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A simple spectral representation of a second-order symmetric tensor and its variation

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ABSTRACT

The spectral decomposition of a second-order, symmetric tensor is widely adopted in many fields of Computational Mechanics. As an example, in elasto-plasticity under large strain and rotations, given the Cauchy deformation tensor, it is a fundamental step to compute the logarithmic strain tensor.

Recently, this approach has also been adopted in small-strain isotropic plasticity to reconstruct the stress tensor as a function of its eigenvalues, allowing the formulation of predictor–corrector return algorithms in the invariants space. These algorithms not only reduce the number of unknowns at the constitutive level, but also allow the correct handling of stress states in which the plastic normals are undefined, thus ensuring a better convergence with respect to the standard approach.

While the eigenvalues of a symmetric, second-order tensor can be simply computed as a function of the tensor invariants, the computation of its eigenbasis can be more difficult, especially when two or more eigenvalues are coincident. Moreover, when a Newton–Raphson algorithm is adopted to solve nonlinear problems in Computational Mechanics, also the tensorial derivatives of the eigenbasis, whose computation is still more complicated, are required to assemble the tangent matrix.

A simple and comprehensive method is presented, which can be adopted to compute a closed form representation of a second-order tensor, as well as their derivatives with respect to the tensor itself, allowing a simpler and numerically accurate implementation of spectral decomposition of a tensor in Computational Mechanics applications.

1. Introduction

This paper presents important developments regarding the eigenvalues and eigenvectors of a symmetric second-order tensor and the determination of the associated basis required for its spectral representation. The results here presented apply to situations involving isotropic scalar-valued functions and isotropic tensor-valued functions of a symmetric second-order tensor.

For instance, the findings of this article are useful for the integration of constitutive laws of isotropic materials and in finite deformations (e.g., to compute the logarithmic strain tensor from the displacement gradient).

The numerical integration of isotropic elasto-plastic constitutive laws can be more efficiently carried out by formulating the return algorithms in terms of eigenvalues of the elastic strain tensor (e.g. Borja et al., 2003 and de Souza Neto et al., 2008), or in the invariants elastic strain space (Panteghini and Lagioia, 2018, 2022). Differently from the standard approach (de Souza Neto et al., 2008), an invariant-based return algorithm allows the correct handling of stress states in which the plastic normals are undefined.

These two integration algorithms require the spectral representation of the stress, as well as the determination of its derivatives to assemble the stiffness matrix. Unfortunately, their determination using the approach described in the literature is very cumbersome (see e.g., de Souza Neto et al., 2008; Borja et al., 2003), particularly when two or three eigenvalues coincide. In this case, in fact, the derivative of the stress spectral representation is usually computed as a limit case, which requires the employment of the de L'Hôpital rule to be solved (see, e.g. Ogden, 1984 or de Souza Neto et al., 2008).

These difficulties certainly make these invariant-based integration algorithms, even if more efficient, less attractive with respect to standard return algorithms formulated in terms of full tensorial components.

About the applications in large strain theories, to avoid the complexity of the standard procedure, commercial codes (e.g. SIMULIA Abaqus Dassault Systèmes, 2020) often employ approximate formulations to numerically integrate the logarithmic strain in finite deformation analyses. Some Authors suggest, for specific isotropic functions, to resort to their numerical approximation based on series expansion

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(e.g. Ortiz et al., 2001; de Souza Neto, 2001; Hudobivnik and Korelc, 2016). However, it should be noted that these series-based procedures, even if simpler and numerically efficient, can be hardly adopted when the isotropic functions are not known explicitly (i.e., for instance, in the case of the integration of the isotropic elastoplastic materials described above).

The writer has later discovered that Ogden (1984) incidentally describes, in an exercise contained in his book, a very important result, which to the best of his knowledge, seems to have been missed by the vast majority of the research community. He suggests a very simple method for retrieving a closed-form expression for the basis of the spectral decomposition of a second-order tensor which does not require the computation of the originating eigenvectors. This result has later been reported also by Miehe (1993), who, however, states that “the formulation above is restricted to the case of distinct eigenvalues of the tensor”. Moreover, the same Author (Miehe, 1998) points out that such an approach requires the inversion of the second-order tensor, which severely restricts the applicability of the method. de Souza Neto et al. (2008) describe a very cumbersome method to evaluate both the basis and their spin. They also state that “...a methodology similar to that adopted here was introduced by Miehe (1993, 1998a), where a particularly compact representation for the function derivative is used. However, the compact representation allows only the computation of the derivative at invertible arguments and cannot be used...”.

In this paper it is mathematically shown that indeed the basis required for the spectral representation of a symmetric second-order tensor can be derived without the computationally expensive evaluation of the associated eigenvectors. It is also shown that this can also be directly derived from the secular (or characteristic) equation of the tensor, without any assumptions about the invertibility of the second-order tensor. Most importantly, it is clarified how the result can be particularized to the case of two and three coinciding eigenvalues, hence removing the strong limitation of the approach described by Miehe (1993, 1998) which *de facto* prevents the application of this extremely useful result. This paper also provides the tensor derivatives of the basis, i.e. its *spin*. Moreover, it is presented a simple and generic approach to compute the spectral representation of isotropic tensor-valued functions, as well as their derivatives with respect to the tensor variable itself. The proposed procedures can be practically adopted in computational mechanics since all limitations of the procedures available in the literature have been removed (the approach of de Souza Neto et al., 2008 does not have such limitations but is laborious to implement). Finally, two applications are presented for isotropic elastoplasticity and for the evaluation of the logarithmic strain tensor in finite deformations.

2. Eigenvalues, eigenvectors and spectral representation of a symmetric, second-order tensor T

Given the symmetric, second-order tensor T , its (ordered) eigenvalues λ_i and their corresponding eigenvectors n_i are obtained by solving the eigenvalues–eigenvectors problem (Malvern, 1969):

$$(T - \lambda I)n = 0 \quad \text{under the condition} \quad n^T n = 1 \quad (1)$$

being I the second-order identity tensor. The principal components λ_i can be obtained by solving the third-order scalar equation in λ , namely the *secular equation* (Malvern, 1969):

$$\lambda^3 - I_1 \lambda^2 + I_2 \lambda - I_3 = 0 \quad (2)$$

The coefficients

$$I_1 = \text{tr}(T) \quad (3)$$

$$I_2 = \frac{1}{2} (I_1^2 - T : T^T) \quad (4)$$

$$I_3 = \det(T) \quad (5)$$

are the *invariants* of T , since their values do not depend on the reference system in which T is expressed. The three *ordered* solutions of Eq. (2) are the eigenvalues of the problem described in Eq. (1). As explained in Malvern (1969), they can be computed in closed form as:

$$\begin{aligned} \lambda_I &= \frac{I_1}{3} + \frac{2}{\sqrt{3}} \sqrt{J_2} \sin\left(\theta + \frac{2}{3}\pi\right) \\ \lambda_{II} &= \frac{I_1}{3} + \frac{2}{\sqrt{3}} \sqrt{J_2} \sin(\theta) \\ \lambda_{III} &= \frac{I_1}{3} + \frac{2}{\sqrt{3}} \sqrt{J_2} \sin\left(\theta - \frac{2}{3}\pi\right) \end{aligned} \quad (6)$$

where

$$J_2 = \frac{1}{2} t : t \quad (7)$$

$$J_3 = \det(t)$$

are the invariants of the second-order, deviatoric symmetric tensor $t = T - (I_1/3)I$, and the Lode’s angle θ is defined as

$$\theta = \frac{1}{3} \arcsin\left(-\frac{\sqrt{27}}{2} \frac{J_3}{\sqrt{J_2^3}}\right) \quad (8)$$

where $-\pi/6 \leq \theta \leq \pi/6$.

