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Computation of Derivatives of Repeated Eigenvalues and Corresponding Eigenvectors by Simultaneous Iteration

Alan L. Andrew*
La Trobe University,
Bundoora, Victoria 3083, Australia
and
Roger C. E. Tan†
National University of Singapore, 0511 Singapore

I. Introduction

THE past 30 years have seen much effort[1] devoted to the development of numerical methods for computing partial derivatives (sensitivities) of eigenvalues and eigenvectors of matrices, which depend smoothly on a number of real-valued design parameters, $\rho_1, \ldots, \rho_m$. These derivatives are important in the optimum design of structures,[2] in mode tracking[3] and in model updating.[4] Until recently,[1,5–7] most of this work was restricted to the case of simple (i.e., nonrepeated) eigenvalues, although it is well known that eigenvalues often coalesce as a design structure approaches an optimum,[2,8] and, even before optimizing, repeated eigenvalues may occur when a structure has certain symmetry properties.[9] Also, as previously noted,[10] some earlier work on the repeated-eigenvalue case is flawed.

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*Senior Lecturer, School of Mathematics.

†Senior Lecturer, Department of Mathematics and Programme in Computational Science.

This Note presents a new algorithm for computing partial derivatives of repeated eigenvalues and the corresponding eigenvectors. Formally, we consider the problem

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

where $A(\rho)$ is a nondefective $n \times n$ matrix depending smoothly on $\rho = (\rho_1, \ldots, \rho_m) \in \mathbb{R}^m$ and $\lambda_i(\rho)$ and $x_i(\rho)$ are eigenvalues and the corresponding eigenvectors. We denote first- and second-order partial derivatives with respect to ρ_j by the subscripts j and jj, respectively. Our algorithm computes $\lambda_{i,j}(\rho_0)$, $\lambda_{i,jj}(\rho_0)$, and $x_{i,j}(\rho_0)$, $i = 1, \ldots, r$, when $\lambda_1(\rho_0) = \cdots = \lambda_r(\rho_0)$ and, for some constant σ, $|\lambda_1(\rho_0)-\sigma| > |\lambda_{r+1}(\rho_0)-\sigma| \geq \cdots \geq |\lambda_n(\rho_0)-\sigma|$, i.e., the r dominant eigenvalues (or r eigenvalues that can be made dominant by a suitable origin shift[11–13]) coincide at the point $\rho = \rho_0$.

Computation of derivatives of eigenvalues and (especially) eigenvectors is relatively difficult for repeated eigenvalues, partly because of the nonuniqueness of the corresponding eigenvectors.[7] (The even more difficult problem[14] for defective matrices is not considered here.) Differentiability of the eigenvectors requires that an appropriate basis be chosen for the multidimensional eigenspace corresponding to the repeated eigenvalue. This basis will not generally be known a priori. Moreover, there are well-known examples[2,8,9,15] in which, regardless of the choice of this basis, the repeated eigenvalues and the corresponding eigenvectors are not differentiable. Nevertheless, there is also a large class of important examples[15] in which repeated eigenvalues and the corresponding eigenvectors are not only differentiable but also analytic. This Note considers only the case in which all required derivatives exist.

Our main result is the previously promised[13,16] extension of our simultaneous iteration method[12] (sometimes called subspace iteration) for computing partial derivatives of eigenvalues and eigenvectors to the case where the dominant eigenvalue is repeated. We remarked previously[12,13] that the methods described in those papers could be used to compute derivatives of repeated eigenvalues (though not the corresponding eigenvectors). However, this remark was made in the context of the assumption that the eigenvectors were differentiable. As noted above, this requires a particular choice of basis for the eigenspace at $\rho = \rho_0$. This choice was indeed used in the numerical calculations reported previously.[13]

