Direct determination of the rotation in the polar decomposition of the deformation gradient by maximizing a Rayleigh quotient

C. Bouby [1], **D. Fortuné** [2], **W. Pietraszkiewicz** *[3], and **C. Vallée** [2]

[1] LML, Université Lille 1, bd P. Langevin, Cité Scientifique, F-59655 Villeneuve d'Ascq cedex, France
[2] L3MA, SP2MI, bd M. et P. Curie, téléport 2, BP 30179, F-86962 Futuroscope-Chasseneuil cedex, France
[3] Institute of Fluid-Flow Machinery, Polish Academy of Sciences, ul. Gen. J. Fiszera, 80-952, Gdańsk, Poland

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We develop a new effective method of determining the rotation $\mathbf{R}$ and the stretches $\mathbf{U}$ and $\mathbf{V}$ in the polar decomposition $\mathbf{F} = \mathbf{RU} = \mathbf{VR}$ of the deformation gradient. The method is based on a minimum property of $\mathbf{R}$ to have the smallest "distance" from $\mathbf{F}$ in the Euclidean norm. The proposed method does not require to perform any square root and/or inverse operations. With each $\mathbf{F}$ having nine independent components we associate a 4×4 symmetric traceless matrix Q. The rotation is described by quaternion parameters from which a quadrivector X is formed. It is shown that X corresponding to $\mathbf{R}$ maximizes X^TQX over all X satisfying $X^TX = 1$. We prefer to equivalently maximize the Rayleigh quotient Y^TQY/Y^TY over all non-vanishing Y and to deduce X by subsequent normalization $X = Y/\sqrt{Y^TY}$. The maximization of the Rayleigh quotient is performed by a conjugate gradient algorithm with all iterative steps carried out by explicit closed formulae. Efficiency and accuracy of the method is illustrated by a numerical example.

1 Introduction

Within classical continuum mechanics (see [1], for example, also for notation[1]) the local deformation is described by the deformation gradient $\mathbf{F} \in Lin^+$. According to the polar decomposition theorem, there exist unique, symmetric, positive definite stretch tensors $\mathbf{U}$, $\mathbf{V} \in$ *Psym* and a rotation $\mathbf{R} \in Orth^+$ such that

$$\mathbf{F} = \mathbf{RU} = \mathbf{VR} \tag{1}$$

The rotation $\mathbf{R}$ can be found from (1) by first calculating $\mathbf{U} = (\mathbf{F}^T\mathbf{F})^{\frac{1}{2}}$ or $\mathbf{V} = (\mathbf{F}\mathbf{F}^T)^{\frac{1}{2}}$, and then $\mathbf{R} = \mathbf{F}\mathbf{U}^{-1} = \mathbf{V}^{-1}\mathbf{F}$. Such a direct analysis requires to perform square root and inverse operations on symmetric tensors, and this may bring computational difficulties. Alternative procedures for calculating $\mathbf{R}$ from $\mathbf{F}$ without using the square root operation were worked out by Hoger and Carlson [2], Zubov and Rudev [3], Lu and Papadopoulos [4], and Dui [5], where references to other papers are given.

Over sixty years ago Grioli [6] pointed out an interesting minimum property: the rotation $\mathbf{R}$ following from the polar decomposition (1) has the smallest "distance" from $\mathbf{F}$ within Lin equipped with an Euclidean norm. Martin and Podio-Guidugli [7] generalized this result to any linear transformation of a finite-dimensional Euclidean real vector space into itself, and provided in [8] a new proof of the theorem (1). The minimum property of $\mathbf{R}$ was also used in discussing various local measures of mean rotation [9, 10], and in the analysis of fitting a rotation to given data [11].

In this paper the minimum property of the rotation in (1) is used to determine $\mathbf{R}$ directly from $\mathbf{F}$ by maximizing a Rayleigh quotient. In Section 2 we provide an alternative concise proof of the minimum property of $\mathbf{R}$ in (1). Then an arbitrary rotation $\mathbf{\Omega} \in Orth^+$ is parametrized in Section 3 by four quaternion parameters m_1, m_2, m_3, m, [12–17], from which a quadrivector (column matrix) X satisfying the condition $X^TX = 1$ is formed. In Section 4 we introduce a 4×4 symmetric traceless matrix Q with nine independent components established linearly and uniquely from nine independent components of $\mathbf{F}$. The quadrivector X corresponding to $\mathbf{R}$ in (1) is then shown to follow from maximization of the Rayleigh quotient Y^TQY/Y^TY over all non-vanishing quadrivectors Y, with normalization of the result to $X = Y/\sqrt{Y^TY}$. The maximum of the Rayleigh quotient is attained when Y becomes an eigenvector of Q corresponding to its greatest eigenvalue known to be $tr\mathbf{U}$ (or $tr\mathbf{V}$). The characteristic polynomial of Q is revealed in Section 5 to coincide with the fourth-degree polynomial derived by Hoger and Carlson [2] to extract $tr\mathbf{U}$ as a root.