It is well known that the second-order symmetric tensor T can be expressed as a function of its eigenvalues λ_i and the corresponding eigenvectors n_i by resorting to the spectral theorem¹:

$$T = \sum \lambda_i n_i \otimes n_i = \lambda_i N_i \quad (9)$$

where N_i is the eigenbasis of T related to λ_i .

It is well known (see, e.g. Bertram, 2021) that, in closed form, an equivalent spectral representation of T as a function of its m *distinct* eigenvalues and eigenbasis, i.e.

$$T = \sum_{i=1}^m \lambda_i \tilde{N}_i$$

can be obtained by resorting to the Sylvester’s formula:

$$\tilde{N}_i = \begin{cases} \prod_{j=1, j \neq i}^m \frac{1}{\lambda_i - \lambda_j} (T - \lambda_j I) & \text{if } m > 1 \\ I & \text{if } m = 1 \end{cases} \quad (10)$$

Let us observe that, if $m = 3$ (no repeated eigenvalues), $N_i = \tilde{N}_i$. The strong limitation of this approach is represented by the non-differentiability of Eq. (10) in the case of $m \neq 3$. This is due to the fact that a repeated eigenvalue results to be not differentiable. Moreover, also in the case of $m = 3$, the differentiation, even if conceptually not complicated, is not very easy, resulting in a rather long expression (here, for brevity, the results of this differentiation are not reported. The Reader may refer to de Souza Neto, 2001).

3. A simple, closed-form expression for the eigenbasis of T

We will consider three cases, as a function of the multiplicity of the eigenvalues λ_i :

1. $\lambda_I > \lambda_{II} > \lambda_{III}$
2. $\lambda_I > \lambda_{II} = \lambda_{III}$ or $\lambda_I = \lambda_{II} > \lambda_{III}$
3. $\lambda_I = \lambda_{II} = \lambda_{III}$

¹ Let us consider that, unless otherwise specified, it is always intended $\sum f_i = \sum_{i=I,II,III} f_i$.

A general property of the eigenbasis N_i

We will initially prove that it results:

$$\sum N_i = I \quad (11)$$

Let us consider that the i -th eigenvalue and eigenvector of T will satisfy Eq. (1), i.e.

$$T n_i = \lambda_i n_i \quad (12)$$

Since n_i is a unit vector, it results

$$n_i^T T n_i = T : (n_i \otimes n_i) = \lambda_i (n_i^T n_i) = \lambda_i$$

one can compute the first invariant I_1 in the principal coordinate system as

$$I_1 = \text{tr}(T) = T : I = \sum \lambda_i = T : \sum N_i$$

From this equation it must result

$$T : I = T : \sum N_i$$

This condition yields

$$\sum N_i = I$$

Case (i): $\lambda_1 > \lambda_{II} > \lambda_{III}$

Let us observe that it is well known (see, e.g., Ogden, 1984; Bertram, 2021; Vallée et al., 2006, or Itskov, 2015) that the spectral theorem

$$T = \sum \lambda_i (n_i \otimes n_i) = \sum \lambda_i N_i \quad (13)$$

can be written as

$$T = \sum \lambda_i \frac{d\lambda_i}{dT}$$

i.e., that it simply results:

$$N_i = \frac{d\lambda_i}{dT}$$

By considering the symmetry of T , the derivatives of the invariants I_1 , I_2 and I_3 , defined by Eq. (3), (4) and (5) with respect to T are:

$$\frac{dI_1}{dT} = I \quad (14)$$

$$\frac{dI_2}{dT} = I_1 I - T \quad (15)$$

$$\frac{dI_3}{dT} = I_3 T^{-1} = \text{adj}(T) \quad (16)$$

where $\text{adj}(T)$ denotes the adjugate matrix of T . By substituting the property (11) and the spectral theorem (13) into Eq. (14) and (15) respectively, one obtains:

$$\frac{dI_1}{dT} = \sum N_i \quad (17)$$

$$\frac{dI_2}{dT} = I_1 I - \sum \lambda_i N_i \quad (18)$$

Finally, by resorting to the spectral theorem (13), one can write Eq. (16) as²

$$\frac{dI_3}{dT} = \sum (\lambda_j \lambda_k N_i)_{i \neq j \neq k} \quad (22)$$

Let us consider now that the values of I_1 , I_2 and I_3 are independent with respect to the reference system, hence one can compute them also in terms of principal components. It results:

$$I_1 = \lambda_1 + \lambda_{II} + \lambda_{III}$$

$$I_2 = \lambda_1 \lambda_{II} + \lambda_1 \lambda_{III} + \lambda_{II} \lambda_{III}$$

$$I_3 = \lambda_1 \lambda_{II} \lambda_{III}$$

The derivatives of the invariants I_1 , I_2 and I_3 can also be computed by differentiating these last three expressions, observing that $\lambda_i = \lambda_i(T)$. It results:

$$\frac{dI_1}{dT} = \frac{d\lambda_1}{dT} + \frac{d\lambda_{II}}{dT} + \frac{d\lambda_{III}}{dT} = \sum \frac{d\lambda_i}{dT} \quad (23)$$

$$\frac{dI_2}{dT} = I_1 \sum \frac{d\lambda_i}{dT} - \sum \lambda_i \frac{d\lambda_i}{dT} = I_1 I - \sum \lambda_i \frac{d\lambda_i}{dT} \quad (24)$$

$$\frac{dI_3}{dT} = \lambda_{II} \lambda_{III} \frac{d\lambda_1}{dT} + \lambda_1 \lambda_{III} \frac{d\lambda_{II}}{dT} + \lambda_1 \lambda_{II} \frac{d\lambda_{III}}{dT} = \sum \left(\lambda_j \lambda_k \frac{d\lambda_i}{dT} \right)_{i \neq j \neq k} \quad (25)$$

One can now compute the eigenbasis N_i as a function of the derivatives of the eigenvalues λ_i with respect to T by solving the linear system of equations obtained by equating Eq. (17), (18) and (22) with Eq. (23), (24) and (25) respectively. One obtains

$$\begin{cases} \sum N_i = \sum \frac{d\lambda_i}{dT} \\ \sum \lambda_i N_i = \sum \lambda_i \frac{d\lambda_i}{dT} \\ \sum (\lambda_j \lambda_k N_i)_{i \neq j \neq k} = \sum \left(\lambda_j \lambda_k \frac{d\lambda_i}{dT} \right)_{i \neq j \neq k} \end{cases} \quad (26)$$

which, under the assumption $\lambda_1 > \lambda_{II} > \lambda_{III}$ ³ simply gives

$$N_i = \frac{d\lambda_i}{dT}$$

so that the spectral theorem (13) can be re-written as:

$$T = \sum \lambda_i (n_i \otimes n_i) = \sum \lambda_i \frac{d\lambda_i}{dT}$$

² Let us observe that, by multiplying Eq. (1) by $\text{adj}(T) = I_3 T^{-1}$ one obtains

$$I_3 T^{-1} T n = \lambda I_3 T^{-1} n$$

which gives

$$\text{adj}(T) n = \frac{I_3}{\lambda} n \quad (19)$$

Hence, the eigenvectors n of $\text{adj}(T)$ and T are coincident, whilst the i th eigenvalue μ_i of $\text{adj}(T)$ associated with n_i can be computed from λ_i as:

$$\mu_i = \frac{I_3}{\lambda_i} = (\lambda_j \lambda_k)_{i \neq j \neq k} \quad (20)$$