We use an idea of Mills-Curran,[7] who considered only the symmetric case, to modify the simultaneous iteration method[12] so that an arbitrary basis for the eigenspace corresponding to $\lambda_1(\rho_0) = \cdots = \lambda_r(\rho_0)$ can be used to compute $\lambda_{i,j}(\rho_0)$, $\lambda_{i,jj}(\rho_0)$, and $x_{i,j}(\rho_0)$, $i = 1, \ldots, r$, provided the $\lambda_{i,j}(\rho_0)$ are well separated. Using techniques that have been developed for direct methods,[5] our algorithm can be modified to deal with problems where the eigenvalue derivatives also are repeated. Although an iterative method is available for the simpler problem of computing derivatives of multidimensional invariant subspaces,[17] previous iterative methods for computing derivatives of individual eigenvectors[11–13,16,18,19] require that the corresponding eigenvalues be simple. When comparing our iterative method with direct[5,7] or modal-expansion[6] methods, note that the extrapolation methods previously used for simple eigenvalues[12,13,16,18] also can be used with the algorithm presented here for repeated eigenvalues, and this can increase its efficiency dramatically.

Our new algorithm is described and a summary (Theorem 1) of its main properties is given in Sec. II; Sec. III illustrates the algorithm by a simple example. More theoretical matters will be addressed in a later paper.[20] These include 1) a proof of Theorem 1 and an analysis of the rate of convergence of the iteration; 2) extension of Algorithm 1 to the case in which the $\lambda_{i,j}(\rho_0)$ are not well separated and to problems with repeated subdominant eigenvalues and to the computation of higher-order derivatives[13]; 3) consideration of questions of existence of derivatives; 4) theory of extrapolation procedures required for a valid comparison with other methods; and 5) an analysis of the numerical stability of the algorithm.

II. Simultaneous-Iteration Algorithm

The derivatives of eigenvectors depend on the normalizing condition used.[15] For definiteness, we consider the case

$$x_i^*(\rho)x_i(\rho) = 1, \qquad i = 1, \ldots, n \tag{2}$$

where the asterisk denotes complex conjugate transpose. Algorithm 1, below, is readily modified to deal with other normalizing conditions by making appropriate changes to the diagonal elements of the matrix C in step 5.

For simplicity, Algorithm 1 is shown without an origin shift, but if an origin shift is required (e.g., to compute derivatives of eigenvectors corresponding to the smallest eigenvalue) then, as before,[12,13,16] A and λ_1 should be replaced by $A - \sigma I$ and $\lambda_1 - \sigma$. Simultaneous iteration also can be used to simultaneously compute derivatives of s eigenvalues and eigenvectors where $s \geq r$ and $|\lambda_s| > |\lambda_{s+1}|$. For simplicity, we consider here only the case $s = r$, but, as with simple eigenvalues[12,16] the general case $s \geq r$ is useful if $|\lambda_r|$ is very close to $|\lambda_{r+1}|$ or if derivatives of more than r eigenvectors are required.

Algorithm 1 uses only the values at $\rho = \rho_0$ of $A, A_{,j}, A_{,jj}, \lambda_1$, and any r linearly independent right and left eigenvectors, $\hat{x}_i$ and y_i^*, respectively, corresponding to λ_1. Let $\hat{X}$ be the $n \times r$ matrix with ith column $\hat{x}_i$, and Y^* the $r \times n$ matrix with ith row y_i^*. Then, $A\hat{X} = \lambda_1 \hat{X}$ and $Y^* A = \lambda_1 Y^*$ at ρ_0. From these data, Algorithm 1 computes the required basis $x_1(\rho_0), \ldots, x_r(\rho_0)$ of the eigenspace corresponding to $\lambda_1(\rho_0)$ and the partial derivatives $\lambda_{i,j}(\rho_0), \lambda_{i,jj}(\rho_0)$, and $x_{i,j}(\rho_0), i = 1, \ldots, r$. Derivatives of left eigenvectors can be calculated similarly from the same data. If $\hat{X}(\rho_0) = X(\rho_0)$, whose columns are $x_1(\rho_0), \ldots, x_r(\rho_0)$, then the recurrence relation in step 2 of Algorithm 1 is shown readily (because $s = r$) to be equivalent to the recurrence relations

