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COMPUTATION OF EIGENVALUE AND EIGENVECTOR DERIVATIVES FOR A GENERAL COMPLEX-VALUED EIGENSYSTEM*

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Abstract. In many engineering applications, the physical quantities that have to be computed are obtained by solving a related eigenvalue problem. The matrix under consideration and thus its eigenvalues usually depend on some parameters. A natural question then is how sensitive the physical quantity is with respect to (some of) these parameters, i.e., how it behaves for small changes in the parameters. To find this sensitivity, eigenvalue and/or eigenvector derivatives with respect to those parameters need to be found. A method is provided to compute first order derivatives of the eigenvalues and eigenvectors for a *general* complex-valued, non-defective matrix.

Key words. Eigenvalue derivatives, Eigenvector derivatives, Repeated eigenvalues.

AMS subject classifications. 65F15.

1. Introduction.

In many engineering applications, e.g., diffraction grating theory [6], the computation of eigenvalues and eigenvectors is an important step in the qualitative and quantitative analysis of the physical quantities involved. These quantities usually depend on some predefined problem dependent parameters. For example, in diffraction grating theory, where an electromagnetic field is incident on a periodic structure, the physical quantity to be computed is the reflected electromagnetic field, which, among other things, depends on the shape of the diffraction grating. Once these parameters have been assigned a value, eigenvalues and eigenvectors can be computed by standard methods such as the QR algorithm. However, we are usually even more interested in the sensitivity of the physical quantity with respect to (some of) the parameters, that is, how this quantity behaves for small changes in the parameters. To find this sensitivity also eigenvalue and/or eigenvector derivatives with respect to those parameters must be computed.

To be more specific, let $\mathbf{A} \in \mathbb{C}^{N\times N}$ be a non-defective matrix given as a function of a certain parameter p. Let $\mathbf{\Lambda} \in \mathbb{C}^{N\times N}$ be the eigenvalue matrix of $\mathbf{A}$ and $\mathbf{X} \in \mathbb{C}^{N\times N}$ a corresponding eigenvector matrix of $\mathbf{A}$, i.e.,

$$\mathbf{A}(p)\mathbf{X}(p) = \mathbf{X}(p)\mathbf{\Lambda}(p). \tag{1.1}$$

It is well known that eigenvectors are not uniquely determined. If the eigenvalues are distinct, then the eigenvectors are determined up to a constant multiplier, whereas if an eigenvalue has geometric multiplicity higher than 1, then any linear combination of the associated eigenvectors will be an eigenvector again. This implies that an eigenvector derivative cannot be computed uniquely unless the eigenvectors are fixed.

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For the case that all eigenvalues are *distinct*, one of the first methods to compute eigenvector derivatives analytically for *real-valued* $\mathbf{A}$ can be found in [8]. A numerical way of retrieving the eigenvector derivatives is given in [2, 9]. This numerical method is fast when only a small number of eigenvalue derivatives and their corresponding eigenvector derivatives have to be computed. If the eigenvalues and eigenvectors are already available and only their corresponding derivatives should be computed, then an analytical approach will usually be much faster. For an overview of the methods available for distinct eigenvalues for an arbitrary complex-valued matrix, consider [7].

Repeated eigenvalues have also been analysed before, though not for the general case yet. For real-valued matrices, Mills–Curran [5] shows how the eigenvector derivatives for a symmetric real-valued matrix can be found. However, it is assumed that the eigenvalue derivatives are distinct. In [4], the theory is extended by assuming that there are still eigenvalue derivatives which are repeated, but the second order derivatives of the eigenvalues have to be distinct. In [3], this theory is generalized to complex-valued, Hermitian matrices. Here it is assumed that for an eigenvalue with multiplicity r, all its eigenvalue derivatives up to kth order are also equal and the $(k+1)$st order derivatives are distinct again.

The generalization towards a *general* non-defective matrix has not been provided yet. This paper presents an algorithm to compute the first order analytical derivatives of both eigenvalues and eigenvectors for such a general non-defective matrix. It is assumed that all eigenvalues and their associated eigenvectors are either known analytically or from a numerical procedure, and that the eigenvector derivatives exist.

This paper is set up as follows. As a prelude, Section 2 gives the basic problem. To have more insight into the problem, some simple cases will be discussed in Section 3 first before discussing the mathematical details of the generalization in Section 4. Afterwards some examples are presented in Section 5 to illustrate the method in Section 4.

2. The basic theory. Let the non-defective matrix $\mathbf{A}(p)$ and its eigenvalue and eigenvector matrix $\mathbf{\Lambda}(p)$ and $\mathbf{X}(p)$ respectively, be differentiable in a neighbourhood of $p = p_0$. Usually, the eigensystem (1.1) is differentiated directly with respect to p without taking into account that the eigenvector matrix $\mathbf{X}$ is not unique. Below we show that this can go wrong. The p-dependency is discarded for notational convenience. The derivative with respect to p is denoted by a prime. So from (1.1) we have

$$\mathbf{A}'\mathbf{X} - \mathbf{X}\mathbf{\Lambda}' = -\mathbf{A}\mathbf{X}' + \mathbf{X}'\mathbf{\Lambda}. \tag{2.1}$$

In (2.1), both the eigenvalue derivative matrix $\mathbf{\Lambda}'$ and the eigenvector derivative matrix $\mathbf{X}'$ occur. To find an expression for $\mathbf{\Lambda}'$, the inverse of the eigenvector matrix $\mathbf{X}$ is needed. Premultiplying by $\mathbf{X}^{-1}$ in (2.1) results in

$$\mathbf{X}^{-1}\mathbf{A}'\mathbf{X} - \mathbf{\Lambda}' = -\mathbf{X}^{-1}\mathbf{A}\mathbf{X}' + \mathbf{X}^{-1}\mathbf{X}'\mathbf{\Lambda}. \tag{2.2}$$

Since $\mathbf{A}$ is assumed to be non-defective, the eigenvectors span the complete $\mathbb{C}^{N\times N}$. For ease of notation, let us define a matrix $\mathbf{C} := \mathbf{X}^{-1}\mathbf{X}'$, i.e.,

$$\mathbf{X}' = \mathbf{X}\mathbf{C}. \tag{2.3}$$

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Rather than determining $\mathbf{X}'$, we will try to find $\mathbf{C}$. ¿From (2.2) we derive

$$\mathbf{X}^{-1}\mathbf{A}'\mathbf{X} - \mathbf{\Lambda}' = -\mathbf{\Lambda}\mathbf{C} + \mathbf{C}\mathbf{\Lambda}. \tag{2.4}$$

Often the eigenvalues and eigenvectors of $\mathbf{A}(p)$ are needed for some specific value $p = p_0$. If the eigenvalues are distinct, then the eigenvectors are unique up to a multiplicative constant, but this constant drops out in the computation of the diagonal elements of $\mathbf{\Lambda}'$. However, if some eigenvalues are repeated, then every linear combination of the corresponding eigenvectors is an eigenvector again. Once the eigenvalues and eigenvectors of $\mathbf{A}(p_0)$ have been determined, the set of eigenvectors does not guarantee the continuity of the eigenvalue derivatives as is shown by the following example.