The spectral representation of $\text{adj}(T)$ is then:

$$\text{adj}(T) = \sum (\lambda_j \lambda_k N_i)_{i \neq j \neq k} \quad (21)$$

³ Let us observe that the determinant of the matrix of the system (26) reads:

$$\det \begin{bmatrix} 1 & 1 & 1 \\ \lambda_1 & \lambda_{II} & \lambda_{III} \\ \lambda_{II} \lambda_{III} & \lambda_1 \lambda_{III} & \lambda_1 \lambda_{II} \end{bmatrix} = -(\lambda_1 - \lambda_{II})(\lambda_1 - \lambda_{III})(\lambda_{II} - \lambda_{III})$$

It is always nonzero if $\lambda_1 > \lambda_{II} > \lambda_{III}$.

Case (ii): $\lambda_1 > \lambda_{II} = \lambda_{III}$ or $\lambda_1 = \lambda_{II} > \lambda_{III}$

If one or more eigenvalues of T are coincident, the linear system (26) will not admit a unique solution. Let $\hat{\lambda}$ be the non-repeated eigenvalue of T and \hat{N} the correspondent eigenbasis. The first invariant I_1 is equal to:

$$I_1 = \hat{\lambda} + 2\lambda_{II}$$

so that, it results:

$$\lambda_{II} = \frac{1}{2} (I_1 - \hat{\lambda})$$

Eq. (11) can be rewritten as:

$$\hat{N} + 2N_{II} = I$$

hence, it results:

$$N_{II} = \frac{1}{2} (I - \hat{N}) \quad (27)$$

The spectral theorem can be rewritten as:

$$T = \hat{\lambda}\hat{N} + \frac{1}{2} (I_1 - \hat{\lambda}) (I - \hat{N}) = \frac{3}{2} \left(\hat{\lambda} - \frac{I_1}{3} \right) \hat{N} + \frac{1}{2} (I_1 - \hat{\lambda}) I \quad (28)$$

Eq. (28) can be further simplified by computing the deviatoric part \hat{t} of $\hat{\lambda}$ as $\hat{t} = \hat{\lambda} - I_1/3$. One obtains

$$T = \frac{I_1}{3} I + \frac{3}{2} \hat{t} \left(\hat{N} - \frac{1}{3} I \right) \quad (29)$$

This last equation clearly shows that, when two eigenvalues are coincident, the deviatoric part of \hat{N} , defined as $\hat{N}^d = \hat{N} - I/3$, is simply proportional to the deviatoric part of the tensor T , i.e.

$$\hat{N}^d = \frac{1}{\hat{\lambda} - \lambda_{II}} t = \mp \frac{1}{q} t \quad \text{for } \theta = \pm \frac{\pi}{6} \quad (30)$$

where $q = \sqrt{3J_2}$. This result is a consequence of the multiplicity of the deviatoric principal components. When two eigenvalues of T coincide, the two coincident deviatoric principal components result to be minus half of the (only) independent one, since their sum must vanish. Eq. (28) results to be the sum of two independent terms: the volumetric and the deviatoric parts. The basis of the volumetric part is obviously proportional to the identity tensor I , whilst that of the deviatoric part can only be proportional to the tensor itself.

$$T = \frac{I_1}{3} I + \frac{3}{2} \hat{t} \hat{N}^d$$

It should be noted that, as in Case (i), it is still possible to demonstrate that

$$\hat{N} = \frac{d\hat{\lambda}}{dT}$$

To prove this result, let us compute the second invariant J_2 of the deviatoric tensor t as a function of the principal component $\hat{\lambda}$:

$$J_2 = \frac{t : t}{2} = \frac{(\hat{\lambda} - I_1/3)^2 + 2(\lambda_{II} - I_1/3)^2}{2} = \frac{3(\hat{\lambda} - I_1/3)^2}{4} \quad (31)$$

By differentiating this expression with respect to T , one obtains

$$\frac{dJ_2}{dT} = t = T - \frac{I_1}{3} I = \frac{3}{2} \left(\hat{\lambda} - \frac{I_1}{3} \right) \left(\frac{d\hat{\lambda}}{dT} - \frac{1}{3} I \right) \quad (32)$$

so that, solving for T one obtains:

$$T = \frac{3}{2} \left(\hat{\lambda} - \frac{I_1}{3} \right) \frac{d\hat{\lambda}}{dT} + \frac{1}{2} (I_1 - \hat{\lambda}) I$$

By equating this last expression with Eq. (28) and solving for \hat{N}^d one obtains:

$$\hat{N} = \frac{d\hat{\lambda}}{dT} \quad (33)$$

⁴ This can be done under the condition $\hat{\lambda} \neq I_1/3$ that, observing Eq. (31) is equivalent to $J_2 \neq 0$.

Case (iii): $\lambda_1 = \lambda_{II} = \lambda_{III}$

Finally, let us consider the case of three coincident eigenvalues $\lambda = \lambda_1 = \lambda_{II} = \lambda_{III}$. The tensor T is purely volumetric in any reference system. By observing that it results $l_i = 0 \quad \forall i$ and $I_1 = 3\lambda$, Eq. (29) simply becomes

$$T = \lambda I \quad (34)$$

From Eq. (11) it results

$$N_I = N_{II} = N_{III} = \frac{1}{3} I$$

4. Computation the eigenbasis directly from the secular equation

Since the three eigenbasis are equal to the derivatives of its conjugate principal components with respect to the tensor T , one can determine them by simply differentiating Eqs. (6) with respect to T . Using the chain rule, one obtains:

$$N_i = \frac{d\lambda_i}{dT} = \frac{1}{3} I + \frac{\sqrt{3}}{3} \left(\frac{\sin \beta_i}{\sqrt{J_2}} \frac{dJ_2}{dT} + 2J_2 \cos \beta_i \frac{d\theta}{dT} \right)$$

where $\beta_I = \theta + (2/3)\pi$, $\beta_{II} = \theta$, $\beta_{III} = \theta - (2/3)\pi$, and⁵

$$\frac{dJ_2}{dT} = t$$

$$\frac{d\theta}{dT} = \frac{1}{\cos 3\theta} \left(\frac{\sin 3\theta}{3} t^{-1} - \frac{\sqrt{3}}{6\sqrt{J_2}} I - \frac{\sin 3\theta}{2J_2} t \right) \quad (36)$$

The computation of the spin of the eigenbasis, i.e. dN_i/dT is even more tiring.