$$M(k) = (X^*X)^{-1}X^*[A_{,j}X + AU(k) - U(k)\Lambda]$$
$$U(k+1) = [A_{,j}X + AU(k) - XM(k)]\Lambda^{-1}, \quad k = 0, 1, 2, \ldots \tag{3}$$

where $\Lambda = \mathrm{diag}[\lambda_1(\rho_0), \ldots, \lambda_s(\rho_0)]$, which we previously proposed[11] and analyzed[12] for simple eigenvalues, and M in step 3 is the last $M(k)$ from Eq. (3). With simple eigenvalues, the matrix X of eigenvectors corresponding to $\lambda_1, \ldots, \lambda_s$ is already known once the eigenproblem for $A(\rho_0)$ is solved, whereas with multiple eigenvalues we know only some basis for the eigenspace. Algorithm 1 uses the known matrix $\hat{X}$ instead of X, and hence produces $\hat{U}(k)$ (defined below) instead of $U(k)$. In addition, the recurrence relation is written differently here to emphasize that P, T, Q_0 and each $Q(k)$ need to be calculated only once, and is simplified by the fact that, in the special case $s = r$ considered here, $\lambda_1(\rho_0) = \cdots = \lambda_r(\rho_0)$ so that $\Lambda = \lambda_1(\rho_0)I$. In the statement of Algorithm 1, all functions are evaluated at $\rho = \rho_0$.

Algorithm 1:

1) Compute $P = \hat{X}(\hat{X}^*\hat{X})^{-1}\hat{X}^*$, $Q_0 = A_{,j}\hat{X}$ and $T = (Q_0 - PQ_0)/\lambda_1$. Set the $n \times r$ matrix $\hat{U}(1) = T$. [It can be shown that this is equivalent to setting $\hat{U}(0) = 0$.] Select a tolerance $\delta > 0$ and a maximum number of iterations $K \in \mathbb{N}$.

2) For $k = 1, 2, \ldots,$ until $\|\hat{U}(k+1) - \hat{U}(k)\|_1 < \delta$ or $k > K$, compute $Q(k) = A\hat{U}(k)$ and

$$\hat{U}(k+1) = T + \{Q(k) + P[\lambda_1\hat{U}(k) - Q(k)]\}/\lambda_1$$

3) From the last $\hat{U}(k)$ computed in step 2, compute the $r \times r$ matrix

$$M = (\hat{X}^*\hat{X})^{-1}\hat{X}^*[Q_0 + A\hat{U}(k) - \lambda_1\hat{U}(k)]$$

Using the EIG command of MATLAB or otherwise, compute a diagonal matrix $\Lambda_1 = \mathrm{diag}(\omega_1, \ldots, \omega_r)$ and a matrix R satisfying $R\Lambda_1 = MR$ (i.e., the ω_i are the eigenvalues of M, and the columns of R are the corresponding eigenvectors). Then, ω_i is the accepted value of $\lambda_{i,j}$.

4) Let μ_i be the two-norm of the ith column of $\hat{X}R$. Compute the matrices X and V obtained from $\hat{X}R$ and $\hat{U}(k)R$, respectively, by dividing their ith columns by $\mu_i, i = 1, \ldots, r$. [This ensures that the columns of X satisfy Eq. (2).] Compute

$$E = (Y^*X)^{-1}Y^*(A_{,jj}X + 2A_{,j}V - 2V\Lambda_1)$$

The ith diagonal element of E is the accepted value of $\lambda_{i,jj}$.

5) Compute the matrix $C = (c_{il})$ defined by

$$c_{il} = \frac{e_{il}}{2(\omega_l - \omega_i)}, \qquad i, l = 1, \ldots, r, \quad i \neq l$$

and

$$c_{ii} = -x_i^* v_i - \sum_{\substack{p=1 \\ p \neq i}}^{r} c_{pi} x_i^* x_p, \qquad i = 1, \ldots, r$$

where c_{il} and e_{il} are the elements in the ith row and lth column of C and E, and x_i and v_i are the ith columns of X and V, respectively. Compute $V + XC$. The ith column of this matrix is the accepted value of $x_{i,j}$.

