Comput. Methods Appl. Mech. Engrg. 197 (2008) 4007–4015

Contents lists available at ScienceDirect

Comput. Methods Appl. Mech. Engrg.

journal homepage: www.elsevier.com/locate/cma

A robust algorithm for finding the eigenvalues and eigenvectors of 3×3 symmetric matrices

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ARTICLE INFO

Article history:
Received 23 October 2006
Received in revised form 21 March 2008
Accepted 25 March 2008
Available online 10 June 2008

Keywords:
Eigenvalues
Eigenvectors
Principal coordinates

ABSTRACT

Many concepts in continuum mechanics are most easily understood in principal coordinates; using these concepts in a numerical analysis requires a robust algorithm for finding the eigenvalues and eigenvectors of 3×3 symmetric matrices. A robust algorithm for solving this eigenvalue problem is presented along with an analysis of the algorithm. The special case of two or three nearly identical eigenvalues is examined in detail using an asymptotic analysis. Numerical results are shown that compare this algorithm with existing methods found in the literature. The behavior of this algorithm is shown to be more reliable than the other methods with a minimal computational cost.

1. Introduction

Many concepts in continuum mechanics are simplified when they are formulated and presented in principal coordinates. Hill [4] makes use of the "method of principal axes" in presenting a number of important concepts for solid mechanics, constitutive modeling and bifurcation theory. The method of principal axes is used to provide "a sure way through tensor algebra which can otherwise relapse into labyrinthine complexity". This statement is as true today as it was when it was published. Numerical methods for solid mechanics generally use Cartesian coordinate systems, and in doing so the form of the computational problem is quite simple. However, some of the mechanics that goes into developing the numerical problem, in particular kinematics and constitutive modeling, may be better suited to a formulation in principal coordinates. Some of these problems can be solved in other ways (see [1,3]), and some can be approximated (see [7]), but the best solution is to be able to solve the eigenvalue problem. To use principal coordinates in computational mechanics, a robust algorithm – one that gives accurate results for all conceivable cases – for finding the eigenvalues and eigenvectors of a symmetric, second-order tensor (or equivalently a 3×3 matrix) must be developed.

Since accurate solutions to the eigenvalue problem for 3×3 symmetric matrices are valuable for computational mechanics, a number of authors have developed algorithms for finding the eigenvalues and eigenvectors for these problems. Hartmann [2] provides a good review of what currently exists. The review includes two analytical methods presented by Simo and Hughes [8] and calculations are compared with a numerical solution from the LAPACK library. It is shown that while the analytical methods are faster than the numerical routine from LAPACK, for many problems the eigenvalues returned by the numerical algorithm in LAPACK are much more accurate than the analytical algorithms in Simo and Hughes [8]. Hartmann concludes that "the analytical solutions of the eigenvalue problem of symmetric second-order tensors should only be of interest in theoretical calculations". The method presented in this paper is based on an analytical solution and the accuracy exceeds that of the LAPACK library while at the same time being comparable in speed to other analytical methods. The method presented here is slightly more computationally expensive than other analytical methods, but not to the point of being a serious disadvantage. Another drawback to some of the work that has been presented in the literature is that it is not general. For example, finding the square root of a 3×3 symmetric positive definite matrix, as in [1] or [3], does not allow one to find the logarithm of that matrix. The algorithm presented here is extremely general, allowing one to calculate square roots or any other isotropic tensor function once the eigenvalues and eigenvectors are found.

In this paper we present a robust algorithm for finding the eigenvalues and eigenvectors of a 3×3 symmetric matrix. The algorithm is based on an analytical solution of the problem presented in Malvern [6]. Section 2 reviews the general algorithm from Malvern. The algorithm is analyzed by looking at the asymptotic behavior of the solution when either 2 or 3 eigenvalues are nearly identical. Based on this analysis an accurate algorithm is

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doi:10.1016/j.cma.2008.03.031

developed that solves the eigenvalue and eigenvector problem simultaneously. Furthermore, no tolerances are necessary to determine when two eigenvalues are “close”. Section 3 provides an analysis of the algorithm, comparing it to a method based on Malvern, a LAPACK routine, and the algorithms presented in Hartmann [2] and Simo and Hughes [8]. The algorithm in this paper is the only algorithm that rivals the numerical results of the LAPACK routine. Furthermore, it is shown that this algorithm is much faster than the LAPACK routine and comparable to the speed of other analytical solutions. Conclusions and areas of application are presented in Section 4.

