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ARTICLE

Jacobian from Principal Values to Global Values for Eigenvalue Problem: Application to User Subroutine for Material Tangent Stiffness

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ABSTRACT: This work presents the analytical demonstration of an exact Jacobian matrix for a 2nd-order tensor for the third dimension when differentiating the principal values direction as a function of the global value direction. This operation is a requirement when it is necessary to apply an eigenvalue problem for materials that search for the principal stress, strain or material axes, when evaluating their constitutive behaviour during non-linear analysis. This work will be divided into two parts. In the 1st part, it will be the deduction of the 2D case and comparing the general Jacobian with known values using Mohr's Circle. In the 2nd part, it will be the proof of the 3D case using indirect derivatives with Invariants. This last analytical case is compared with numerical calculations of 3D cases using the disturbance method.

KEYWORDS: Principal strain values; exact Jacobian; user subroutine; tangent stiffness; numerical derivative; disturbance method

1 Introduction

It is possible to express mechanical systems with static and dynamic equilibrium using sets of both linear and nonlinear equations. Eigenvalues and related eigenvectors are commonly used in linear models to explain the behaviour of the mechanical system. Most systems can be modelled using linearised formulations and are applicable to general 3D dimensions, in which eigenvalue problems can be applied. The physical significance of the principal values is problem dependent, but its solution is normally standard and based in numerical methods.

In some materials the constitutive equations rely on some source space transformation, usually searching for the principal stress, strain or material directions, commonly associated with either a crack or damage pattern. This is the case for the classical Mazars damage model [1], in which the principal strains are computed throughout the entire iterative process. Meaning, for example, if a researcher wants to implement such a user-material subroutine like UMATs in ABAQUS, it is necessary to calculate the exact Jacobian to achieve quadratic convergence with Newton-Raphson algorithm. To perform an exact Jacobian, it is necessary to compute the sub-Jacobian from principal values to global values for an eigenvalue problem. Previous authors have stated this problem [2], using simplified Jacobians, or even simply ignoring the Jacobian with quadratic convergence and applying a Secant matrix. The method that uses viscous damping has provided accurate results [3], but it comes with a very high computational cost [4], which tends to increase even more for 3D finite element models [5].

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1.1 Objectives

The main purpose of this work is to provide an exact Jacobian from principal values to global values for eigenvalue problems, admitting the matrix is at least 3 × 3 symmetric. The problem will be presented for computational mechanics applied to structural engineering, mainly for user subroutines for damaged material tangent stiffness. This manuscript is not intended to be an exhaustive and intensive mathematical demonstration of the proposed formulation, but rather an engineering approach to a known problem, using simple tools with intuitive background.

1.2 Research Significance

According to the author's best knowledge, there is no analytical expression for an exact Jacobian from principal values to global values for eigenvalue problems, using information from invariants. With this, it will be possible to assemble an exact Jacobian for the constitutive tangent stiffness of the Mazars damage model [6]. Therefore, providing a numerical tool that will allow a quadratic convergence when using classical Newton-Raphson or arch-length algorithms.

2 Applications in Science

In stress-strain with Hooke's Law for elastic deformation, it is referred to as a stiffness matrix or compliance matrix depending on whether stress or strain is the independent variable. The condition of stress or strain at a location in a generalized body is expressed using a second-order tensor or a 3 × 3 matrix. The eigenvalues of this matrix reflect the primary stresses or strains, whereas the eigenvectors represent the directions in the space of the corresponding eigenvalues [7].

There are other possibilities, like dynamic systems, in which the equations are expressed by combining the mass, damping and stiffness matrix [8,9]. These can be expressed also as tensors, and with eigenvalue problem it can be possible to search for vibration modes and shapes [10,11]. In the field of geometrically non-linear analysis, the eigenvalue problem can indeed find buckling modes and shapes that are needed during the design of twin-wall structures [12].

Numerous other applications in science, beyond the field of structural mechanics, can also take advantage of the eigenvalue solution procedure, such as the matrix of atomic orbitals [13], numerical analysis of chemical reactions [14], monitoring electrical networks [15], Markov chain model [16], structural health monitoring [17] and damage assessment [18,19] and, more recently, facial recognition patterns [20].

For determining eigenvalues and eigenvectors, several effective numerical techniques are available, and these are effective for a particular level of accuracy. The Ritz method [21], the Stodola iterative algorithm [22], the power iteration approach [23], the iterative Jacobi method [24], and the QR iteration [25] are the most popular algorithms. Most available software libraries possess either these algorithms or variants of them, like Numerical Recipes [26], NumPy and SciPy [27], Intel MKL [28], modern and legacy LAPACK [29], GNU scientific library [30], and the most recent Armadillo [31]. All of these algorithms are optimized for large matrices and, in some cases, may not be computationally efficient for eigenvalue problems in simple 3 × 3 or 2 × 2 matrices. In addition, all of them are numerical algorithms without a clear analytical definition, therefore, these cannot be used to calculate an analytical derivative.

For the particular case of 2 × 2 matrices, an analytical expression is possible using Mohr's circle, in which an exact analytical derivative can be calculated [4]. This case can also be extrapolated for 3 × 3 if one of the principal values is already known. For the 3 × 3 matrices, an analytical expression was deduced [32] for the particular case of a symmetric matrix, but with expressions that are case dependent and are hard to assess when performing the analytical derivative.

The derivatives of eigenvalues and eigenvectors with explicit formulas, were accomplished by [33,34] using matrix decomposition. Although it was demonstrated the uniqueness of the solution, there were still some difficulties to address for the cases with repeated eigenvalues, that needed alternative algorithms [35]. Some authors [36], have provided sufficient conditions for a positive definite Jacobian constructed from three eigen pairs, complete with an analytic formula and numerical algorithm. Recently the work of [37] offer closed form, basis-free expressions for first and higher-order derivatives via spectral decomposition. New robust algorithms have also been proposed [38,39], but without a clear final analytical expression that could be easily differentiated. According to the author's best knowledge, there is no Jacobian from principal values to global values for the eigenvalue problem.

