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Computational Aspects of the Symmetric Eigenvalue Problem of Second Order Tensors

S. Hartmann

This article is dedicated to the memory of our friend and colleague Jürgen Olschewski who devoted his life to scientific research.

The symmetric eigenvalue problem of second order tensors or 3×3 matrices, respectively, is a frequently treated topic in the field of Computational Mechanics because there exist analytical solutions. However, there are several known difficulties in the numerical computation of the analytical formulae which are recapitulated in this article. In order to show this, a sensitivity analysis is applied and a comparison of different procedures to calculate the eigenvalues, eigenvectors and eigendyades is carried out.

1 Introduction

The eigenvalue problem of symmetric second order tensors or their 3×3 matrix representation is of interest in finite element computations, for instance, where the calculation of principal stresses, strains or particular isotropic tensor functions is required. There, the computation of the eigenvalue problem is carried out several million times, which requires fast and, of course, accurate results. In the past, several analytical formulae for the computation of the right or left stretch tensors $\mathbf{U} = \sqrt{\mathbf{C}}$ and $\mathbf{V} = \sqrt{\mathbf{B}}$ and their inverses $\mathbf{U}^{-1}$ and $\mathbf{V}^{-1}$ have been carried out, where $\mathbf{C} = \mathbf{F}^T\mathbf{F}$ is the Right Cauchy-Green tensor, $\mathbf{B} = \mathbf{F}\mathbf{F}^T$ the Left Cauchy-Green tensor and $\mathbf{F}$, $\det \mathbf{F} > 0$, the deformation gradient (see, for example, Hoger and Carlson (1984); Ting (1985); Franca (1989)). At first sight it is an interesting fact that the eigenvalues and eigenvectors can be determined analytically. However, it is known that the eigenvalue computation, which is based on the solution of the characteristic polynomial, is not suitable to calculate the eigenvalues because it is connected with numerical difficulties in the case of eigenvalues being close to each other (see, for example, Schwarz et al. (1972)). Nevertheless, this topic has been treated in several publications. Franca (1989) and Simo and Hughes (1998) discuss such problems, where Franca (1989) has the objective of calculating the square root of a positive definite second order tensor. Although their benchmark example of eigenvalues with a highly different order is beyond the order of physical applications, such states may occur during an iterative solution scheme as in the non-linear finite element method. (Simo and Hughes, 1998, p.244) mentioned that the eigenvalue computation near the identity tensor yields solutions which might be wrong. Therefore, they change some analytical expressions, which, however, does not change the basic problem. In this article we investigate and recall some of these problems by employing a sensitivity analysis yielding analytical expressions of invariants which are equivalent to two or three equal eigenvalues. Furthermore, two known but stabilized algorithms are compared with the fully numerical computation of the eigenvalue problem in order to show the principal problems.

A second and subsequent problem is linked to the eigenvector computation or, if it is more of interest, the computation of the eigendyades because its precision depends essentially on the accuracy of the eigenvalues. In the Appendix a special procedure to compute the eigenvectors is summarized. As mentioned in Morman (1986), Simo and Taylor (1991), Miehe (1998) and Miehe (1993) the eigendyades can be computed not only by the eigenvector computation but much more efficiently by the evaluation of isotropic tensor function. This computation is taken into account as well.

In the following we use bold-faced roman letters for second order tensors, $\mathbf{B} = b_{ij}\vec{e}_i \otimes \vec{e}_j$, where we restrict ourselves to cartesian coordinates and geometrical vectors with an arrow, $\vec{n} = n_i\vec{e}_i$. Here, the vectors $\vec{e}_i$ define orthogonal unity vectors. Matrices are symbolized by bold-faced, capital, sans-serif letters, $\mathsf{\mathbf{B}} \in \mathbb{R}^{3\times3}$, and column vectors by $\mathsf{\mathbf{n}} \in \mathbb{R}^3$.

At first, we recall some basic relationships which are necessary for the subsequent considerations. In the symmetric eigenvalue problem

$$\mathbf{B}\vec{n} = \lambda\vec{n} \qquad \text{or} \qquad \boldsymbol{\mathsf{B}}\,\boldsymbol{\mathsf{n}} = \lambda\boldsymbol{\mathsf{n}}, \qquad \boldsymbol{\mathsf{B}} = \boldsymbol{\mathsf{B}}^T \in \mathbb{R}^{3\times3} \text{ and } \boldsymbol{\mathsf{n}} \in \mathbb{R}^3, \tag{1}$$

we look for the directions $\vec{n}$ which are mapped onto themselves by the tensor $\mathbf{B} = \mathbf{B}^T$. The proportionality factor λ is called the *eigenvalue* and the direction $\vec{n}$ concerned denotes the *eigenvector*. By means of a rearrangement of Eq.(1),

$$(\mathbf{B} - \lambda\mathbf{I})\vec{n} = \vec{0}, \quad \text{or} \quad (\boldsymbol{\mathsf{B}} - \lambda\boldsymbol{\mathsf{I}})\boldsymbol{\mathsf{n}} = \boldsymbol{\mathsf{0}}, \tag{2}$$

it is obvious that for $\vec{n} \neq \vec{0}$ the determinant of the tensor $\mathbf{B} - \lambda\mathbf{I}$ has to vanish, leading to the characteristic polynomial of third order

$$P(\lambda) = \det(\mathbf{B} - \lambda\mathbf{I}) = -\lambda^3 + \mathrm{I}_\mathbf{B}\lambda^2 - \mathrm{II}_\mathbf{B}\lambda + \mathrm{III}_\mathbf{B} = 0. \tag{3}$$

$\mathbf{I}$ and $\boldsymbol{\mathsf{I}} \in \mathbb{R}^{3\times3}$ are the identity tensor and identity matrix, respectively. The polynomial coefficients define the principal invariants

$$\mathrm{I}_\mathbf{B} = \mathrm{tr}\,\mathbf{B}, \qquad \mathrm{II}_\mathbf{B} = \frac{1}{2}\left((\mathrm{tr}\,\mathbf{B})^2 - \mathrm{tr}\,\mathbf{B}^2\right), \qquad \mathrm{III}_\mathbf{B} = \det\mathbf{B} \tag{4}$$

with the trace operator $\mathrm{tr}\,\mathbf{B} = b_{ii}$ (double ii symbolize the sum from 1 to 3). The analytical solution of the polynomial corresponds to *Cardano*'s formula. An extensive derivation of these formulae is given, for example, in Smirnow (1986), see also Bronstein and Semendjajew (1987). It is a well-known fact that in the case of symmetric tensors only real roots exist. In this case the solution reduces to the *casus irreducibilis*

$$\lambda_k = \frac{1}{3}\left(\mathrm{I}_\mathbf{B} + 2\sqrt{\mathrm{I}_\mathbf{B}^2 - 3\mathrm{II}_\mathbf{B}}\cos\frac{\beta + (k-1)2\pi}{3}\right), \quad k = 1,\ldots,3 \tag{5}$$

$$\beta = \arccos\frac{2\mathrm{I}_\mathbf{B}^3 - 9\mathrm{I}_\mathbf{B}\mathrm{II}_\mathbf{B} + 27\mathrm{III}_\mathbf{B}}{2\sqrt{(\mathrm{I}_\mathbf{B}^2 - 3\mathrm{II}_\mathbf{B})^3}}. \tag{6}$$