A more elegant and simpler approach can be obtained by working directly on the secular Eq. (2). Each of the eigenvalues λ_i will satisfy Eq. (2), i.e.

$$f(T) = \lambda_i^3 - I_1 \lambda_i^2 + I_2 \lambda_i - I_3 = 0$$

Let us observe that this nonlinear equation can be seen as an implicit function of the i th eigenvalue λ_i with respect to the tensor T . Hence, the derivative of λ_i with respect to T can be obtained as the derivative of the implicit function $f(T)$. It must result

$$df(T) = \left[(3\lambda_i^2 - 2I_1 \lambda_i + I_2) \frac{d\lambda_i}{dT} - I \lambda_i^2 + (I_1 I - T) \lambda_i + I_3 T^{-1} \right] : dT = 0 \quad \forall dT$$

This implies the condition:

$$(3\lambda_i^2 - 2I_1 \lambda_i + I_2) \frac{d\lambda_i}{dT} - I \lambda_i^2 + (I_1 I - T) \lambda_i + I_3 T^{-1} = 0$$

The eigenbasis N_i can be obtained by simply solving this last equation for $d\lambda_i/dT$. By observing that $J_2 = (1/3)I_1^2 - I_2$, after some simple algebraic manipulations, one obtains⁶:

$$N_i = \frac{d\lambda_i}{dT} = \frac{\lambda_i [(I_1 - I_1) I + T] + I_3 T^{-1}}{J_2 (4 \sin^2 \beta_i - 1)} \quad (38)$$

⁵ It should be noted that Eq. (36) requires the computation of t^{-1} . An expression more suitable for the implementation, being undefined only for $J_2 = 0$ or $\theta = \pm\pi/6$, is

$$\frac{d\theta}{dT} = -\frac{1}{\cos 3\theta} \left(\frac{\sqrt{3}}{2\sqrt{J_2^3}} \frac{dJ_3}{dT} + \frac{\sqrt{3}}{6\sqrt{J_2}} I + \frac{\sin 3\theta}{2J_2} t \right) \quad (35)$$

where, by using the Cayley–Hamilton theorem (see, e.g., Bertram, 2021):

$$\frac{dJ_3}{dT} = \text{adj}(t) = tt - J_2 I$$

⁶ A very compact way to write this derivative is $I_3 T^{-1}$. However, it should be noted that this expression is not completely correct from a formal point of view, since it is undefined when $I_3 = 0$. The invariant I_3 , being defined as $\det T$, is simply the adjugate matrix of T , that is always defined. By using the

The spin of the eigenbasis can be obtained by differentiating Eq. (38) by the tensor T . One obtains

$$\frac{dN_i}{dT} = \frac{d^2\lambda_i}{dT \otimes dT} = \frac{1}{J_2(4\sin^2\beta_i - 1)} \left[-4\sqrt{3}J_2 \sin\beta_i (N_i \otimes N_i) + (2\lambda_i - I_1)(N_i \otimes I + I \otimes N_i) + (N_i \otimes T + T \otimes N_i) + \lambda_i(I - I \otimes I) + \frac{d^2I_3}{dT \otimes dT} \right] \quad (39)$$

where I is the fourth-order identity tensor, and (see e.g. Zienkiewicz and Taylor, 2013)

$$\left(\frac{d^2I_3}{dT \otimes dT} \right)_{ijkl} = \delta_{jk}(T)_{il} + \delta_{il}(T)_{jk}$$

being δ_{ij} the Kronecker delta operator.

It should be noted that, whilst Sylvester's formula given in Eq. (10) cannot be directly differentiated in the case of two coincident λ_i , here, the spin of the basis associated with the non-repeated eigenvalue $\hat{\lambda}$ can still be computed using Eq. (39). It is the only spin required to compute the derivative of Eq. (29). However, by exploiting the *proportionality* between the deviatoric part of the tensor and the basis itself, it can be more easily obtained by means of Eq. (30). As explained in the previous section, when all the eigenvalues coincide, the three eigenbasis N_i are simply equal to $I/3$. Their spin is not defined, but, as explained in the next section, it is still possible to evaluate the derivative of the spectral representation of the tensor when its invariants are isotropic functions.

5. Isotropic functions

In many mechanical applications it is *a priori* known that two second-order, symmetric tensors S and T share the same principal directions. Under these conditions, the two tensors are called *co-axial*. These applications usually involve isotropic tensor functions, i.e., the invariants of the tensor T are function of the those of the tensor S .

In these applications, once the principal components η_i of the tensor S are computed as a function of those of T , say λ_i , it is finally required to compute the Cartesian components of S .

Let S be a symmetric, second-order tensor, co-axial with T . Let us assume that the generic eigenvalues $\eta_i(\lambda_I, \lambda_{II}, \lambda_{III})$ of S can be computed as a function of the eigenvalues λ_i of T . Since S and T are co-axial, they will share the same eigenbasis N_i and it results

$$S = \sum \eta_i(\lambda_I, \lambda_{II}, \lambda_{III}) N_i \quad (40)$$

The derivative of this expression with respect to the tensor T will be

$$\frac{dS}{dT} = \sum_{i=1}^3 \left(\eta_i \frac{dN_i}{dT} + \sum_{j=1}^3 \frac{\partial \eta_i}{\partial \lambda_j} N_i \otimes N_j \right) \quad (41)$$

Let us consider the case in which two eigenvalues λ_i of T coincide. As explained in the section above, under this condition it results that the deviatoric part of S , say s , results to be *proportional* to the deviatoric part of T , say t . Hence, one can compute S as

$$S = \frac{I_{1S}}{3} I + \frac{q_S}{q_T} t \quad (42)$$

Cayley–Hamilton theorem (see, e.g., Bertram, 2021), the adjugate matrix of T can be expressed as:

$$\frac{dI_3}{dT} = \text{adj}(T) = TT - I_1T + I_2I$$

Eq. (38) becomes

$$N_i = \frac{d\lambda_i}{dT} = \frac{\lambda_i [(\lambda_i - I_1) I + T] + \frac{dI_3}{dT}}{J_2(4\sin^2\beta_i - 1)} \quad (37)$$

where $q_T = \sqrt{(3/2)t : t}$, $I_{1S} = \text{tr}(S) = I_{1S}(I_{1T}, q_T)$ and $q_S = \sqrt{(3/2)s : s} = q_S(I_{1T}, q_T)$, and $I_{1T} = \text{tr}(T)$ is the first invariant of T .

Let us compute dS/dT . It should be noted that, when the eigenvalues are repeated, the eigenbasis as well as the eigenvalues are not differentiable, in spite of the differentiability of S . The derivative dS/dT , in the case of repeated eigenvalues, is usually computed as limit of Eq. (41), that require the employment of the de l'Hôpital rule to be solved (see e.g. Ogden, 1984 and de Souza Neto, 2001). A simpler procedure, based on the proportionality between s and t in this special case, is here described. Let us observe that, being s and t proportional, it must result

$$\theta_S = \theta_T$$

and then

$$\frac{\partial \theta_S}{\partial \theta_T} = 1$$

Moreover, considering that Eq. (47) gives:

$$q_S(\theta_S) = \sqrt[3]{-\frac{27}{2} \frac{J_{3S}}{\sin(3\theta_S)}}$$

it results

$$\frac{\partial q_S}{\partial \theta_T} = \frac{\partial q}{\partial \theta_S} \frac{\partial \theta_S}{\partial \theta_T} = \frac{3\sqrt[3]{4} J_{3S} \cos(3\theta_S) \sqrt[3]{\sin^2(3\theta_S)}}{2 \sqrt[3]{J_{3S}^2 \sin^2(3\theta_S)}} = 0 \text{ for } \theta_S = \theta_T = \pm \frac{\pi}{6}$$

Analogously

$$\frac{\partial I_{1S}}{\partial \theta_T} = \frac{\partial I_{1S}}{\partial \theta_S} \frac{\partial \theta_S}{\partial \theta_T} = 0 \quad \forall \theta_T$$

Hence, observing that from Eq. (30) it results that

$$\frac{dq_T}{dT} = \frac{3}{2q_T} t = \mp \frac{3}{2} \hat{N}^d \text{ for } \theta_T = \pm \frac{\pi}{6} \quad (43)$$

by differentiating Eq. (42) with respect to T one obtains:

$$\frac{dS}{dT} = \frac{1}{3} \frac{\partial I_{1S}}{\partial I_{1T}} I \otimes I \mp \frac{1}{2} \frac{\partial I_{1S}}{\partial q_T} I \otimes \hat{N}^d + \frac{q_S}{q_T} \left(I - \frac{1}{3} I \otimes I \right) + \frac{3}{2} \left(\frac{\partial q_S}{\partial q_T} - \frac{q_S}{q_T} \right) \hat{N}^d \otimes \hat{N}^d \mp \frac{\partial q_S}{\partial I_{1T}} \hat{N}^d \otimes I \text{ for } \theta_T = \pm \frac{\pi}{6} \quad (44)$$

where I is the fourth-order identity tensor.