3 Jacobian Formulation

For this section, the author will demonstrate that it is indeed possible to calculate the exact Jacobian from a transformation of the global values to the principal values from an eigenvalue problem. It will be initially performed for a 2D second-order symmetric tensor, in which an exact solution is already known in the scientific community, to prove the methodology of cross derivatives is a valid alternative to direct derivation. Later, it will be performed for a 3D second-order symmetric tensor, in which it will be demonstrated that it retrieves for particular cases the 2D second-order symmetric tensor solution. To simplify the presentation of the Jacobian, the global and principal values will be represented as ε_i and ε_I, respectively by specific notations.

This problem will be presented for the case of damage mechanics [40] in which the stiffness Jacobian is necessary to calculate for the Mazars damage model [1]. This derivative is general, and this example is only used to situate the interpretation of the problem.

For the implementation of new user subroutines like UMATs in software like ABAQUS, ANSYS or DIANA, it is necessary to calculate a tangent stiffness to execute a Newton-Raphson with near quadratic convergence. To perform this, a Jacobian matrix between stress and strain needs to be calculated (1). Due to the sub-dependency of several variables (2), it is necessary to perform the chain rule in partial differentiation (3). It is beyond the scope of this work to demonstrate all these derivative passages (4), and further reading of [4] is necessary. For an exact Jacobian, a sub-Jacobian for the global values vs. principal values is necessary (5). For the sake of simplicity these representations will be used throughout the description and presentation of this work.

$$C_{ij}^{T} = (1-d)\, C_{ij} - \frac{\partial d}{\partial \varepsilon_j} C_{ik}\varepsilon_k \tag{1}$$

$$d = d\left(\varepsilon_{eq}\right) \quad \varepsilon_{eq} = \varepsilon_{eq}\left(\varepsilon_I, \varepsilon_{II}, \varepsilon_{III}\right) \tag{2}$$

$$\frac{\partial d}{\partial \varepsilon_j} = \frac{\partial d}{\partial \varepsilon_{eq}} \times \frac{\partial \varepsilon_{eq}}{\partial \varepsilon_j} \tag{3}$$

$$\frac{\partial \varepsilon_{eq}}{\partial \varepsilon_j} = \frac{\partial \varepsilon_{eq}}{\partial \varepsilon_I} \times \frac{\partial \varepsilon_I}{\partial \varepsilon_j} + \frac{\partial \varepsilon_{eq}}{\partial \varepsilon_{II}} \times \frac{\partial \varepsilon_{II}}{\partial \varepsilon_j} + \frac{\partial \varepsilon_{eq}}{\partial \varepsilon_{III}} \times \frac{\partial \varepsilon_{III}}{\partial \varepsilon_j} \tag{4}$$

$$\frac{\partial \varepsilon_P}{\partial \varepsilon_i} \quad \text{and} \quad \frac{\partial \varepsilon_P}{\partial \varepsilon_{ij}} \tag{5}$$

3.1 Problem Formulation

This particular case has been widely used by several authors [41] to numerically simplify real 3D cases under certain boundary conditions. The Jacobian for the transformation of the global values to the principal values in an eigenvalue problem was already demonstrated in the work of [4]. This was performed using

classical Mohr-Circle geometry transformation, in which there is always a connection between ε_i and ε_I (16), using the circle radius (R) and circle geometric centre (C). These derivatives are easy to obtain and can be demonstrated for the case of 2D plane strain (17).

$$\varepsilon_{ij} v_j = \varepsilon_P v_j \quad \Longleftrightarrow \quad \left(\varepsilon_{ij} - \varepsilon_P \delta_{ij}\right) v_j = 0 \tag{6}$$

It is always possible to relate the principal values direction with the global values direction (7), for the particular case of a real symmetric tensor (8). In any case, these are dependent on the cosine transformation tensor sphere angles (9).

$$\varepsilon_{pq} = T_{ip} T_{jq} \varepsilon_{ij} \quad \Longleftrightarrow \quad [\varepsilon_P] = [T]^t [\varepsilon] [T] \tag{7}$$

$$T_{ip} T_{jq} = \delta_{pq} \quad \text{and} \quad det\,[T] = 1.0 \tag{8}$$

$$T_{ip} = \cos\left(\vec{e}_i, \vec{e}_p^{\,\prime}\right) \tag{9}$$

Using linear transformation rules, it can be demonstrated that T_{ip} is equal to the principal vector directions from an eigenvalue problem (10), in which a matrix is assembled by grouping the vectors vertically (11). Again, admitting a general eigenvalue, this can be rewritten in a scalar form using tensor notation (12).

$$T_{ip} = v_{ip} \tag{10}$$

$$[T] = [\{\vec{v}_1\}, \{\vec{v}_2\}, \{\vec{v}_3\}] \tag{11}$$

$$\varepsilon_P = \varepsilon_i v_{iP}^2 + \varepsilon_{ij} v_{iP} v_{jP} \tag{12}$$

The exact partial derivative for the first eigenvalue ε_I, for a symmetric tensor can be achieve using expression (13), in which all eigenvectors also dependent on the ε_i and ε_{ij} in the global axis. Since the eigenvectors for tensors above 3×3 are generally computed numerically, these partial derivatives are not straightforward.

$$\frac{\partial \varepsilon_I}{\partial \varepsilon_i} = v_{iI}^2 + 2\varepsilon_j \frac{\partial v_{jI}}{\partial \varepsilon_i} + 2\varepsilon_{kj} \frac{\partial \left(v_{kI} v_{jI}\right)}{\partial \varepsilon_i} \quad \frac{\partial \varepsilon_I}{\partial \varepsilon_{ij}} = 2\varepsilon_m \frac{\partial v_{mI}}{\partial \varepsilon_{ij}} + 2 v_{iI} v_{jI} + 2\varepsilon_{km} \frac{\partial \left(v_{kI} v_{mI}\right)}{\partial \varepsilon_{ij}} \tag{13}$$