It can be shown[20] that, if $U(0) = 0$ in Eq. (3), then $U(k) = \hat{U}(k)G, k = 0, 1, \ldots,$ for some matrix G independent of k. Using this result and ideas from Refs. 7 and 12, the following theorem can be proved.[20]

Theorem 1. Let $A(\rho)$ and its eigenvalues and eigenvectors $\lambda_i(\rho)$ and $x_i(\rho)$ be sufficiently smooth functions of ρ in some neighborhood of $\rho = \rho_0$; let $\lambda_1(\rho_0) = \cdots = \lambda_r(\rho_0)$, $|\lambda_1(\rho_0)| > |\lambda_{r+1}(\rho_0)| \geq \cdots \geq |\lambda_n(\rho_0)|$ and let $\lambda_{i,j}(\rho_0) \neq \lambda_{l,j}(\rho_0)$ for all $i \neq l, i, l = 1, \ldots, r$. Then, the sequence $\{\hat{U}(k)\}$ defined in step 2 of Algorithm 1 converges. If also the limit of that sequence were used in place of the specific $\hat{U}(k)$ used in step 3 of Algorithm 1, then, in the absence of roundoff, the columns of X obtained in step 4 would give the basis for the eigenspace that makes the eigenvectors differentiable at ρ_0, and the values accepted for $\lambda_{i,j}, \lambda_{i,jj}$, and $x_{i,j}$ in steps 3, 4, and 5, respectively, of Algorithm 1 would be the exact values.

III. Numerical Example

If $A = SDS^{-1}$ with D diagonal, then the eigenvalues of A are the diagonal elements of D and the corresponding eigenvectors (prior to normalization) are the corresponding columns of S. In particular, for any region in which the elements of S, S^{-1}, and D are twice differentiable, the eigenvalues and eigenvectors of A are twice differentiable (even when the eigenvalues are repeated), and the smoothness requirements of Theorem 1 are satisfied. This provides a method of constructing test examples with known closed-form solution though, as with simple eigenvalues,[13] the computational effort required to construct such matrices using computer algebra packages greatly exceeds that required by Algorithm 1. We tested Algorithm 1 on several such matrices and found that, provided δ was taken sufficiently small, our computed solutions differed from the exact solution only in the last computed digit, indicating that, although Theorem 1 refers to results obtained using the limit of the sequence $\{\hat{U}(k)\}$, the specific $\hat{U}(k)$ used in Algorithm 1 is sufficient for good results.

For simplicity, we illustrate Algorithm 1 here using a small example constructed in the manner described above, with $m = 1$ (so that ρ is a scalar). Our tests also showed Algorithm 1 to be useful for larger matrices. Consider the example given by

$$S = \begin{bmatrix} \rho & 1 & 1 & 1 \\ 1 & 2\rho & 1 & 1 \\ 1 & 1 & 3\rho & 1 \\ 1 & 1 & 1 & 4\rho \end{bmatrix}$$

and

$$D = \mathrm{diag}(2\rho^2 + \rho + 1, \rho^2 + 2\rho + 1, 0.75\rho^2 + 0.5\rho + 0.3, 0.5\rho^2 + 0.3\rho + 0.1)$$

The normalized eigenvectors corresponding to the first two columns of S are $\pm(\rho, 1, 1, 1)^T/(3 + \rho^2)^{1/2}$ and $\pm(1, 2\rho, 1, 1)^T/(3 + 4\rho^2)^{1/2}$ and, at $\rho = 1$ (where the corresponding eigenvalues are repeated), their derivatives are $\pm(3, -1, -1, -1)^T/8$ and

$\pm(-4, 6, -4, -4)^T/7^{3/2}$, respectively. (Note that the sign, which is not determined by Eq. (2), must be the same for $x_{i,j}$ as for x_i.)

We applied Algorithm 1 with $\rho_0 = 1$ using MATLAB, which uses double precision, but, for convenience of display, results shown here are rounded to four decimal places.

