Revisiting the generalized polar decomposition of Mueller matrices

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Mueller polarimetry is a powerful imaging modality which has been successfully applied to various application fields. Decomposition of Mueller matrices in elementary components is classically considered in order to unfold complex physical phenomena taking place in probed samples or scenes. In this context, the generalized polar decomposition, also known as the Lu and Chipman decomposition, is playing a prominent role. In this article, we show that the set of candidate generalized polar decompositions is richer than the set used so far. Negative-determinant Mueller matrices are naturally addressed in the proposed framework. We show that taking into account those supplementary polar decompositions addresses issues raised in the literature. Application is carried out on synthetic and on measured Mueller matrices.

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1. INTRODUCTION

Mueller polarimetry is a powerful imaging modality which has successfully met many application fields such as medicine, biology, engineering, and material science (see e.g., [1–7]). This probing technique gives access into the structure of the sample of interest. Information is held by a Mueller matrix, which is a 4×4 real matrix modeling the relation between an incoming Stokes vector and the corresponding outgoing Stokes vector. Because of its intrinsic advantages, the Stokes-Mueller formalism is one of the most used in polarimetry. It is in fact capable of representing any state of polarization by a Stokes vector while the Mueller matrix is capable of accounting for any possible linear interaction between a medium and the incident light that provides the outgoing Stokes vector. Thus, for a given geometric configuration, the Mueller matrix contains all the energetic and polarimetric information related to the medium.

The interpretation of Mueller matrices has been and still is of wide scientific interest, with a view to unfolding and interpreting complex physical phenomena taking place in structured media. In this context, the generalized polar decomposition (GPD), also known as the Lu and Chipman decomposition [8] (see also [9, 10]) is playing a central role. Many other decompositions have been proposed (see e.g., [9–13]). In the GPD, a given Mueller matrix M is decomposed as a product $M = M_{\Delta} M_R M_D$, where M_{Δ} , M_R , and M_D are Mueller matrices of a depolarizer, a retarder, and a diattenuator. Such a decomposition allows to

decouple the different polarimetric effects. With this point of view, the medium of interest is modeled as a succession of three layers [10], which gives insight into the physical structure of interest. Besides, it may also be mentioned that the physical parameters of the set $\{M_{\Delta}, M_R, M_D\}$ may constitute interesting features for machine learning algorithms, with a view to tissue classification and early diagnosis [14, 15].

Scientific interest has been devoted to the particular case of negative-determinant Mueller matrices (see e.g., [16] and the references therein; see e.g., [17] for the physical meaning of negative determinant Mueller matrices). In this case, a Mueller matrix is still decomposed as a product $M = M_{\Delta} M_R M_D$, but the decomposition is different from the Lu and Chipman one.

In the original work [8], the choice between different potential decompositions is achieved by minimizing the retardance. In this article, minimizing the retardance is merely a way to address identifiability issues; the authors do not claim that this approach yields an estimation closer to the ground truth than a concurrent approach. We may question whether minimizing the retardance is the best choice to be made from a physical point of view. For example, in [section 3, 16], the authors make a choice with respect to the orientation of the rotation axis, and this may be in contradiction with the minimization of the retardance. Another approach, also to be found in [section 3, 16], is to employ continuity arguments on the depolarization image. This would certainly be an interesting point of view for the estimation of a GPD. Finally, in the present work, indetermination is always

solved by minimizing the retardance, to be consistent with [8]. Considering other criteria, such as the rotation axis orientation or as continuity considerations, is left for future work.

The contribution of this article resides in showing that the original GPD stems from a subset of the admissible candidates. Considering the entire set of GPD candidates may change the GPD retained, since minimization of the retardance is achieved on a richer set of candidates. In the case of negative-determinant Mueller matrices, the solution of [16] appears naturally as a candidate. Nevertheless, for some negative-determinant Mueller matrices, the proposed approach also reaches a lower retardance than the one in [16].

In this work, we focus on decomposition, optimization, and estimation issues. We leave physical interpretations aside, this aspect being widely covered in the literature (see e.g., [8–10]).