To simplify the presentation, the first principal value is given by (14) for a symmetric tensor. Admitting as a simplification that v_{iI} to be constant, the derivative for the diagonal and non-diagonal terms can be approximated as (15).

$$\varepsilon_I = \varepsilon_1 v_{1I}^2 + \varepsilon_2 v_{2I}^2 + \varepsilon_3 v_{3I}^2 + 2\varepsilon_{12} v_{1I} v_{2I} + 2\varepsilon_{23} v_{2I} v_{3I} + 2\varepsilon_{31} v_{3I} v_{1I} \tag{14}$$

$$\frac{\partial \varepsilon_I}{\partial \varepsilon_i} = v_{iI}^2 \quad \text{and} \quad \frac{\partial \varepsilon_I}{\partial \varepsilon_{ij}} = 2 v_{iI} v_{jI} \tag{15}$$

It is important to note that this assumes a weak variation of the cosine transformation tensor with sphere angles close to 0. For the particular case of a pure shear distortion tensor, the error of this approximation is very coarse, since the non-diagonal terms can have a bigger importance. For this reason, this methodology is not enough to obtain an analytical approximation of the exact Jacobian from principal values to global values for the eigenvalue problem.

3.2 2D Jacobian Derivative

This particular case has been widely used by several authors [41] to numerically simplify real 3D cases under certain boundary conditions. The Jacobian for the transformation of the global values to the principal values in an eigenvalue problem was already demonstrated in the work of [4]. This was performed using classical Mohr-Circle geometry transformation, in which there is always a connection between ε_i and ε_I (16), using the circle radius (R) and circle geometric centre (C). These derivatives are easy to obtain and can be demonstrated for the case of 2D plane strain (17).

$$\begin{cases} \varepsilon_I = C + R \\ \varepsilon_{II} = C - R \end{cases} \quad with \quad \begin{aligned} R &= \sqrt{\left(\frac{\varepsilon_1 - \varepsilon_2}{2}\right)^2 + \varepsilon_{12}^2} \\ C &= \frac{(\varepsilon_1 + \varepsilon_2)}{2} \end{aligned} \tag{16}$$

$$\frac{\partial \varepsilon_P}{\partial \varepsilon_i} = \begin{cases} \dfrac{\partial \varepsilon_I}{\partial \varepsilon_1} = \dfrac{1}{4} \times \left(2 + \dfrac{\varepsilon_1 - \varepsilon_2}{R}\right) \\ \dfrac{\partial \varepsilon_I}{\partial \varepsilon_2} = \dfrac{1}{4} \times \left(2 - \dfrac{\varepsilon_1 - \varepsilon_2}{R}\right) \\ \dfrac{\partial \varepsilon_I}{\partial \varepsilon_{12}} = \dfrac{\varepsilon_{12}}{R} \end{cases} \quad \begin{cases} \dfrac{\partial \varepsilon_{II}}{\partial \varepsilon_1} = \dfrac{\partial \varepsilon_I}{\partial \varepsilon_2} \\ \dfrac{\partial \varepsilon_{II}}{\partial \varepsilon_2} = \dfrac{\partial \varepsilon_I}{\partial \varepsilon_1} \\ \dfrac{\partial \varepsilon_{II}}{\partial \varepsilon_{12}} = -\dfrac{\partial \varepsilon_I}{\partial \varepsilon_{12}} \end{cases} \tag{17}$$

An alternative method is to apply a cross derivative using the tensor invariants. Since the tensor is 2D, it only possesses two invariants. These are always valid either for the global values (18) or principal values (19), in which the main difference is the non-diagonal term.

$$\begin{cases} \varepsilon_1 + \varepsilon_2 = I_1 \\ \varepsilon_1 \times \varepsilon_2 - \varepsilon_{12}^2 = I_2 \end{cases} \tag{18}$$

$$\begin{cases} \varepsilon_I + \varepsilon_{II} = I_1 \\ \varepsilon_I \times \varepsilon_{II} = I_2 \end{cases} \tag{19}$$

When applying the cross derivatives, the invariant derivatives are exactly the same, either in the global values (20) or principal values (21).

$$\begin{aligned} \frac{\partial I_1}{\partial \varepsilon_i} &= 1 \quad & \frac{\partial I_1}{\partial \varepsilon_{ij}} &= 0 \\ \frac{\partial I_2}{\partial \varepsilon_i} &= \varepsilon_{j \neq i} \quad & \frac{\partial I_2}{\partial \varepsilon_{ij}} &= -2\varepsilon_{ij} \end{aligned} \tag{20}$$

$$\begin{cases} \dfrac{\partial \varepsilon_I}{\partial \varepsilon_i} + \dfrac{\partial \varepsilon_{II}}{\partial \varepsilon_i} = \dfrac{\partial I_1}{\partial \varepsilon_i} \\ \dfrac{\partial \varepsilon_I}{\partial \varepsilon_i} \times \varepsilon_{II} + \varepsilon_I \times \dfrac{\partial \varepsilon_{II}}{\partial \varepsilon_i} = \dfrac{\partial I_2}{\partial \varepsilon_i} \end{cases} \tag{21}$$

Since the linear system presents two independent variables, it is possible to solve it (22), if the $\varepsilon_I - \varepsilon_{II} \neq 0$. If this last case is not verified, then the global values and principal values are easy to derivate since they present a linear relationship between them and the Mohr's circle is reduced to a point.

