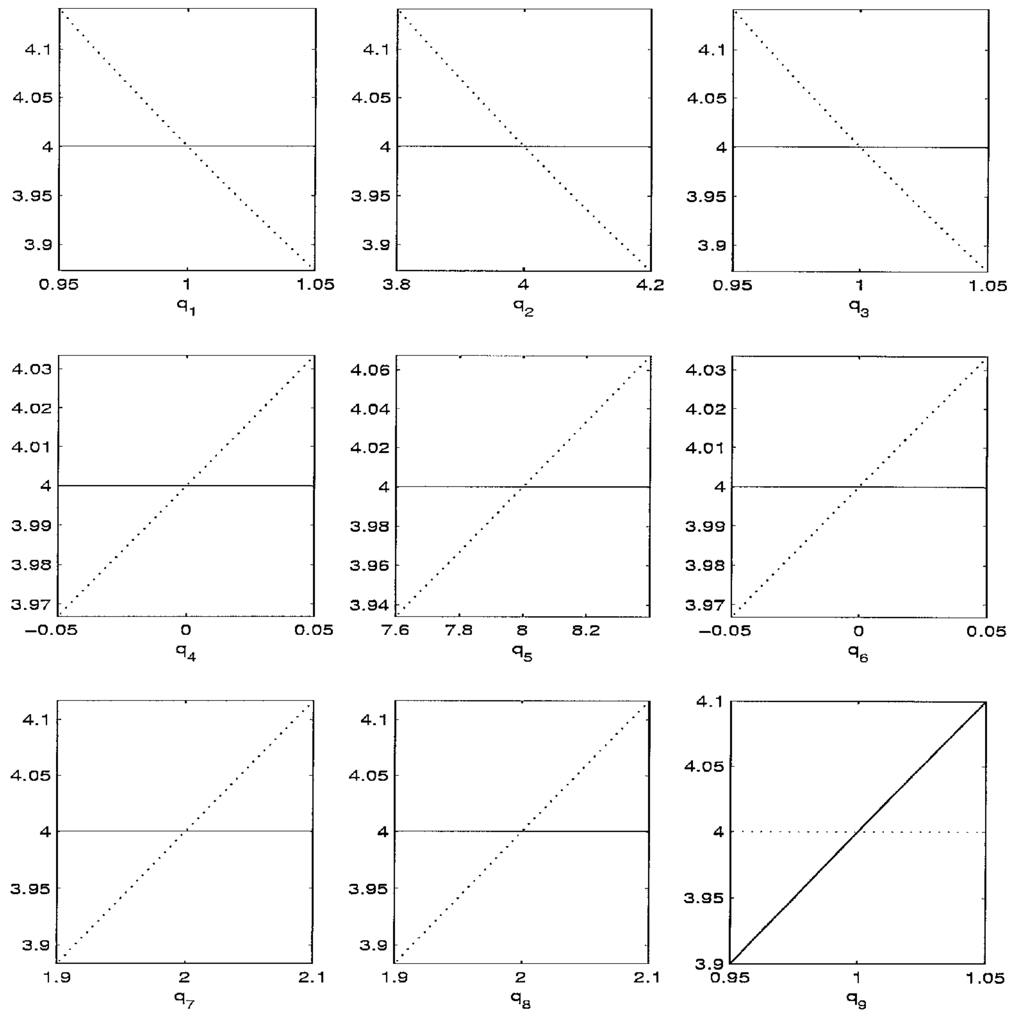

Fig. 5 Graphs $\lambda_2(q_r)$ (——) and $\lambda_3(q_r)$ (· · · ·) for the undamped model with repeated eigenvalues.