Example 2.1. Let

$$\mathbf{A}(p) := \begin{bmatrix} 1 & p \\ p & 1 \end{bmatrix}.$$

Then the eigenvalue matrix $\mathbf{\Lambda}(p)$ and an eigenvector matrix $\mathbf{X}(p)$ can be found as

$$\mathbf{\Lambda}(p) = \begin{bmatrix} 1-p & 0 \\ 0 & 1+p \end{bmatrix}, \quad \mathbf{X}(p) = \begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix},$$

respectively. For $p = 0$, the eigenvalues become repeated and a valid eigenvector matrix would be

$$\mathbf{X}(0) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}.$$

Note that for $p = 0$ the right-hand side of (2.4) vanishes completely, and therefore, $\mathbf{\Lambda}'(0)$ should be equal to $\mathbf{X}^{-1}(0)\mathbf{A}'(0)\mathbf{X}(0)$, but

$$\mathbf{X}^{-1}(0)\mathbf{A}'(0)\mathbf{X}(0) = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.$$

As can be seen, this product is not even a diagonal matrix. Of course, the problem is caused by a wrong choice of $\mathbf{X}$. □

The main focus of this paper is choosing an eigenvector matrix such that $\mathbf{\Lambda}'$ is continuous with respect to parameter p. To do this, let us trivially assume that an eigenvector matrix $\bar{\mathbf{X}}$ has already been found, e.g., by Lapack [1]. Then there exists a non-unique matrix $\mathbf{\Gamma} \in \mathbb{C}^{N\times N}$ such that

$$\mathbf{X} = \bar{\mathbf{X}}\mathbf{\Gamma}, \tag{2.5}$$

with $\mathbf{\Gamma} \in \mathbb{C}^{N\times N}$. Since $\mathbf{X}$ should also be an eigenvector matrix of $\mathbf{A}$, it has to satisfy (1.1), and therefore, $\mathbf{\Gamma}$ has to satisfy the following condition,

$$\mathbf{\Lambda}\mathbf{\Gamma} = \mathbf{\Gamma}\mathbf{\Lambda}. \tag{2.6}$$

Substitution of (2.5) into (2.4) results in

$$\bar{\mathbf{X}}^{-1}\mathbf{A}'\bar{\mathbf{X}}\mathbf{\Gamma} - \mathbf{\Gamma}\mathbf{\Lambda}' = -\mathbf{\Gamma}\mathbf{\Lambda}\mathbf{C} + \mathbf{\Gamma}\mathbf{C}\mathbf{\Lambda}. \tag{2.7}$$

The latter relationship will be the starting point for the computation of eigenvalue and eigenvector derivatives which will be done in the following two sections.

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3. Review of simple cases. Since the derivation of a general formulation is rather involved, we start with the three simplest situations, viz. distinct eigenvalues, repeated eigenvalues with distinct derivatives and, finally, repeated eigenvalues with repeated first order derivatives and distinct second order derivatives.

3.1. Distinct eigenvalues. For distinct eigenvalues, it follows from (2.6) that $\mathbf{\Gamma}$ must be a diagonal matrix. If (2.7) is considered element by element, then it has the following form,

$$\mathbf{y}_k^* \mathbf{A}' \mathbf{x}_l \gamma_l - \delta_{kl} \gamma_l \lambda_l' = \gamma_k \left(\lambda_l - \lambda_k \right) c_{kl},$$

where λ_k is the kth element on the diagonal of $\mathbf{\Lambda}$, $\mathbf{y}_k^*$ and $\mathbf{x}_k$ are the kth left and right eigenvectors, respectively, c_{kl} is the entry (k, l) of matrix $\mathbf{C}$, and $\delta_{kl} = 1$ if $k = l$ and 0 otherwise. Note that * denotes the complex conjugate transpose, that is, $\mathbf{y}^* = \bar{\mathbf{y}}^T$. As a result, we can extract λ_k' and c_{kl} as follows,

$$\lambda_k' = \mathbf{y}_k^* \mathbf{A}' \mathbf{x}_k, \quad k = 1, \ldots, N, \tag{3.1}$$

$$c_{kl} = \frac{\mathbf{y}_k^* \mathbf{A}' \mathbf{x}_l \gamma_l}{\gamma_k \left(\lambda_l - \lambda_k \right)}, \quad k \neq l. \tag{3.2}$$

Thus, for distinct eigenvalues, all eigenvalue derivatives can be found and the off-diagonal entries of matrix $\mathbf{C}$ are determined when the entries of $\mathbf{\Gamma}$ are known. There are no constraints for the diagonal entries of $\mathbf{\Gamma}$, and therefore, they can be chosen arbitrarily. This corresponds to the fact that eigenvectors are unique up to a multiplicative constant for distinct eigenvalues, i.e., these constants can be chosen freely. A reasonable way is to choose an mth element of the kth eigenvector equal to 1 for all p, viz.

$$x_{mk} = 1 \Rightarrow \bar{x}_{mk} \gamma_k = 1 \Rightarrow \gamma_k = \frac{1}{\bar{x}_{mk}}, \tag{3.3}$$

for m with $1 \leq m \leq N$ and $k = 1, \ldots, N$. With this normalization condition, there is always an m such that eigenvector $\mathbf{x}_k$ is uniquely determined, as $\mathbf{x}_k \neq 0$. The index m is chosen as follows,

$$|x_{mk}||y_{mk}| = \max_{1 \leq j \leq N} |x_{jk}||y_{jk}|. \tag{3.4}$$

This prevents both x_{mk} and y_{mk} from becoming very small. At this point, the eigenvectors are uniquely determined and since the normalization condition (3.3) applies to each eigenvector and all values of p, the following holds,

$$x_{mk}' = 0 \quad \text{for all } p.$$

By using (2.3), an expression can be found for the coefficient c_{kk} in terms of the off-diagonal entries of the matrix $\mathbf{C}$,

$$x_{mk}' = \sum_{l=1}^{N} x_{ml} c_{lk} = 0 \quad \Rightarrow \quad c_{kk} = -\frac{1}{x_{mk}} \sum_{\substack{l=1 \\ l \neq k}}^{N} x_{ml} c_{lk} = -\sum_{\substack{l=1 \\ l \neq k}}^{N} x_{ml} c_{lk}. \tag{3.5}$$

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In terms of the given eigenvectors, this implies that

$$c_{kk} = -\sum_{\substack{l=1 \\ l\neq k}}^{N} \bar{x}_{ml}\gamma_l c_{lk}.$$

Thus, the diagonal coefficients c_{kk} can be determined uniquely since (3.2) ensures the off-diagonal entries of $\mathbf{C}$ to be available, and so matrix $\mathbf{X}'$ can uniquely be determined using (2.3).