* Corresponding author: e-mail: pietrasz@imp.gda.pl, Phone: +00 48 58 346 08 81, ext.263, Fax: +00 48 58 341 61 44

[1] Lin = the set of all tensors (of the second order, which transform vectors into vectors), Lin^+ = the set of all tensors with positive determinant, Sym = the set of all symmetric tensors, $Psym$ = the set of all symmetric, positive definite tensors, $Orth^+$ = the set of all rotations.

Finally, the effective determination of $\mathbf{R}$ by maximizing the Rayleigh quotient is performed numerically in Section 6 on an example with the help of a conjugate gradient algorithm.

2 Minimum property of the rotation in the polar decomposition

Property: *Let $\mathbf{F} \in Lin^+$. Then among all rotations $\mathbf{\Omega} \in Orth^+$, the rotation $\mathbf{R}$ in the polar decomposition of $\mathbf{F}$ is the closest to $\mathbf{F}$: $\mathbf{R}$ minimizes in Lin the distance $\{tr[(\mathbf{F}-\mathbf{\Omega})^T(\mathbf{F}-\mathbf{\Omega})]\}^{\frac{1}{2}}$.*

Proof. By setting $\| \mathbf{A} \| = [tr(\mathbf{A}^T\mathbf{A})]^{\frac{1}{2}}$, for any $\mathbf{A} \in Lin$ we equip the vector space Lin by the Euclidean norm. Let $\mathbf{\Omega} \in Orth^+$ be a rotation. Then the square of the distance between $\mathbf{F}$ and $\mathbf{\Omega}$ in the norm $\| \,.\, \|$ is

$$\begin{aligned} \| \mathbf{F}-\mathbf{\Omega} \|^2 &= tr[(\mathbf{F}-\mathbf{\Omega})^T(\mathbf{F}-\mathbf{\Omega})] = tr(\mathbf{F}^T\mathbf{F}) + tr(\mathbf{\Omega}^T\mathbf{\Omega}) - tr(\mathbf{F}^T\mathbf{\Omega}) - tr(\mathbf{\Omega}^T\mathbf{F}) \\ &= \| \mathbf{F} \|^2 + 3 - 2tr(\mathbf{F}^T\mathbf{\Omega}) \end{aligned} \tag{2}$$

The problem of minimization of (2) can then be equivalently stated as follows:

$$\text{Given } \mathbf{F} \in Lin^+, \text{ find } \max_{\mathbf{\Omega}\in Orth^+} \; 2tr(\mathbf{F}^T\mathbf{\Omega}) \tag{3}$$

The necessary condition for (3) to attain a maximum is

$$2tr(\mathbf{F}^T\delta\mathbf{\Omega}) = 0 \tag{4}$$

for any variation $\delta\mathbf{\Omega} \in Lin$ satisfying the constraint

$$\delta\mathbf{\Omega}^T\mathbf{\Omega} + \mathbf{\Omega}^T\delta\mathbf{\Omega} = \mathbf{0} \tag{5}$$

Due to linearity of both (4) and (5) relative to $\delta\mathbf{\Omega}$ there exists a tensor $\mathbf{\Lambda} \in Sym$ - a Lagrange multiplier [18] - such that

$$2tr(\mathbf{F}^T\delta\mathbf{\Omega}) = tr[\mathbf{\Lambda}(\delta\mathbf{\Omega}^T\mathbf{\Omega} + \mathbf{\Omega}^T\delta\mathbf{\Omega})] = 2tr(\mathbf{\Lambda}\mathbf{\Omega}^T\delta\mathbf{\Omega})$$

or

$$tr[(\mathbf{F}^T - \mathbf{\Lambda}\mathbf{\Omega}^T)\delta\mathbf{\Omega}] = 0 \qquad \text{for any } \delta\mathbf{\Omega} \in Lin \tag{6}$$

Relation (6) holds only if $\mathbf{F}^T = \mathbf{\Lambda}\mathbf{\Omega}^T$, or $\mathbf{F} = \mathbf{\Omega}\mathbf{\Lambda}$, which gives

$$\mathbf{F}^T\mathbf{F} = \mathbf{\Lambda}^2, \;\; tr(\mathbf{F}^T\mathbf{\Omega}) = tr\mathbf{\Lambda} \tag{7}$$