$$\begin{cases} \dfrac{\partial \varepsilon_I}{\partial \varepsilon_i} = \dfrac{\dfrac{\partial I_1}{\partial \varepsilon_i} \times \varepsilon_I - \dfrac{\partial I_2}{\partial \varepsilon_i}}{\varepsilon_I - \varepsilon_{II}} \\ \dfrac{\partial \varepsilon_{II}}{\partial \varepsilon_i} = \dfrac{\dfrac{\partial I_1}{\partial \varepsilon_i} \times \varepsilon_{II} - \dfrac{\partial I_2}{\partial \varepsilon_i}}{\varepsilon_{II} - \varepsilon_I} \end{cases} \tag{22}$$

An important observation is, as expected, from a mathematical point of view, the order of the principal values is irrelevant when deducing the analytical expressions. This is the case, and a single expression can be written independent of the first or second eigenvalue (23). In this case, ε_P is the analysed principal axis, and $\varepsilon_{Q \neq P}$ is the perpendicular one.

$$\frac{\partial \varepsilon_P}{\partial \varepsilon_i} = \frac{\dfrac{\partial I_1}{\partial \varepsilon_i} \times \varepsilon_P - \dfrac{\partial I_2}{\partial \varepsilon_i}}{\varepsilon_P - \varepsilon_{Q \neq P}} \tag{23}$$

Although the invariants derivatives are not equal for the diagonal and non-diagonal, these can be simplified respectively as (24) and (25).

$$\begin{cases} \dfrac{\partial \varepsilon_I}{\partial \varepsilon_i} = \dfrac{\varepsilon_I - \varepsilon_{j \neq i}}{\varepsilon_I - \varepsilon_{II}} \\ \dfrac{\partial \varepsilon_{II}}{\partial \varepsilon_i} = \dfrac{\varepsilon_{II} - \varepsilon_{j \neq i}}{\varepsilon_{II} - \varepsilon_I} \end{cases} \tag{24}$$

$$\begin{cases} \dfrac{\partial \varepsilon_I}{\partial \varepsilon_{ij}} = \dfrac{2\varepsilon_{ij}}{\varepsilon_I - \varepsilon_{II}} \\ \dfrac{\partial \varepsilon_{II}}{\partial \varepsilon_{ij}} = \dfrac{2\varepsilon_{ij}}{\varepsilon_{II} - \varepsilon_I} \end{cases} \tag{25}$$

There is a limitation to the application to this expression, in this case the denominator cannot be zero. If this happens both eigenvalues are equal and the solution is indeterminate. It is possible to demonstrate that the solution in the Mohr circle is a single point, and the derivatives can be calculated by solving the indeterminate form, resulting in this case (26).

$$\frac{\partial \varepsilon_{I,II}}{\partial \varepsilon_1} = \frac{\partial \varepsilon_{I,II}}{\partial \varepsilon_2} = 1 \quad \frac{\partial \varepsilon_{I,II}}{\partial \varepsilon_{12}} = 0 \tag{26}$$

At first glance it seems the derivatives (24) and (25) are different from (17). However, with mathematical algebraic tricks, it can be demonstrated they are exactly the same. For simplicity of presentation, the derivative of the 1st eigenvalue relative to the 1st value in the global axis (27) will be demonstrated.

$$\frac{\partial \varepsilon_I}{\partial \varepsilon_1} = \frac{1}{2} + \frac{\varepsilon_1 - \varepsilon_2}{2\left(\varepsilon_I - \varepsilon_{II}\right)} \quad \text{since} \quad 2R = \varepsilon_I - \varepsilon_{II} \quad \text{and} \quad \varepsilon_I \geq \varepsilon_{II} \tag{27}$$

By adding new numerators (28) and using the same fraction denominators in (29) to (30), it is possible to rewrite the numerators in terms of the invariants (31).

$$\Longleftrightarrow \frac{\partial \varepsilon_I}{\partial \varepsilon_1} = \frac{\varepsilon_I - \varepsilon_{II} + \varepsilon_1 - \varepsilon_2}{2\left(\varepsilon_I - \varepsilon_{II}\right)} \tag{28}$$

$$\Longleftrightarrow \frac{\partial \varepsilon_I}{\partial \varepsilon_1} = \frac{\varepsilon_1 - \varepsilon_{II} - \varepsilon_I + \varepsilon_2}{2\left(\varepsilon_I - \varepsilon_{II}\right)} + \frac{\varepsilon_I + \varepsilon_I - \varepsilon_2 - \varepsilon_2}{2\left(\varepsilon_I - \varepsilon_{II}\right)} \tag{29}$$

$$\Longleftrightarrow \frac{\partial \varepsilon_I}{\partial \varepsilon_1} = \frac{\varepsilon_1 + \varepsilon_2 - \left(\varepsilon_I + \varepsilon_{II}\right)}{2\left(\varepsilon_I - \varepsilon_{II}\right)} + \frac{\varepsilon_I + \varepsilon_I - \varepsilon_2 - \varepsilon_2}{2\left(\varepsilon_I - \varepsilon_{II}\right)} \tag{30}$$

$$\Longleftrightarrow \frac{\partial \varepsilon_I}{\partial \varepsilon_1} = \frac{I_1 - \left(I_1\right)}{2\left(\varepsilon_I - \varepsilon_{II}\right)} + \frac{2\left(\varepsilon_I - \varepsilon_2\right)}{2\left(\varepsilon_I - \varepsilon_{II}\right)} \tag{31}$$

One of the numerators is nullified, and it is possible to get (32), which is exactly the same derivative of (17).

$$\Longrightarrow \frac{\partial \varepsilon_I}{\partial \varepsilon_1} = \frac{\varepsilon_I - \varepsilon_2}{\varepsilon_I - \varepsilon_{II}} \tag{32}$$

This can easily be demonstrated for the case of principal values derivatives relative to the non-diagonal terms (33). By direct substitution of the Mohr-Circle radius (R), it is possible to verify the same derivative (34) as the previous one presented in (17).

$$\frac{\partial \varepsilon_I}{\partial \varepsilon_{12}} = \frac{\varepsilon_{12}}{R} \quad \text{since} \quad R = \frac{\varepsilon_I - \varepsilon_{II}}{2} \quad \text{and} \quad \varepsilon_I \geq \varepsilon_{II} \tag{33}$$

$$\frac{\partial \varepsilon_I}{\partial \varepsilon_{12}} = \frac{2\varepsilon_{12}}{\varepsilon_I - \varepsilon_{II}} \tag{34}$$

It is then demonstrated that the cross derivatives are indeed possible to be used and provide equal values of the direct analytical derivatives in the 2D case.

