Simplified Calculation of Eigenvector Derivatives

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A simplified procedure is presented for the determination of the derivatives of eigenvectors of *n*th order algebraic eigensystems. The method is applicable to symmetric or nonsymmetric systems, and requires knowledge of only one eigenvalue and its associated right and left eigenvectors. In the procedure, the matrix of the original eigensystem of rank (*n*-1) is modified to convert it to a matrix of rank *n*, which then is solved directly for a vector which, together with the eigenvector, gives the eigenvector derivative to within an arbitrary constant. The norm of the eigenvector is used to determine this constant and complete the calculation. The method is simple, since the modified *n* rank matrix is formed without matrix multiplication or extensive manipulation. Since the matrix has the same bandedness as the original eigensystems, it can be treated efficiently using the same banded equation solution algorithms that are used to find the eigenvectors.

Introduction

THE investigation of large algebraic eigensystems by means of digital computers has become economically feasible in recent years because of advances in computer efficiency and improvements in computational algorithms. Smith et al.[1] presented an extensive listing of available computer programs for solving algebraic eigensystems, primarily based on a set of ALGOL procedures published by Wilkinson and Reinsch.[2] Dong et al.[3] and Bathe and Wilson[4] developed algorithms, based on the Stodola-Vianello (power) iteration method,[5] for determining eigenvalues and associated eigenvectors of a specified portion of the spectrum of eigenvalues of an *n*th-order real symmetric eigensystem. The advantage of these algorithms is that only a reduced eigensystem of order equal to the number of eigenvalues required by the program user actually must be solved. Thus, very large systems can be solved efficiently for eigendata most useful to the analyst. Dong recently extended his algorithm to cases of nonsymmetric systems[6] by use of an approach similar to that of Clint and Jennings,[7] but requiring only the use of right eigenvectors.

The increased effectiveness of these algorithms has made possible studies of the sensitivity of eigendata to changes in system parameters, in order to investigate system design problems,[8,9] system identification (modeling) problems,[10] and random systems.[11] In a recent paper, Taylor and Kane[12] give a comprehensive review of research on eigendata sensitivity analysis, i.e., the determination of derivatives of eigendata with respect to system parameters, and present a procedure for determining derivatives of eigenvectors of arbitrary eigensystems. This work is an extension of an approach first presented by Fox and Kapoor[13] for real symmetric eigensystems, and later employed by Plaut and Huseyin[14] for nonsymmetric systems. Rogers[15] has generalized the second approach in Ref. 13 to include nonsymmetric systems.

The determination of eigenvalue derivatives is shown in Refs. 12-16 to be a straightforward and simple calculation, but the calculation of eigenvector derivatives is found to be much more complicated, and two approaches for determining these derivatives are presented. In the first, the eigenvector derivative is expressed as a sum of all the eigenvectors defined by the eigensystem. Although analytically simple, this approach becomes prohibitively expensive for large *n*th-order eigensystems, since the determination of all *n* eigenvectors is a formidable task. The second approach requires only the specified eigenvalue and associated eigenvector, but requires the premultiplication of an $(n+1)\times n$ matrix by its transpose to form an *n*th-order system of linear equations, the solution of which gives the eigenvector derivative. This matrix multiplication is a lengthy operation, and destroys any bandedness associated with the original eigensystem, a serious difficulty since most algorithms exploit the banded form of the eigensystem to reduce computational effort, computer storage requirements, and thus the need for using external memory. Also, the *n*th-order system of equations which must be solved for the eigenvector derivative often is poorly conditioned and difficult to solve. The problems associated with either of these two approaches are greatly compounded when eigenvector calculations must be repeated many times, as is typical of practical optimization problems.[8-10] Thus, the procedures employed in Refs. 8-13 for the calculation of eigenvector derivatives, although analytically straightforward, become very lengthy, and therefore costly when applied to large eigensystems.