By $\det \mathbf{F} > 0$ and from $(7)_1$ it follows that

$$\det(\mathbf{F}^T\mathbf{F}) = (\det\; \mathbf{F})^2 = \det(\mathbf{\Lambda}^2) = (\det \mathbf{\Lambda})^2 > 0$$

Therefore, $\mathbf{\Lambda}$ is invertible. Among two $\mathbf{\Lambda}$'s satisfying $(7)_1$ only $\mathbf{\Lambda} = (\mathbf{F}^T\mathbf{F})^{\frac{1}{2}}$ allows $tr\mathbf{\Lambda} = tr(\mathbf{F}^T\mathbf{\Omega})$ to attain the maximum. Such $\mathbf{\Lambda} \in Psym$ coincides with the square root $\mathbf{U}$ of $\mathbf{C} = \mathbf{F}^T\mathbf{F}$. Therefore,

$$\mathbf{\Omega} = \mathbf{F}\mathbf{\Lambda}^{-1} = \mathbf{F}\mathbf{U}^{-1} = \mathbf{R} \tag{8}$$

and among all $\mathbf{\Omega} \in Orth^+$ the rotation $\mathbf{R}$ defined by (1) is the closest to $\mathbf{F}$ in the sense of the norm $\| \,.\, \|$. □

3 Representation of a rotation

Property: *For any rotation $\mathbf{\Omega} \in Orth^+$ there exist a 3-dimensional vector $\mathbf{m}$ and a scalar m satisfying the constraint $\mathbf{m}\cdot\mathbf{m} + m^2 = 1$ such that*

$$\mathbf{\Omega} = (m^2 - \mathbf{m}\cdot\mathbf{m})\mathbf{I} + 2\mathbf{m}\otimes\mathbf{m} + 2m(\mathbf{m}\times\mathbf{I}) \tag{9}$$

where $\mathbf{I}$ is the identity tensor in Lin, $\cdot$ is the scalar product, $\otimes$ is the tensor product, and $\times$ is the cross product.

Proof. Let $\mathbf{\Omega}$ be represented by the Gibbs formula [19]

$$\mathbf{\Omega} = (cos\theta)\mathbf{I} + (sin\theta)\mathbf{n}\times\mathbf{I} + (1-cos\theta)\mathbf{n}\otimes\mathbf{n} \tag{10}$$

where the unit vector $\mathbf{n}$ directed along the axis of rotation satisfies $\mathbf{\Omega}\mathbf{n} = \mathbf{n}$ and θ is the angle of rotation about $\mathbf{n}$. Let us introduce the Euler-Rodrigues parameters $\mathbf{m}$ and m defined by [17]

$$\mathbf{m} = (sin\frac{\theta}{2})\mathbf{n}, \qquad m = cos\frac{\theta}{2}$$

which satisfy the condition $\mathbf{m}\cdot\mathbf{m} + m^2 = 1$ Then $sin\theta$ and $cos\theta$ can be expressed through $\theta/2$ by elementary trigonometric identities, and the rotation (10) can be directly transformed into (9). □

4 Maximization of the Rayleigh quotient

Choosing an orthonormal basis $\mathbf{e}_i,\ \ i = 1,2,3,$ in the 3-dimensional vector space, in this Section we show how the quadrivector (column matrix) $X = (m_1\ m_2\ m_3\ m)^T$, built from three components $m_i = \mathbf{e}_i \cdot \mathbf{m}$ of the vector $\mathbf{m}$ and the scalar m associated with the rotation $\mathbf{R}$ in the polar decomposition (1), can be determined by maximizing a Rayleigh quotient.

Property: *Let* $\mathbf{F} \in Lin^+$, $\mathbf{S} = \frac{1}{2}(\mathbf{F}+\mathbf{F}^T) \in Sym$ *and* $\mathbf{w}$ *be the axial vector of the skew-symmetric tensor* $\mathbf{F}-\mathbf{F}^T$ *given by* $\mathbf{F}-\mathbf{F}^T = \mathbf{w}\times\mathbf{I}$. *For any orthonormal basis* $\mathbf{e}_i$ *the components of the quadrivector* X *associated with the rotation* $\mathbf{R}$ *in the polar decomposition of* $\mathbf{F}$ *maximize the quadratic form* X^TQX *associated with the* 4×4 *symmetric traceless matrix*

$$Q = \begin{pmatrix} 2S-(trS)I & W \\ W^T & trS \end{pmatrix} \tag{11}$$

built from the matrices S *and* W *associated with* $\mathbf{S}$ *and* $\mathbf{w}$, *respectively.*