3.2. Repeated eigenvalues with distinct eigenvalue derivatives. For repeated eigenvalues, condition (2.6) indicates that matrix $\mathbf{\Gamma}$ does have to be diagonal anymore. Every linear combination of such eigenvectors is still an eigenvector. Now let $\lambda_1 = \ldots = \lambda_M$ for some $M \leq N$. Introduce the following partitioning of $\mathbf{\Lambda}$, the corresponding eigenvector matrices $\bar{\mathbf{X}}$ and $\bar{\mathbf{Y}}^*$ and the matrix $\mathbf{\Gamma}$,

$$\mathbf{\Lambda} = \begin{bmatrix} \mathbf{\Lambda}_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{\Lambda}_2 \end{bmatrix}, \quad \bar{\mathbf{X}} = \begin{bmatrix} \bar{\mathbf{X}}_1 & \bar{\mathbf{X}}_2 \end{bmatrix}, \quad \bar{\mathbf{Y}}^* = \begin{bmatrix} \bar{\mathbf{Y}}_1^* \\ \bar{\mathbf{Y}}_2^* \end{bmatrix}, \tag{3.6}$$
$$\mathbf{\Gamma} = \begin{bmatrix} \mathbf{\Gamma}_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{\Gamma}_2 \end{bmatrix}, \quad \mathbf{C} = \begin{bmatrix} \mathbf{C}_{11} & \mathbf{C}_{12} \\ \mathbf{C}_{21} & \mathbf{C}_{22} \end{bmatrix},$$

where $\mathbf{\Lambda}_2 = \lambda\mathbf{I} \in \mathbb{C}^{M\times M}$ consists of all M repeated eigenvalues and all other eigenvalues are in $\mathbf{\Lambda}_1 \in \mathbb{C}^{(N-M)\times(N-M)}$. Matrix $\mathbf{\Lambda}_1$ can still contain repeated eigenvalues, but none of the eigenvalues of this matrix is equal to λ. The block row $\bar{\mathbf{X}}_2 \in \mathbb{C}^{N\times M}$ consists of the right eigenvectors belonging to the repeated eigenvalues and $\bar{\mathbf{X}}_1 \in \mathbb{C}^{N\times(N-M)}$ consists of the right eigenvectors belonging to the other eigenvalues.

For notational convenience, a left eigenvector matrix $\mathbf{Y}^*$ is introduced which is defined as

$$\mathbf{Y}^* := \mathbf{X}^{-1}.$$

Likewise the matrix $\bar{\mathbf{Y}}^*$ is divided into two block rows $\bar{\mathbf{Y}}_1^* \in \mathbb{C}^{(N-M)\times N}$ and $\bar{\mathbf{Y}}_2^* \in \mathbb{C}^{M\times N}$, respectively. The matrices $\mathbf{\Gamma}$ and $\mathbf{C}$ are partitioned in a similar way, but note that (2.6) implies that the off-diagonal blocks of $\mathbf{\Gamma}$ are $\mathbf{0}$. As a result, (2.7) can be described by a set of four smaller equations,

$$\bar{\mathbf{Y}}_1^*\mathbf{A}'\bar{\mathbf{X}}_1\mathbf{\Gamma}_1 - \mathbf{\Gamma}_1\mathbf{\Lambda}_1' = -\mathbf{\Gamma}_1\mathbf{\Lambda}_1\mathbf{C}_{11} + \mathbf{\Gamma}_1\mathbf{C}_{11}\mathbf{\Lambda}_1, \tag{3.7a}$$
$$\bar{\mathbf{Y}}_1^*\mathbf{A}'\bar{\mathbf{X}}_2\mathbf{\Gamma}_2 = \mathbf{\Gamma}_1\left(\lambda\mathbf{I} - \mathbf{\Lambda}_1\right)\mathbf{C}_{12}, \tag{3.7b}$$
$$\bar{\mathbf{Y}}_2^*\mathbf{A}'\bar{\mathbf{X}}_1\mathbf{\Gamma}_1 = -\mathbf{\Gamma}_2\mathbf{C}_{21}\left(\lambda\mathbf{I} - \mathbf{\Lambda}_1\right), \tag{3.7c}$$
$$\bar{\mathbf{Y}}_2^*\mathbf{A}'\bar{\mathbf{X}}_2\mathbf{\Gamma}_2 - \mathbf{\Gamma}_2\mathbf{\Lambda}_2' = \mathbf{0}. \tag{3.7d}$$

Clearly, (3.7d) is an eigenvalue problem itself, $\mathbf{\Lambda}_2'$ containing the eigenvalues of matrix $\bar{\mathbf{Y}}_2^*\mathbf{A}'\bar{\mathbf{X}}_2$ and $\mathbf{\Gamma}_2$ being the eigenvector matrix. Assuming that all eigenvalues of $\mathbf{\Lambda}_2'$ are distinct, the column vectors of $\mathbf{\Gamma}_2$ are determined up to a constant multiplier.

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Since $\bar{\mathbf{\Gamma}}_2$ can be computed by Lapack [1], we have $\mathbf{\Gamma}_2 = \bar{\mathbf{\Gamma}}_2\mathbf{\Psi}$, with $\mathbf{\Psi}$ a diagonal matrix. Now, the choice (3.3) gives an expression for the diagonal entries of $\mathbf{\Gamma}_2$,

$$x_{mk} = 1 \Rightarrow \left(\sum_{l=1}^{M} \bar{x}_{ml}\gamma_{lk}\right)\psi_k = 1 \Rightarrow \psi_k = \frac{1}{\sum_{l=1}^{M} \bar{x}_{ml}\gamma_{lk}}. \tag{3.8}$$

If $\mathbf{\Lambda}_1$ still contains repeated eigenvalues, then the same procedure can be performed until $\mathbf{\Gamma}_1$ has been determined uniquely.

Once $\mathbf{\Gamma}$ is known, the eigenvectors are determined uniquely and the eigenvector derivatives can be computed. Also $\mathbf{C}_{12}$ and $\mathbf{C}_{21}$ can be found from (3.7b) and (3.7c), viz.

$$\mathbf{C}_{12} = (\lambda\mathbf{I} - \mathbf{\Lambda}_1)^{-1}\mathbf{\Gamma}_1^{-1}\bar{\mathbf{Y}}_1^*\mathbf{A}'\bar{\mathbf{X}}_2\mathbf{\Gamma}_2, \tag{3.9a}$$

$$\mathbf{C}_{21} = -\mathbf{\Gamma}_2^{-1}\bar{\mathbf{Y}}_2^*\mathbf{A}'\bar{\mathbf{X}}_1\mathbf{\Gamma}_1(\lambda\mathbf{I} - \mathbf{\Lambda}_1)^{-1}. \tag{3.9b}$$

Since the eigenvalues of $\mathbf{\Lambda}_2$ are repeated, but their derivatives are not, (2.1) needs to be differentiated once more to determine $\mathbf{C}_{22}$. When the result is premultiplied by $\mathbf{Y}^*$, (2.5) and (2.3) are used for $\mathbf{X}$ and $\mathbf{X}'$, respectively, and matrix $\mathbf{D}$ is introduced to write $\mathbf{X}''$ in a similar way as in (2.3) such that

$$\mathbf{X}'' = \mathbf{X}\mathbf{D}, \tag{3.10}$$

we have

$$\bar{\mathbf{Y}}_2^*\mathbf{A}''\bar{\mathbf{X}}_2\mathbf{\Gamma}_2 - \mathbf{\Gamma}_2\mathbf{\Lambda}_2'' = -2\mathbf{\Gamma}_2(\mathbf{\Lambda}_2'\mathbf{C}_{22} - \mathbf{C}_{22}\mathbf{\Lambda}_2') - 2\mathbf{\Gamma}_2\bar{\mathbf{Y}}_2^*\mathbf{A}'\bar{\mathbf{X}}_1\mathbf{\Gamma}_1\mathbf{C}_{12}. \tag{3.11}$$

Then (3.11) gives an expression for the off-diagonal entries of $\mathbf{C}_{22}$, since $\mathbf{C}_{12}$ is already available from (3.9a).