Positive definite tensors have merely positive eigenvalues and the three cases of Fig. 1 may occur, i.e. three distinct

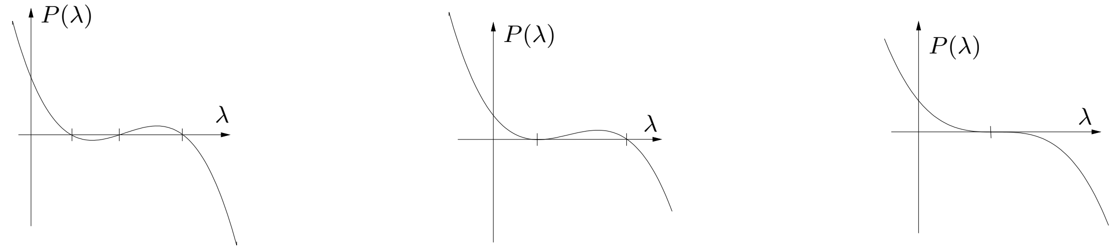

Figure 1: Curves of characteristic polynoms in the case of single and multiple eigenvalues (for positive definite tensors)

eigenvalues, $\lambda_1 \neq \lambda_2 \neq \lambda_3 \neq \lambda_1$, one multiple eigenvalue, $\lambda_1 = \lambda_2 \neq \lambda_3$, and three multiple eigenvalues, $\lambda \equiv \lambda_1 = \lambda_2 = \lambda_3$. The first question treats the computation of the eigenvalues (5), which is studied in the subsequent section. On the basis of these results we have to compute the eigenvectors $\vec{n}_k$, $k = 1, 2, 3$, or, if it is of interest, the eigendyades $\mathbf{N}_k = \vec{n}_k \otimes \vec{n}_k$, which are investigated in the sections following the next one.

2 Computation of eigenvalues

In this section we recall and discuss the numerical computation of the analytical expressions (5)-(6). In Tab. 1 an algorithm (standard version) is proposed, where we incorporate some stabilization aspects mentioned by (Press et al., 1992, p.179) for a numerically stable algorithm in wide ranges of a given tensor $\mathbf{B}$ and further interrogation commands regarding different tolerances. These commands are incorporated in the algorithmic boxes.

(Simo and Hughes, 1998, p. 244) emphasize that the computation of Eq.(5) leads to sensitive solutions "near the origin", $\mathbf{B} \approx \mathbf{I}$, and propose changing the $\arccos$ function into the $\arctan$ function

$$\arccos x = \arctan\frac{\sqrt{1 - x^2}}{x}. \tag{7}$$

This statement must be enlarged and investigated in more detail because the difficulties are only transferred but not avoided. Therefore, we have to study the basic problem of the computation of the analytical expressions and

Table 1: Eigenvalue computation using the $\arccos$-function

Given: $\mathsf{B} = \mathsf{B}^T \in \mathbb{R}^{3\times3}$
SOLVE $\mathrm{I}_{\mathsf{B}} = \operatorname{tr}\mathsf{B}$, $\mathrm{II}_{\mathsf{B}} = \frac{1}{2}(\mathrm{I}_{\mathsf{B}}^2 - \operatorname{tr}\mathsf{B}^2)$, $\mathrm{III}_{\mathsf{B}} = \det\mathsf{B}$, $p = \mathrm{I}_{\mathsf{B}}^2 - 3\mathrm{II}_{\mathsf{B}}$
IF $(p < 0)$ THEN $p = 0$
SOLVE $s = \sqrt{p}$
IF $(s < \text{tol})$ THEN $\lambda_1 = \lambda_2 = \lambda_3 = \frac{\mathrm{I}_{\mathsf{B}}}{3}$ RETURN
SOLVE $q = 2\mathrm{I}_{\mathsf{B}}^3 - 9\mathrm{I}_{\mathsf{B}}\mathrm{II}_{\mathsf{B}} + 27\mathrm{III}_{\mathsf{B}}$
IF $(\lvert q\rvert < \text{tol})$ THEN $q = 0$
SOLVE $t = \frac{q}{2s^3}$
IF $(\lvert t\rvert > 1)$ THEN $t = \text{sign}(t)$
SOLVE $\beta = (\arccos t)/3$, $r = \frac{2}{3}s$, $\lambda_k = \frac{\mathrm{I}_{\mathsf{B}}}{3} + r\cos\left(\beta + \frac{2\pi}{3}(k-1)\right)$ for $k = 1,2,3$

look at a perturbation of the eigenvalue calculation. In Tab. 2 a modified version of the algorithm of Simo and Hughes (1998) is given because in some situations the original procedure does not work very well. Here, various tolerance interrogations are introduced as well in order to obtain a more stable algorithm. The procedures of Tab. 1 and Tab. 2 are compared in an example which is discussed in the subsequent section.

3 Sensitivity analysis of the eigenvalue computation

In the following, we try to find out which cases could lead to problems in the eigenvalue computation on the basis of analytical considerations. To this end, we look at the Gateaux derivative, defined by

$$\mathsf{D}_{x_i} f(\ldots, x_i, \ldots)[\mathrm{d}x_i] = \frac{\mathrm{d}}{\mathrm{d}s} f(\ldots, x_i + s\mathrm{d}x_i, \ldots)|_{s=0}, \tag{8}$$

of the eigenvalues λ_k in Eq.(5), by a change of the original tensor $\mathbf{B}$, $\mathsf{D}_{\mathbf{B}}\,\lambda_k(\mathbf{B})[\mathbf{H}]$. This term represents the main part of an error in the tensor $\mathbf{B}$

$$\lambda_k(\mathbf{B} + \mathbf{H}) = \lambda_k(\mathbf{B}) + \mathsf{D}_{\mathbf{B}}\,\lambda_k(\mathbf{B})[\mathbf{H}] + \ldots \tag{9}$$

Then, in respect of Eq.(5), we have

$$\begin{aligned}\mathsf{D}_{\mathbf{B}}\,\lambda_k(\mathbf{B})[\mathbf{H}] &= \mathsf{D}_{\mathbf{B}}\,\lambda_k(\mathrm{I}_{\mathbf{B}}(\mathbf{B}), \mathrm{II}_{\mathbf{B}}(\mathbf{B}), \mathrm{III}_{\mathbf{B}}(\mathbf{B}))[\mathbf{H}] = \\ &= \mathsf{D}_{\mathrm{I}_{\mathbf{B}}}\,\lambda_k(z)[\mathsf{D}_{\mathbf{B}}\,\mathrm{I}_{\mathbf{B}}(\mathbf{B})[\mathbf{H}]] + \mathsf{D}_{\mathrm{II}_{\mathbf{B}}}\,\lambda_k(z)[\mathsf{D}_{\mathbf{B}}\,\mathrm{II}_{\mathbf{B}}(\mathbf{B})[\mathbf{H}]] + \mathsf{D}_{\mathrm{III}_{\mathbf{B}}}\,\lambda_k(z)[\mathsf{D}_{\mathbf{B}}\,\mathrm{III}_{\mathbf{B}}(\mathbf{B})[\mathbf{H}]] = \\ &= \frac{\partial\lambda_k}{\partial\mathrm{I}_{\mathbf{B}}}h_1 + \frac{\partial\lambda_k}{\partial\mathrm{II}_{\mathbf{B}}}h_2 + \frac{\partial\lambda_k}{\partial\mathrm{III}_{\mathbf{B}}}h_3\end{aligned} \tag{10}$$