This paper gives an alternate and simplified procedure for calculating eigenvector derivatives of arbitrary *n*th-order symmetric or nonsymmetric eigensystems, requiring only the left and right eigenvectors and the associated eigenvalue under consideration. In this procedure, the *n*th-order (*n*-1) rank system of equations, which relates the eigenvector derivative to the derivative of the matrix of the eigensystem, is directly and simply modified to form a system of equations of rank *n*. The solution of this set of equations, together with the eigenvector and its norm, is sufficient to determine the eigenvector derivative completely.

The procedure in which the (*n*-1) rank matrix is converted to a matrix of rank *n* requires only "zeroing" out certain row and column entries of the matrix of the eigensystem, and gives a matrix with exactly the same banded characteristics as the original system. The modified equations, therefore, may be solved by use of the same banded equation solving algorithms used in the eigensystem analysis. A simple matrix is presented to indicate the simplicity of the procedure.

Analytical Review

Consider an algebriac eigensystem of the form

$$[A-\lambda_i I]\{X_i\}=\{0\} \tag{1}$$

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where $[I]$ is the unit matrix, $[A]$ is a real nonsymmetric nonsingular $n \times n$ matrix, and λ_i and $\{X_i\}$ are the ith eigenvalue and right eigenvector, respectively. The left eigenvector $\{Y_i\}$ associated with λ_i is defined by the equation

$$\{Y_i\}^T[A-\lambda_i I] = \{0\}^T \tag{2a}$$

or

$$[A^T-\lambda_i I]\{Y_i\} = \{0\} \tag{2b}$$

The left and right eigenvectors are equal when $[A]=[A]^T$, i.e., when $[A]$ is symmetric. The n eigenvalues associated with $[A]$ are determined by solution of the nth order polynomial defined by

$$\det[A-\lambda I] = 0 \tag{3}$$

Assuming that the n eigenvalues are distinct, then n independent right eigenvectors exist and are biorthonormal to a set of n independent left eigenvectors, i.e.,

$$\{Y_i\}^T\{X_j\} = \delta_{ij} \tag{4}$$

where δ_{ij} is the Kronecker delta.† This relation may be written in matrix notation by first defining $n \times n$ matrices $[X]$ and $[Y]$ the ith columns of which are $\{X_i\}$ and $\{Y_i\}$, respectively. Then,

$$[Y]^T[X] = [I] \tag{5}$$

so that

$$[Y]^T = [X]^{-1} \tag{6}$$

The eigensystem, Eq. (1), may be written in the form

$$[A][X] = [X][\lambda] \tag{7}$$

where $[\lambda]$ is a diagonal matrix of eigenvalues, the entry in ith row being the eigenvalue associated with the eigenvector in the ith column of $[X]$. Then,

$$[Y]^T[A][X] = [X]^{-1}[A][X] = [\lambda] \tag{8}$$

Note that Eq. (4) is not a gage condition (norm) for $\{X_i\}$ when $\{X_i\} \neq \{Y_i\}$, since $\{Y_i\}$ always can be scaled so that Eq. (4) holds.

Solution for Eigenvector Derivatives

The derivative of the eigenvector with respect to a system parameter p is obtained by taking the derivative of Eq. (1) with respect to p,

$$(\partial/\partial p)([A-\lambda_i I]\{X_i\}) = \{0\} \tag{9}$$

which gives

$$[A-\lambda_i I]\left\{\frac{\partial X_i}{\partial p}\right\} = -\left[\frac{\partial A}{\partial p} - \frac{\partial \lambda_i}{\partial p} I\right]\{X_i\} \tag{10}$$

The eigenvalue derivative is obtained by premultiplying Eq. (10) by $\{Y_i\}^T$, and noting Eqs. (2a) and (4)

$$\frac{\partial \lambda_i}{\partial p} = \{Y_i\}^T\left[\frac{\partial A}{\partial p}\right]\{X_i\} \tag{11}$$

Then Eq. (10) becomes

$$[A-\lambda_i I]\left\{\frac{\partial X_i}{\partial p}\right\} = \{X_i\}\left(\{Y_i\}^T\left[\frac{\partial A}{\partial p}\right]\{X_i\}\right) - \left[\frac{\partial A}{\partial p}\right]\{X_i\} \tag{12a}$$

$$\equiv \{F_i\} \tag{12b}$$

†Note that the left and right eigenvectors and the eigenvalue may be complex.