3.3. Repeated eigenvalue with repeated eigenvalue derivatives. If eigenvalue system (3.7d) has repeated eigenvalues too, implying that some of the derivatives of the repeated eigenvalue under consideration are also equal, the column vectors of $\mathbf{\Gamma}_2$ are not unique either. As a consequence, introduce a partitioning as follows,

$$\mathbf{\Lambda} = \begin{bmatrix} \mathbf{\Lambda}_1 & & \mathbf{0} \\ & \tilde{\mathbf{\Lambda}}_2 & \\ \mathbf{0} & & \tilde{\mathbf{\Lambda}}_3 \end{bmatrix}, \quad \bar{\mathbf{X}} = \begin{bmatrix} \bar{\mathbf{X}}_1 & \tilde{\bar{\mathbf{X}}}_2 & \tilde{\bar{\mathbf{X}}}_3 \end{bmatrix}, \bar{\mathbf{Y}}^* = \begin{bmatrix} \bar{\mathbf{Y}}_1^* \\ \tilde{\bar{\mathbf{Y}}}_2^* \\ \tilde{\bar{\mathbf{Y}}}_3^* \end{bmatrix}, \tag{3.12}$$

$$\mathbf{\Gamma} = \begin{bmatrix} \mathbf{\Gamma}_1 & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \tilde{\mathbf{\Gamma}}_2 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \tilde{\mathbf{\Gamma}}_3 \end{bmatrix}, \quad \mathbf{C} = \begin{bmatrix} \mathbf{C}_{11} & \tilde{\mathbf{C}}_{12} & \tilde{\mathbf{C}}_{13} \\ \tilde{\mathbf{C}}_{21} & \tilde{\mathbf{C}}_{22} & \tilde{\mathbf{C}}_{23} \\ \tilde{\mathbf{C}}_{31} & \tilde{\mathbf{C}}_{32} & \tilde{\mathbf{C}}_{33} \end{bmatrix},$$

where $\tilde{\mathbf{\Lambda}}_3 \in \mathbb{C}^{P\times P}$, with $P \le M$, is the eigenvalue matrix containing those eigenvalues whose derivatives are equal. Then $\tilde{\mathbf{\Lambda}}_2 \in \mathbb{C}^{(M-P)\times(M-P)}$ is the eigenvalue matrix that contains the remaining repeated eigenvalues, while $\mathbf{\Lambda}_1$ remains unchanged. A corresponding partitioning is also carried out for $\bar{\mathbf{X}}$, $\bar{\mathbf{Y}}^*$, $\mathbf{\Gamma}$ and $\mathbf{C}$.

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The primary goal is to determine $\mathbf{\Gamma}$. Since $\tilde{\mathbf{\Gamma}}_2$ consists of eigenvectors of (3.7d) corresponding to the distinct eigenvalue derivatives, only $\tilde{\mathbf{\Gamma}}_3$ has to be determined. However, we need an extra relation. Therefore, (2.1) is differentiated once more with respect to p and premultiplied by the left eigenvector matrix $\mathbf{Y}^*$. Substitute (2.5), (2.3) and (3.10), which are the expressions for $\mathbf{X}$, $\mathbf{X}'$ and $\mathbf{X}''$, respectively, and introduce a similar expression for $\mathbf{X}'''$. To find $\mathbf{\Gamma}_3$, we use the partitioning given by (3.12),

$$\tilde{\tilde{\bar{\mathbf{Y}}}}_3^* \mathbf{A}'' \tilde{\tilde{\bar{\mathbf{X}}}}_3 \mathbf{\Gamma}_3 - \mathbf{\Gamma}_3 \mathbf{\Lambda}_3'' = -2\mathbf{\Gamma}_3 \mathbf{C}_{31} \left(\lambda \mathbf{I} - \mathbf{\Lambda}_1\right) \mathbf{C}_{13}. \tag{3.13}$$

For simplicity of notation, which will be of high importance in the generalization of the theory, we omit the tilde again. Unfortunately, $\mathbf{C}_{31}$ and $\mathbf{C}_{13}$ cannot be computed since $\mathbf{\Gamma}_3$ is not yet determined. However, (3.7c) and (3.7b) give expressions for $\mathbf{C}_{13}$ and $\mathbf{C}_{31}$ in terms of $\mathbf{\Gamma}_1$ and $\mathbf{\Gamma}_3$. Insertion of these expressions into (3.13) again gives an eigenproblem with $\mathbf{\Gamma}_3$ the eigenvector matrix and $\mathbf{\Lambda}_3''$ the eigenvalue matrix. Hence,

$$\left(\bar{\mathbf{Y}}_3^* \mathbf{A}'' \bar{\mathbf{X}}_3 - 2\bar{\mathbf{Y}}_3^* \mathbf{A}' \bar{\mathbf{X}}_1 \left(\lambda \mathbf{I} - \mathbf{\Lambda}_1\right)^{-1} \bar{\mathbf{Y}}_1^* \mathbf{A}' \bar{\mathbf{X}}_3\right) \mathbf{\Gamma}_3 - \mathbf{\Gamma}_3 \mathbf{\Lambda}_3'' = \mathbf{0}. \tag{3.14}$$

If the second order derivatives of the eigenvalues are distinct, then $\mathbf{\Gamma}_3$ consists of column vectors that are unique up to a multiplicative constant. Again, (3.3) ensures an expression for the diagonal entries of $\mathbf{\Gamma}_3$. Since $\mathbf{\Gamma}_2$ has already been determined in (3.7d), and for $\mathbf{\Gamma}_1$, the same procedure can be performed until $\mathbf{\Gamma}_1$ has been determined uniquely, the desired eigenvector matrix has been found.

To determine the eigenvector derivatives, the coefficient matrix $\mathbf{C}$ needs to be computed. The blocks $\mathbf{C}_{12}$, $\mathbf{C}_{13}$, $\mathbf{C}_{21}$, $\mathbf{C}_{31}$ are computed like in (3.7b) and (3.7c), respectively. The matrices $\mathbf{C}_{23}$ and $\mathbf{C}_{32}$ can be found from

$$\bar{\mathbf{Y}}_2^* \mathbf{A}'' \bar{\mathbf{X}}_3 \mathbf{\Gamma}_3 = 2\mathbf{\Gamma}_2 \left(\lambda' \mathbf{I} - \mathbf{\Lambda}_2'\right) \mathbf{C}_{23} + 2\mathbf{\Gamma}_2 \mathbf{C}_{21} \left(\lambda \mathbf{I} - \mathbf{\Lambda}_1\right) \mathbf{C}_{13}, \tag{3.15a}$$

$$\bar{\mathbf{Y}}_3^* \mathbf{A}'' \bar{\mathbf{X}}_2 \mathbf{\Gamma}_2 = -2\mathbf{\Gamma}_3 \mathbf{C}_{32} \left(\lambda' \mathbf{I} - \mathbf{\Lambda}_2'\right) + 2\mathbf{\Gamma}_3 \mathbf{C}_{31} \left(\lambda \mathbf{I} - \mathbf{\Lambda}_1\right) \mathbf{C}_{12}. \tag{3.15b}$$

The matrix $\mathbf{C}_{33}$ follows from differentiating equation (2.1) twice, viz.