Finally, when all the eigenvalues coincide, Eq. (42) reduces to:

$$S = \frac{I_{1S}}{3} I \quad (45)$$

whilst its derivative can be computed by particularizing Eq. (44). By observing that when $t \rightarrow 0$, $N_i \rightarrow I/3$, so that its deviatoric part $\hat{N}^d \rightarrow 0$. Observing that $q_S \rightarrow 0$ when $q_T \rightarrow 0$, using a Taylor expansion for $q_T \rightarrow 0$, it will result:

$$q_S(I_{1T}, 0) \approx \frac{\partial q_S}{\partial q_T} q_T$$

so that $q_S/q_T \rightarrow \partial q_S/\partial q_T$, and finally:

$$\frac{dS}{dT} = \frac{1}{3} \frac{\partial I_{1S}}{\partial I_{1T}} I \otimes I + \frac{\partial q_S}{\partial q_T} \left(I - \frac{1}{3} I \otimes I \right) \quad (46)$$

6. Applications

6.1. Isotropic elastoplastic materials under small-strains and displacements

Let us consider a generic elastoplastic isotropic material, in which the principal directions of the elastic strains and of the stress coincide.

Let us assume a backward Euler integration scheme in which the solution is computed at discrete times. The increment that any variable (\cdot) takes when the pseudo-time t passes from the beginning to the end of a generic time interval $[t_n, t_{n+1}]$ will be indicated with $\Delta(\cdot) = (\cdot)_{n+1} - (\cdot)_n$, whilst all the quantities, if not otherwise indicated, are referred to time t_{n+1} .

At the time t_n all the quantities are known. Let $\Delta\epsilon$ be the strain tensor increment applied during the time interval $[t_n, t_{n+1}]$. The solution of the problem requires the computation at time t_{n+1} of the stress σ , of the plastic deformation tensor ϵ^p , as well as of the constitutive model's state variables. In order to achieve quadratic convergence on the *structural* Newton's loop, also the consistent Jacobian Matrix $d\Delta\sigma/d\Delta\epsilon$ must be computed.

Let $\epsilon^* = \epsilon_n^e + \Delta\epsilon$ be the elastic strain predictor, whilst $\Delta\epsilon^p$ is the plastic strain increment, that can be computed as a function of an *isotropic* plastic potential $g(p, q, \theta_\sigma)$ as

$$\Delta\epsilon^p = \frac{\partial g(p, q, \theta_\sigma)}{\partial \sigma} \Delta\gamma$$

where $\Delta\gamma$ is the plastic multiplier. Since $g(p, q, \theta_\sigma)$ is an isotropic function of σ , its derivative with respect to σ will be co-axial with the stress (de Souza Neto et al., 2008; Panteghini and Lagioia, 2018). Then, since the elastic strain ϵ^e is co-axial with σ because of the assumption of isotropy, it results that also

$$\epsilon^* = \epsilon^e + \Delta\epsilon^p$$

is co-axial with σ . For these reasons, the principal directions of stress are *a priori* known, being coincident with those of the predictor ϵ^* . Let e^* be the deviatoric part of the elastic predictor ϵ^* , and

$$\begin{aligned} \epsilon_v^* &= \text{tr}(\epsilon^*) \\ \epsilon_q^* &= \sqrt{\frac{2}{3}} e^* : e^* \\ \theta_\epsilon^* &= \frac{1}{3} \arcsin\left(-4 \frac{\det e^*}{\epsilon_q^{*3}}\right) \end{aligned}$$

its invariants, i.e. the volumetric strain predictor, the equivalent von Mises strain predictor, and the strain predictor Lode's angle.

In general, if a standard return algorithm in the full tensorial space is employed, numerical problems and convergence difficulties can arise when two or more eigenvalues coincide. Instead, the value of the hydrostatic pressure p , the equivalent von Mises stress q , and the stress Lode's angle θ_σ at the end of the increment, defined as

$$p = \frac{1}{3} \text{tr}(\sigma)$$

$$q = \sqrt{\frac{3}{2}} s : s$$

$$\theta_\sigma = \frac{1}{3} \arcsin\left(-\frac{27}{2} \frac{\det s}{q^3}\right) \quad (47)$$

can be more easily computed by formulating a return algorithm in the invariants strain space (Panteghini and Lagioia, 2018). Once p , q and θ_σ have been obtained as a function of the strain invariant predictors ϵ_v^* , ϵ_q^* and θ_ϵ^* , it is necessary to compute the stress tensor σ . Let us observe that, because of the isotropy, as described above, the stress tensor σ results to be co-axial with the elastic trial ϵ^* . Hence, if $\epsilon_q^* \neq 0$ and $|\theta_\epsilon^*| \neq \pi/6$, one can compute the stress tensor from its invariants and from the eigenbasis N_i^* of the elastic strain predictor ϵ^* by resorting to the spectral theorem. It results

$$\sigma = \sum \left[p(\epsilon_v^*, \epsilon_q^*, \theta_\epsilon^*) + \frac{2}{3} q(\epsilon_v^*, \epsilon_q^*, \theta_\epsilon^*) \sin \beta_i(\epsilon_v^*, \epsilon_q^*, \theta_\epsilon^*) \right] N_i^*$$

where

$$\begin{aligned} \beta_I &= \theta_\sigma(\epsilon_v^*, \epsilon_q^*, \theta_\epsilon^*) + \frac{2}{3} \pi \\ \beta_{II} &= \theta_\sigma(\epsilon_v^*, \epsilon_q^*, \theta_\epsilon^*) \\ \beta_{III} &= \theta_\sigma(\epsilon_v^*, \epsilon_q^*, \theta_\epsilon^*) - \frac{2}{3} \pi \end{aligned}$$

and N_i^* is computed from Eq. (37) as a function of the invariants of ϵ^* and its principal components. The consistent jacobian matrix⁷ can be computed from Eq. (41) as

$$\begin{aligned} \frac{d\Delta\sigma}{d\Delta\epsilon} &= \sum \left[p + \frac{2}{3} q \sin \beta_i \right] \frac{dN_i^*}{d\epsilon^*} + N_i^* \\ &\otimes \left\{ \left[\frac{\partial p}{\partial \epsilon_v^*} + \frac{2}{3} \left(\frac{\partial q}{\partial \epsilon_q^*} \sin \beta_i + q \frac{\partial \theta_\sigma}{\partial \epsilon_q^*} \cos \beta_i \right) \right] I \right. \\ &+ \frac{2}{3\epsilon_q^*} \left[\frac{\partial p}{\partial \epsilon_q^*} + \frac{2}{3} \left(\frac{\partial q}{\partial \epsilon_q^*} \sin \beta_i + q \frac{\partial \theta_\sigma}{\partial \epsilon_q^*} \cos \beta_i \right) \right] e^* \\ &\left. + \left[\frac{\partial p}{\partial \theta_\epsilon^*} + \frac{2}{3} \left(\frac{\partial q}{\partial \theta_\epsilon^*} \sin \beta_i + q \frac{\partial \theta_\sigma}{\partial \theta_\epsilon^*} \cos \beta_i \right) \right] \frac{\partial \theta_\epsilon^*}{\partial \epsilon^*} \right\} \end{aligned}$$

where the eigenbasis spin $dN_i^*/d\epsilon^*$ and $\partial\theta_\epsilon^*/\partial\epsilon^*$ are computed as a function of the invariants and principal components of ϵ^* from Eqs. (35) and (39) respectively.