The matrix on the left-hand side of Eq. (12) is of rank $(n-1)$, but the n equations are consistent, since the $\{Y_i\}^T\{F_i\} = 0$. Although these equations cannot be solved uniquely for the eigenvector derivative, the portion of the eigenvector derivative which cannot be determined uniquely from Eq. (12) can be detailed by expressing $\{\partial X_i/\partial p\}$ as a sum of all n right eigenvectors,

$$\left\{\frac{\partial X_i}{\partial p}\right\} = \sum_{k=1}^{n} c_k\{X_k\} = [X]\{C\} \tag{13}$$

where $\{C\}$ is the vector of constants c_i. Substitution of Eq. (13) into Eq. (12) and premultiplication by $[Y]^T$ gives

$$[Y]^T[A-\lambda_i I][X]\{C\} = [Y]^T\{F_i\} \tag{14a}$$

or

$$[(\lambda-\lambda_i)]\{C\} = [Y]^T\{F_i\} \tag{14b}$$

where $[(\lambda-\lambda_i)]$ denotes a diagonal matrix with elements $(\lambda_k-\lambda_i)$ at row and column k. Then

$$c_k = \frac{\{Y_k\}^T\{F_i\}}{\lambda_k-\lambda_i} \qquad i \neq k \tag{15}$$

and c_i is arbitrary. This procedure shows that the eigenvector derivative has a unique expression in terms of all of the system eigenvectors, excluding the ith one, i.e.,

$$\left\{\frac{\partial X_i}{\partial p}\right\} = \sum_{k=1}^{n} c_k\{X_k\} + c_i\{X_i\} \tag{16a}$$

$$\equiv \{V_i\} + c_i\{X_i\} \tag{16b}$$

The first vector, when substituted in Eq. (12), gives $\{F_i\}$ and the second (the ith eigenvector) is the homogeneous solution. In order to determine c_i, it is necessary to consider the norm for $\{X_i\}$, usually in the form

$$\{X_i^c\}^T[M]\{X_i\} = 1 \tag{17}$$

where $[M]$ is a symmetric nonsingular matrix, and the superscript c denotes complex conjugate. Taking the partial derivative of Eq. (17) with respect to parameter p gives

$$2Re\left(\{X_i^c\}^T[M]\left\{\frac{\partial X_i}{\partial p}\right\}\right) + \{X_i^c\}^T\left[\frac{\partial M}{\partial p}\right]\{X_i\} = 0 \tag{18}$$

where the symbol Re denotes the real part of the complex number. Substitution of Eq. (16b) into Eq. (18) gives

$$c_i = -Re(\{X_i^c\}^T[M]\{V_i\}) + \tfrac{1}{2}\{X_i^c\}^T\left[\frac{\partial M}{\partial p}\right]\{X_i\} \tag{19}$$

which completes the calculation for the eigenvector derivative. Thus, both Eq. (12) and Eq. (19), the norm condition, must be used. Finally $\{\partial Y_i/\partial p\}$ is determined by solving the set of equations

$$[A^T-\lambda_i I]\left\{\frac{\partial Y_i}{\partial p}\right\} = -\left[\frac{\partial A^T}{\partial p} - \frac{\partial \lambda_i}{\partial p} I\right]\{Y_i\} \tag{20a}$$