$$\begin{aligned} \mathbf{Y}_3^* \mathbf{A}''' \mathbf{X}_3 - \mathbf{\Lambda}_3''' = & -6\mathbf{C}_{31} \left(\lambda \mathbf{I} - \Lambda_1\right) \mathbf{C}_{11} \mathbf{C}_{13} - 6\mathbf{C}_{31} \left(\lambda \mathbf{I} - \Lambda_1\right) \mathbf{C}_{12} \mathbf{C}_{23} \\ & - 6\mathbf{C}_{31} \left(\lambda \mathbf{I} - \Lambda_1\right) \mathbf{C}_{13} \mathbf{C}_{33} + 3\mathbf{D}_{31} \left(\lambda \mathbf{I} - \mathbf{\Lambda}_1\right) \mathbf{C}_{13} \\ & + 3\mathbf{C}_{31} \left(\lambda \mathbf{I} - \mathbf{\Lambda}_1\right) \mathbf{D}_{13} - 6\mathbf{C}_{31} \left(\lambda' \mathbf{I} - \mathbf{\Lambda}_1'\right) \mathbf{C}_{13} \\ & - 6\mathbf{C}_{32} \left(\lambda' \mathbf{I} - \mathbf{\Lambda}_2'\right) \mathbf{C}_{23} + 3\left(\mathbf{C}_{33} \mathbf{\Lambda}_3'' - \mathbf{\Lambda}_3'' \mathbf{C}_{33}\right). \end{aligned} \tag{3.16}$$

Note that $\mathbf{D}$ has the same partitioning as $\mathbf{C}$. Now that all off-diagonal entries of $\mathbf{C}$ have been found, we use (3.5) to determine the diagonal entries to fill the coefficient matrix completely.

4. Generalization. The cases discussed in the previous section provide us a way to generalize the theory of finding the first order derivatives of the eigenvectors for eigenvalues with the property that (some of) their derivatives up to the kth order are repeated, but the $(k + 1)$st order derivatives are distinct. This generalization will

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be given in this section, and for readability, we try to keep the notation as simple as possible.

Let $\mathbf{A}$, its eigenvalue and eigenvector matrix $\mathbf{\Lambda}$ and $\mathbf{X}$, be n times continuously differentiable. Then from Leibniz' rule we have

$$\mathbf{A}^{(n)}\mathbf{X} - \mathbf{X}\mathbf{\Lambda}^{(n)} = -\sum_{k=1}^{n} \binom{n}{k} \left(\mathbf{A}^{(n-k)}\mathbf{X}^{(k)} - \mathbf{X}^{(k)}\mathbf{\Lambda}^{(n-k)}\right). \tag{4.1}$$

As before, let the non-uniqueness of $\mathbf{X}$ be expressed by

$$\mathbf{X} = \bar{\mathbf{X}}\mathbf{\Gamma}, \tag{4.2}$$

where $\mathbf{\Gamma}$ is a nonsingular matrix to be determined. Note that because $\mathbf{X}$ is an eigenvector matrix, $\mathbf{\Gamma}$ has to satisfy (2.6). Since $\mathbf{A}$ is non-defective, the kth derivative of the eigenvector matrix can be expressed in terms of the eigenvectors of $\mathbf{A}$,

$$\mathbf{X}^{(k)} := \mathbf{X}\mathbf{C}_k, \qquad k = 1, \ldots, n. \tag{4.3}$$

Upon substituting (4.2) and (4.3) into (4.1), we obtain

$$\begin{aligned} &\bar{\mathbf{Y}}^*\mathbf{A}^{(n)}\mathbf{X}\mathbf{\Gamma} - \mathbf{\Gamma}\mathbf{\Lambda}^{(n)} = \\ &\quad -\mathbf{\Gamma}\sum_{k=0}^{n-1} \beta_0 \left(\mathbf{\Lambda}^{(k)}\mathbf{C}_{n-k} - \mathbf{C}_{n-k}\mathbf{\Lambda}^{(k)}\right) \\ &\quad +\mathbf{\Gamma}\sum_{k=0}^{n-1}\sum_{\gamma=1}^{n}\sum_{m_1=1}^{\alpha_1}\cdots\sum_{m_\gamma=1}^{\alpha_{\gamma-1}} (-1)^\gamma \beta_\gamma \left(\mathbf{\Lambda}^{(k)}\mathbf{C}_{m_1} - \mathbf{C}_{m_1}\mathbf{\Lambda}^{(k)}\right)\mathbf{C}_{m_2}\cdots\mathbf{C}_{m_\gamma}\mathbf{C}_{m_{\gamma+1}}, \end{aligned} \tag{4.4}$$

where

$$\alpha_p := n - k - \sum_{j=1}^{p-1} m_j - 1, \qquad p = 1, \ldots, \gamma, \tag{4.5a}$$

$$\beta_\gamma := \binom{n}{k}\binom{n-k}{m_1}\binom{n-k-m_1}{m_2}\cdots\binom{n-k-m_1-\ldots-m_{\gamma-1}}{m_\gamma}, \tag{4.5b}$$

$$m_{\gamma+1} := n - k - \sum_{j=1}^{\gamma} m_j. \tag{4.5c}$$

To determine $\mathbf{\Gamma}$, a generalization of the partitioning of the matrices $\mathbf{\Lambda}$, $\mathbf{X}$, $\mathbf{Y}^*$ and $\mathbf{C}_k$ for $k = 1, \ldots, n-1$, has to be introduced. Thus, let the eigenvalue matrix $\mathbf{\Lambda}$ be partitioned as

$$\mathbf{\Lambda} = \begin{bmatrix} \mathbf{\Lambda}_1 & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \mathbf{\Lambda}_2 & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{\Lambda}_3 & \cdots & \mathbf{0} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \ldots & \mathbf{\Lambda}_{n+1} \end{bmatrix}, \tag{4.6}$$

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such that

$$\mathbf{\Lambda} = \begin{bmatrix} \mathbf{\Lambda}_1 & \mathbf{0} \\ \mathbf{0} & \lambda\mathbf{I} \end{bmatrix}, \mathbf{\Lambda}' = \begin{bmatrix} \mathbf{\Lambda}_1' & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{\Lambda}_2' & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \lambda'\mathbf{I} \end{bmatrix}, \ldots, \tag{4.7}$$

$$\mathbf{\Lambda}^{(n)} = \begin{bmatrix} \mathbf{\Lambda}_1^{(n)} & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \mathbf{\Lambda}_2^{(n)} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{\Lambda}_3^{(n)} & \cdots & \mathbf{0} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \ldots & \mathbf{\Lambda}_{n+1}^{(n)} \end{bmatrix}.$$

Notice that $\mathbf{\Lambda}_1$ can still contain repeated eigenvalues, but not the eigenvalue λ in (4.7). On the other hand, nothing is prescribed anymore for the derivatives, which means that some diagonal entry of $\mathbf{\Lambda}_1'$ might be equal to λ'. According to the partitioning of $\mathbf{\Lambda}$ the following partitioning of $\bar{\mathbf{X}}$, $\bar{\mathbf{Y}}^*$ and $\mathbf{C}_k$ is introduced,

$$\bar{\mathbf{X}} = \begin{bmatrix} \bar{\mathbf{X}}_1 & \cdots & \bar{\mathbf{X}}_{n+1} \end{bmatrix}, \quad \bar{\mathbf{Y}}^* = \begin{bmatrix} \bar{\mathbf{Y}}_1^* \\ \vdots \\ \bar{\mathbf{Y}}_{n+1}^* \end{bmatrix}, \tag{4.8}$$

$$\mathbf{C}_m = \begin{bmatrix} \mathbf{C}_{m,11} & \mathbf{C}_{m,12} & \cdots & \mathbf{C}_{m,1(n+1)} \\ \mathbf{C}_{m,21} & \mathbf{C}_{m,22} & \cdots & \mathbf{C}_{m,2(n+1)} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{C}_{m,(n+1)1} & \mathbf{C}_{m,(n+1)2} & \cdots & \mathbf{C}_{m,nn} \end{bmatrix}.$$