The article is structured as follows. In the second section, we recall the GPD and define the variables at stake. In the third section, we revisit the GPD construction and we derive the complete set of GPD candidates attached to a given Mueller matrix. Simulations using random synthetic Mueller matrices are proposed to supplement the derivations. In the fourth section, we apply the proposed decomposition methodology to a biological sample. Conclusion is drawn in the last section.

2. THE GENERALIZED POLAR DECOMPOSITION

The goal of this section is to recall the GPD of a Mueller matrix, as taken from [8]. All notations are standard and stem from the literature.

A Mueller matrix M can be written as $M = m_{00} \begin{bmatrix} 1 & D^t \\ P & m \end{bmatrix}$ [8, 9, 18], and is decomposed as $M = M_\Delta M_R M_D$, where M_Δ , M_R , and M_D represent respectively a depolarizer, a retarder, and a diattenuator. The matrices at stake write

$$M_\Delta = \begin{bmatrix} 1 & 0^t \\ P_\Delta & m_\Delta \end{bmatrix}, \quad M_R = \begin{bmatrix} 1 & 0^t \\ 0 & m_R \end{bmatrix}, \quad M_D = m_{00} \begin{bmatrix} 1 & D^t \\ D & m_D \end{bmatrix}.$$

The diattenuator vector D has norm D ($0 \leq D \leq 1$). The polarizance vector P has norm P ($0 \leq P \leq 1$). We define the unit vectors $\hat{D}$ and $\hat{P}$ along D and P : $D = D \hat{D}$, $P = P \hat{P}$. We have:

$$m_D = \sqrt{1 - D^2} \mathbf{I} + (1 - \sqrt{1 - D^2}) \hat{D} \hat{D}^t.$$

Matrix M_D can therefore be calculated from m_{00} and from the diattenuator vector D . Besides, the equations given above yield:

$$\begin{cases} P = P_\Delta + m_\Delta m_R D, \\ m = P_\Delta D^t + m_\Delta m_R m_D. \end{cases}$$

From $m_D D = D$, we get

$$\begin{aligned} P &= P_\Delta + m_\Delta m_R m_D D = P_\Delta + (m - P_\Delta D^t) D \\ &= (1 - D^2) P_\Delta + m D. \end{aligned} \quad (1)$$

By definition, submatrices m_R and m_Δ are respectively a 3D rotation matrix and a symmetric matrix [8].

It should be noticed that M_Δ is not a physically admissible Mueller matrix (see e.g., [section 5.12.1, page 39, 9]; see [section 5.4, 9] for the characterization of Mueller matrices). More precisely, Lu and Chipman decompose M as

$$M = M_\Delta M_R M_D = M_\Delta M_R \left[m_{00} \begin{bmatrix} 1 & D^t \\ D & m_D \end{bmatrix} \right].$$

Gil [9] decomposes M as

$$M = [c M_\Delta] [b M_R] \left[a \begin{bmatrix} 1 & D^t \\ D & m_D \end{bmatrix} \right],$$

with the physical admissibility conditions $a b c = m_{00}$, $a, b, c \geq 0$, $a(1 + D) \leq 1$, $b \leq 1$, $c(1 + \|P_\Delta\|) \leq 1$. In the framework of Gil, Lu and Chipman choose $a = m_{00}$, $b = 1$, $c = 1$. With $c = 1$, condition $c(1 + \|P_\Delta\|) \leq 1$ cannot be met, unless $\|P_\Delta\| = 0$. This point may be addressed by post processing the Lu and Chipman decomposition, by distributing m_{00} on a , b , and c , without any further impact on the decomposition.

We define matrix M' as $M' = M_\Delta M_R$ [Eq. 48, 8]. Thus we get $M' = \begin{bmatrix} 1 & 0^t \\ P_\Delta & m' \end{bmatrix}$, where $m' = m_\Delta m_R$.