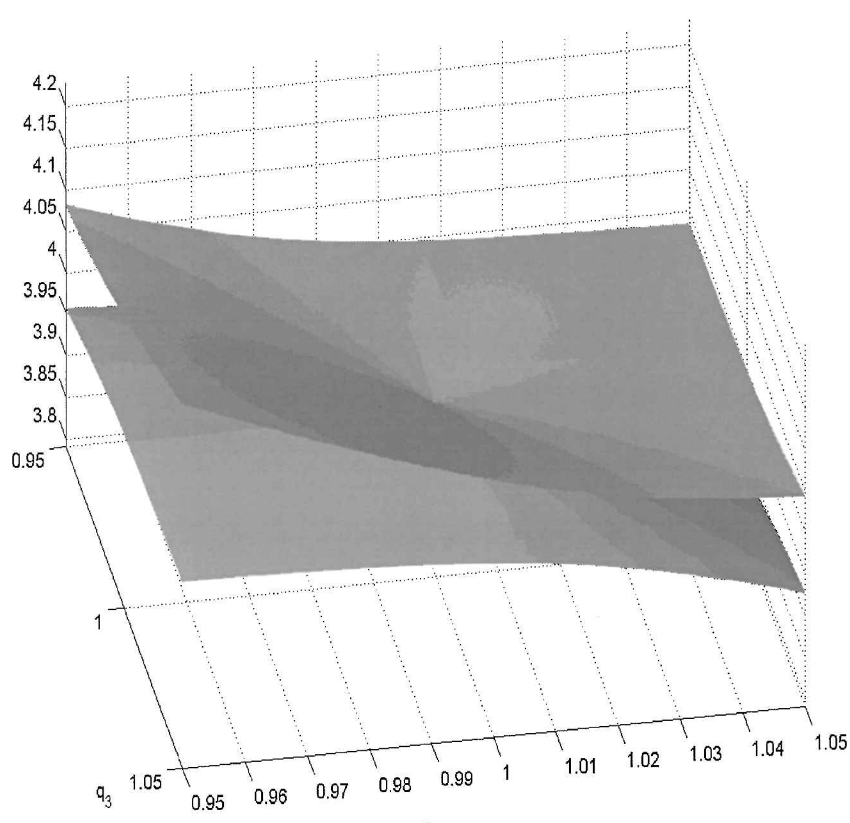

Fig. 6 Surfaces $\lambda_2(q_3, q_9)$ and $\lambda_3(q_3, q_9)$ with noncontinuous derivatives at $(q_3, q_9) = (1, 1)$.

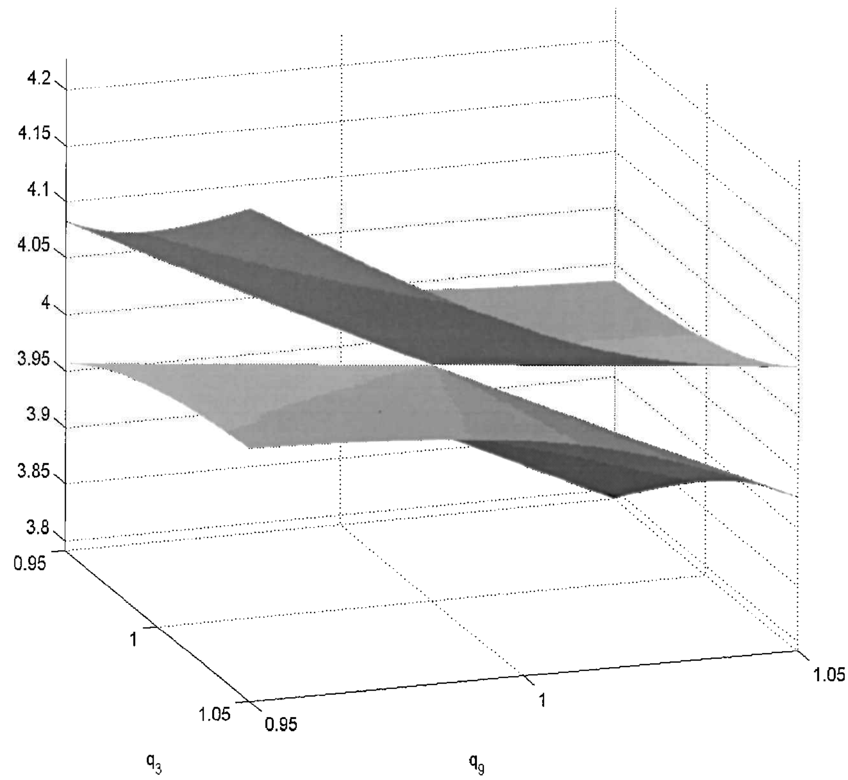

Fig. 7 Different viewing angle of surfaces $\lambda_2(q_3, q_9)$ and $\lambda_3(q_3, q_9)$ with noncontinuous derivatives at $(q_3, q_9) = (1, 1)$.