To determine $\mathbf{\Gamma}_{n+1}$, the partitioning of $\mathbf{\Lambda}$, $\mathbf{X}$, $\mathbf{Y}^*$ and $\mathbf{C}$ has to be substituted in (4.4). Then $\mathbf{\Gamma}_{n+1}$ will follow from the $(n+1, n+1)$ block,

$$\begin{aligned} &\mathbf{Y}_{n+1}^* \mathbf{A}^{(n)} \mathbf{X}_{n+1} \mathbf{\Gamma}_{n+1} - \mathbf{\Gamma}_{n+1} \mathbf{\Lambda}_{n+1}^{(n)} = \\ &\quad \mathbf{\Gamma} \sum_{k=0}^{n-1} \sum_{\gamma=1}^{n} \sum_{m_1=1}^{\alpha_1} \ldots \sum_{m_\gamma=1}^{\alpha_\gamma} \sum_{p_1=1}^{n+1} \ldots \sum_{p_\gamma=1}^{n} (-1)^\gamma \beta_\gamma \\ &\qquad \times \mathbf{C}_{m_1,(n+1)p_1} \left(\lambda^{(k)} \mathbf{I} - \mathbf{\Lambda}_{p_1}^{(k)} \right) \mathbf{C}_{m_2,p_1 p_2} \cdots \mathbf{C}_{m_{\gamma+1},p_\gamma(n+1)}. \end{aligned} \tag{4.9}$$

Not all coefficient matrices can be computed since the eigenvectors are still not fixed. However, an analytical expression for each coefficient matrix can be derived from (4.4) by considering the right derivative and block matrices. As a result, we obtain the following,

$$\mathbf{Y}_{n+1}^* \mathbf{A}^{(n)} \mathbf{X}_{n+1} \mathbf{\Gamma}_{n+1} - \mathbf{\Gamma}_{n+1} \mathbf{\Lambda}_{n+1}^{(n)} = -\mathcal{L}(n, n-1, n+1, n+1) \mathbf{\Gamma}_{n+1}, \tag{4.10}$$

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where the right-hand side is found by using the following recurrence relation for $\mathcal{L}$,

(4.11)

$$\begin{aligned}&\mathcal{L}(n,m,p,q) := \\ &\quad\sum_{\ell=1}^{m}\sum_{k=\ell}^{n-1}\frac{\gamma_{k\ell}}{\ell}\left(\mathbf{Y}_p^*\mathbf{A}^{(k)}\mathbf{X}_\ell-\delta_{p\ell}\lambda^{(k)}\mathbf{I}+\mathcal{L}(k,\ell-1,p,\ell)\right)\left(\lambda^{(\ell-1)}\mathbf{I}-\mathbf{\Lambda}_\ell^{(\ell-1)}\right)^{-1} \\ &\qquad\times\left(\mathcal{L}(n-k+\ell-1,\ell,\ell,q)+\mathbf{Y}_\ell^*\mathbf{A}^{(n-k+\ell-1)}\mathbf{X}_q-\delta_{\ell q}\lambda^{(n-k+l-1)}\mathbf{I}\right).\end{aligned}$$

In this relation, the constant $\gamma_{k\ell}$ is defined as

$$\gamma_{k\ell} := \begin{cases}\binom{n}{k} & \text{if } k \geq n-k+\ell-1 \\ \binom{n}{n-k+\ell-1} & \text{if } k < n-k+\ell-1\end{cases}, \tag{4.12}$$

and

$$\mathbf{X}_q := \begin{cases}\bar{\mathbf{X}}_1 & \text{if } q=1 \\ \bar{\mathbf{X}}_q\mathbf{\Gamma}_q & \text{if } 1<q<n+1 \\ \bar{\mathbf{X}}_{n+1} & \text{if } q=n+1\end{cases}. \tag{4.13}$$

By computing the eigenvalues and eigenvectors of (4.10) the matrix $\mathbf{\Gamma}_{n+1}$ can be determined for every n.

To determine an eigenvector matrix that is continuously differentiable, (4.10) has to be solved recursively. When repeated eigenvalues occur, (4.10) has to be evaluated for the first order derivative. If (some of) the eigenvalues of the resulting matrix are still the same, then (4.10) has to be evaluated once more for the second order derivative. This process has to be repeated until (4.10) does not result in any repeated eigenvalues. At each iteration step the eigenvectors have to be updated by multiplication of the $\mathbf{\Gamma}$ matrix. This iterative process is illustrated in Figure 4.1. After that all the blocks of $\mathbf{\Gamma}$ have been determined, the only thing left is the normalization of the eigenvectors as in (3.3) taking (3.4) into account and computing the coefficient matrix $\mathbf{C}_1$.

After a continuously differentiable eigenvector matrix has been found, i.e., in fact $\mathbf{\Gamma}$, the coefficient matrix $\mathbf{C}_1$ can be determined. For this, the same recurrence relation as in the conjecture is used. Also these relations are a result of extending the procedure of the simple cases presented in the previous section,

$$\begin{aligned}C_{1,mn} &:= \frac{1}{m}\left(\lambda^{(m-1)}\mathbf{I}-\mathbf{\Lambda}_m^{(m-1)}\right)^{-1}\mathbf{\Gamma}_m^{-1} \\ &\qquad\times\left\{\mathbf{Y}_m^*\mathbf{A}^{(m)}\mathbf{X}_n+\mathcal{L}(m,m-1,m,n)\right\} \text{ if } m<n,\end{aligned} \tag{4.14a}$$

$$\begin{aligned}C_{1,mn} &:= \frac{1}{n}\mathbf{\Gamma}_m^{-1}\left\{\mathbf{Y}_m^*\mathbf{A}^{(n)}\mathbf{X}_n+\mathcal{L}(m,m-1,m,n)\right\} \\ &\qquad\times\left(\lambda^{(n-1)}\mathbf{I}-\mathbf{\Lambda}_n^{(n-1)}\right)^{-1} \text{ if } m>n.\end{aligned} \tag{4.14b}$$

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For the diagonal matrices $\mathbf{C}_{1,mm}$ for $m = 1, \dots, n+1$, it holds that only the off-diagonal entries can be determined by the following formula,

$$\begin{aligned}(4.15)\qquad & \mathbf{\Lambda}_m^{(m-1)}\mathbf{C}_{1,mm} - \mathbf{C}_{1,mm}\mathbf{\Lambda}_m^{(m-1)} := \\ & \frac{1}{m}\mathbf{\Gamma}_m^{-1}\left\{\mathbf{Y}_m^*\mathbf{A}^{(m)}\mathbf{X}_m - \mathbf{\Lambda}_m^{(m)} + \mathcal{L}(m, m-1, m, m)\right\}.\end{aligned}$$

Finally, the diagonal entries of $\mathbf{C}_1$ can then be found by

$$(4.16)\qquad c_{kk} = -\sum_{\substack{l=1\\ l\neq k}}^{N} x_{ml}c_{lk},$$

analogously as for the simple cases in the previous section. After the determination of $\mathbf{C}_1$, the first order derivative of the eigenvector matrix $\mathbf{X}'$ can be found.