with $z = (\mathrm{I}_{\mathbf{B}}, \mathrm{II}_{\mathbf{B}}, \mathrm{III}_{\mathbf{B}})$ and

$$\begin{aligned} h_1 &\equiv \mathsf{D}_{\mathbf{B}}\,\mathrm{I}_{\mathbf{B}}(\mathbf{B})[\mathbf{H}] = \mathbf{I}\cdot\mathbf{H}, \\ h_2 &\equiv \mathsf{D}_{\mathbf{B}}\,\mathrm{II}_{\mathbf{B}}(\mathbf{B})[\mathbf{H}] = (\mathrm{I}_{\mathbf{B}}\mathbf{I} - \mathbf{B})\cdot\mathbf{H}, \\ h_3 &\equiv \mathsf{D}_{\mathbf{B}}\,\mathrm{III}_{\mathbf{B}}(\mathbf{B})[\mathbf{H}] = \mathrm{III}_{\mathbf{B}}\mathbf{B}^{-1}\cdot\mathbf{H} = (\operatorname{adj}\mathbf{B})\cdot\mathbf{H}. \end{aligned}$$

Here, we have assumed a symmetric tensor $\mathbf{B}$. Then

$$\operatorname{adj}\mathbf{B} = \mathbf{B}^2 - \mathrm{I}_{\mathbf{B}}\mathbf{B} + \mathrm{II}_{\mathbf{B}}\mathbf{I} \tag{11}$$

Table 2: Eigenvalue computation using the $\arctan$-function

Given: $\mathbf{B} = \mathbf{B}^T \in \mathbb{R}^{3\times 3}$
SOLVE $$\begin{aligned} \mathrm{I}_{\mathbf{B}} &= \mathrm{tr}\,\mathbf{B} \\ \mathrm{II}_{\mathbf{B}} &= \frac{1}{2}(\mathrm{I}_{\mathbf{B}}^2 - \mathrm{tr}\,\mathbf{B}^2) \\ \mathrm{III}_{\mathbf{B}} &= \det \mathbf{B} \\ p &= \mathrm{II}_{\mathbf{B}} - \frac{1}{3}\mathrm{I}_{\mathbf{B}}^2 \\ q &= -\frac{2}{27}\mathrm{I}_{\mathbf{B}}^3 + \frac{1}{3}\mathrm{I}_{\mathbf{B}}\mathrm{II}_{\mathbf{B}} - \mathrm{III}_{\mathbf{B}} \end{aligned}$$
IF $(p > -\mathrm{tol})$ THEN $\lambda_1 = \lambda_2 = \lambda_3 = \frac{\mathrm{I}_{\mathbf{B}}}{3}$ RETURN
SOLVE $$t = \frac{-q}{2\sqrt{(-p)^3/27}}$$
IF $(\|t\| > 1)$ THEN $t = \mathrm{sign}(t)$
SOLVE $$\begin{aligned} s &= 2\sqrt{\frac{-p}{3}} \\ r &= \frac{\sqrt{1-t^2}}{t} \\ \beta &= \frac{1}{3}\arctan r \\ \lambda_k &= \frac{\mathrm{I}_{\mathbf{B}}}{3} + s\cos\left(\beta + \frac{2\pi}{3}(k-1)\right) \quad \text{for } k = 1,2,3 \end{aligned}$$

defines the adjoint of a tensor. The partial derivatives in (10) are given by

$$\frac{\partial \lambda_k}{\partial \mathrm{I}_{\mathbf{B}}} = \frac{1}{3}\left(1 + \frac{2\mathrm{I}_{\mathbf{B}}}{p}\cos\alpha_k - \frac{2}{3}p\sin\alpha_k\,\frac{\partial\beta}{\partial \mathrm{I}_{\mathbf{B}}}\right), \tag{12}$$

$$\frac{\partial \lambda_k}{\partial \mathrm{II}_{\mathbf{B}}} = \frac{1}{3}\left(-\frac{3}{p}\cos\alpha_k - \frac{2}{3}p\sin\alpha_k\,\frac{\partial\beta}{\partial \mathrm{II}_{\mathbf{B}}}\right), \tag{13}$$

$$\frac{\partial \lambda_k}{\partial \mathrm{III}_{\mathbf{B}}} = -\frac{2}{3}p\sin\alpha_k\,\frac{\partial\beta}{\partial \mathrm{III}_{\mathbf{B}}}, \tag{14}$$

where we introduce the abbreviations $p = \sqrt{\mathrm{I}_{\mathbf{B}}^2 - 3\mathrm{II}_{\mathbf{B}}}$ and $\alpha_k = \frac{1}{3}(\beta + (k-1)2\pi)$. Furthermore, we need the derivatives $\frac{\partial\beta}{\partial \mathrm{I}_{\mathbf{B}}}$, $\frac{\partial\beta}{\partial \mathrm{II}_{\mathbf{B}}}$ and $\frac{\partial\beta}{\partial \mathrm{III}_{\mathbf{B}}}$ for β given in Eq.(6). Because from the form $\beta = \arccos\left(\frac{g(\mathrm{I}_{\mathbf{B}},\mathrm{II}_{\mathbf{B}},\mathrm{III}_{\mathbf{B}})}{h(\mathrm{I}_{\mathbf{B}},\mathrm{II}_{\mathbf{B}})}\right)$ with

$$g(\mathrm{I}_{\mathbf{B}},\mathrm{II}_{\mathbf{B}},\mathrm{III}_{\mathbf{B}}) \equiv 2\mathrm{I}_{\mathbf{B}}^3 - 9\mathrm{I}_{\mathbf{B}}\mathrm{II}_{\mathbf{B}} + 27\mathrm{III}_{\mathbf{B}} \qquad \text{and} \qquad h(\mathrm{I}_{\mathbf{B}},\mathrm{II}_{\mathbf{B}}) \equiv 2\sqrt{\left(\mathrm{I}_{\mathbf{B}}^2 - 3\mathrm{II}_{\mathbf{B}}\right)^3} \tag{15}$$

we have

$$\frac{\partial\beta}{\partial x} = -\frac{1}{\sqrt{1-\left(\frac{g}{h}\right)^2}}\,\frac{\frac{\partial g}{\partial x}\,h - g\frac{\partial h}{\partial x}}{h^2}, \qquad x = \mathrm{I}_{\mathbf{B}},\mathrm{II}_{\mathbf{B}} \tag{16}$$

$$\frac{\partial\beta}{\partial \mathrm{III}_{\mathbf{B}}} = -\frac{1}{\sqrt{1-\left(\frac{g}{h}\right)^2}}\,\frac{1}{h}\,\frac{\partial g}{\partial \mathrm{III}_{\mathbf{B}}}. \tag{17}$$

Now, we see in Eqns.(12) and (13) that for the case $p \to 0$, i.e.

$$\mathrm{I}_{\mathbf{B}}^2 - 2\mathrm{II}_{\mathbf{B}} \longrightarrow 0 \tag{18}$$

the derivatives are not limited. Additionally, in Eqns.(16) and (17) the case $h \approx g$

$$2\mathrm{I}_{\mathbf{B}}^3 - 9\mathrm{I}_{\mathbf{B}}\mathrm{II}_{\mathbf{B}} + 27\mathrm{III}_{\mathbf{B}} \approx 2\left(\mathrm{I}_{\mathbf{B}}^2 - 3\mathrm{II}_{\mathbf{B}}\right)^{3/2} \tag{19}$$

might cause numerical difficulties. Other cases could be very large invariants $\mathrm{I}_{\mathbf{B}}$, $\mathrm{II}_{\mathbf{B}}$ or $\mathrm{III}_{\mathbf{B}}$ which are beyond physical orders and therefore not of interest.