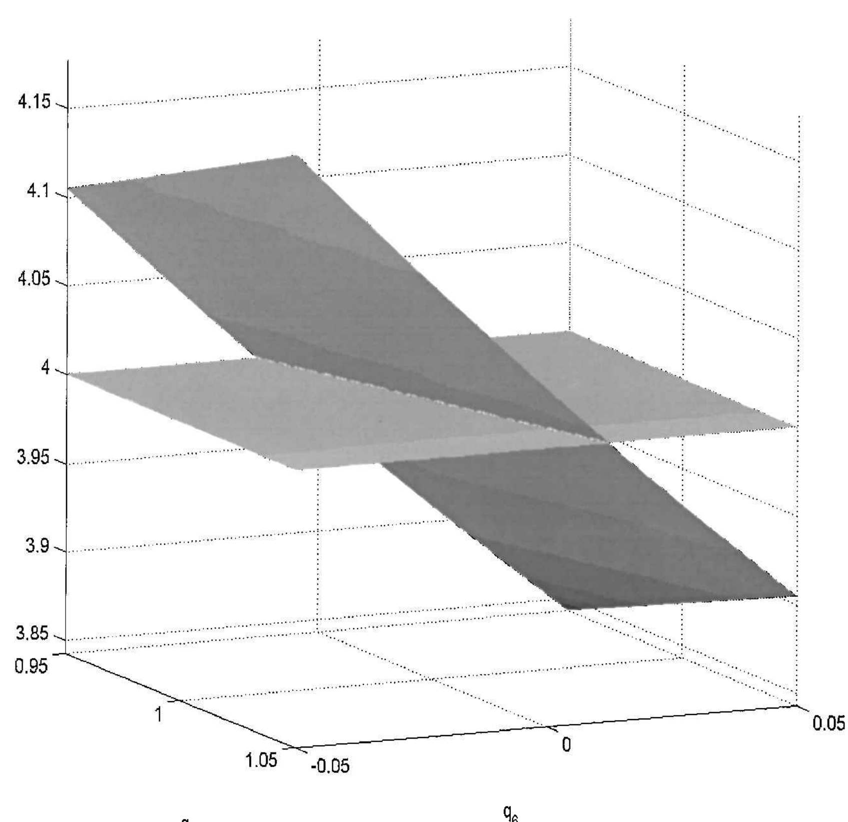

Fig. 8 Surfaces $\lambda_2(q_3, q_6)$ and $\lambda_3(q_3, q_6)$ with continuous derivatives at $(q_3, q_6) = (1, 0)$.

$$\{1, 4, 7\}, \{2, 5, 8\}, \{3, 6, 9\} \tag{84}$$

The derivatives of λ_2 and λ_3 with respect to the parameters of each subset are consistent with the derivatives with respect to each single parameter. In detail one finds

$$\lambda_{3,r}(q^0) = 0, \qquad r = 1, \ldots, 12 \tag{85}$$

$$\lambda_{2,1}(q^0) = \lambda_{2,3}(q^0) = 0.0333 - 0.6660j \tag{86}$$

$$\lambda_{2,2} = 0.0083 - 0.1665j \tag{87}$$

$$\lambda_{2,r}(q^0) = -0.3333 + 0.0083j, \qquad r = 4, \ldots, 9 \tag{88}$$

$$\lambda_{2,10}(q^0) = \lambda_{2,11} = -1.0833 + 0.0271j \tag{89}$$

$$\lambda_{2,12}(q^0) = -1 + 0.025j \tag{90}$$

The derivatives w.r.t. parameters q_{10}, q_{11}, q_{12} do not occur in either subset. Hence for these parameters only the singleton sets are permissible. The subsets of cardinality 3 are indeed permissible because the matrix derivatives associated with parameters q_1, q_2, and q_3 are equal to those associated with parameters q_4, q_5, and q_6, respectively.