Let us define vectors v_{D1} , v_{D2} , v_{D3} , v_{D4} respectively as

$$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ \hat{D} \end{bmatrix}, \quad \begin{bmatrix} 0 \\ \hat{D}_{\perp 1} \end{bmatrix}, \quad \begin{bmatrix} 0 \\ \hat{D}_{\perp 2} \end{bmatrix}, \quad \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -\hat{D} \end{bmatrix},$$

where $\hat{D}_{\perp 1}$ and $\hat{D}_{\perp 2}$ are two orthonormal vectors, orthogonal to $\hat{D}$. Those four vectors are unit-normed and are eigenvectors of M_D , with eigenvalues

$$S_D = m_{00} \begin{bmatrix} 1 + D; \sqrt{1 - D^2}; \sqrt{1 - D^2}; 1 - D \end{bmatrix},$$

appearing in decreasing order (see [Eqs. 20 & 21, 8]). Therefore, if we define matrix V_D as $V_D = [v_{D1} v_{D2} v_{D3} v_{D4}]$, $(V_D, \text{diag}(S_D), V_D)$ is a singular value decomposition (SVD) of M_D : $M_D = V_D \text{diag}(S_D) V_D^t$. As a consequence, M_D is invertible if and only if $D < 1$.

Two cases are to be distinguished: the M_D invertible case, and the M_D singular case.

A. The M_D invertible case

If M_D is invertible, M' is uniquely defined as $M' = M M_D^{-1}$, and we get P_Δ from

$$P_\Delta = \frac{1}{1 - D^2} (P - m D).$$

Let (V, S, U) be a SVD of m' , i.e., $m' = V S U^t$. If m' is invertible, m_Δ is determined using [Eq. 52, 8], or equivalently using [Eq. B2, 8] as

$$m_\Delta = \pm V S V^t,$$

where the $+$ sign is used if $\det m' > 0$, whereas the $-$ sign is used if $\det m' < 0$. See also [Eq. 230, 9].

Finally, $m_R = m_\Delta^{-1} m'$ and the Lu and Chipman GPD (LC-GPD) is complete. Equivalently, we may use

$$m_R = \pm V U^t,$$

with the same rule as above for choosing the sign.

If m' is singular, m_Δ is singular as well and m_R is not unique. This case is addressed in [Appendix B, 8]. We do not detail this case here, since this will be one of the topics of the next section.

B. The M_D singular case

If M_D is singular (i.e., if $D = 1$ and $D = \hat{D}$), then matrix M writes $M = m_{00} \begin{bmatrix} 1 & D^t \\ P & P D^t \end{bmatrix}$ (see section A in the appendix). The LC-GPD writes [Eq. A3, 8]

$$M_\Delta = \begin{bmatrix} 1 & 0^t \\ 0 & P \mathbf{I} \end{bmatrix}, \quad M_R = \begin{bmatrix} 1 & 0^t \\ 0 & \mathcal{R}(D, \hat{P}) \end{bmatrix},$$

where $\mathcal{R}(\mathbf{u}_1, \mathbf{u}_2)$ is the minimal angle rotation matrix that transforms unit-length vector $\mathbf{u}_1$ to unit-length vector $\mathbf{u}_2$ ($\mathbf{u}_1$ and $\mathbf{u}_2$ are supposed linearly independent). This is a rotation around $\mathbf{u}_1 \times \mathbf{u}_2$ normalized to unit-length, and the rotation angle θ is the angle formed by $\mathbf{u}_1$ and $\mathbf{u}_2$ (see e.g., [19]). Let $\mathbf{u} = \frac{1}{\|\mathbf{u}_1 \times \mathbf{u}_2\|} \mathbf{u}_1 \times \mathbf{u}_2 = [u_x \ u_y \ u_z]^t$. If we define the skew-symmetric matrix $[\mathbf{u}]_\times$ as

$$[\mathbf{u}]_\times = \begin{bmatrix} 0 & -u_z & u_y \\ u_z & 0 & -u_x \\ -u_y & u_x & 0 \end{bmatrix},$$