Case (18) occurs in the case of spherical tensors, i.e. nearly three equal eigenvalues. In order to show this, we look at the second invariant of the deviator of the tensor $\mathbf{B}$, namely $\mathbf{B}^D = \mathbf{B} - \frac{1}{3}(\mathrm{tr}\,\mathbf{B})\mathbf{I}$,

$$J_2(\mathbf{B}) = \frac{1}{2}\left((\mathrm{tr}\,\mathbf{B}^D)^2 - \mathbf{B}^D \cdot \mathbf{B}^D\right) = -\frac{1}{2}\mathbf{B}^D \cdot \mathbf{B}^D = -\frac{1}{3}(\mathrm{I}_{\mathbf{B}}^2 - 3\mathrm{II}_{\mathbf{B}}) \leq 0, \tag{20}$$

i.e. in the case of a vanishing deviator relation (18) occurs. Then, the tensor becomes a spherical tensor and we have three equal eigenvalues. The dot symbolizes the inner product of two second order tensors, $\mathbf{A} \cdot \mathbf{B} = a_{ij}b_{ij}$.

The second problematic case (19) concerns two equal eigenvalues, $\lambda_i = \lambda_j \neq \lambda_k$. In order to show this, we first look at the right-hand side of Eq.(19) leading to

$$2\left(\mathrm{I}_{\mathbf{B}}^2 - 3\mathrm{II}_{\mathbf{B}}\right)^{3/2} = 2(\lambda_k - \lambda_i)^3 = 2(\lambda_k^3 - 3\lambda_k^2\lambda_i + 3\lambda_k\lambda_i^2 - \lambda_i^3). \tag{21}$$

The left-hand side is given by means of

$$\mathrm{I}_{\mathbf{B}} = 2\lambda_i + \lambda_k \quad \rightarrow \quad \mathrm{I}_{\mathbf{B}}^3 = 8\lambda_i^3 + 12\lambda_i^2\lambda_k + 6\lambda_i\lambda_k^2 + \lambda_k^3 \tag{22}$$

$$\mathrm{II}_{\mathbf{B}} = \lambda_i^2 + 2\lambda_i\lambda_k \quad \rightarrow \quad \mathrm{I}_{\mathbf{B}}\mathrm{II}_{\mathbf{B}} = 2\lambda_i^3 + 5\lambda_i^2\lambda_k + 2\lambda_i\lambda_k^2 \tag{23}$$

$$\mathrm{III}_{\mathbf{B}} = \lambda_i^2\lambda_k \tag{24}$$

and leads to the relation

$$2\mathrm{I}_{\mathbf{B}}^3 - 9\mathrm{I}_{\mathbf{B}}\mathrm{II}_{\mathbf{B}} + 27\mathrm{III}_{\mathbf{B}} = 2(\lambda_k^3 - 3\lambda_k^2\lambda_i + 3\lambda_k\lambda_i^2 - \lambda_i^3), \tag{25}$$

which is equivalent to Eq.(21). Incidentally, for two equal eigenvalues there is a connection between the third invariant of the deviator

$$J_3(\mathbf{B}) = \det \mathbf{B}^D = \frac{1}{27}\left(2\mathrm{I}_{\mathbf{B}}^3 - 9\mathrm{I}_{\mathbf{B}}\mathrm{II}_{\mathbf{B}} + 27\mathrm{III}_{\mathbf{B}}\right) \tag{26}$$

and the second invariant J_2 of Eq.(20), namely

$$27J_3 \approx 2(-3J_2)^{3/2}. \tag{27}$$

As a result we have obtained two relations of invariants, namely relation (27) and $J_2 \rightarrow 0$. Both define indicators that the eigenvalue computation could fail if procedures based on analytical expressions are applied.

Using the $\arctan$ function instead of the $\arccos$ function temporarily avoids the case $g/h > 1$ in $\arccos(g/h)$ (see definitions (15)) which might be caused by numerical inaccuracies. However, the argument $1 - t^2$ could be negative due to numerical inaccuracies, see Tab. 2. In other words, the sensitivity of the eigenvalue problem does not vanish.

A proposed perturbation of the eigenvalues $\tilde{\lambda}_1 = \lambda_1(1+\delta)$, $\tilde{\lambda}_2 = \lambda_2(1-\delta)$ and $\tilde{\lambda}_3 = \lambda_3/((1+\delta)(1-\delta))$, see Miehe (1993), overcomes the distinction of different equations of the solution. However, the computation of the eigenvectors or eigendyades, and accordingly the calculation of isotropic tensor functions fundamentally depends on the precision of the eigenvalues and therefore we have to accept additional inaccuracies.

The numerical sensitivity of the closed form solution of symmetric eigenvalue problems is already known (see, for example, (Schwarz et al., 1972, p.106 ff.) and (Kielbasinski and Schwetlick, 1988, p.354 ff.)) because an accumulation of points occurs near multiple roots and therefore the points are difficult to distinguish. It is worth thinking about the purely numerical solution utilizing iterative solution schemes, because these procedures are much more stable. In order to emphasize the basic problem, we investigate an example of a perturbed spherical tensor and compare different procedures.