If ϵ_q^* is not nil, at least two eigenvalues of the strain predictor ϵ^* are distinct. Specifically, if $\theta_\epsilon^* = \pm\pi/6$, two eigenvalues of ϵ^* will be coincident. In this case, from Eq. (30) it will result that e^* will be *proportional* to the deviatoric part of the eigenbasis associated with its non-repeated eigenvalue. Hence, from Eq. (42) one simply obtains:

$$\sigma = p(\epsilon_v^*, \epsilon_q^*, \theta_\epsilon^*) I + \frac{2}{3\epsilon_q^*} q(\epsilon_v^*, \epsilon_q^*, \theta_\epsilon^*) e^*$$

Also the eigenbasis of the deviatoric part of the plastic strain increment $\Delta\epsilon^p$ and of the elastic strains will coincide with those of e^* , and then it will result:

$$\begin{aligned} \Delta\epsilon^p &= \frac{\epsilon_v^p}{3} I + \frac{\epsilon_q^p}{\epsilon_q^*} e^* \\ \epsilon^e &= \frac{\epsilon_v^e}{3} I + \frac{\epsilon_q^e}{\epsilon_q^*} e^* \end{aligned}$$

The jacobian matrix can be obtained by simplifying Eq. (44) using Eq. (30). It yields:

$$\begin{aligned} \frac{d\Delta\sigma}{d\Delta\epsilon} &= \frac{\partial p}{\partial \epsilon_v^*} I \otimes I + \frac{2}{3\epsilon_q^*} \left[\frac{\partial p}{\partial \epsilon_q^*} (I \otimes e^*) + \frac{\partial q}{\partial \epsilon_q^*} (e^* \otimes I) \right. \\ &\left. + \frac{2}{3\epsilon_q^*} \left(\frac{\partial q}{\partial \epsilon_q^*} - \frac{q}{\epsilon_q^*} \right) (e^* \otimes e^*) + q \left(I - \frac{1}{3} I \otimes I \right) \right] \end{aligned}$$

If ϵ_q^* is nil, the strain predictor ϵ^* will be a volumetric tensor, since its spectral decomposition has the same structure of Eq. (34). Moreover, $\epsilon_q^* = 0$ implies $e^* = \mathbf{0}$. Since the material is isotropic, the eigenbasis

⁷ This *general* approach has been recently adopted by the Author in Panteghini and Lagioia (2022), while in his older works (see, e.g., Panteghini and Lagioia, 2014, 2018) in order to avoid the computation of the spin of the eigenbasis, the jacobian matrix was obtained by means of a "simplified" procedure based on the inversion of a 6x6 matrix. Unfortunately, this procedure is model-specific and requires the smoothness in the deviatoric plane of the yield function and of the plastic potential.

Moreover, by employing the approach described in Panteghini and Lagioia (2014, 2018), three different *full tensorial* jacobian matrices must be implemented for a single constitutive model, as a function of the principal stress multiplicity, with a consequent major complexity and increase in coding time. The approach here described, instead, can be used for several constitutive models (not necessarily smooth) in a Finite Element code, formulating the return algorithm of each model only in the invariants space. Once the invariants of the stress (and their derivatives, that can be computed a single time even in the case of different eigenvalues multiplicity) are computed as a function of the invariants of elastic predictors, one can obtain the stress tensor and the consistent jacobian matrix by employing the generic subroutines that compute the spectral representation and its derivatives. These subroutines, being generic, can be used for several constitutive models, as well as for computing the logarithmic strain and its derivatives in the case of large strains framework.

of σ and ε^* will be the same, resulting to be coincident with the second-order identity tensor I . Then, from Eq. (34) it will result

$$\sigma = p(\varepsilon_v^*)I$$

The derivative of the eigenbasis is undefined. However, as explained in the section above, the Jacobian Matrix can be obtained as a limit case of Eq. (44), i.e., using Eq. (46). Let us observe that, under purely volumetric conditions, the convexity of the elastic potential requires (Lagioia and Panteghini, 2019):

$$\frac{\partial p}{\partial \varepsilon_v^*} = \frac{\partial q}{\partial \varepsilon_v^*} = 0$$

It results:

$$\frac{d\Delta\sigma}{d\Delta\varepsilon} = \frac{\partial p}{\partial \varepsilon_v^*} I \otimes I + \frac{2}{3} \frac{\partial q}{\partial \varepsilon_v^*} \left(I - \frac{1}{3} I \otimes I \right)$$

6.2. Computation of logarithmic strain tensor from displacement gradient

In the framework of large strains and rotations, let p denote the reference coordinate system. Indicating with $u(p)$ the vector function describing the displacement of each material point, it results that its final position will be (i.g. de Souza Neto et al., 2008)

$$x = p + u(p)$$

The deformation gradient F is defined as

$$F = \nabla_p x = I + \nabla_p u(p)$$

By applying the polar decomposition (i.g. de Souza Neto et al., 2008) to the deformation gradient F , one obtains:

$$F = VR$$

where the orthogonal tensor R describes the local rotation, whilst the symmetric, positive definite tensor V is the left stretch tensor, where

$$V^2 = B = FF^T$$

B being the left Cauchy–Green tensor. The logarithmic strain tensor can be computed as:

$$\varepsilon = \ln V = \frac{1}{2} \ln B$$

i.e.,

$$\varepsilon = \frac{1}{2} \sum \ln(\lambda_i^B) N_i^B \quad (48)$$

where λ_i^B and N_i^B are the i -th principal component and eigenbasis of the tensor B respectively.

The invariants of B , I_{1B} , J_{2B} and θ_B can be computed using Eqs. (3), (7) and (8), whilst the principal components λ_i^B can be obtained using Eqs. (6).

If λ_i^B are distinct, i.e., if $J_{2B} \neq 0$ and $|\theta_B| \neq \pi/6$, all the eigenbasis N_i^B of the left Cauchy–Green tensor can be computed as a function of its invariants and its principal components using Eq. (37). The logarithmic strain tensor can be computed using Eq. (48). The jacobian matrix $d\varepsilon/dB$ can be computed by using Eq. (41):

$$\frac{d\varepsilon}{dB} = \frac{1}{2} \sum \left[\ln(\lambda_i^B) \frac{dN_i^B}{dB} + \frac{1}{\lambda_i^B} N_i^B \otimes N_i^B \right]$$

where dN_i^B/dB can be computed using Eq. (39).