P r o o f. With the representation (9) of $\mathbf{R}$, $tr(\mathbf{F}^T\mathbf{R})$ becomes

$$tr(\mathbf{F}^T\mathbf{R}) = (m^2-\mathbf{m}\cdot\mathbf{m})tr(\mathbf{F}^T) + 2\mathbf{m}\cdot\mathbf{F}\mathbf{m} + 2m\ tr[\mathbf{F}^T(\mathbf{m}\times\mathbf{I})]$$

Splitting the deformation gradient $\mathbf{F}$ into its symmetric and skew-symmetric parts, we obtain

$$\mathbf{m}\cdot\mathbf{F}\mathbf{m} = \mathbf{m}\cdot\mathbf{S}\mathbf{m}, \quad tr\mathbf{F}^T = tr\mathbf{S}, \quad tr[\mathbf{F}^T(\mathbf{m}\times\mathbf{I})] = -\frac{1}{2}tr[(\mathbf{w}\times\mathbf{I})(\mathbf{m}\times\mathbf{I})] = \mathbf{w}\cdot\mathbf{m}$$

Then

$$tr(\mathbf{F}^T\mathbf{R}) = (m^2-\mathbf{m}\cdot\mathbf{m})tr\mathbf{S} + 2\mathbf{m}\cdot\mathbf{S}\mathbf{m} + 2m\mathbf{w}\cdot\mathbf{m} \tag{12}$$

In the orthonormal basis $\mathbf{e}_i$ the vectors $\mathbf{m}$, $\mathbf{w}$ and the tensors $\mathbf{S}$, $\mathbf{I}$, $\mathbf{m}\times\mathbf{I}$ are represented by the corresponding matrices

$$M = \begin{pmatrix} m_1 \\ m_2 \\ m_3 \end{pmatrix}, \quad W = \begin{pmatrix} w_1 \\ w_2 \\ w_3 \end{pmatrix} \tag{13}$$

$$S = \begin{pmatrix} S_{11} & S_{12} & S_{13} \\ S_{12} & S_{22} & S_{23} \\ S_{13} & S_{23} & S_{33} \end{pmatrix}, \quad I = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad M\times I = \begin{pmatrix} 0 & -m_3 & m_2 \\ m_3 & 0 & -m_1 \\ -m_2 & m_1 & 0 \end{pmatrix}$$

Introducing the 4×4 matrix Q by (11) it is seen that $trQ = 0$. With the quadrivector X defined above (11), the expression (12) becomes $tr(\mathbf{F}^T\mathbf{R}) = X^TQX$. Now the minimum property of $\mathbf{R}$ in terms of M and m reads

$$\text{Given } Q, \quad \text{find} \quad \max_{X,\ X^TX=1} \quad X^TQX$$

which is equivalent to

$$\text{Given } Q, \quad \text{find} \quad \max_{Y,\ Y\neq 0} \quad Y^TQY/Y^TY. \tag{14}$$

□

The expression $\phi(Y) = Y^TQY/Y^TY$, usually called the Rayleigh quotient in the literature [20–22], attains its maximum for the eigenvector Y associated with the greatest eigenvalue of Q. We already know by (7) and (8) that this eigenvalue is $tr\mathbf{U}$. When Y is found from (14) we normalize it to $X = Y/\sqrt{Y^TY}$ satisfying $X^TX = 1$. Then $\mathbf{R}$, $\mathbf{U}$, and $\mathbf{V}$ can be found from algebraic relations

$$\begin{aligned} \mathbf{R} &= (m^2-\mathbf{m}\cdot\mathbf{m})\mathbf{I} + 2\mathbf{m}\otimes\mathbf{m} + 2m(\mathbf{m}\times\mathbf{I}) \\ \mathbf{U} &= \mathbf{R}^T\mathbf{F} = (m^2-\mathbf{m}\cdot\mathbf{m})\mathbf{F} + 2\mathbf{m}\otimes(\mathbf{F}^T\mathbf{m}) - 2m(\mathbf{m}\times\mathbf{F}) \\ \mathbf{V} &= \mathbf{F}\mathbf{R}^T = (m^2-\mathbf{m}\cdot\mathbf{m})\mathbf{F} + 2(\mathbf{F}\mathbf{m})\otimes\mathbf{m} - 2m\mathbf{F}(\mathbf{m}\times\mathbf{I}) \end{aligned} \tag{15}$$

5 Characteristic polynomial of Q

One root of the characteristic polynomial of the 4×4 matrix Q is $tr\mathbf{U}$, as it was found by Hoger and Carlson [2] for a fourth degree polynomial derived for this purpose. In this Section we prove that the two polynomials coincide.