4 Example

Let us look at the matrix

$$\mathbf{B} = \begin{bmatrix} 1 & & \\ & 1 + \frac{\epsilon}{4} & \frac{\sqrt{3}\epsilon}{4} \\ & \frac{\sqrt{3}\epsilon}{4} & 1 + \frac{3\epsilon}{4} \end{bmatrix}, \tag{28}$$

which is used to study the behaviour of different methods using the factor ϵ, $0 < \epsilon < 1$. We have the exact eigenvalues $\lambda_1 = 1$, $\lambda_2 = 1$ and $\lambda_3 = 1 + \epsilon$ and the eigenvectors

$$\mathbf{n}_1 = \left\{ \begin{array}{c} 1 \\ 0 \\ 0 \end{array} \right\}, \quad \mathbf{n}_2 = \left\{ \begin{array}{c} 0 \\ -\sqrt{3}/2 \\ 1/2 \end{array} \right\}, \quad \mathbf{n}_3 = \left\{ \begin{array}{c} 0 \\ -1/2 \\ -\sqrt{3}/2 \end{array} \right\}.$$

Selecting an arbitrary B_{11}, so that we have three distinct eigenvalues, does not alter the problem under consideration. Now, we apply the algorithms of Tab. 1 and 2 and an iterative solution scheme; here, the double precision version of the LAPACK driver routine DSYEV of (Anderson et al., 1992, p.211) is applied. The calculations are carried out on a PENTIUM III/600 PC under LINUX operating system utilizing the g77 FORTRAN compiler. The eigenvalues are investigated for different perturbations ϵ, where we obtain the results of Tab. 3. In the case

Table 3: Eigenvalue computation using different methods

$\epsilon = 10^{-3}$	λ_1	λ_2	λ_3
exact	0.1000000000000000E+01	0.1000000000000000E+01	0.1001000000000000E+01
arccos method	0.9999999999997780E+00	0.9999999999997780E+00	0.1001000000000445E+01
arctan method	0.9999999999998613E+00	0.9999999999998613E+00	0.1001000000000278E+01
LAPACK-routine	0.1000000000000000E+01	0.1000000000000000E+01	0.1001000000000000E+01
$\epsilon = 10^{-5}$	λ_1	λ_2	λ_3
exact	0.1000000000000000E+01	0.1000000000000000E+01	0.1000010000000000E+01
arccos method	0.9999975598691122E+00	0.1000003333333333E+01	0.1000009106797554E+01
arctan method	0.9999976429858176E+00	0.1000003170570670E+01	0.1000009186443512E+01
LAPACK-routine	0.1000000000000000E+01	0.1000000000000000E+01	0.1000010000000000E+01
$\epsilon = 10^{-7}$	λ_1	λ_2	λ_3
exact	0.1000000000000000E+01	0.1000000000000000E+01	0.1000000100000000E+01
arccos method	0.9999999718730994E+00	0.1000000033333333E+01	0.1000000094793567E+01
arctan method	0.1000000033333333E+01	0.1000000033333333E+01	0.1000000033333333E+01
LAPACK-routine	0.9999999999999999E+00	0.1000000000000000E+01	0.1000000100000000E+01

of $\epsilon = 10^{-3}$ the results are quite satisfactory. The accuracy of the closed solution decreases rapidly for smaller $\epsilon = 10^{-3}$, i.e. as the eigenvalues become closer the results deteriorate. For a tolerance $\text{tol} = 10^{-14}$ the arctan version yields three equal eigenvalues in the case of $\epsilon = 10^{-7}$ (see Tab. 1 and 2). The iterative solution leads to the most reliable technique (in respect of the error bounds of the numerical symmetric eigenvalue problem, see (Anderson et al., 1992, pp.53-54) and the literature cited therein).

If we look at the computation time, the analytical solutions might be preferred. In a finite element calculation the eigenvalue problem has to be computed several million times. Therefore, we solve the eigenvalue problem 20,000,000 times. Tab. 4 shows a comparison between the algorithm of Tab. 2, called (a), and the iterative LAPACK routine, called (b). The collapse of the arctan version for $\epsilon = 10^{-7}$ lies in the detection of multiple eigenvalues and leads to a fast but inaccurate solution. The closed form solution is twice as fast as the iterative method. However, the total computational costs are very small in comparison to practical finite element applications. Moreover, the applied LAPACK algorithms have been developed for large eigenvalue problems and calculate all machine precision numbers in each call. Thus, the comparison is questionable. A specially adapted iterative scheme can save much more time. However, this lies beyond the scope of the article.

The aforementioned problems do not only occur for two equal eigenvalues. As mentioned before, inaccurate results occur in the case of three multiple eigenvalues as well. In such cases, an iterative method has to be given priority.

A further important aspect touches on the affect of inaccuracies on the eigenvector $\vec{n}_k$ and eigendyade computation $\mathbf{N}_k = \vec{n}_k \otimes \vec{n}_k$, which are shown in Appendix A and B. In the case of the eigenvector computation we revert to the aforementioned example. The calculation of the eigenvectors shown in Tab. 5 only turns out to be reliable under certain circumstances, because we have to calculate the difference of two non-precise eigenvalues (see Tab. 3). If the user-defined tolerance tol in Tab. 5 is too small, we obtain basic inaccuracies in the eigenvectors. This might yield $\mathbf{B}^* = \mathbf{Q}^T\mathbf{B}\mathbf{Q}$ to be a non-diagonal matrix, i.e. the off-diagonal coefficients are of the order of the eigenvalues. On the other hand, if tol is too large, the algorithm detects three equal eigenvalues.

If we look at the efficiency of the eigenvector computation, we again solve the eigenvalues and eigenvectors 20,000,000 times to produce the results of Tab. 4. In case (b) we apply the eigenvalue calculation of Tab. 2 and the eigenvector computation of Tab. 5 and compare them with the iterative LAPACK routine. The iterative scheme is twice as slow as the closed form solution, but has the advantage of a robust calculation.

Table 4: Comparison of computation time from the point of view of closed form solution and iterative method (a) eigenvalue computation (b) eigenvalue and eigenvector computation

		$\epsilon = 10^{-3}$	$\epsilon = 10^{-5}$	$\epsilon = 10^{-7}$
closed form solution	(a)	52 [s]	59 [s]	22 [s]
	(b)	1.21 [min]	1.24 [min]	26 [s]
iterative solution	(a)	1.48 [min]	1.48 [min]	1.48 [min]
	(b)	2.55 [min]	2.55 [min]	3.00 [min]

The third aspect of the sensitivity of the eigenvalue computation treats its influence on the eigendyade computation during the calculation of an isotropic tensor function. In Appendix B the numerical calculation is summarized. In order to get an impression of the sensitivity of the calculation, we deal again with the example (28) and look for $\mathbf{f}(\mathbf{B}) = \exp\mathbf{B} = \sum_{k=1}^{3}(\exp\lambda_k)\vec{n}_k \otimes \vec{n}_k$ with the analytical solution

$$\mathbf{f}(\mathbf{B}) = \frac{1}{4}\begin{bmatrix} 4e & & \\ & e(3+e^{\epsilon}) & \sqrt{3}e(e^{\epsilon}-1) \\ & \sqrt{3}e(e^{\epsilon}-1) & e(1+3e^{\epsilon}) \end{bmatrix}. \tag{29}$$

In the case of $\epsilon = 10^{-8}$ and the tolerance tol $= 10^{-10}$, which is used in Tab. 7, the analytical and the numerical solution do not correspond. The algorithm behaves in a very unstable manner. Therefore, we had to assume a higher tolerance tol, which, however, could yield only diagonal terms in $\mathbf{f}(\mathbf{B})$.

Finally, we study the necessary computational work of isotropic tensor functions. In the case of $\epsilon = 10^{-3}$, see Eq.(29), the calculation of $\mathbf{f}(\mathbf{B}) = \exp\mathbf{B}$ using $\mathbf{B}$ in Eq.(28) needs for 2×10^7 evaluations 1.51 [min] if one uses the eigenvector calculation of Tab. 5. By means of the direct eigendyade calculation of the algorithm in Tab. 7 only 1.16 [min] is required. The eigenvalues were calculated by means of the $\arccos$-method contained in Tab. 1.