When two principal components of B are coincident, i.e. if $J_{2B} = 0$ and $|\theta_B| = \pi/6$, one can compute ε by exploiting the proportionality between the deviatoric part b of B and e . Let us start by computing the invariants $q_\varepsilon = \sqrt{3J_{2\varepsilon}}$ and $I_{1\varepsilon}$ of ε as a function of $q_B = \sqrt{3J_{2B}}$ and I_{1B} . Let us observe that it results

$$q_B = \pm (\lambda_{II}^B - \hat{\lambda}^B) \quad \text{for } \theta_B = \pm \frac{\pi}{6}$$

By solving this expression for λ_{II}^B one obtains

$$\lambda_{II}^B = \hat{\lambda}^B \pm q_B \quad \text{for } \theta_B = \pm \frac{\pi}{6} \quad (49)$$

Substituting this result into the definition of $I_{1B} = \hat{\lambda}^B + 2\lambda_{II}^B$ and solving for $\hat{\lambda}^B$ gives

$$\hat{\lambda}^B = \frac{I_{1B} \mp 2q_B}{3} \quad \text{for } \theta_B = \pm \frac{\pi}{6}$$

By substituting this expression into Eq. (49) one obtains

$$\lambda_{II}^B = \frac{I_{1B} \pm q_B}{3} \quad \text{for } \theta_B = \pm \frac{\pi}{6}$$

One can now compute the invariants of ε as a function of those of B . It results:

$$\begin{aligned} I_{1\varepsilon} &= \hat{\lambda}^\varepsilon + 2\lambda_{II}^\varepsilon = \frac{1}{2} \left[\ln \left(\frac{I_{1B} \mp 2q_B}{3} \right) + 2 \ln \left(\frac{I_{1B} \pm q_B}{3} \right) \right], \\ q_\varepsilon &= \pm (\lambda_{II}^\varepsilon - \hat{\lambda}^\varepsilon) = \pm \frac{1}{2} (\ln \lambda_{II}^B - \ln \hat{\lambda}^B) = \pm \frac{1}{2} \ln \left(\frac{I_{1B} \pm q_B}{I_{1B} \mp 2q_B} \right) \\ &\quad \text{for } \theta_\varepsilon = \theta_B = \pm \frac{\pi}{6} \end{aligned} \quad (50)$$

The logarithmic strain tensor ε can be finally computed using Eq. (42). It results:

$$\varepsilon = \frac{I_{1\varepsilon}}{3} I + \frac{q_\varepsilon}{q_B} b$$

Its derivative can be obtained by applying Eq. (44). It results:

$$\begin{aligned} \frac{d\varepsilon}{dB} &= \frac{1}{3} \frac{\partial I_{1\varepsilon}}{\partial I_{1B}} I \otimes I \mp \frac{1}{2} \frac{\partial I_{1\varepsilon}}{\partial q_B} I \otimes \hat{N}_B^d + \frac{q_\varepsilon}{q_B} \left(I - \frac{1}{3} I \otimes I \right) \\ &+ \frac{3}{2} \left(\frac{\partial q_\varepsilon}{\partial q_B} - \frac{q_\varepsilon}{q_B} \right) \hat{N}_B^d \otimes \hat{N}_B^d \mp \frac{\partial q_\varepsilon}{\partial I_{1B}} \hat{N}_B^d \otimes I \quad \text{for } \theta_\varepsilon = \theta_B = \pm \frac{\pi}{6} \end{aligned}$$

where, from Eq. (30):

$$\hat{N}_B^d = \mp \frac{1}{q_B} b \quad \text{for } \theta_B = \pm \frac{\pi}{6}$$

and, by computing the derivatives of Eq. (50):

$$\begin{aligned} \frac{\partial I_{1\varepsilon}}{\partial I_{1B}} &= \frac{3(\pm q_B - I_{1B})}{(I_{1B} \pm q_B)(\pm 4q_B - 2I_{1B})} \\ \frac{\partial I_{1\varepsilon}}{\partial q_B} &= \frac{3q_B}{(\pm 2q_B - I_{1B})(I_{1B} \pm q_B)} \quad \text{for } \theta_\varepsilon = \theta_B = \pm \frac{\pi}{6} \\ \frac{\partial q_\varepsilon}{\partial q_B} &= \frac{3q_B}{(I_{1B} \pm q_B)(\pm 4q_B - 2I_{1B})} \\ \frac{\partial q_\varepsilon}{\partial I_{1B}} &= -\frac{3I_{1B}}{(I_{1B} \pm q_B)(\pm 4q_B - 2I_{1B})} \end{aligned} \quad (51)$$

Finally, if $J_{2B} = 0$, then the logarithmic strain will be purely volumetric, and it will result $\lambda_i^B = \lambda^B$. Eqs. (50) become:

$$I_{1\varepsilon} = \frac{3}{2} \ln \left(\frac{I_{1B}}{3} \right) = \frac{3}{2} \ln \lambda^B \quad (52)$$

$$q_\varepsilon = 0$$

By applying Eq. (45) it will result:

$$\varepsilon = \frac{1}{2} \ln \lambda^B I$$

To compute the derivative of ε with respect to B , let us start substituting Eqs. (52) into Eqs. (51). It results:

$$\begin{aligned} \frac{\partial I_{1\varepsilon}}{\partial I_{1B}} &= \frac{3}{2I_{1B}} = \frac{1}{2\lambda^B} \\ \frac{\partial I_{1\varepsilon}}{\partial q_B} &= \frac{\partial q_\varepsilon}{\partial I_{1B}} = 0 \\ \frac{\partial q_\varepsilon}{\partial q_B} &= \frac{3}{2I_{1B}} = \frac{1}{2\lambda^B} \end{aligned}$$

By substituting these expressions into Eq. (46) one obtains:

$$\frac{d\varepsilon}{dB} = \frac{1}{2\lambda^B} I$$

7. Some notes about the numerical implementation

Let us observe that the correct determination of the eigenvalues multiplicity is a key point in the proposed method. In the numerical implementation, this can be problematic if direct checks of the values of λ_i or of the Lode's angle θ are employed. As pointed out by Harari and Albocher (2023), this issue is caused by an increase of floating point error for $\theta \rightarrow \pm\pi/6$ related to the inverse sine function $\arcsin(x)$, which enters in Eq. (8). This function results to be numerically ill conditioned for $x \rightarrow \pm 1$ because its derivative is unbounded.

The eigenvalues multiplicity can be accurately determined by checking the value of J_2 and of the argument of arcsin function in the Lode's angle definition (Eq. (8)). Hence:

- $\lambda_I > \lambda_{II} > \lambda_{III}$ occurs when $J_2 \neq 0$ and $-2J_2\sqrt{J_2} < 3\sqrt{3}J_3 < 2J_2\sqrt{J_2}$ (that is analytically equivalent to the condition $\theta \neq \pm\pi/6$);
- $\lambda_I > \lambda_{II} = \lambda_{III}$ occurs when $J_2 \neq 0$ and $3\sqrt{3}J_3 = 2J_2\sqrt{J_2}$ (equivalent to the condition $\theta = -\pi/6$);
- $\lambda_I = \lambda_{II} > \lambda_{III}$ occurs when $J_2 \neq 0$ and $3\sqrt{3}J_3 = -2J_2\sqrt{J_2}$ (equivalent to the condition $\theta = \pi/6$);
- $\lambda_I = \lambda_{II} = \lambda_{III}$ occurs when $J_2 = 0$ (while θ is undefined).