Let us consider $\mathbf{C} = \mathbf{F}^T\mathbf{F} \in$ *Psym*. Then the Cayley-Hamilton theorem allows one to determine the square root $\mathbf{U}$ of $\mathbf{C}$ provided that $tr\mathbf{U}$ is known. Indeed,

$$\mathbf{U}^2 = \mathbf{C}, \quad \mathbf{U}^3 = \mathbf{C}\mathbf{U}, \quad tr(\mathbf{U}^2) = tr\mathbf{C}, \quad det\mathbf{U} = \sqrt{det\mathbf{C}}$$

and the Cayley-Hamilton theorem applied to $\mathbf{U}$ yields

$$\big[\mathbf{C} + \frac{tr\mathbf{C} - (tr\mathbf{U})^2}{2}\mathbf{I}\big]\mathbf{U} = (tr\mathbf{U})\mathbf{C} + \sqrt{det\mathbf{C}}\;\mathbf{I}$$

If one knows $tr\mathbf{U}$, then $\mathbf{U}$ can be obtained by inverting the tensor $\mathbf{C} + \dfrac{(tr\mathbf{C}) - (tr\mathbf{U})^2}{2}\mathbf{I}$.

To find $tr\mathbf{U}$, Hoger and Carlson [2] succeeded to show that it is the root of a fourth-degree polynomial. Let us summarize their idea.

If λ_1, λ_2, λ_3 are the eigenvalues of $\mathbf{U}$, then taking the square of the algebraic identity

$$(\lambda_1 + \lambda_2 + \lambda_3)^2 - (\lambda_1^2 + \lambda_2^2 + \lambda_3^2) = 2(\lambda_1\lambda_2 + \lambda_2\lambda_3 + \lambda_3\lambda_1)$$

one can be aware that

$$[(tr\mathbf{U})^2 - tr\mathbf{C}]^2 = 2[(tr\mathbf{C})^2 - tr(\mathbf{C}^2)] + 8\sqrt{det\mathbf{C}}(tr\mathbf{U})$$

from which it follows that $tr\mathbf{U}$ is the root of the fourth degree polynomial [2]

$$\lambda^4 - 2(tr\mathbf{C})\lambda^2 - 8\sqrt{det\mathbf{C}}\;\lambda + 2tr(\mathbf{C}^2) - (tr\mathbf{C})^2 \tag{16}$$

This polynomial has no cubic term, hence the sum of the four roots is zero. We also note that if we change λ_1 to $-\lambda_1$ and λ_2 to $-\lambda_2$, the scalars $tr\mathbf{C}$, $tr(\mathbf{C}^2)$, and $\det\mathbf{C}$ remain unchanged. Thus the value $\lambda_3 - \lambda_1 - \lambda_2$ is still the root of (16). Therefore, the four roots of (16) are

$$\lambda_1 + \lambda_2 + \lambda_3, \quad \lambda_1 - \lambda_2 - \lambda_3, \quad \lambda_2 - \lambda_3 - \lambda_1, \quad \lambda_3 - \lambda_1 - \lambda_2 \tag{17}$$

From (17) it is apparent that $tr\mathbf{U} = \lambda_1 + \lambda_2 + \lambda_3$ is the greatest root of (16). This provides an answer to the discussion by Sawyers [23].

Property: *When a rotation* $\mathbf{\Omega}$ *represented by* (9) *transforms the deformation gradient* $\mathbf{F}$ *into* $\mathbf{F}' = \mathbf{\Omega}^T\mathbf{F}$, *then the matrix* Q *associated with* $\mathbf{F}$ *is transformed into* $Q' = \Lambda^T Q \Lambda$ *associated with* $\mathbf{F}'$, *where* Λ *is the quaternion* [12–17]

$$\Lambda = \begin{pmatrix} mI + M\times I & M \\ -M^T & m \end{pmatrix} = \begin{pmatrix} m & -m_3 & m_2 & m_1 \\ m_3 & m & -m_1 & m_2 \\ -m_2 & m_1 & m & m_3 \\ -m_1 & -m_2 & -m_3 & m \end{pmatrix} \tag{18}$$

$$= m_1\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix} + m_2\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} + m_3\begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix} + m\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Proof. Let $X' = (M'^T\ m')^T$ be a quadrivector associated with a quaternion Λ' and a rotation $\mathbf{\Omega}'$. Then the quadrivector

$$X'' = \Lambda X' = \begin{pmatrix} M'' \\ m'' \end{pmatrix} = \begin{pmatrix} mM' + m'M + M \times M' \\ mm' - M^TM' \end{pmatrix} \tag{19}$$

is associated with the quaternion product $\Lambda'' = \Lambda\Lambda'$, as one can easily check. Interpreting (19) in terms of $\mathbf{\Omega}$, $\mathbf{\Omega}'$, $\mathbf{\Omega}''$, one can also recognize Rodrigues' rules [17] for calculating the rotation product $\mathbf{\Omega}'' = \mathbf{\Omega}\mathbf{\Omega}'$.