5 Conclusions

In this article we have related investigations derived in Numerical Mathematics in the context of the symmetric eigenvalue problem of 3×3 matrices to methods applied in Computational Mechanics. In this respect a sensitivity analysis is applied to the eigenvalue computation using the analytical solution which is based of the characteristic polynomial. As a result two expression are found expressing difficulties for spherical tensors and a relation between the second and third invariant of the deviator. Both relations are connected to three and two equal eigenvalues and could be indicators for switching between procedures based on the analytical expressions and fully numerical algorithms.

Additionally, different procedures of the eigenvalue computation of symmetric second order tensors are compared, namely the original formulation of Cardano's rule using the $\arccos$ function, a reformulation using the $\arctan$ function and a fully numerical method. The analytical formulations always yield larger inaccuracies for nearly equal eigenvalues as it is estimated by the sensitivity analysis. The extratime of the fully numerical method is neglectable to the total time of computation in a practical finite element application.

In conlusion, the analytical solutions of the eigenvalue problem of symmetric second order tensors should only be of interest in theoretical considerations. In practical applications, however, the numerical procedures have to be preferred since they yield much more accurate and trustworthy solutions.

Appendix

A Computation of eigenvectors

The calculation of the eigenvectors $\vec{n}_k$, which correspond to the eigenvalues λ_k, is well-known. However, a concrete implementation is not known to the author and, accordingly, shown in the following. In the case of the eigenvector calculation one has to solve the homogeneous linear system of equation $(2)_2$ and prescribe one or two components of the eigenvectors $\mathbf{n}_k$. However, we have to introduce different cases depending on the number of equal eigenvalues.

In the case of three different eigenvalues $\lambda_1 \neq \lambda_2 \neq \lambda_3 \neq \lambda_1$ the matrix $\mathbf{B} - \lambda_k \mathbf{I}$ has a maximum of rank 2 and leads to three different eigenvectors with unique directions. Here, we propose the following procedure: first of all, we set the first coefficient of the eigenvector identical to 1 and solve a resulting linear system of two equations. Here, we choose

$$\begin{bmatrix} b_{11}-\lambda & b_{12} & b_{31} \\ b_{12} & b_{22}-\lambda & b_{23} \\ b_{31} & b_{23} & b_{33}-\lambda \end{bmatrix} \left\{ \begin{array}{c} 1 \\ v_2 \\ v_3 \end{array} \right\} = \left\{ \begin{array}{c} 0 \\ 0 \\ 0 \end{array} \right\},$$

and solve the last two equations

$$\begin{bmatrix} b_{22}-\lambda & b_{23} \\ b_{23} & b_{33}-\lambda \end{bmatrix} \left\{ \begin{array}{c} v_2 \\ v_3 \end{array} \right\} = \left\{ \begin{array}{c} -b_{12} \\ -b_{31} \end{array} \right\} \tag{30}$$

producing the solution

$$\left\{ \begin{array}{c} v_2 \\ v_3 \end{array} \right\} = \left\{ \begin{array}{c} \dfrac{b_{31}b_{23} - (b_{33}-\lambda)b_{12}}{(b_{22}-\lambda)(b_{33}-\lambda) - b_{23}^2} \\ \dfrac{b_{12}b_{23} - (b_{22}-\lambda)b_{31}}{(b_{22}-\lambda)(b_{33}-\lambda) - b_{23}^2} \end{array} \right\}. \tag{31}$$

If $(b_{22}-\lambda)(b_{33}-\lambda) - b_{23}^2 = 0$, then both equations are linear dependent. In this case we choose $v_2 = 1$ and obtain

$$\begin{bmatrix} b_{11}-\lambda & b_{12} & b_{31} \\ b_{12} & b_{22}-\lambda & b_{23} \\ b_{31} & b_{23} & b_{33}-\lambda \end{bmatrix} \left\{ \begin{array}{c} v_1 \\ 1 \\ v_3 \end{array} \right\} = \left\{ \begin{array}{c} 0 \\ 0 \\ 0 \end{array} \right\}$$

with the resulting equations

$$\begin{bmatrix} b_{11}-\lambda & b_{31} \\ b_{23} & b_{33}-\lambda \end{bmatrix} \left\{ \begin{array}{c} v_1 \\ v_3 \end{array} \right\} = \left\{ \begin{array}{c} -b_{12} \\ -b_{23} \end{array} \right\} \tag{32}$$

and the solution

$$\left\{ \begin{array}{c} v_1 \\ v_3 \end{array} \right\} = \left\{ \begin{array}{c} \dfrac{b_{23}b_{31} - (b_{33}-\lambda)b_{12}}{(b_{11}-\lambda)(b_{33}-\lambda) - b_{31}^2} \\ \dfrac{b_{12}b_{31} - (b_{11}-\lambda)b_{23}}{(b_{11}-\lambda)(b_{33}-\lambda) - b_{31}^2} \end{array} \right\}. \tag{33}$$

If the denominator of (32) is also identical to zero, we must choose $v_3 = 1$ and solve

$$\begin{bmatrix} b_{11}-\lambda & b_{12} & b_{31} \\ b_{12} & b_{22}-\lambda & b_{23} \\ b_{31} & b_{23} & b_{33}-\lambda \end{bmatrix} \left\{ \begin{array}{c} v_1 \\ v_2 \\ 1 \end{array} \right\} = \left\{ \begin{array}{c} 0 \\ 0 \\ 0 \end{array} \right\},$$

i.e.

$$\begin{bmatrix} b_{11}-\lambda & b_{12} \\ b_{12} & b_{22}-\lambda \end{bmatrix} \left\{ \begin{array}{c} v_1 \\ v_2 \end{array} \right\} = \left\{ \begin{array}{c} -b_{31} \\ -b_{23} \end{array} \right\} \tag{34}$$

with the result

$$\left\{ \begin{array}{c} v_1 \\ v_2 \end{array} \right\} = \left\{ \begin{array}{c} \dfrac{b_{23}b_{12} - (b_{22}-\lambda)b_{31}}{(b_{11}-\lambda)(b_{22}-\lambda) - b_{12}^2} \\ \dfrac{b_{31}b_{12} - (b_{11}-\lambda)b_{23}}{(b_{11}-\lambda)(b_{22}-\lambda) - b_{12}^2} \end{array} \right\}. \tag{35}$$

This procedure has to be carried out for each eigenvalue, so that we obtain three different eigenvectors. However, it is more convenient to calculate only two eigenvectors and solve the last one by means of the cross product, because all eigenvectors should lead to a right-handed coordinate system.