The only thing that still has to be done is to find $\mathbf{\Lambda}_1'$. If $\mathbf{\Lambda}_1$ still contains repeated eigenvalues, then the whole process described in this section has to be performed for $\mathbf{\Lambda}_1$ again. If $\mathbf{\Lambda}_1$ only consists of distinct eigenvalues, then $\mathbf{\Lambda}_1$ is computed by determining the diagonal of $\mathbf{Y}_1^*\mathbf{A}'\mathbf{X}_1$, since

$$(4.17)\qquad \mathbf{Y}_1^*\mathbf{A}'\mathbf{X}_1 - \mathbf{\Lambda}_1' = -\mathbf{\Lambda}_1\mathbf{C}_{1,11} + \mathbf{C}_{1,11}\mathbf{\Lambda}_1.$$

By comparing the diagonal entries on both left and right-hand side, the statement follows.

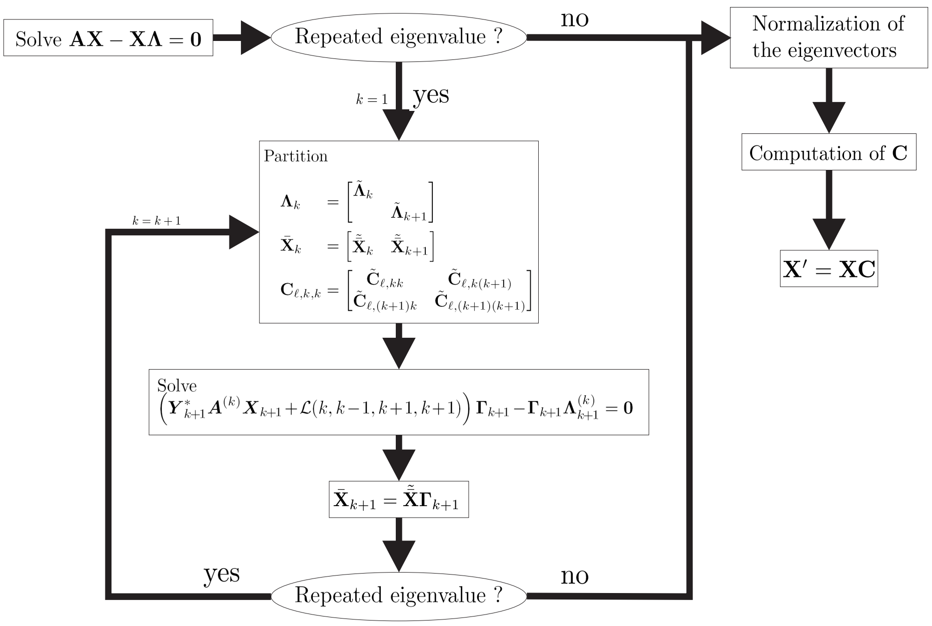

FIG. 4.1. *A flowchart representation of the way to compute* $\mathbf{\Gamma}$.

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Finally, a last remark has to be given. The fact that $\mathbf{\Lambda}_1$ can still contain repeated eigenvalues ensures that $\mathbf{\Gamma}_1$ does not have to be a diagonal matrix, but this matrix is unknown. However, the fact that $\mathbf{\Gamma}$ commutes with $\mathbf{\Lambda}$ and that no higher order derivative of $\mathbf{\Lambda}_1$ occurs, $\mathbf{\Gamma}_1$ disappears from (4.10), and therefore, definition (4.13) is justified.

5. Examples. In this section, the generalization of the method presented in the previous section will be illustrated by some examples. The first three examples show that the three simple cases discussed in Section 3 fit with the general algorithm. The fourth example is a numerical example.

Example 5.1. If all eigenvalues of $\mathbf{\Lambda}$ are distinct, then the only thing left for the eigenvectors is to normalize them according to (3.3), taking (3.4) into account. To compute the coefficient matrix $\mathbf{C}_1$ and the eigenvalue derivative matrix $\mathbf{\Lambda}'$, writing out (4.15) in coordinates for $m = 1$ results in (3.1) and (3.2), but now the values of γ_k for $k = 1, \ldots, N$ are already known from the normalization. The diagonal entries of $\mathbf{C}_1$ do not follow from (4.15), but from (4.16) which is identical to (3.5), where again all γ_k are known. □

Example 5.2. If $\mathbf{\Lambda}$ contains a repeated eigenvalue, then a partitioning (4.6) has to be performed on $\mathbf{\Lambda}$ for $n = 1$ and a similar one on the eigenvector matrix $\bar{\mathbf{X}}$ and coefficient matrix $\mathbf{C}$. This partitioning is equal to (3.6). Next, (4.10) has to be evaluated for $n = 1$. In this case, matrix $\mathcal{L}$ is equal to zero, and therefore, (4.10) indeed reduces to (3.7d). Since this eigensystem does not yield any repeated eigenvalues again, also here the normalization of the eigenvectors takes place and the computation of $\mathbf{C}_1$ can be carried out by using (4.14b), (4.14a), (4.15) and (4.16) again. □

Example 5.3. If both $\mathbf{\Lambda}$ and the eigenvalues of system (3.7d) contain repeated eigenvalues, then partitioning (4.6) has to be performed for $n = 2$. Similarly, partitioning (4.8) is applied to the eigenvector matrix $\bar{\mathbf{X}}$ and coefficient matrix $\mathbf{C}$. The result resembles the partitioning of (3.12). The evaluation of (4.10) returns the first nontrivial case, since $\mathcal{L}$ is nonzero, viz.

$$\mathcal{L}(2,1,3,3) = 2\mathbf{Y}_3^*\mathbf{A}'\mathbf{X}_1\left(\lambda\mathbf{I} - \mathbf{\Lambda}_1\right)^{-1}\mathbf{Y}_1^*\mathbf{A}'\mathbf{X}_3 = 2\bar{\mathbf{Y}}_3^*\mathbf{A}'\bar{\mathbf{X}}_1\left(\lambda\mathbf{I} - \mathbf{\Lambda}_1\right)^{-1}\bar{\mathbf{Y}}_1^*\mathbf{A}'\bar{\mathbf{X}}_3\mathbf{\Gamma}_3.$$

With this $\mathcal{L}$, (4.10) reduces to (3.14). Because this eigensystem is assumed to have only distinct eigenvalues, we can proceed by normalizing the eigenvectors and computing $\mathbf{C}_1$ in a similar way as in the previous simple case. □

Example 5.4. This example illustrates the method given by Figure 4.1 for a matrix of which we can compute the eigenvalues and eigenvectors analytically. Therefore, the results of the numerical method presented in this paper can be verified immediately, because the derivatives of the eigenvalues and eigenvectors are also available analytically. Let $\mathbf{A}$ be given by

$$A(p) := \frac{1}{2(1+p^2)}\begin{bmatrix} a_{11}(p) & a_{12}(p) & a_{13}(p) \\ a_{21}(p) & a_{22}(p) & a_{23}(p) \\ a_{31}(p) & a_{23}(p) & a_{33}(p) \end{bmatrix},$$