The relation $\mathbf{F}' = \mathbf{\Omega}^T\mathbf{F}$ implies that

$$tr(\mathbf{F}'^T\mathbf{\Omega}') = tr[\mathbf{F}^T(\mathbf{\Omega}\mathbf{\Omega}')] \quad \text{for any } \ \mathbf{\Omega}' \in Orth^+$$

or equivalently

$$X'^TQ'X' = (\Lambda X')^TQ(\Lambda X') \quad \text{for any } \ X'$$

As a consequence, $Q' = \Lambda^TQ\Lambda$. □

Remark: The transformation of $\mathbf{F}$ into $\mathbf{\Omega}^T\mathbf{F}$ is an action of $Orth^+$ on Lin^+. If two rotations $\mathbf{\Omega}_1$ and $\mathbf{\Omega}_2$ are successively applied, $\mathbf{F}$ is transformed into

$$\mathbf{\Omega}_2^T(\mathbf{\Omega}_1^T\mathbf{F}) = (\mathbf{\Omega}_1\mathbf{\Omega}_2)^T\mathbf{F}$$

which corresponds to the direct action of the compound rotation $\mathbf{\Omega} \equiv \mathbf{\Omega}_1\mathbf{\Omega}_2$.

Likewise, the transformation of Q into $\Lambda^T Q \Lambda$ is an action of the quaternion group on the linear space of 4×4 symmetric traceless matrices. Therefore, if two quaternions Λ_1 and Λ_2 are successively applied, Q is transformed into

$$\Lambda_2^T(\Lambda_1^T Q \Lambda_1)\Lambda_2 = (\Lambda_1\Lambda_2)^T Q(\Lambda_1\Lambda_2)$$

which corresponds to the direct action of the compound quaternion $\Lambda \equiv \Lambda_1\Lambda_2$. The property indicates that the action of rotations on $\mathbf{F}$ is transferred towards the action of quaternions on Q.

Property: *The characteristic polynomial $det(Q - \lambda I_4)$ of the matrix Q coincides with the polynomial* (16).

P r o o f. Let $I_4 = \begin{pmatrix} I & 0 \\ 0 & 1 \end{pmatrix}$ be the unit 4 × 4 matrix. For any quaternion Π as a matrix of SO(4) we have

$$det[\Pi^T(Q - \lambda I_4)\Pi] = det(Q - \lambda I_4)$$

In particular, if X is the quadrivector representing the rotation $\mathbf{R}$ in the polar decomposition (1) (see Section 2), then the quaternion Λ defined by (18) is such that

$$\Lambda^T Q \Lambda = \begin{pmatrix} 2U - (trU)I & 0 \\ 0 & trU \end{pmatrix}$$

where $U = (U_{ij})$ is the symmetric positive definite matrix with $U_{ij} = \mathbf{e}_i \cdot \mathbf{U}\mathbf{e}_j$. Therefore

$$det(Q - \lambda I_4) = det \begin{pmatrix} 2U - (trU)I - \lambda I & 0 \\ 0 & trU - \lambda \end{pmatrix}$$

Moreover, there exists a rotation matrix $P \in$ SO(3) which makes $P^T U P$ diagonal

$$P^T U P = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix}$$

with $\lambda_1, \lambda_2, \lambda_3$ to be the eigenvalues of U. Introducing the 4×4 matrix $\Pi = \begin{pmatrix} P & 0 \\ 0 & 1 \end{pmatrix} \in$ SO(4) we can show that

$$\begin{aligned} \Pi^T \begin{pmatrix} 2U - (trU)I & 0 \\ 0 & trU \end{pmatrix} \Pi &= \begin{pmatrix} 2P^T U P - (trU)I & 0 \\ 0 & trU \end{pmatrix} \\ &= \begin{pmatrix} \lambda_1 - \lambda_2 - \lambda_3 & 0 & 0 & 0 \\ 0 & \lambda_2 - \lambda_3 - \lambda_1 & 0 & 0 \\ 0 & 0 & \lambda_3 - \lambda_1 - \lambda_2 & 0 \\ 0 & 0 & 0 & \lambda_1 + \lambda_2 + \lambda_3 \end{pmatrix} \end{aligned}$$

Therefore, the characteristic polynomial of Q equal to $det(Q - \lambda I_4) = det[\Pi^T \Lambda^T (Q - \lambda I_4)\Lambda\Pi]$ can be written in the explicit form

$$det(Q - \lambda I_4) = (\lambda_1 - \lambda_2 - \lambda_3 - \lambda)(\lambda_2 - \lambda_3 - \lambda_1 - \lambda)(\lambda_3 - \lambda_1 - \lambda_2 - \lambda)(\lambda_1 + \lambda_2 + \lambda_3 - \lambda)$$