If we have two identical eigenvalues, then we obtain a single eigenvector resulting from the unique eigenvalue and an additional rank deficiency, so that we can choose a further coefficient of the eigenvector. Then, we obtain further equations from the linear systems (30), (32) and (34): $v_1 = v_2 = 1$:

$$\begin{bmatrix} b_{22}-\lambda & b_{23} \\ b_{23} & b_{33}-\lambda \end{bmatrix} \left\{ \begin{array}{c} 1 \\ v_3 \end{array} \right\} = \left\{ \begin{array}{c} -b_{12} \\ -b_{31} \end{array} \right\} \Longrightarrow v_3 = \frac{-b_{23}-b_{31}}{b_{33}-\lambda} \tag{36}$$

$v_2 = v_3 = 1$:

$$\begin{bmatrix} b_{11}-\lambda & b_{31} \\ b_{31} & b_{33}-\lambda \end{bmatrix} \left\{ \begin{array}{c} v_1 \\ 1 \end{array} \right\} = \left\{ \begin{array}{c} -b_{12} \\ -b_{23} \end{array} \right\} \Longrightarrow v_1 = \frac{-b_{31}-b_{12}}{b_{11}-\lambda} \tag{37}$$

$v_3 = v_1 = 1$:

$$\begin{bmatrix} b_{11}-\lambda & b_{12} \\ b_{12} & b_{22}-\lambda \end{bmatrix} \left\{ \begin{array}{c} 1 \\ v_2 \end{array} \right\} = \left\{ \begin{array}{c} -b_{31} \\ -b_{23} \end{array} \right\} \Longrightarrow v_2 = \frac{-b_{12}-b_{23}}{b_{22}-\lambda} \tag{38}$$

Again, the third eigenvector can be solved by the cross product.

In the case of three identical eigenvalues, we obtain a further rank deficiency. Then, the eigenvectors are arbitrary. We choose $[\mathbf{n}_1\mathbf{n}_2\mathbf{n}_3] = [\mathbf{e}_1\mathbf{e}_2\mathbf{e}_3]$. Since the "length" of the eigenvectors is arbitrary, we normalize them by

$$\mathbf{n}_i = \frac{\mathbf{v}_i}{\|\mathbf{v}_i\|} \text{ with } \|\mathbf{v}_i\| = \sqrt{v_{(i)1}^2 + v_{(i)2}^2 + v_{(i)3}^2}. \tag{39}$$

The algorithm is depicted in Tab. 5 and 6.

Table 5: Calculation of the matrix $\mathbf{Q} = [\mathbf{n}_1\mathbf{n}_2\mathbf{n}_3]$ containing the eigenvectors columnwise

Given $\mathbf{B} = \mathbf{B}^T \in \mathbb{R}^{3\times 3}$, $\lambda_1, \lambda_2, \lambda_3$
Control number of equal eigenvalues
Compute $d_1 = \lvert\lambda_1 - \lambda_2\rvert$, $d_2 = \lvert\lambda_2 - \lambda_3\rvert$, $d_3 = \lvert\lambda_3 - \lambda_1\rvert$
3 equal eigenvalues
IF $((d_1 < \text{tol})$ and $(d_2 < \text{tol})$ and $(d_3 < \text{tol}))$ THEN $\mathbf{Q} = \mathbf{I}$ RETURN
2 equal eigenvalues
IF $(d_1 < \text{tol})$ THEN
Compute $\mathbf{n}_3, \mathbf{n}_1$ according to Tab. 6 and $\mathbf{n}_2 = \mathbf{n}_3 \times \mathbf{n}_1$
ELSE IF $(d_2 < \text{tol})$ THEN
Compute $\mathbf{n}_1, \mathbf{n}_2$ according to Tab. 6 and $\mathbf{n}_3 = \mathbf{n}_1 \times \mathbf{n}_2$
ELSE IF $(d_3 < \text{tol})$ THEN
Compute $\mathbf{n}_2, \mathbf{n}_1$ according to Tab. 6 and $\mathbf{n}_3 = \mathbf{n}_1 \times \mathbf{n}_2$
Distinct eigenvalues
ELSE
Compute $\mathbf{n}_1, \mathbf{n}_2$ according to Tab. 6 and $\mathbf{n}_3 = \mathbf{n}_1 \times \mathbf{n}_2$
END IF
RETURN

B Computation of eigendyades

We finally look at the computation of the eigendyades $\mathbf{N}_k = \vec{n}_k \otimes \vec{n}_k$, i.e. particular tensor functions $\mathbf{f}(\mathbf{B})$ like $\ln \mathbf{B}$, $\exp \mathbf{B}$ or $\mathbf{B}^{1/2}$. In the case of distinct eigenvalues these tensor functions are represented by

$$\mathbf{f}(\mathbf{B}) = \sum_{k=1}^{3} f(\lambda_k)\vec{n}_k \otimes \vec{n}_k = \left(\mathrm{III}_{\mathbf{B}}\lambda_k^{-1}\mathbf{I} + (\lambda_k - \mathrm{I}_{\mathbf{B}})\mathbf{B} + \mathbf{B}^2\right) D_k^{-1}, \tag{40}$$

Table 6: Computation of eigenvectors for given eigenvalue λ_k.

Given: $\mathbf{B} = \mathbf{B}^T \in \mathbb{R}^{3\times3}$ and λ	
Compute	$D = (b_{22} - \lambda)(b_{33} - \lambda) - b_{23}^2$
IF $(\|D\| > \text{tol})$ THEN	$\begin{Bmatrix} v_1 \\ v_2 \\ v_3 \end{Bmatrix} = \frac{1}{D} \begin{Bmatrix} D \\ b_{31}b_{23} - (b_{33} - \lambda)b_{12} \\ b_{12}b_{23} - (b_{22} - \lambda)b_{31} \end{Bmatrix}$ GOTO 1
Compute	$D = (b_{11} - \lambda)(b_{33} - \lambda) - b_{31}^2$
IF $(\|D\| > \text{tol})$ THEN	$\begin{Bmatrix} v_1 \\ v_2 \\ v_3 \end{Bmatrix} = \frac{1}{D} \begin{Bmatrix} b_{23}b_{31} - (b_{33} - \lambda)b_{12} \\ D \\ b_{12}b_{31} - (b_{11} - \lambda)b_{23} \end{Bmatrix}$ GOTO 1
Compute	$D = (b_{11} - \lambda)(b_{22} - \lambda) - b_{12}^2$
IF $(\|D\| > \text{tol})$ THEN	$\begin{Bmatrix} v_1 \\ v_2 \\ v_3 \end{Bmatrix} = \frac{1}{D} \begin{Bmatrix} b_{23}b_{12} - (b_{22} - \lambda)b_{31} \\ b_{31}b_{12} - (b_{11} - \lambda)b_{23} \\ D \end{Bmatrix}$ GOTO 1
Compute	$D = b_{33} - \lambda$
IF $(\|D\| > \text{tol})$ THEN	$\begin{Bmatrix} v_1 \\ v_2 \\ v_3 \end{Bmatrix} = \frac{1}{D} \begin{Bmatrix} D \\ D \\ -b_{23} - b_{31} \end{Bmatrix}$ GOTO 1
Compute	$D = b_{11} - \lambda$
IF $(\|D\| > \text{tol})$ THEN	$\begin{Bmatrix} v_1 \\ v_2 \\ v_3 \end{Bmatrix} = \frac{1}{D} \begin{Bmatrix} -b_{31} - b_{12} \\ D \\ D \end{Bmatrix}$ GOTO 1
Compute	$D = b_{22} - \lambda$
IF $(\|D\| > \text{tol})$ THEN	$\begin{Bmatrix} v_1 \\ v_2 \\ v_3 \end{Bmatrix} = \frac{1}{D} \begin{Bmatrix} D \\ -b_{12} - b_{23} \\ D \end{Bmatrix}$ GOTO 1
1	$n = \|\mathbf{v}\| = \sqrt{v_1^2 + v_2^2 + v_3^2}$
	$\boxed{\mathbf{n} = \frac{1}{n}\mathbf{v}}$