For $\rho_0 = 1$,

$$A = \begin{bmatrix} 6.2583 & 0 & -1.2250 & -1.0333 \\ 2.2583 & 4.0000 & -1.2250 & -1.0333 \\ 4.7083 & 0 & 0.3250 & -1.0333 \\ 5.3583 & 0 & -1.2250 & -0.1333 \end{bmatrix}$$

$$A_{,j} = \begin{bmatrix} -0.8806 & 1.2583 & 1.4667 & 0.8972 \\ -4.8806 & 5.2583 & 1.4667 & 0.8972 \\ -9.8222 & 3.7083 & 4.6917 & 1.7139 \\ -10.9639 & 4.3583 & 3.0167 & 3.2306 \end{bmatrix}$$

$$A_{,jj} = \begin{bmatrix} 53.3991 & -18.7944 & -11.5306 & -7.3130 \\ 45.7324 & -14.7944 & -10.5306 & -6.6463 \\ 89.8880 & -36.4778 & -17.6472 & -12.1185 \\ 101.0102 & -41.3611 & -21.2639 & -12.4574 \end{bmatrix}$$

Because $\rho_0 = 1$, inspection of D shows that A has eigenvalues $\lambda_1 = \lambda_2 = 4$, $\lambda_3 = 1.55$, $\lambda_4 = 0.9$, and that $\lambda_{1,j} = 5$, $\lambda_{2,j} = 4$, $\lambda_{1,jj} = 4$ and $\lambda_{2,jj} = 2$. MATLAB computed right and left eigenvectors corresponding to the repeated eigenvalue λ_1 as

$$\hat{X} = \begin{bmatrix} -0.5657 & 0 \\ 0.2002 & 1.00000 \\ -0.5657 & 0 \\ -0.5657 & 0 \end{bmatrix} \quad \text{and} \quad Y = \begin{bmatrix} 0.4158 & -0.9503 \\ 0.8151 & 0 \\ -0.3357 & 0.2592 \\ -0.2238 & 0.1728 \end{bmatrix}$$

With these starting values and with $\delta = 10^{-5}$ and $K \geq 13$, it is readily checked that Algorithm 1 exits step 2 at $k = 13$ with

$$\hat{U}(k+1) = \begin{bmatrix} -0.8877 & -0.6667 \\ 0 & 0 \\ 0.4438 & 0.3333 \\ 0.4438 & 0.3333 \end{bmatrix}$$

giving

$$M = \begin{bmatrix} 6.3539 & 1.7678 \\ -1.8027 & 2.6461 \end{bmatrix}$$

whose eigenvalues, 5.0000 and 4.0000, give $\lambda_{1,j}$ and $\lambda_{2,j}$ and whose eigenvectors give R for use in step 4. The remaining steps give

$$X = \begin{bmatrix} -0.5000 & 0.3780 \\ -0.5000 & 0.7559 \\ -0.5000 & 0.3780 \\ -0.5000 & 0.3780 \end{bmatrix}, \qquad V = \begin{bmatrix} -0.3333 & 0.0000 \\ 0 & 0 \\ 0.1667 & 0.0000 \\ 0.1667 & 0.0000 \end{bmatrix}$$

$$E = \begin{bmatrix} 4.0000 & -3.0237 \\ 0.8819 & 2.0000 \end{bmatrix}, \quad \text{and} \quad C = \begin{bmatrix} 0.4167 & 1.5119 \\ 0.4410 & 1.4286 \end{bmatrix}$$

Then, the diagonal elements of E give $\lambda_{1,jj}$ and $\lambda_{2,jj}$, and the columns of

$$V + XC = \begin{bmatrix} -0.3750 & -0.2160 \\ 0.1250 & 0.3240 \\ 0.1250 & -0.2160 \\ 0.1250 & -0.2160 \end{bmatrix}$$

give the derivatives of the corresponding normalized eigenvectors.

IV. Conclusion

An earlier simultaneous-iteration method for computing derivatives of eigenvalues and the corresponding eigenvectors of nonsymmetric matrices depending smoothly on some real parameters is extended to the case of repeated eigenvalues. The proposed algorithm is illustrated by a numerical example and its properties are summarized.

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