2. Eigenvalue problem

2.1. Solution of eigenvalue problem for a 3 × 3 matrix

The eigenvalue problem for a real symmetric 3×3 matrix is well known

$$\mathbf{A} \cdot \mathbf{v} = \lambda \mathbf{v}, \tag{1}$$

where $\mathbf{A} \in \mathrm{R}^{3\times3}$, the eigenvector $\mathbf{v} \in \mathrm{R}^3$ and the eigenvalue $\lambda \in \mathrm{R}$. There are three eigenvalues, λ_i, and three associated eigenvectors, $\mathbf{v}_i$.[1] We are interested in symmetric matrices, $\mathbf{A} = \mathbf{A}^{\mathrm{T}}$, so the eigenvectors can be normalized such that $\mathbf{v}_i \cdot \mathbf{v}_j = \delta_{ij}$.[2]

The solution of the eigenvalue problem is based on the presentation by Malvern [6, pp. 91–93]. Instead of solving the original problem (1), the eigenvalue problem is solved for the deviatoric matrix. The deviatoric matrix, $\mathbf{A}'$, associated with $\mathbf{A}$ is

$$\mathbf{A}' = \mathbf{A} - \frac{1}{3}\mathbf{I}\mathrm{tr}\mathbf{A}, \tag{2}$$

where $\mathrm{tr}\mathbf{A}$ is the trace of $\mathbf{A}$ and $\mathbf{I}$ is the identity matrix. It is easy to see that the eigenvalues of the deviatoric matrix are just shifted from those of the original matrix, $\mathbf{A}$, and that the eigenvectors for the two matrices are the same. The eigenvalue problem for the deviatoric matrix given by (2) is

$$\begin{aligned} &\mathbf{A}' \cdot \mathbf{v} = \eta \mathbf{v}, \\ &\eta_i = \lambda_i - \tfrac{1}{3}\mathrm{tr}\mathbf{A}. \end{aligned} \tag{3}$$

Since $\mathrm{tr}\mathbf{A}' = 0$, the characteristic equation for the eigenvalues, η_i, is

$$\eta^3 - J_2\eta - J_3 = 0, \tag{4}$$

where J_2 and J_3 are the second and third invariants of the deviatoric matrix $\mathbf{A}'$[3]

$$J_2 = \frac{1}{2}\mathrm{tr}(\mathbf{A}' \cdot \mathbf{A}'); \quad J_3 = \det \mathbf{A}'. \tag{5}$$

The characteristic equation is a reduced cubic equation – it is missing its quadratic term – and a solution can be found using the substitution

$$\eta = 2\sqrt{\frac{J_2}{3}}\cos\alpha \tag{6}$$

in (4) and solving the resulting equation for the angle α. The solution for α is

$$\cos 3\alpha = \frac{J_3}{2}\left(\frac{3}{J_2}\right)^{3/2}. \tag{7}$$

There are three solutions to (7), α, $\alpha + 2\pi/3$ and $\alpha + 4\pi/3$, and they are shown in Fig. 1. Solving for the three angles and substituting them into (6) gives the three eigenvalues of $\mathbf{A}'$; the eigenvalues of the original matrix, $\mathbf{A}$, are found using (3).