3.3 3D Jacobian Derivative

For the 3D case, the same hypothesis of the existence of a cross derivative with tensor invariants will be used. Since the tensor possesses 3D axes, three invariants are needed (35). For the principal axes this can be simplified due to the inexistence of diagonal terms (36).

$$\begin{cases} \varepsilon_1 + \varepsilon_2 + \varepsilon_3 = I_1 \\ \varepsilon_1 \times \varepsilon_2 + \varepsilon_2 \times \varepsilon_3 + \varepsilon_3 \times \varepsilon_1 - \varepsilon_{12}^2 - \varepsilon_{23}^2 - \varepsilon_{31}^2 = I_2 \\ \varepsilon_1 \times \varepsilon_2 \times \varepsilon_3 + 2 \times \varepsilon_{12} \times \varepsilon_{23} \times \varepsilon_{31} - \varepsilon_1 \times \varepsilon_{23}^2 - \varepsilon_2 \times_{31}^2 - \varepsilon_3 \times \varepsilon_{12}^2 = I_3 \end{cases} \tag{35}$$

$$\begin{cases} \varepsilon_I + \varepsilon_{II} + \varepsilon_{III} = I_1 \\ \varepsilon_I \times \varepsilon_{II} + \varepsilon_{II} \times \varepsilon_{III} + \varepsilon_{III} \times \varepsilon_I = I_2 \\ \varepsilon_I \times \varepsilon_{II} \times \varepsilon_{III} = I_3 \end{cases} \tag{36}$$

Since the invariants are the same independent of the chosen axes, the derivatives of the invariants are also the same, independently of these being defined in the global (37) or principal values (38).

$$\begin{aligned} \frac{\partial I_1}{\partial \varepsilon_i} &= 1 & \frac{\partial I_1}{\partial \varepsilon_{ij}} &= 0 \\ \frac{\partial I_2}{\partial \varepsilon_i} &= \varepsilon_j + \varepsilon_k & \frac{\partial I_2}{\partial \varepsilon_{ij}} &= -2\varepsilon_{ij} \\ \frac{\partial I_3}{\partial \varepsilon_i} &= \varepsilon_j \times \varepsilon_k - \varepsilon_{jk}^2 & \frac{\partial I_3}{\partial \varepsilon_{ij}} &= 2\left(\varepsilon_{ik} \times \varepsilon_{jk} - \varepsilon_k \times \varepsilon_{ij}\right) \end{aligned} \tag{37}$$

$$\begin{cases} \dfrac{\partial \varepsilon_I}{\partial \varepsilon_i} + \dfrac{\partial \varepsilon_{II}}{\partial \varepsilon_i} + \dfrac{\partial \varepsilon_{III}}{\partial \varepsilon_i} = \dfrac{\partial I_1}{\partial \varepsilon_i} \\ \dfrac{\partial \varepsilon_I}{\partial \varepsilon_i} \times \varepsilon_{II} + \varepsilon_I \times \dfrac{\partial \varepsilon_{II}}{\partial \varepsilon_i} + \dfrac{\partial \varepsilon_{II}}{\partial \varepsilon_i} \times \varepsilon_{III} + \varepsilon_{II} \times \dfrac{\partial \varepsilon_{III}}{\partial \varepsilon_i} + \dfrac{\partial \varepsilon_{III}}{\partial \varepsilon_i} \times \varepsilon_I + \varepsilon_{III} \times \dfrac{\partial \varepsilon_I}{\partial \varepsilon_i} = \dfrac{\partial I_2}{\partial \varepsilon_i} \\ \dfrac{\partial \varepsilon_I}{\partial \varepsilon_i} \times \varepsilon_{II} \times \varepsilon_{III} + \varepsilon_I \times \dfrac{\partial \varepsilon_{II}}{\partial \varepsilon_i} \times \varepsilon_{III} + \varepsilon_I \times \varepsilon_{II} \times \dfrac{\partial \varepsilon_{III}}{\partial \varepsilon_i} = \dfrac{\partial I_3}{\partial \varepsilon_i} \end{cases} \tag{38}$$

Once again, this is a set of three independent variables in a linear system of 3×3, and the solution of the dependent terms (39) can be achieved using standard Cramer's rule [42]. Again, it can point to the non-dependence of choosing either the first or last principal value to execute the derivative, which means there is a radial effect that can be written as (40) for the principal value (P) depending on the other principal values (Q, T).

$$\begin{cases} \dfrac{\partial \varepsilon_I}{\partial \varepsilon_i} = \dfrac{\dfrac{\partial I_1}{\partial \varepsilon_i}\varepsilon_I^2 - \dfrac{\partial I_2}{\partial \varepsilon_i}\varepsilon_I + \dfrac{\partial I_3}{\partial \varepsilon_i}}{\varepsilon_I^2 - \varepsilon_I \times \varepsilon_{II} - \varepsilon_I \times \varepsilon_{III} + \varepsilon_{II} \times \varepsilon_{III}} \\ \dfrac{\partial \varepsilon_{II}}{\partial \varepsilon_i} = \dfrac{\dfrac{\partial I_1}{\partial \varepsilon_i}\varepsilon_{II}^2 - \dfrac{\partial I_2}{\partial \varepsilon_i}\varepsilon_{II} + \dfrac{\partial I_3}{\partial \varepsilon_i}}{\varepsilon_{II}^2 - \varepsilon_{II} \times \varepsilon_I - \varepsilon_{II} \times \varepsilon_{III} + \varepsilon_{III} \times \varepsilon_I} \\ \dfrac{\partial \varepsilon_{III}}{\partial \varepsilon_i} = \dfrac{\dfrac{\partial I_1}{\partial \varepsilon_i}\varepsilon_{III}^2 - \dfrac{\partial I_2}{\partial \varepsilon_i}\varepsilon_{III} + \dfrac{\partial I_3}{\partial \varepsilon_i}}{\varepsilon_{III}^2 - \varepsilon_{III} \times \varepsilon_I - \varepsilon_{III} \times \varepsilon_{II} + \varepsilon_{II} \times \varepsilon_I} \end{cases} \tag{39}$$