$$\equiv \{G_i\} \tag{20b}$$

The vector $\{G_i\}$ is orthogonal to the right eigenvector $\{X_i\}$. Following the procedure used to determine $\{\partial X_i/\partial p\}$, the quantity $\{\partial Y_i/\partial p\}$ is obtained by writing

$$\left\{\frac{\partial Y_i}{\partial p}\right\} = \sum_{k=1}^{n} d_k\{Y_k\} \equiv [Y]\{D\} \tag{21}$$

$$= \{W_i\} + d_i\{Y_i\} \tag{22}$$

In a procedure analogous to the determination of the constants c_k, $k \neq i$, the constants d_k, $k \neq 1$, may be obtained, so that $\{W_i\}$ is determined uniquely. Since Eq. (4) determines the norm of $\{Y_i\}$ if Eq. (17) holds, the constant d_i is determined by Eq. (4), which is, after differentiation,

$$\{X_i\}^T\left(\{W_i\}+d_i\{Y_i\}\right)+\left\{\frac{\partial X_i}{\partial p}\right\}^T\{Y_i\}=0 \tag{23}$$

or

$$d_i=-\left(\{V_i\}^T\{Y_i\}+\{W_i\}^T\{X_i\}+c_i\right) \tag{24}$$

This analytical procedure, first presented in Ref. 13 for symmetric eigensystems, becomes impractical for large systems, since the calculation of all n eigenvectors is a very lengthy task.

In the same manner in which the nth-order problem may be approximated by a limited number of eigenvectors (e.g., use of a limited number of so-called modes in structural dynamics problems), the eigenvector derivatives also may be approximated by using only a limited number of eigenvectors in the expansion, Eq. (13). Unfortunately, the quality of such an approximation, which is difficult to assess for a single calculation in which $m<n$ eigenvectors are employed, often has been unacceptable for test problems.

In the second procedure in Ref. 13, the nth-order (n-1) rank system in Eq. (12) is combined with Eq. (18) to form the $(n+1)\times n$ system

$$\begin{bmatrix} A-\lambda_i I \\ \hline 2Re\{X_i^c\}^T[M] \end{bmatrix}\{\partial X_i/\partial p\}=\begin{Bmatrix} F_i \\ \hline -\{X_i^c\}^T[\partial M/\partial p]\{X_i\} \end{Bmatrix} \tag{25}$$

Equation (25) is premultiplied by the transpose of the $(n+1)\times n$ matrix of coefficients on the left side of the equation to give an nth-order system, the matrix of which is of rank n. Although only the given eigenvalue and left and right eigenvectors are required, the procedure has several weaknesses:

1) The inner product of two $(n+1)\times n$ matrices must be performed, which is a lengthy computation.

2) Even when the nth-order eigensystem is banded, the $n\times n$ matrix that is developed by the inner product is fully populated. This results in additional computational expenses, since most modern computer codes for the solution of linear equations exploit the bandedness of the matrix, and since the increased storage requirements of the fully populated system may require use of external memory.

3) The $n\times n$ matrix that results is poorly conditioned and difficult to solve for $\{\partial X_i/\partial p\}$.

In the next section, a simplified procedure is presented which may be used to determine eigenvector derivatives. This procedure requires only the eigenvalue and associated right and left eigenvectors under consideration.

Simplified Calculation for Eigenvector Derivative

The basic requirement for determining the eigenvector derivative is to determine a vector $\{V_i\}$ [see Eqs. (16b)], which, when substituted in the left-hand side of Eq. (12), gives $\{F_i\}$. The eigenvector derivative then must be in the form of Eq. (16b), since the eigenvector $\{X_i\}$ is a solution of the Eq. (12) with $\{F_i\}=0$.