this matrix being such that $[\mathbf{u}]_\times \mathbf{w} = \mathbf{u} \times \mathbf{w}$ for any vector $\mathbf{w}$, we have

$$\mathcal{R}(\mathbf{u}_1, \mathbf{u}_2) = \cos \theta \mathbf{I} + \sin \theta [\mathbf{u}]_\times + (1 - \cos \theta) \mathbf{u} \mathbf{u}^t,$$

which may also be written (Rodrigues formula, see e.g., [19])

$$\mathcal{R}(\mathbf{u}_1, \mathbf{u}_2) = \mathbf{I} + \sin \theta [\mathbf{u}]_\times + (1 - \cos \theta) [\mathbf{u}]_\times^2,$$

where we used the relation $[\mathbf{u}]_\times^2 = \mathbf{u} \mathbf{u}^t - \mathbf{I}$. Changing the sign of $\mathbf{u}$ amounts to changing the sign of θ .

In the appendix of this article, we will also use the notation $\mathcal{R}(\mathbf{u}, \theta)$ for the rotation of angle θ around vector $\mathbf{u}$.

In fact, M_R in [8] is written $\begin{bmatrix} 1 & \mathbf{0}^t \\ \mathbf{0} & \mathcal{R}(\hat{\mathbf{P}}, D) \end{bmatrix}$, which amounts to changing the sign of the rotation angle. But on the other hand, matrix m_R in [8] is the rotation of angle $-R$ [Eq. 15, 8]. Therefore, in [8] we have a double sign flip which cancels out.

3. REVISITING THE GENERALIZED POLAR DECOMPOSITION

We aim at devising the set of all GPDs attached to a given Mueller matrix. One decomposition will have to be selected among all GPDs. As in [8], we will retain the one minimizing the retardance R , which is the rotation angle associated to m_R .

This section is divided in four parts. We first address the M_D invertible case, we then deal with the M_D singular case. In the third part, we focus on accounting for physical constraints. The fourth section proposes two case studies on synthetic Mueller matrices.

Definition: Δ RF. (m_Δ, m_R) is a Δ R factorization (Δ RF) of a given matrix m' if

$$m' = m_\Delta m_R, \quad m_R m_R^t = \mathbf{I}, \quad \det m_R = 1, \quad m_\Delta = m_\Delta^t.$$

A. The M_D invertible case

In this case, M' and m' are uniquely defined. We aim at decomposing m' as $m' = m_\Delta m_R$. Let $(V^{(p)}, S, U^{(p)})$ be a particular SVD of m' , such as given by a numerical software, or as chosen by the investigator. The singular values being unique (see e.g., [section 2, 20]), we drop (p) and write S instead of $S^{(p)}$. Then m' admits at least one Δ RF, which may be computed from the SVD [Eqs. B2 & B3, 8]:

$$\begin{cases} m_\Delta^{(p)} &= e^{(p)} V^{(p)} S V^{(p)t}, \\ m_R^{(p)} &= e^{(p)} V^{(p)} U^{(p)t}, \\ e^{(p)} &= \pm 1. \end{cases} \quad (2)$$

The sign of $e^{(p)}$ is such that $\det m_R^{(p)} = 1$.

We aim at devising the set of all Δ RFs attached to m' . Let $(m_\Delta^{(g)}, m_R^{(g)})$ be a general Δ RF of m' (i.e., any Δ RF of m'). Matrix $m_\Delta^{(g)}$ being real symmetric, it may be written $m_\Delta^{(g)} = V_\Delta S_\Delta V_\Delta^t$ (spectral theorem for normal matrices, see e.g., [section 2.5, 21]), where we suppose, without loss of generality, that the diagonal matrix S_Δ is such that $|s_{\Delta 1}| \geq |s_{\Delta 2}| \geq |s_{\Delta 3}|$ (modification of the order of the $|s_{\Delta i}|$'s is achieved by permutation of the columns of V_Δ). Thereby

$$\begin{cases} m' m'^t &= m_\Delta^{(g)} m_\Delta^{(g)t}, \\ m' m'^t &= V^{(p)} S^2 V^{(p)t}, \\ m_\Delta^{(g)} m_\Delta^{(g)t} &= V_\Delta S_\Delta^2 V_\Delta^t. \end{cases}$$