This polynomial has the same roots and the same highest term as the polynomial (16). Therefore, both polynomials coincide. □

Remark: Although the matrix Q has been built linearly and uniquely from components of the tensor $\mathbf{F}$, the invariants of Q depend solely on the invariants of $\mathbf{C} = \mathbf{F}^T\mathbf{F}$ and remain unchanged when $\mathbf{F}$ is changed into $\mathbf{\Omega}^T\mathbf{F}$ by any rotation $\mathbf{\Omega}$. From the point of view of the principle of material frame-indifference, for example, the matrix Q seems to be better suited than $\mathbf{F}$ to describe the deformation in continuum mechanics.

6 Maximization of the Rayleigh quotient by the conjugate gradient algorithm

To apply the method of Section 4, we have to maximize numerically the Rayleigh quotient $\phi(Y)$ on all non-vanishing quadrivectors Y and then to normalize the resultant quadrivector to $X = Y/\sqrt{Y^TY}$. This procedure can be performed by a conjugate gradient algorithm. We have used here the Polak-Ribière implementation [24] with the following steps:

Step 1: initialize Y_0, $Z_0 = G_0 = grad\ \phi(Y_0)$
Step 2: start iterations
Step 3: search for μ_i maximizing $\phi(Y_i + \mu Z_i)$ with regard to μ
Step 4: compute $Y_{i+1} = Y_i + \mu_i Z_i$
Step 5: compute $G_{i+1} = grad\ \phi(Y_{i+1})$
Step 6: compute $\nu_{i+1} = G^T_{i+1}(G_{i+1} - G_i)/G^T_i G_i$
Step 7: determine the new search direction $Z_{i+1} = G_{i+1} + \nu_{i+1} Z_i$
Step 8: stop iterations when $G^T_{i+1} G_{i+1}$ is small enough

At the very beginning, an initial value Y_0 of the maximization problem is improved in the ascent direction of the gradient G_0 by choosing μ_0 which maximizes $\phi(Y_0 + \mu G_0)$. Thus, following a straight line, one arrives at $Y_1 = Y_0 + \mu_0 G_0$ as close to the maximum as possible. Then, an ascent direction $Z_1 = G_1 + \nu_1 G_0$, expected to be better than G_1, is chosen in the plane determined by G_1 and $Z_0 = G_0$. An optimal direction corresponds to the choice $\nu_1 = G^T_1(G_1 - G_0)/G^T_0 G_0$ as proposed by Polak and Ribière [24]. Then μ_1 is chosen by maximizing $\phi(Y_1 + \mu Z_1)$ and $Y_2 = Y_1 + \mu_1 Z_1$ is determined. Now $G_2 = grad\ \phi(Y_2)$, $\nu_2 = G^T_2(G_2 - G_1)/G^T_1 G_1$, $Z_2 = G_2 + \nu_2 Z_1$, and μ_2 can be calculated, which allows one to compute $Y_3 = Y_2 + \mu_2 Z_2$. And so on ...

In the particular case of the quotient of two quadratic forms discussed here we are able to perform steps 3 and 5 by explicit formulae.

In the fifth step the gradient of the Rayleigh quotient is given by the closed formula

$$grad\ \phi(Y) = \frac{2}{Y^TY}[QY - \phi(Y)Y] \tag{20}$$

Therefore, there is no need to calculate the gradient G_{i+1} at Y_{i+1} by numerical derivative.

In the third step we should find μ requiring $\phi(Y + \mu Z)$ to attain a maximum. Therefore, we have to fulfill the condition

$$\frac{d}{d\mu}\phi(Y + \mu Z) = [grad\ \phi\ (Y + \mu Z)]^T Z = 0 \tag{21}$$

Thanks to the closed formula (20), the condition (21) leads to

$$\frac{2}{[(Y + \mu Z)^T(Y + \mu Z)]^2}(a\mu^2 + b\mu + c) = 0 \tag{22}$$

with the trinomial coefficients

$$\begin{aligned} a &= (Y^TZ)(Z^TQZ) - (Z^TZ)(Z^TQY) \\ b &= (Y^TY)(Z^TQZ) - (Z^TZ)(Y^TQY) \\ c &= (Y^TY)(Z^TQY) - (Y^TZ)(Y^TQY) \end{aligned} \tag{23}$$

Taking into account the identity $(Y^TZ)b = (Y^TY)a + (Z^TZ)c$, the discriminant $\Delta = b^2 - 4ac$ of the trinomial in (22) can be expressed as

$$\Delta = \frac{[(Y^TY)(Z^TZ) - (Y^TZ)^2]b^2 + [(Y^TY)a - (Z^TZ)c]^2}{(Y^TY)(Z^TZ)} \tag{24}$$

Due to the Cauchy-Schwarz-Buniakowski inequality $(Y^TY)(Z^TZ) - (Y^TZ)^2$ is positive, therefore Δ is always positive. In computing Δ according to (24) we need to divide by Y^TY and Z^TZ. This is not allowed when Y or Z vanishes. But in such singular cases the coefficients a, b, and c vanish by definitions (23) as well and then the value of Δ becomes zero.