The difficulty in determining $\{V_i\}$ is that the matrix $[A-\lambda_i I]$ on the left-hand side of Eq. (12) is of rank $(n-1)$ and cannot be inverted. However, the homogeneous solution $\{X_i\}$ is known. This solution contains important information, best illustrated by noting that this solution may be obtained by partitioning the matrix

$$\begin{bmatrix} (A-\lambda_i I)_{11} & A_{1k} & A_{13} \\ \hline A_{k1} & (A-\lambda_i I)_{kk} & A_{k3} \\ \hline A_{31} & A_{3k} & (A-\lambda_i I)_{33} \end{bmatrix}\begin{Bmatrix} X_1 \\ \hline x_k \\ \hline X_3 \end{Bmatrix}=\begin{Bmatrix} 0 \\ \hline 0 \\ \hline 0 \end{Bmatrix} \tag{26}$$

where A_{1k}, A_{3k} are single column matrices, A_{k1} and A_{k3} are single row matrices, and $(A-\lambda_i I)_{kk}$ is the k, k element of $[A-\lambda_i I]$, X_1 and X_3 are partitioned subvectors, and x_k the kth component of the eigenvector $\{X_i\}$. Then

$$\begin{bmatrix} (A-\lambda_i I)_{11} & A_{13} \\ \hline A_{k1} & A_{k3} \\ \hline A_{31} & (A-\lambda_i I)_{33} \end{bmatrix}\begin{Bmatrix} X_1 \\ \hline X_3 \end{Bmatrix}=-x_k\begin{Bmatrix} A_{1k} \\ \hline (A-\lambda_i I)_{kk} \\ \hline A_{3k} \end{Bmatrix} \tag{27}$$

If x_k is nonzero and assigned a specified value, say 1, then the subvectors $\{X_1\}$, $\{X_3\}$ must be uniquely determined by solving the $n\times(n-1)$ system of rank $(n-1)$. The set of equations cannot be of rank $(n-2)$ since if this were the case $\{X_1\}$ and $\{X_3\}$ could be determined only to within an arbitrary constant, with x_k fixed. This cannot occur when only one right eigenvector exists, since each component is fixed once x_k is fixed. [If x_k is zero, then Eq. (26) must be repartitioned and another component in the eigenvector taken as the pivotal element to appear on the right side of Eq. (27)].

This argument also shows that when $x_k \neq 0$ the kth column of the $n\times n$ matrix in Eq. (26) is a linear combination of the remaining $(n-1)$ and that the remaining $(n-1)$ are linearly independent, since the matrix on the left-hand side of Eq. (27) is of rank $(n-1)$.

There is no assurance that the kth equation in Eq. (27) is a linear combination of the remaining $(n-1)$ equations (see the example in the following section). However, since Eq. (2b) holds, the same partitioning scheme can be applied to determine $\{Y_i\}$, starting with the kth component of $\{Y_i\}$ as arbitrary. By a similar argument to that given in the preceding showing that the kth column must be linearly dependent on the remaining $(n-1)$ columns if $x_k \neq 0$, the remaining components of $\{Y_i\}$ may be determined in terms of $y_k \neq 0$, since the kth *row* is then linearly dependent on the remaining $(n-1)$ rows. Thus, if y_k is nonzero, the kth row may be deleted in Eq. (27), and the calculation for $\{X_1\}$ and $\{X_3\}$ may be carried out simply by solving the system

$$\begin{bmatrix} (A-\lambda_i I)_{11} & A_{13} \\ \hline A_{31} & (A-\lambda_i I)_{33} \end{bmatrix}\begin{Bmatrix} X_1 \\ \hline X_3 \end{Bmatrix}=-x_k\begin{Bmatrix} A_{1k} \\ \hline A_{3k} \end{Bmatrix} \tag{28}$$

Since both x_k and y_k must be nonzero, a reasonable value k is that for which $|x_k| \cdot |y_k|$ is maximum. (If $[A]$ is symmetric, $x_k=y_k$ and the location of the component x_k with maximum absolute value should be used as the pivotal element.) However, if x_k is very small as compared to the largest component in the eigenvector $\{X_i\}$, the numerical

solution of Eq. (28) will blow up, or give inaccurate results, even if y_k is large. Fortunately, since the eigenvectors are known at the outset, they can be examined to find a value k so that both x_k and y_k are of acceptable magnitude. Then x_k can be used as the pivotal element, and Eq. (28) may be solved without difficulty for the remaining components.