$$\frac{\partial \varepsilon_P}{\partial \varepsilon_i} = \frac{\dfrac{\partial I_1}{\partial \varepsilon_i}\varepsilon_P^2 - \dfrac{\partial I_2}{\partial \varepsilon_i}\varepsilon_P + \dfrac{\partial I_3}{\partial \varepsilon_i}}{\varepsilon_P^2 - \varepsilon_P \times \varepsilon_{Q \neq P} - \varepsilon_P \times \varepsilon_{T \neq P} + \varepsilon_{Q \neq P} \times \varepsilon_{T \neq P}} \tag{40}$$

Again, separating the diagonal and non-diagonal terms of the global variables, this last expression (40) can be simplified into (41) and (42), respectively.

$$\frac{\partial \varepsilon_P}{\partial \varepsilon_i} = \frac{\varepsilon_P^2 - \left(\varepsilon_j + \varepsilon_k\right) \times \varepsilon_P + \varepsilon_j \times \varepsilon_k - \varepsilon_{jk}^2}{\varepsilon_P^2 - \varepsilon_P \times \varepsilon_{Q \neq P} - \varepsilon_P \times \varepsilon_{T \neq P} + \varepsilon_{Q \neq P} \times \varepsilon_{T \neq P}} \tag{41}$$

$$\frac{\partial \varepsilon_P}{\partial \varepsilon_{ij}} = \frac{2\left(\varepsilon_{ij} \times \varepsilon_P + \varepsilon_{ik} \times \varepsilon_{jk} - \varepsilon_k \times \varepsilon_{ij}\right)}{\varepsilon_P^2 - \varepsilon_P \times \varepsilon_{Q \neq P} - \varepsilon_P \times \varepsilon_{T \neq P} + \varepsilon_{Q \neq P} \times \varepsilon_{T \neq P}} \tag{42}$$

It is possible to retrieve the 2D derivative solution (23) as a particular case of the 3D by admitting $\varepsilon_{III} = 0$ and $I_3 = 0$. This demonstrates that the analytical expression is not dependent on the rank of the tensor, therefore validating the solution. In addition, the denominator can be written as (43), meaning stability is guaranteed in the case of eigenvalue degeneracy.

$$\varepsilon_P \times \left(\varepsilon_P - \varepsilon_{Q \neq P} - \varepsilon_{T \neq P}\right) + \varepsilon_{Q \neq P} \times \varepsilon_{T \neq P} \tag{43}$$

3.4 Limitations

There are particular aspects that need to be verified when applying these expressions since some singularities may occur. These are related to the non-nullity of the denominators, in which this needs to be verified (44).

$$\varepsilon_P^2 - \varepsilon_P \times \varepsilon_{Q\neq P} - \varepsilon_P \times \varepsilon_{T\neq P} + \varepsilon_{Q\neq P} \times \varepsilon_{T\neq P} \neq 0 \tag{44}$$

If this condition is not checked, then there is a possibility of all eigenvalues being equal. If this last condition is also not verified, then the Mohr's circle is reduced to a point, and the derivatives are straight forward. In this case the solution is indeterminate, and its resolution can be achieved therefore obtaining the following expressions (45).

$$\frac{\partial \varepsilon_P}{\partial \varepsilon_i} = 1 \quad \frac{\partial \varepsilon_P}{\partial \varepsilon_{ij}} = 0 \tag{45}$$

4 Numerical Examples

In this section, some numerical examples will be presented to test the proposed analytical derivatives. According to [32], a generalization expression (12) can be used to calculate analytically any principal value, which means it is possible to also compute a numerical derivative (46). This will be presented as an academic example to numerically validate the analytically proposed Jacobians.

These proposed derivative expressions will be compared with known approximated values and numerical methods using the disturbance method [4]. The Disturbance Method uses the standard derivative Formula (47), but it fixes the value of the disturbance $h = 10^{-3}$ for each column and row index i, j separately (46). This means for a symmetric tensor, this must be performed separately $6 + 1$ times, including the calculation of a fully principal tensor separately (ε_P), which may be computationally very expensive.

$$\varepsilon_P\left(\varepsilon_1, \varepsilon_2, \varepsilon_3, \varepsilon_{12}, \varepsilon_{23}, \varepsilon_{31}\right) \tag{46}$$

$$f'(x) = \lim_{h \longrightarrow 0} \frac{f(x+h) - f(x)}{h} \tag{47}$$

For $\mathbb{R}^2$, the partial derivative of the function $f(x, y)$ is given by (48). For the expression (12), this can be extrapolated for each row for a given principal strain, and each column for the respective strain at the global axis. It is then possible to calculate approximately the numerical Jacobian for each row and column.

$$\begin{aligned} \frac{\partial f(x,y)}{\partial x} &= \lim_{h \longrightarrow 0} \frac{f(x+h,y) - f(x,y)}{h} \\ \frac{\partial f(x,y)}{\partial y} &= \lim_{h \longrightarrow 0} \frac{f(x,y+h) - f(x,y)}{h} \end{aligned} \tag{48}$$