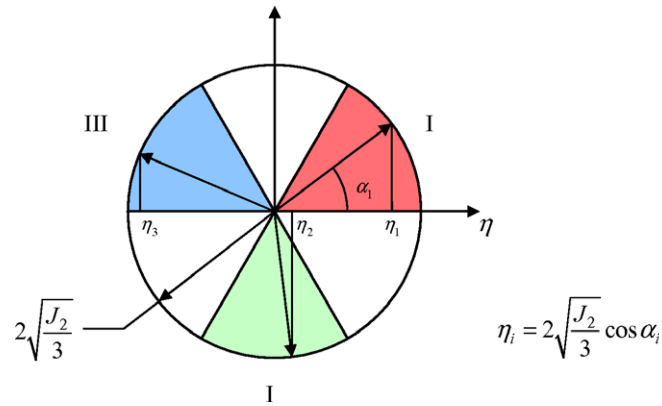

Fig. 1. The general case for finding three distinct eigenvalues. The special case of two nearly identical eigenvalues occurs as $\alpha_1 \to 0$ and $\alpha_1 \to \pi/3$. The special case of three nearly identical eigenvalues is approached as $J_2 \to 0$. As $J_2 \to 0$ the radius of the circle approaches zero.

Looking at Fig. 1 it is easy to see that the three angles associated with the roots of (5) result in eigenvalues that sum to zero, a requirement since $\mathrm{tr}\mathbf{A}' = 0$. Furthermore, the three roots lie in distinct sectors of the circle, each angle separated by $2\pi/3$, and by finding one root we could easily find the other two. In fact, this is entirely valid theoretically. However, in a numerical algorithm when two eigenvalues are nearly identical it is difficult to retain accuracy solving the problem in this manner. The following analysis provides a method of finding an accurate numerical solution when two eigenvalues are “close”.

2.2. Analysis of two nearly identical eigenvalues

Numerically, the solution presented above breaks down when we have two nearly identical eigenvalues. This is seen by making an asymptotic expansion of the eigenvalues. In addition to highlighting the problem when two eigenvalues are nearly identical, the expansion also provides a simple solution.

The analysis starts with two distinct eigenvalues, λ_1 and λ_2. Define the third eigenvalue relative to λ_2, e.g. $\lambda_3 = \lambda_2 + \Delta\lambda$. Substituting this representation into (3) the eigenvalues of the deviatoric matrix, $\mathbf{A}'$, are[4]

$$\begin{aligned} &\bar\eta_1 = \bar\eta(1-\varepsilon); \quad \bar\eta_2 = -\tfrac{1}{2}\bar\eta(1+2\varepsilon); \quad \bar\eta_3 = -\tfrac{1}{2}\bar\eta(1-4\varepsilon), \\ &\bar\eta = \tfrac{2}{3}(\lambda_1 - \lambda_2); \quad \varepsilon = \tfrac{\Delta\lambda}{3\bar\eta}. \end{aligned} \tag{8}$$

We will examine the case where $|\varepsilon| \ll 1$.

Substituting (8) into (5) we have

$$\begin{aligned} &J_2 = \tfrac{3}{4}\bar\eta^2(1 - 2\varepsilon + 4\varepsilon^2), \\ &J_3 = \tfrac{1}{4}\bar\eta^3(1 - 3\varepsilon - 6\varepsilon^2 + 8\varepsilon^3). \end{aligned} \tag{9}$$

These expressions are used in (7) to find an asymptotic expansion for $\cos 3\alpha$ in terms of ε

$$\cos 3\alpha = \mathrm{sgn}(\bar\eta)\left(1 - \frac{27}{2}\varepsilon^2 - 27\varepsilon^3 + \mathrm{O}(\varepsilon^4)\right). \tag{10}$$

Since the leading order term in the expansion is O(1) and $\varepsilon \ll 1$, we can truncate the terms of order ε^2 and higher on the right-hand side of (10). When considering numerical applications, this is valid since adding a small number to an O(1) term will result in a loss of precision. Therefore, to first order, when $\varepsilon \ll 1$ the solutions of (10) are

[1] Latin indices, $i, j, k, \ldots$, have values from 1 to 3.

[2] δ_{ij} is the Kronecker delta. $\delta_{ij} = 1$ if $i = j$ and $\delta_{ij} = 0$ if $i \neq j$.

[3] Notice that there is a sign difference in the definition of J_2 compared to the standard definition of the second invariant. This is to ensure that $J_2 > 0$ which simplifies some of the expressions that follow.

[4] The superimposed bar on the eigenvalues in (8) denote the exact solutions to the eigenvalue problem for $\mathbf{A}'$.