Although no need exists for computing eigenvectors, since they are already known, the previous argument shows that knowledge of the left and right eigenvectors is sufficient to determine which $(n-1)$ submatrix in the matrix $[A-\lambda_i I]$ is of rank $(n-1)$, and also which $(n-1)$ submatrix may be expected to give accurate results. But matrix $[A-\lambda_i I]$ is the matrix that appears on the left-hand side of Eq. (12). Therefore, in order to determine a solution $\{V_i\}$ to Eq. (12), the matrix on the left-hand side may be partitioned as for Eq. (26), taking as the pivotal element the component of $\{V_i\}$ at the location k where $|x_k| \cdot |y_k|$ is maximum. The partitioned system is then

$$\left[\begin{array}{c|c} (A-\lambda_i I)_{11} & A_{13} \\ \hline A_{31} & (A-\lambda_i I)_{33} \end{array}\right] \left\{\begin{array}{c} V_1 \\ \hline V_3 \end{array}\right\} = -v_k \left\{\begin{array}{c} A_{1k} \\ \hline A_{3k} \end{array}\right\} + \left\{\begin{array}{c} F_1 \\ \hline F_3 \end{array}\right\} \tag{29}$$

Note that, if $v_k \neq 0$ and $\{F\} = \{0\}$, a repeated calculation for the eigenvector results. Therefore, since the eigenvector is known, set $v_k = 0$ for simplicity, and solve Eq. (29) for $\{V_1\}$, $\{V_3\}$. The complete solution for the eigenvector derivative is then

$$\left\{\frac{\partial X_i}{\partial p}\right\} = \left\{\begin{array}{c} V_1 \\ \hline 0 \\ \hline V_3 \end{array}\right\} + c_i \left\{\begin{array}{c} X_1 \\ \hline x_k \\ \hline X_3 \end{array}\right\} \tag{30}$$

where c_i is given by the norm, Eq. (19).

In practice, the partitioning operation need not be used. A simpler procedure is to set elements

$$(A-\lambda_i I)_{ki} = 0, \quad (A-\lambda_i I)_{ik} = 0, \quad i = 1,\ldots,n, \quad i \neq k,$$

$$(A-\lambda_i I)_{kk} = 1 \quad f_k = 0,$$

and directly solve the $n \times n$ set of equations

$$\left[\begin{array}{c|c|c} (A-\lambda_i I)_{11} & 0 & A_{13} \\ \hline 0 & 1 & 0 \\ \hline A_{31} & 0 & (A-\lambda_i I)_{33} \end{array}\right] \left\{\begin{array}{c} V_1 \\ \hline v_k \\ \hline V_3 \end{array}\right\} = \left\{\begin{array}{c} F_1 \\ \hline 0 \\ \hline F_3 \end{array}\right\} \tag{31}$$

The matrix on the left-hand side of Eq. (31) is of rank n, and has a determinant equal to the determinant of the matrix defined by Eq. (29). The left-hand side of Eq. (31) has exactly the same bandedness as the original eigensystem, and can be solved directly using the same banded-equation solving routines used in the solution to the eigenvalue problem.