Finally, it has been found that, in the case of non-repeated eigenvalues, the accuracy of the proposed method for the computation of the spectral decomposition can be deeply improved by enforcing the constraint given by Eq. (11) instead of computing the three eigenbasis independently. In particular:

- if $\theta > \pi/9$, compute N_{II} and N_{III} from Eq. (37). Then, $N_I = I - N_{II} - N_{III}$
- if $-\pi/9 \leq \theta \leq \pi/9$, compute N_I and N_{III} from Eq. (37). Then, $N_{II} = I - N_I - N_{III}$
- if $\theta < -\pi/9$, compute N_I and N_{II} from Eq. (37). Then, $N_{III} = I - N_I - N_{II}$

Further improvements of the accuracy can be achieved by computing the deviatoric invariants J_2 and θ , as well as the eigenvalues λ_i , using the more accurate expressions reported by Harari and Albocher (2023) instead of Eqs. (7), (6) and (8) respectively.

8. A simple numerical benchmark

In order to study the numerical accuracy of the proposed method, let us consider a simple benchmark. Let us observe that, given a generic "reference" deviatoric tensor t , one can compute its the eigenbasis and eigenvalues. Hence, one can reconstruct a tensor \tilde{t} using Eq. (9). Due to the floating point errors introduced by the spectral decomposition of t , it results $\tilde{t} \neq t$. The relative error can be estimated as:

$$e = \frac{|\tilde{t} - t|}{|t|}$$

In order to evaluate the accuracy of the proposed method in the whole range of the admissible values of the Lode's angle θ_T , a discrete set of reference deviatoric tensors t are computed from their reference principal components, that are functions of a given value of the invariant q_T and of the set of the Lode's angle θ_T . Each "reference" generic tensor t is finally obtained by rotating the diagonal tensor containing the reference principal components of t using a given rotation matrix R , i.e.,

$$t = R \begin{bmatrix} \hat{\lambda}_I^T & 0 & 0 \\ 0 & \hat{\lambda}_{II}^T & 0 \\ 0 & 0 & \hat{\lambda}_{III}^T \end{bmatrix} R^T$$

where $\hat{\lambda}_i^T = (2/3)q_T \sin(\beta_i)$.

Fig. 1 shows the error e as a function of the Lode's angle θ_T , assuming $q_T = 100$. and

$$R = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & \frac{\sqrt{2}}{2} \\ -\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} & 0 \\ -\frac{1}{2} & -\frac{1}{2} & \frac{\sqrt{2}}{2} \end{bmatrix}$$

The Lode's angle interval $[-\pi/6, \pi/6]$ has been subdivided into 10^5 increments. The relative error has been compared with that obtained employing the SPRIND subroutine implemented in SIMULIA Abaqus (Dassault Systèmes, 2020), that computes the eigenvalues and the eigenvectors of a second-order, symmetric tensor.⁸

Fig. 1a shows a comparison between the SPRIND subroutine and the proposed approach, without enforcing the constraint given by Eq. (11) (i.e., by individually computing each of the eigenbasis N_i from Eq. (37)).

Fig. 1b reports the comparison between the SPRIND subroutine and the proposed approach, by enforcing the constraint given by Eq. (11) as described in Section 7. Also the results obtained by computing the deviatoric invariants and the principal components following Harari and Albocher (2023) are presented. As pointed out in the previous section, in the case of non-repeated eigenvalues, the accuracy is deeply improved by enforcing the constraint given by Eq. (11): the maximum relative error results to be three orders of magnitude smaller than that obtained using the SPRIND subroutine. Finally, Fig. 1b shows that, when Eq. (11) is enforced, the accuracy of the proposed formulation is almost constant in the whole interval of Lode's angle θ_T . The SPRIND subroutine, instead, results to be less accurate when $\theta_T \rightarrow \pm\pi/6$. Further improvements can be achieved by computing the invariants and the principal components as a function of the discriminant of the characteristic equation, as proposed by Harari and Albocher (2023).

The run time required to perform the benchmark (10^5 spectral decompositions) using the proposed formulation (and enforcing constraint (11)) on a 2014 Laptop is equal to 0.02s, without employing any code optimization or parallel coding. If the approach described in Harari and Albocher (2023) is employed, the computational time is equal to 0.0216s. For comparison, the same benchmark run using the SPRIND subroutine requires 0.019s.

9. Conclusions

The spectral representation of a symmetric, second-order tensor is an important tool in many applications of computational mechanics.

While the computation of the eigenvalues of a symmetric, second-order tensor is a relatively simple task, obtaining a closed-form expression for the eigenbasis is more complicate, especially when some eigenvalue is repeated. Moreover, in many computational mechanics applications, the derivative of the spectral representation is also required. The exact closed-form expressions available in the literature for both the eigenbasis and their derivative are quite hard to implement (see, e.g., de Souza Neto et al., 2008). For this reason, many Authors suggest to resort to series expansions, that, however, are available only for specific functions (see, e.g., de Souza Neto, 2001; Ortiz et al., 2001) or require automatic differentiation techniques for a generic function (Hudobivnik and Korelc, 2016).

These approximate techniques are hard to apply when the isotropic tensor-valued functions are not known explicitly, such as, for instance, in the numerical integration of elastoplastic isotropic constitutive laws formulated in invariants space (Borja et al., 2003; Panteghini and Lagioia, 2018, 2022).

⁸ Let us observe that this subroutine does not compute any tensorial derivatives of the eigenvectors.

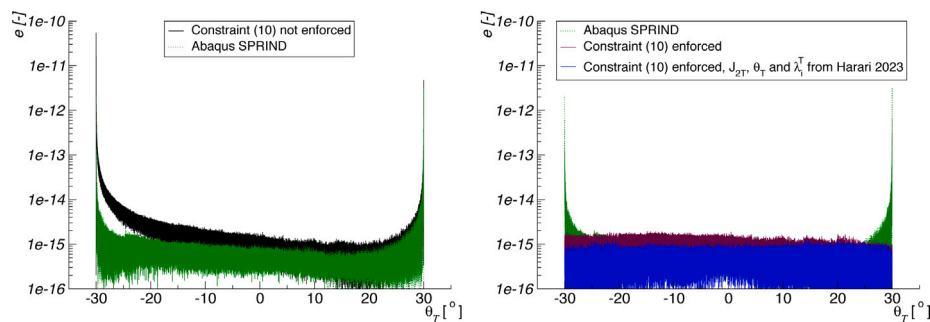


Fig. 1. Relative error e as a function of the Lode's angle θ_r .

In this paper, starting from a incidental result reported by Ogden (1984) working only in the case of not coincident eigenvalues, an exact, simple and clear approach has been developed. Differently from that described by Miehe (1993, 1998) no particular requirements about the invertibility of the tensor, or its eigenvalues multiplicity are necessary.

Two applications have been presented: (i) the computation of stress tensor and of the stiffness matrix in the case of the numerical integration of an elastoplastic isotropic material in the invariant stress space, and (ii) the calculation of the logarithmic strain tensor from the displacement gradient, as well as its derivative with respect to the left Cauchy–Green tensor.

Finally, to show the numerical accuracy of the proposed formulation, a simple numerical benchmark has been presented and discussed.

CRediT authorship contribution statement

Andrea Panteghini: Conceptualization, Data curation, Formal analysis, Funding acquisition, Investigation, Methodology, Project administration, Resources, Software, Supervision, Validation, Visualization, Writing – original draft, Writing – review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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