To solve the eigenvalues, the free open software wxMaxima [43], will be used. Although wxMaxima works mainly with symbolic formulations, it is still possible to achieve numerical results with good approximation. Since it uses symbolic operations during the eigenvalues, the software will always present principal values in the complex domain. However, due to the used tensors being symmetric, the presented values of the imaginary part are always 0. To achieve maximum accuracy during the disturbance method, double float digits will be forced, and these are the best possible solution according to the user's manual. To shorten the presentation, this numerical derivative will only be applied to the Jacobian row ε_I and column ε_1, according to (49).

$$\left.\frac{\partial \varepsilon_I}{\partial \varepsilon_1}\right|_{\varepsilon_1+h} \simeq \left.\frac{\varepsilon_P\left(\varepsilon_j + h, \varepsilon_{i(i\neq j)}\right) - \varepsilon_P\left(\varepsilon_j, \varepsilon_{i(i\neq j)}\right)}{h}\right|_h \tag{49}$$

This methodology can indeed be used to provide a numerical Jacobian from principal values to global values for the eigenvalue problem. However, these need to be applied at least 7 times for a 3D problem in which the eigenvalues need to be fully calculated each time. Since the eigenvalue problem is an iterative process by itself, to solve it at least 7 times would be a very expensive computational cost, which is unreliable in incremental non-linear analysis.

For this reason, the pursuit for an analytical exact Jacobian from principal values to global values for the eigenvalue problem, may present an optimal solution, in future implementations.

4.1 Polynomial 2D Tensor

Initially only a 2D tensor will be tested, to verify the analytical formulation for the plane strain hypothesis. The tensor will be 2 × 2 with all indexes different from zero, which is the most difficult case to numerically derivate. This will provide a full, robust test to study the accuracy of the analytical derivatives.

The tensor will be time dependent (50) just like in a non-linear computational analysis, and the derivative will be calculated for the time $t = 3.0$ (51). With this tensor 2 × 2 it is possible to calculate the two principal values for the same time set (52).

$$[\varepsilon(t)] = \begin{bmatrix} t & 1/t \\ 1/t & \sqrt{t} \end{bmatrix} \tag{50}$$

$$[\varepsilon(3)] = \begin{bmatrix} 3 & 1/3 \\ 1/3 & \sqrt{3} \end{bmatrix} \tag{51}$$

$$\left[\varepsilon_p(3)\right] = \left[3.082289949715476 \quad 1.6497608578534002\right] \tag{52}$$

With these values it is possible to calculate the 1st row and the 1st column of the Jacobian from principal values to global values for the eigenvalue problem. Initially it is possible to calculate the derivatives of the 1st and 2nd invariants I_1, I_2 (53) with respect to ε_1 (54).

$$\frac{\partial I_1}{\partial \varepsilon_1} = 1.0 \quad \frac{\partial I_2}{\partial \varepsilon_1} = \sqrt{3} \tag{53}$$

$$\frac{\partial \varepsilon_I}{\partial \varepsilon_1} = \frac{\varepsilon_I^2 - \sqrt{3} \times \varepsilon_I}{\varepsilon_I^2 - \varepsilon_I \times \varepsilon_{II}} = 0.9426316977408544 \tag{54}$$

To use the disturbance method for the strain ε_1, it is necessary to apply a small disturbance $h = 10^{-3}$ in the same index of the column and row (55). It is now possible to calculate the new principal values, with values very close to the previous one since the disturbance is very small (56).

$$[\varepsilon_{1_h}(3)] = \begin{bmatrix} 3+h & 1/3 \\ 1/3 & \sqrt{3} \end{bmatrix} \tag{55}$$

$$\left[\varepsilon_p(3, \varepsilon_{1h})\right] = \left[3.0832325436637693 \quad 1.6498182639051067\right] \tag{56}$$

Later the numerical partial derivative is calculated, using the expression (23). The difference between the analytical value (57), and the numerical value is below 0.005%. It is then possible to confirm that the analytical derivative provides accurate results when compared with numerical models.

$$\frac{\partial \varepsilon_I}{\partial \varepsilon_1} \simeq \frac{3.0832325436637693 - 3.082289949715476}{10^{-3}} = 0.9425939482934353 \tag{57}$$

To evaluate that the error tends to zero, a variation of the exponent z used in the disturbance coefficient (58), varies from 1 to 7 and is displayed in Fig. 1 with a vertical logarithmic scale. The analytical expression seems to be correct, since the error tends to zero with the increase of the exponent z, with values lower than 0.0000002%.

$$h = 10^{-z} \tag{58}$$

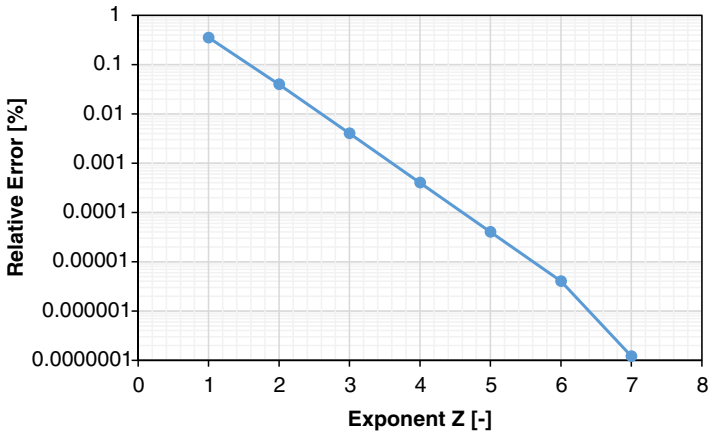


Figure 1: Variation of the error with the increase of the exponent z for the 2D tensor.