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with

$$\begin{aligned}
a_{11}(p) &= 2\cos(p)(-2+2p^2+(1+p^2)\cos(2p)-4p^2\sin(p)),\\
a_{12}(p) &= 8p(-2\cos(p)+\sin(2p)),\\
a_{13}(p) &= (-3+5p^2)\cos(p)-(1+p^2)\cos(3p)-4p^2\sin(2p),\\
a_{21}(p) &= 4p(-2\cos(p)+\sin(2p)),\\
a_{22}(p) &= -2\cos(p)(-5+3p^2+8\sin(p)),\\
a_{23}(p) &= 4p(-2\cos(p)+\sin(2p)),\\
a_{31}(p) &= (-3+5p^2)\cos(p)-(1+p^2)\cos(3p)-4p^2\sin(2p),\\
a_{32}(p) &= 8p(-2\cos(p)+\sin(2p)),\\
a_{33}(p) &= 2\cos(p)(-2+2p^2+(1+p^2)\cos(2p)-4p^2\sin(p)).
\end{aligned}$$

The (analytical) eigenvalues are then

$$\lambda_1(p) = \cos(3p), \quad \lambda_2(p) = 5\cos(p) - 4\sin(2p), \quad \lambda_3(p) = -3\cos(p). \tag{5.1}$$

For $p = \pi/2$, we see that $\lambda_1^{(k)} = \lambda_2^{(k)} = \lambda_3^{(k)}$ for $k = 0, 1, 2$, and $\lambda_1^{(k)} = \lambda_2^{(k)}$ for $k = 0, 1, \ldots, 5$. The eigenvectors can also be found analytically, and if normalization (3.4) at $p = \pi/2$ is used, then they are given by

$$\mathbf{X} = \begin{bmatrix} -1 & 1 & 1/p \\ 0 & -1/p & 1 \\ 1 & 1 & 1/p \end{bmatrix}. \tag{5.2}$$

In general, the analytical expressions for the eigenvalues and eigenvectors is hard, if not impossible to obtain. At $p = \pi/2$, $\mathbf{A}$ reduces to the identity matrix. Since any 3×3 matrix is a candidate for an eigenvector matrix, we just take the identity matrix. Because the analytical form of the eigenvector matrix is available, we already know that this choice of the eigenvector matrix is not continuously differentiable. To find a continuously differentiable eigenvector matrix, we use the algorithm illustrated in Figure 4.1. Note that in this example outcomes are given in 4 decimals.

Initialization step:

$$\mathbf{A} = \mathbf{I}_{3\times3},\ \mathbf{\Lambda}_1 = \emptyset,\ \mathbf{\Lambda}_2 = \mathbf{0}_{3\times3},\ \mathbf{X}_1 = \emptyset,\ \bar{\mathbf{X}}_2 = \mathbf{I}_{3\times3}.$$

Step 2:

$$\mathbf{A}' = 3\mathbf{I}_{3\times3},\ \mathbf{\Lambda}_2 = \emptyset,\ \mathbf{\Lambda}_3 = 3\mathbf{I}_{3\times3},\ \mathbf{X}_2 = \emptyset,\ \bar{\mathbf{X}}_3 = \mathbf{I}_{3\times3}.$$

Step 3:

$$\mathbf{A}'' = \mathbf{0}_{3\times3},\ \mathbf{\Lambda}_3 = \emptyset,\ \mathbf{\Lambda}_4 = \mathbf{0}_{3\times3},\ \mathbf{X}_3 = \emptyset,\ \bar{\mathbf{X}}_4 = \mathbf{I}_{3\times3}.$$

Step 4:

$$\mathbf{A}^{(3)} = \begin{bmatrix} -23.5392 & 10.8724 & 3.4608 \\ 5.4362 & -9.9216 & 5.4362 \\ 3.4608 & 10.8724 & -23.5392 \end{bmatrix},$$

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$$\mathbf{\Lambda}_4 = -3,\ \mathbf{\Lambda}_5 = -27\mathbf{I}_{2\times2},\ \mathbf{X}_4 = \begin{bmatrix} 0.4731 \\ 0.7432 \\ 0.4731 \end{bmatrix},\ \bar{\mathbf{X}}_5 = \begin{bmatrix} 0.4187 & -0.9541 \\ -0.3938 & 0.2525 \\ 0.8183 & 0.1608 \end{bmatrix}.$$

Step 5:

$$\mathbf{A}^{(4)} = \begin{bmatrix} -12.5425 & -11.7169 & -12.5425 \\ -5.8584 & 25.0849 & -5.8584 \\ -12.5425 & -11.7169 & -12.5425 \end{bmatrix},$$

$$\mathbf{\Lambda}_5 = \emptyset,\ \mathbf{\Lambda}_6 = \mathbf{0}_{2\times2},\ \mathbf{X}_5 = \emptyset,\ \bar{\mathbf{X}}_6 = \begin{bmatrix} 0.4187 & -0.9541 \\ -0.3938 & 0.2525 \\ 0.8183 & 0.1608 \end{bmatrix}.$$

Step 6:

$$\mathbf{A}^{(5)} = \begin{bmatrix} 202.5537 & -63.9949 & -40.4463 \\ -31.9975 & -36.1074 & -31.9975 \\ -40.4463 & -63.9949 & 202.5537 \end{bmatrix},$$

$$\mathbf{\Lambda}_6 = \begin{bmatrix} 3.2283 & 0 \\ 0 & 243.0000 \end{bmatrix},\ \mathbf{X}_6 = \begin{bmatrix} -0.7161 & 0.5771 \\ 0.4559 & 0 \\ -0.7161 & -0.5771 \end{bmatrix}.$$

Since no repeated eigenvalues occur anymore, the continuously differentiable eigenvector matrix has been determined up to the normalization. When the normalization (3.3) has been performed, $\mathbf{X}$ equals

$$\mathbf{X} = \begin{bmatrix} 1.0000 & -1.0000 & 0.6366 \\ -0.6366 & 0.0000 & 1.0000 \\ 1.0000 & 1.0000 & 0.6366 \end{bmatrix},$$

which, of course, is equal to the analytical solution of $\mathbf{X}$ given in (5.2) for $p = \pi/2$.

The next step is to determine $\mathbf{C}$. Because several blocks in the partitioning of $\mathbf{\Lambda}$ are empty, $\mathbf{C}$ only consists of the following blocks

$$\mathbf{C} = \begin{bmatrix} \mathbf{C}_{44} & \mathbf{C}_{46} \\ \mathbf{C}_{64} & \mathbf{C}_{66} \end{bmatrix}.$$

The blocks $\mathbf{C}_{46}$ and $\mathbf{C}_{64}$ and the off-diagonal entries of $\mathbf{C}_{66}$ can be determined by using (4.14a), (4.14b) and (4.15), respectively. The diagonal entries of $\mathbf{C}$ can be computed by using (4.16). As a consequence, $\mathbf{C}$ equals

$$\mathbf{C} = \begin{bmatrix} -0.2884 & -0.1836 & 0.0000 \\ 0.0000 & 0.0000 & 0.0000 \\ -0.1836 & 0.2884 & 0.0000 \end{bmatrix}.$$

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To conclude this example, the eigenvalue and eigenvector derivative matrix are given by

$$\mathbf{\Lambda}' = \begin{bmatrix} \mathbf{\Lambda}_4' & \\ & \mathbf{\Lambda}_6' \end{bmatrix} = \begin{bmatrix} 3 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 3 \end{bmatrix},$$

$$\mathbf{X}' = \mathbf{XC} = \begin{bmatrix} 0.0000 & 0.0000 & -0.4053 \\ 0.4053 & 0.0000 & 0.0000 \\ 0.0000 & 0.0000 & -0.4053 \end{bmatrix}.$$

Note that the outcome is of course equal to the analytical derivatives of the eigenvalues and eigenvectors as given by (5.1) and (5.2) after substitution of $p = \pi/2$. $\square$

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