Example

In order to illustrate the procedure, consider the eigensystem for a specified value of p to be

$$\begin{bmatrix} 1-\lambda & 0 & -2 & 0 \\ -3 & 2-\lambda & -2 & -2 \\ 0 & 0 & 3-\lambda & 0 \\ 3 & 0 & 2 & 4-\lambda \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{Bmatrix} \tag{32}$$

with eigenvalues $\lambda_i = 1, 2, 3, 4$ and associated eigenvectors

$$[X] = \begin{bmatrix} 1/\sqrt{3} & 0 & -1/2 & 0 \\ 1/\sqrt{3} & 1 & -1/2 & -1/\sqrt{2} \\ 0 & 0 & 1/2 & 0 \\ -1/\sqrt{3} & 0 & 1/2 & 1/\sqrt{2} \end{bmatrix}$$

$$[Y] = \begin{bmatrix} \sqrt{3} & 0 & 0 & \sqrt{2} \\ 0 & 1 & 0 & 0 \\ \sqrt{3} & 0 & 2 & 0 \\ 0 & 1 & 0 & \sqrt{2} \end{bmatrix} \tag{33}$$

where $[M] = [I]$. In order to determine $\{\partial X_1/\partial p\}$, $(\lambda_1 = 1)$, let the right-hand side of Eq. (12) be

$$\{F_1\} = \begin{Bmatrix} 1 \\ 2 \\ -1 \\ 2 \end{Bmatrix} \tag{34}$$

This vector, which could be developed for some form of $[\partial A/\partial p]$, has the essential property $\{Y_1\}^T\{F_1\} = 0$.

Inspection of $\{X_1\}$ and $\{Y_1\}$ shows x_3, y_2, and y_3 to be zero. Therefore, in order to implement the procedure, the first row and column of the matrix in Eq. (32) and the first row of $\{F\}$ are modified to give

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & -2 & -2 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 2 & 3 \end{bmatrix} \begin{Bmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \end{Bmatrix} = \begin{Bmatrix} 0 \\ 2 \\ -1 \\ 2 \end{Bmatrix} \tag{35}$$

Then $v_1 = 0$, $v_2 = 3$, $v_3 = -\frac{1}{2}$, $v_4 = 1$. Note that all of the equations in Eq. (32), with right-hand side given by Eq. (34) (and $\lambda_1 = 1$) are identically satisfied. Then

$$\left\{\frac{\partial X_1}{\partial p}\right\} = \begin{Bmatrix} 0 \\ 3 \\ -1/2 \\ 1 \end{Bmatrix} + c_1 \begin{Bmatrix} 1/\sqrt{3} \\ 1/\sqrt{3} \\ 0 \\ -1/\sqrt{3} \end{Bmatrix} \tag{36}$$

The value $c_1 = -\{X_1\}^T\{V_1\} = -2/3$, see Eq. (19). Note that the procedure would fail if any other row and column were chosen, since the modified 4×4 matrix would be singular.

Conclusion

The simplified procedure for determining eigenvector derivatives, presented herein, becomes more efficient than other procedures when large systems are considered, since only the eigendata associated with λ_i is required, and since the linear equations obtained through the modification procedure have the same banded form as the matrix of the original eigensystem. For numerical reasons, very few zero elements appear in $\{X_i\}$ or $\{Y_i\}$ for a large eigensystem, and so the selection of which row and column k to modify is a simple task.

In order to determine the derivatives of $\{X_i\}$ with respect to j independent parameters $p_1, \ldots, p_j$, the j different vectors $\{F\}$ associated with the matrices $[\partial A/\partial p_k]$, $k = 1, \ldots, j$ must be calculated, and these can all be stored as an $n \times j$ matrix. The modification of $[A-\lambda_1 I]$ and its conversion to upper

triangular form need take place only once, so that the determination of a vector $\{V\}$ associated with each $\{F\}$ requires only a backsubstitution maneuver. Thus, the series of derivatives $\{\partial X_i/\partial p_k\}k=1,\ldots,j$ can be calculated very efficiently by use of the present approach. Efficient computer algorithms, which exploit system bandedness, sparseness of the matrices $[\partial A/\partial p_k]$, and are based on the simplified procedure for calculating eigenvector derivatives, should make such calculations sufficiently accurate and economical to permit efficient optimization studies of large, eigenvector sensitive systems.

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