IV. Conclusions

A method to calculate the derivatives of repeated and nonrepeated eigenvalues has been introduced, which is based on the characteristic polynominal of the underlying eigenvalue problem. In contrast to existing methods, this method does not require the eigenvectors. The case of repeated eigenvalues of arbitrary multiplicity has been discussed. The derivatives of repeated eigenvalues do not exist for any parameterization. The condition for permissible parameters was formulated for pairs of repeated eigenvalues. The application of the method has been demonstrated by several simulation examples.

Appendix A: Proof of Proposition 3

With reference to Eq. (54),

$$\operatorname{tr}(E) = \sum_{i=1}^{n} \operatorname{tr}\{[C^{(i|i)}]^{\mathrm{ad}}\} \tag{A1}$$

$$= \sum_{i=1}^{n} \operatorname{tr}[(H_i^\top C H_i)^{\mathrm{ad}}] \tag{A2}$$

with the selecting matrix $H_i := [e_1, \ldots, e_{i-1}, e_{i+1}, \ldots, e_n] \in \mathbb{N}^{n\times(n-1)}$, which results by elimination of the ith column of the identity matrix I_n. $H_i^\top H_i = I_{n-1}$ for arbitrary $i \in \{1, \ldots, n\}$. To proceed, one needs to introduce the rth compound matrix $\mathcal{C}_r(A) \in \mathbb{C}^{N\times M}$ of an arbitrary $n \times m$ matrix A, where $N := \binom{n}{r}$ and $M := \binom{m}{r}$, and in general

$$\binom{n}{r} := \frac{n!}{r!(n-r)!}, \qquad n \geq r \in \mathbb{N} \tag{A3}$$

The compound matrix $\mathcal{C}_r(A)$ consists of all minors of size r of A (see, for instance, Horn and Johnson,[8] p. 19 ff.), where the N index sets $\alpha_i \subset \{1, \ldots, n\}, i = 1, \ldots, N$ and the M index sets $\beta_k \subset \{1, \ldots, m\}$, $k = 1, \ldots, M$ are of cardinality r and are usually ordered lexicographically. Thus, the element in row i and column k of $\mathcal{C}_r(A)$ is $\det(A_{\alpha_i\beta_k})$, i.e., the determinant of the $r \times r$ matrix resulting from selecting all rows with indices in α_i and all columns with indices in β_k of A. Some properties of compound matrices are

$$\mathcal{C}_r(AB) = \mathcal{C}_r(A)\mathcal{C}_r(B), \qquad A, B \text{ arbitrary} \tag{A4}$$

$$\mathcal{C}_r(A^{-1}) = \mathcal{C}_r(A)^{-1}, \qquad A \text{ nonsingular} \tag{A5}$$

$$\mathcal{C}_r(A^\top) = \mathcal{C}_r(A)^\top \tag{A6}$$

$$(A)^{\mathrm{ad}} = \mathcal{E}\mathcal{C}_{n-1}(A)^\top\mathcal{E}^\top, \qquad A \in \mathbb{C}^{n\times n} \tag{A7}$$

where in the latter equation

$$\mathcal{E} := \begin{bmatrix} 0 & 0 & \cdots & 0 & 1 \\ 0 & 0 & \cdots & -1 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ (-1)^{n-1} & 0 & \cdots & 0 & 0 \end{bmatrix} \in \mathbb{Z}^{n\times n} \tag{A8}$$

Note, that $\mathcal{E}\mathcal{E}^\top = I_n$. The argument of the trace in Eq. (92) now can be written as

$$(H_i^\top C H_i)^{\mathrm{ad}} = \mathcal{E}\mathcal{C}_{n-2}(H_i^\top C H_i)^\top \mathcal{E}^\top \tag{A9}$$

$$= \mathcal{E}\mathcal{C}_{n-2}(H_i)^\top \mathcal{C}_{n-2}(C)^\top \mathcal{C}_{n-2}(H_i)\mathcal{E}^\top \tag{A10}$$

Because Z is diagonalizable, one may write $C = X\Omega X^{-1}$, where $\Omega := \Lambda - \lambda I_n$, which leads to

$$\mathcal{C}_{n-2}(C) = \mathcal{C}_{n-2}(X)\mathcal{C}_{n-2}(\Omega)\mathcal{C}_{n-2}(X)^{-1} \tag{A11}$$