4.2 Polynomial 3D Tensor

A similar tensor was used, by this time with all columns and rows filled in 3 × 3. The most challenging case to numerically deduce is when all the indexes are different from zero. This will offer a comprehensive and reliable test to examine the precision of the analytical derivatives.

$$[\varepsilon(t)] = \begin{bmatrix} 0.5t & 4t & 5t \\ 4t & 2t & t \\ 5t & t & 3t \end{bmatrix} \tag{59}$$

Again, the tensor will be time dependent (59), and the derivative will be calculated for the time $t = 2.0$ (60). The three principal values for the same time set can be computed using this tensor 3 × 3 (61).

$$[\varepsilon(2)] = \begin{bmatrix} 1 & 8 & 10 \\ 8 & 4 & 2 \\ 10 & 2 & 6 \end{bmatrix} \tag{60}$$

$$\left[\varepsilon_p(2, \varepsilon_1)\right] = \begin{bmatrix} 17.270352692563463 & 2.826210087673758 & -9.096562780237221 \end{bmatrix} \tag{61}$$

The first row and the first column of the Jacobian from principal values to global values for the eigenvalue problem can be computed using these numbers (63). First, the derivatives of the 1st, 2nd and 3rd invariants

I_1, I_2, I_e with respect to ε_1 (62) can be computed.

$$\frac{\partial I_1}{\partial \varepsilon_i} = 1 \quad \frac{\partial I_2}{\partial \varepsilon_1} = 10 \quad \frac{\partial I_3}{\partial \varepsilon_i} = 20 \tag{62}$$

$$\frac{\partial \varepsilon_I}{\partial \varepsilon_1} = \frac{\varepsilon_I^2 - 10 \times \varepsilon_I + 20}{\varepsilon_I^2 - \varepsilon_I \times \varepsilon_{II} - \varepsilon_I \times \varepsilon_{III} + \varepsilon_{II} \times \varepsilon_{III}} = 0.38222226997322245 \tag{63}$$

Again, just like in the previous example, a small disturbance $h = 10^{-3}$ must be applied at the same index of the column and row (64) in order to apply the disturbance method for the strain ε_1. Since there is very little disturbance, it is now feasible to calculate the new principal values, which are extremely similar to the prior one (65).

$$[\varepsilon_{1_h}(2)] = \begin{bmatrix} 1+h & 8 & 10 \\ 8 & 4 & 2 \\ 10 & 2 & 6 \end{bmatrix} \tag{64}$$

$$\left[\varepsilon_p(2, \varepsilon_{1h})\right] = \left[17.270734905858873 \quad 2.8262116824568464 \quad -9.09594658831572\right] \tag{65}$$

Finally, the expression (41) is then used to calculate the numerical partial derivative. The numerical value and the analytical value (66) differ by less than 0.005%. The accuracy of the results obtained from the analytical derivative can then be verified by comparing it with numerical models.

$$\frac{\partial \varepsilon_I}{\partial \varepsilon_1} \simeq \frac{17.270734905858873 - 17.270352692563463}{10^{-3}} = 0.38221329540988336 \tag{66}$$

As in the previous example to evaluate that the error lean towards zero, a variation of the exponent z used in the disturbance coefficient (58), varies from 1 to 7 and is displayed in Fig. 2, also with a vertical logarithmic scale. The analytical expression appears to be true, as the error goes to zero with increasing the exponent z, with values less than 0.000002%. It is observed an error increase after exponent 7. This is due to wxmaxima symbolic round off errors in eigenvalue calculation, when decimal float variable is converted to double precision.

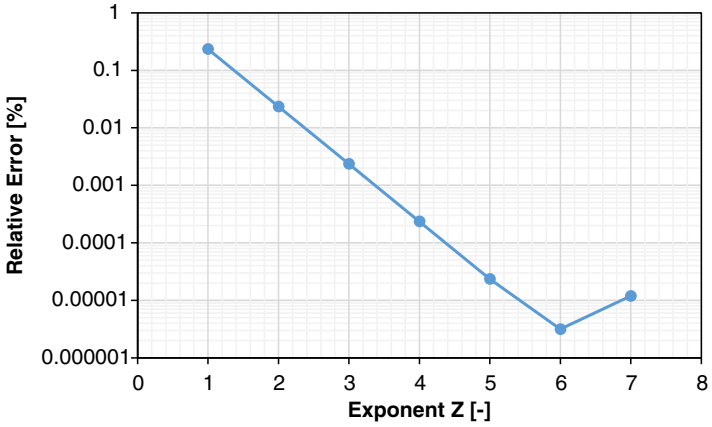


Figure 2: Variation of the error with the increase of the exponent z for the 3D tensor.

5 Conclusions

The main objective of this work was to establish an analytical formulation for the exact Jacobian matrix of a second-order tensor in 3D as a function of its eigenvalue orientation relative to the values in global coordinates. Using simple cross derivatives using the invariants, it was possible to extrapolate a simple general expression for the rows and columns of the Jacobian.

By validating the 2D case against Mohr's circle theory and extending the approach to 3D through invariants and indirect differentiation, it offers a robust methodology for applying eigenvalue analysis to material behaviour problems when an exact tangent stiffness needs to be calculated. The agreement between the analytical 3D formulation and numerical methodology results confirms both the accuracy and applicability of the proposed framework. This comprehensive demonstration provides an essential tool for advanced material modelling and implementation in computational mechanics.

5.1 Further Developments

The genesis of this work happened during the implementation of an exact Jacobian stiffness matrix, during the assembly of a UMAT user subroutine for the finite element software ABAQUS. This UMAT-based Mazars damage model will be implemented in the future with this new 3D exact Jacobian stiffness matrix using an exact Jacobian from principal values to global values for eigenvalue problems.

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Availability of Data and Materials: All data and UMAT files, with the proposed Jacobian will be publicly displayed and ready to be downloaded by the scientific community on GitHub at github.com/marioruiarruda/.

Ethics Approval: Not applicable.

Conflicts of Interest: The authors declare no conflicts of interest.

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