Since Δ is positive, the trinomial in (22) has two real roots: $(-b + \sqrt{\Delta})/2a$ and $(-b - \sqrt{\Delta})/2a$. One of them leads to the maximum value of the Rayleigh quotient, the other one to its minimum value. To identify the root leading to the maximum, we should identify the sign of the second derivative of $\phi(Y + \mu Z)$ with regard to μ, when (21) holds. Taking derivative of the left-hand side of (22) we find

$$\frac{2(2a\mu + b)}{[(Y + \mu Z)^T(Y + \mu Z)]^2} \tag{25}$$

In order to maximize the Rayleigh quotient $\phi(Y + \mu Z)$ the expression (25) must be negative. Therefore, we should choose the root $\mu = (-b - \sqrt{\Delta})/2a$ for which $b + 2a\mu = -\sqrt{\Delta}$.

To validate the proposed algorithm, we analyse again the example studied by Dui and Zhuo [25], where the deformation gradient $\mathbf{F}$ in the basis $\mathbf{e}_i$ was defined by the matrix

$$F = \begin{pmatrix} 2 & 1 & 1 \\ 1 & 3 & 0 \\ 0 & 2 & 1 \end{pmatrix}$$

After performing the polar decomposition of $\mathbf{F}$, the following results were obtained in [25] for the corresponding rotation and right stretch matrices:

$$R = \begin{pmatrix} 0.8795 & 0.0005 & 0.4760 \\ 0.2557 & 0.8429 & -0.4735 \\ -0.4014 & 0.5381 & 0.7412 \end{pmatrix}, \quad U = R^T F = \begin{pmatrix} 2.0147 & 0.8438 & 0.4781 \\ 0.8439 & 3.6054 & 0.5386 \\ 0.4785 & 0.5383 & 1.2172 \end{pmatrix}$$

Please note that the matrix U is symmetric here with accuracy up to 10^{-3}.

With the method proposed in this paper, after 13 iterations the conjugate gradient algorithm has given the following rotation and right stretch matrices:

$$R = \begin{pmatrix} 0.879553 & 0.000445 & 0.475801 \\ 0.255633 & 0.842968 & -0.473345 \\ -0.401296 & 0.537963 & 0.741321 \end{pmatrix}, \quad U = \begin{pmatrix} 2.014739 & 0.843859 & 0.478257 \\ 0.843859 & 3.605276 & 0.538408 \\ 0.478257 & 0.538408 & 1.217122 \end{pmatrix}$$

We have printed the values of R and U with accuracy up to 10^{-6}. In fact, our numerical results are accurate up to 10^{-14}.

7 Conclusions

We have used the minimum property of $\mathbf{R}$ in the polar decomposition (1) to develop a new effective method of determining $\mathbf{R}$ from the given $\mathbf{F}$ without necessity to perform any square root and/or inverse operations on tensors.

In our approach the rotation is replaced by an equivalent quadrivector X composed of four quaternion parameters, and the deformation gradient $\mathbf{F}$ is replaced by an equivalent 4×4 symmetric traceless matrix Q. The characteristic polynomial of Q has been shown to coincide with the one derived by Hoger and Carlson [2] and its greatest root be $tr\mathbf{U}$.

It has been proved that the quadrivector X corresponding to $\mathbf{R}$ in (1) can be found by maximizing the Rayleigh quotient $\phi(Y) = Y^T QY/Y^T Y$ over all non-vanishing Y, with subsequent normalization of the resulting Y to $X = Y/\sqrt{Y^T Y}$. The maximization of $\phi(Y)$ has been performed with the help of a conjugate gradient algorithm. The efficiency and accuracy of the algorithm has been tested on the example discussed by Dui and Zhuo [25]. Our algorithm has been shown to be very efficient with accuracy of the results up to 10^{-14} obtained after 13 iterations.

The algorithm is applicable not only to the 4×4 symmetric traceless matrices discussed here. It can be used to determine the greatest and/or the smallest eigenvalue of a symmetric matrix of any size, for example in determining eigenfrequencies of mechanical vibrations. It is also useful in calculating the square root of any symmetric positive definite tensor, [26].

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