We notice that $(V_\Delta, S_\Delta^2, V_\Delta)$ and $(V^{(p)}, S^2, V^{(p)})$ are two SVDs of the same matrix. As a consequence (see section B in the appendix), $S_\Delta^2 = S^2$ and there exists Q_1 such that $V_\Delta = V^{(p)} Q_1$. With $\varepsilon = \text{diag}([\pm 1 \ \pm 1 \ \pm 1]) = \text{diag}([\varepsilon_1 \ \varepsilon_2 \ \varepsilon_3])$, $S_\Delta = \varepsilon S$. The structure of Q_1 is determined by the structure of the singular values s_1, s_2, s_3 (see the appendix, section B, Eq. 5, which reads $\hat{V} = V Q_1$). Thus, for any $m_\Delta^{(g)}$ and considering any given SVD $(V^{(p)}, S, U^{(p)})$ of m' , there exists (Q_1, ε) such that

$$m_\Delta^{(g)} = V^{(p)} Q_1 \varepsilon S Q_1^t V^{(p)t}.$$

The goal is to capture all $m_\Delta^{(g)}$'s. This amounts to capturing all couples (Q_1, ε) which, associated to the SVD $(V^{(p)}, S, U^{(p)})$, will yield a Δ RF. The symmetry condition on $m_\Delta^{(g)}$ being satisfied for any couple (Q_1, ε) , the stake is to find a matching $m_R^{(g)}$. The ultimate goal being to capture all Δ RFs, we aim at capturing all triples $(Q_1, \varepsilon, m_R^{(g)})$ which, associated to the SVD $(V^{(p)}, S, U^{(p)})$, will yield a Δ RF.

Let us write a $m_R^{(g)}$ candidate as $m_R^{(g)} = V^{(p)} Q_1 \varepsilon U_R^t$. Matrices $V^{(p)}$, Q_1 , and ε being invertible, any 3×3 real matrix may be written $V^{(p)} Q_1 \varepsilon U_R^t$, with a proper U_R . We aim at finding the necessary and sufficient conditions on (Q_1, ε, U_R) such that (Q_1, ε, U_R) will yield a Δ RF of m' .

The necessary conditions are

$$1. \ m_R^{(g)} m_R^{(g)t} = \mathbf{I} \ (\Leftrightarrow m_R^{(g)t} m_R^{(g)} = \mathbf{I}), \text{ which yields } U_R U_R^t = U_R^t U_R = \mathbf{I}. \text{ Matrix } U_R \text{ must be orthonormal;}$$

$$2. \ m' = m_\Delta^{(g)} m_R^{(g)} = [V^{(p)} Q_1 \varepsilon S Q_1^t V^{(p)t}] [V^{(p)} Q_1 \varepsilon U_R^t].$$

Thus $m' = V^{(p)} Q_1 S U_R^t$. On the other hand, we have $m' = V^{(p)} S U^{(p)t}$.

We now have two SVDs of m' : $(V^{(p)} Q_1, S, U_R)$ and $(V^{(p)}, S, U^{(p)})$. Using section B in the appendix, we may state that there exists Q_2 such that $U_R = U^{(p)} Q_2$ (see Eq. 6, which reads $\hat{W} = W Q_2$), and that there exists Q_3 such that $V^{(p)} Q_1 = V^{(p)} Q_3$ (obviously, Q_3 must be equal to Q_1).

$$3. \ \det m_R^{(g)} = 1 \Rightarrow \det (V^{(p)} Q_1 \varepsilon U_R^t) = 1.$$

Considering $\mathbf{U}_R = \mathbf{U}^{(p)} \mathbf{Q}_2$, condition 1 above is satisfied, and condition 3 writes $\det(\mathbf{V}^{(p)} \mathbf{Q}_1 \varepsilon \mathbf{Q}_2^t \mathbf{U}^{(p)t}) = 1$. Those necessary conditions are sufficient: when met, they yield a ΔRF of $\mathbf{m}'$.