Without loss of generality, one may assume that $\lambda_{n-1} = \lambda_n = \lambda$ yielding

$$\mathcal{C}_{n-2}(\Omega) = \rho e_1 e_1^\top \in \mathbb{C}^{N\times N} \tag{A12}$$

where

$$N := \frac{n(n-1)}{2}, \qquad \rho := \prod_{i=1}^{n-2}(\lambda_i - \lambda) \neq 0$$

The trace of E now becomes

$$\operatorname{tr}(E) = \rho \sum_{i=1}^{n} \operatorname{tr}[\mathcal{E}\mathcal{C}_{n-2}(H_i)^\top \mathcal{C}_{n-2}(X)^{-\top} e_1 e_1^\top \mathcal{C}_{n-2}(X)^\top \times \mathcal{C}_{n-2}(H_i)\mathcal{E}^\top] \tag{A13}$$

$$= \rho \sum_{i=1}^{n} e_1^\top \mathcal{C}_{n-2}(X)^\top \mathcal{C}_{n-2}(H_i)\mathcal{C}_{n-2}(H_i)^\top \mathcal{C}_{n-2}(X)^{-\top} e_1 \tag{A14}$$

$$= \rho y^\top \sum_{i=1}^{n} \mathcal{C}_{n-2}[N(i)]z \tag{A15}$$

where $z := \mathcal{C}_{n-2}(X)^{-\top}e_1$ and $y := \mathcal{C}_{n-2}(X)e_1$, which implies $z^\top y = 1$. The matrix $N(i) := H_i H_i^\top$ is diagonal and consists of units in all diagonal places except a zero at position (i, i). The $(n-2)$th compound matrix of $N(i)$ is diagonal, too. Its kth diagonal component is the determinant of $N(i)_{(\alpha_k,\alpha_k)}$, where α_k is the kth subset of cardinality $n-2$ of the index set $\{1, \ldots, n\}$. Defining for $k = 1, \ldots, n(n-1)/2 = N$ and for $i = 1, \ldots, n$

$$(\mathcal{H})_{ki} := \begin{cases} 0, & i \in \alpha_k \\ 1, & \text{else} \end{cases} \tag{A16}$$

one finds

$$\mathcal{C}_{n-2}[N(i)] = \operatorname{diag}(\mathcal{H}e_i) \tag{A17}$$

Because there are $n - (n-2) = 2$ units in each row and $\binom{n}{n-2} - \binom{n-1}{n-3} = \binom{n-1}{n-2} = n-1$ units in each column of $\mathcal{H}$, a simple calculation reveals

$$\operatorname{tr}(E) = \rho y^\top \sum_{i=1}^{n} [\operatorname{diag}(\mathcal{H}e_i)]z \tag{A18}$$

$$= \rho y^\top (2I_N)z = 2\rho \tag{A19}$$

which completes the proof. □

Appendix B: Computation of the Adjoint

If the size of C is large, the direct computation of its adjoint via the determinants may become time consuming. A more efficient way is to calculate the adjoint via the singular value decomposition of C. Using properties (A4) and (A7), one finds

$$C^{\mathrm{ad}} = (L\Sigma R^{\top})^{\mathrm{ad}} \tag{B20}$$

$$= \mathcal{E}\mathcal{C}_{n-1}(R\Sigma L^{\top})\mathcal{E}^{\top} \tag{B21}$$

$$= \mathcal{E}\mathcal{C}_{n-1}(R)\mathcal{E}^{\top}\mathcal{E}\mathcal{C}_{n-1}(\Sigma)\mathcal{E}^{\top}\mathcal{E}\mathcal{C}_{n-1}(L)^{\top}\mathcal{E}^{\top} \tag{B22}$$

$$= (R^{\mathrm{ad}})^{\top}\Sigma^{\mathrm{ad}}L^{\mathrm{ad}} \tag{B23}$$

$$= R\Sigma^{\mathrm{ad}}L^{\top} \tag{B24}$$

The transition to the last equation is possible because, in general, for an unitary matrix U [see Eq. (14)] $U^{\mathrm{ad}} = U^{\top}$.

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