see Ting (1985), Morman (1986), Simo and Taylor (1991) and Miehe (1993), i.e. the eigendyades have the representation of an isotropic tensor function

$$\mathbf{N}_k = \vec{n}_k \otimes \vec{n}_k = \left(\mathrm{III}_{\mathbf{B}}\lambda_k^{-1}\mathbf{I} + (\lambda_k - \mathrm{I}_{\mathbf{B}})\mathbf{B} + \mathbf{B}^2\right) D_k^{-1} \tag{41}$$

with

$$D_k = \prod_{i=1\backslash k}^{3} (\lambda_i - \lambda_k) = 2\lambda_k^2 - \lambda_k \mathrm{I}_{\mathbf{B}} + \mathrm{III}_{\mathbf{B}}\lambda_k^{-1}, \qquad k = 1, \ldots, 3. \tag{42}$$

In this context we have to point out that the equivalent form of Eq.(41)

$$\mathbf{N}_k = \frac{\Pi_{i=1\backslash k}^{3}(\lambda_i \mathbf{I} - \mathbf{B})}{D_k} \tag{43}$$

is already known as Sylvester's theorem, see (Bowen and Wang, 1976, p.144). In the case of two equal eigenvalues $\lambda_1 = \lambda_2 \neq \lambda_3$, see (Morman, 1986, Eq.(15)), we have by means of

$$\mathbf{B} = \sum_{k=1}^{3} \lambda_k \vec{n}_k \otimes \vec{n}_k = \lambda_1 \mathbf{I} + (\lambda_3 - \lambda_1)\vec{n}_3 \otimes \vec{n}_3 \tag{44}$$

the isotropic tensor function

$$\mathbf{f}(\mathbf{B}) = f(\lambda_1)\mathbf{I} + (f(\lambda_3) - f(\lambda_1))\vec{n}_3 \otimes \vec{n}_3 \tag{45}$$

with

$$\mathbf{N}_3 = \vec{n}_3 \otimes \vec{n}_3 = \left(\mathrm{III}_{\mathbf{B}}\lambda_3^{-1}\mathbf{I} + (\lambda_3 - \mathrm{I}_{\mathbf{B}})\mathbf{B} + \mathbf{B}^2\right) D_3^{-1}, \tag{46}$$

$D_3 = 2\lambda_3^2 - \lambda_3 \mathrm{I}_{\mathbf{B}} + \mathrm{III}_{\mathbf{B}}\lambda_3^{-1}$, $D_1 = D_2 = 0$. Now, the eigendyades $\mathbf{N}_1$ and $\mathbf{N}_2$ are not unique. In the case of three equal eigenvalues $\lambda \equiv \lambda_1 = \lambda_2 = \lambda_3$ we have

$$\mathbf{B} = \lambda \mathbf{I} \qquad \text{bzw.} \qquad \mathbf{f}(\mathbf{B}) = f(\lambda)\mathbf{I}. \tag{47}$$

Tab. 7 shows a possible algorithmic treatment of the eigendyade calculation.

Table 7: Computation of isotropic tensor functions in spectral representation

Given $\mathbf{B} = \mathbf{B}^T \in \mathbb{R}^{3\times3}$, $\lambda_1, \lambda_2, \lambda_3$	
Compute	$d_1 = \lambda_1 - \lambda_2, \quad d_2 = \lambda_2 - \lambda_3, \quad d_3 = \lambda_3 - \lambda_1$
3 equal eigenvalues	
IF $((\lvert d_1\rvert < \text{tol})$ and $(\lvert d_2\rvert < \text{tol})$ and $(\lvert d_3\rvert < \text{tol}))$	
	THEN $\boxed{\mathbf{f} = f(\lambda_1)\mathbf{I}}$ RETURN
Compute $\mathbf{B}^2$	
2 equal eigenvalues	
IF $(\lvert d_1\rvert < \text{tol})$ THEN	
Compute	$D_3 = -d_2 d_3$
	$\mathbf{N}_3 = (\lambda_1^2\mathbf{I} - 2\lambda_1\mathbf{B} + \mathbf{B}^2)/D_3$
	$\boxed{\mathbf{f} = f(\lambda_1)\mathbf{I} + (f(\lambda_3) - f(\lambda_1))\mathbf{N}_3}$
ELSE IF $(\lvert d_2\rvert < \text{tol})$ THEN	
Compute	$D_1 = -d_1 d_3$
	$\mathbf{N}_1 = (\lambda_2^2\mathbf{I} - 2\lambda_2\mathbf{B} + \mathbf{B}^2)/D_1$
	$\boxed{\mathbf{f} = f(\lambda_2)\mathbf{I} + (f(\lambda_1) - f(\lambda_2))\mathbf{N}_1}$
ELSE IF $(\lvert d_3\rvert < \text{tol})$ THEN	
Compute	$D_2 = -d_1 d_2$
	$\mathbf{N}_2 = (\lambda_3^2\mathbf{I} - 2\lambda_3\mathbf{B} + \mathbf{B}^2)/D_2$
	$\boxed{\mathbf{f} = f(\lambda_3)\mathbf{I} + (f(\lambda_2) - f(\lambda_3))\mathbf{N}_2}$
END IF	
RETURN	
3 distinct eigenvalues	
Compute	$D_1 = -d_1 d_3, \quad D_2 = -d_1 d_2, \quad D_3 = -d_2 d_3$
	$h_1 = (\lambda_2\lambda_3)/D_1, \quad h_2 = -(\lambda_2 + \lambda_3)/D_1, \quad h_3 = 1/D_1$
	$\mathbf{N}_1 = h_1\mathbf{I} + h_2\mathbf{B} + h_3\mathbf{B}^2$
	$h_2 = (\lambda_1\lambda_3)/D_2, \quad h_2 = -(\lambda_1 + \lambda_3)/D_2, \quad h_3 = 1/D_2$
	$\mathbf{N}_2 = h_1\mathbf{I} + h_2\mathbf{B} + h_3\mathbf{B}^2$
	$h_1 = (\lambda_1\lambda_2)/D_3, \quad h_2 = -(\lambda_1 + \lambda_2)/D_3, \quad h_3 = 1/D_3$
	$\mathbf{N}_3 = h_1\mathbf{I} + h_2\mathbf{B} + h_3\mathbf{B}^2$
Compute	$\boxed{\mathbf{f} = f(\lambda_1)\mathbf{N}_1 + f(\lambda_2)\mathbf{N}_2 + f(\lambda_3)\mathbf{N}_3}$

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Address: Priv.-Doz. Dr.-Ing. Stefan Hartmann, Institut für Mechanik, Universität Kassel, Mönchebergstr.7, D-34125 Kassel.
email: hart@ifm.maschinenbau.uni-kassel.de.