$$\text{Conclusion: provided that } \det(\mathbf{V}^{(p)} \mathbf{Q}_1 \varepsilon \mathbf{Q}_2^t \mathbf{U}^{(p)t}) = 1, \\ \left(\mathbf{V}^{(p)} \mathbf{Q}_1 \varepsilon \mathbf{S} \mathbf{Q}_1^t \mathbf{V}^{(p)t}, \mathbf{V}^{(p)} \mathbf{Q}_1 \varepsilon \mathbf{Q}_2^t \mathbf{U}^{(p)t} \right) \quad (3)$$

is a ΔRF of $\mathbf{m}'$.

Given a particular SVD $(\mathbf{V}^{(p)}, \mathbf{S}, \mathbf{U}^{(p)})$ of $\mathbf{m}'$, we capture the entire set of ΔRFs by allowing $\mathbf{Q}_1$, $\mathbf{Q}_2$, and ε to vary.

Structure. Eight different cases can be distinguished, according to the structure of the singular values s_1, s_2, s_3 (see also section D in the appendix):

- case (a): $s_1 > s_2 > s_3 > 0 (\Rightarrow \mathbf{Q}_1 = \mathbf{Q}_2)$;
- case (b): $s_1 = s_2 > s_3 > 0 (\Rightarrow \mathbf{Q}_1 = \mathbf{Q}_2)$;
- case (c): $s_1 > s_2 = s_3 > 0 (\Rightarrow \mathbf{Q}_1 = \mathbf{Q}_2)$;
- case (d): $s_1 = s_2 = s_3 > 0 (\Rightarrow \mathbf{Q}_1 = \mathbf{Q}_2)$;
- case (e): $s_1 = s_2 > s_3 = 0$;
- case (f): $s_1 > s_2 > s_3 = 0$;
- case (g): $s_1 > s_2 = s_3 = 0$;
- case (h): $s_1 = s_2 = s_3 = 0$.

Properties. Considering for each case (a)–(h) the particular structure of $\mathbf{Q}_1$, $\mathbf{Q}_2$, and $\mathbf{S}$, we see that relations

$$\mathbf{S} \mathbf{Q}_2 = \mathbf{Q}_1 \mathbf{S}, \quad \mathbf{S} \mathbf{Q}_1 = \mathbf{Q}_1 \mathbf{S}, \quad \mathbf{S} \mathbf{Q}_2 = \mathbf{Q}_2 \mathbf{S}$$

hold.

Interpretation: linking the Lu and Chipman decomposition to the proposed decomposition. Let $\mathbf{R}_p = e^{(p)} \mathbf{V}^{(p)} \mathbf{Q}_1 \varepsilon \mathbf{Q}_2^t \mathbf{V}^{(p)t}$. It may easily be checked that matrix $\mathbf{R}_p$ is a rotation matrix, thereby satisfying $\mathbf{R}_p^t \mathbf{R}_p = \mathbf{I}$.

Inserting the product $\mathbf{R}_p^t \mathbf{R}_p$ in the Lu and Chipman decomposition ($\mathbf{m}_{\Delta-\text{LC}}$ and $\mathbf{m}_{R-\text{LC}}$ are taken from Eqs. (2)), we get:

$$\mathbf{m}' = [\mathbf{m}_{\Delta-\text{LC}} \mathbf{R}_p^t] [\mathbf{R}_p \mathbf{m}_{R-\text{LC}}].$$

Using the first equation in the *Properties* above, it can easily be checked that the brackets in the previous equation correspond respectively to matrices $\mathbf{m}_{\Delta-\text{PA}}$ and $\mathbf{m}_{R-\text{PA}}$ obtained with the proposed approach ($\mathbf{m}_{\Delta-\text{PA}}$ and $\mathbf{m}_{R-\text{PA}}$ are found in Eq. 3). In fact, relation

$$\mathbf{m}_{R-\text{PA}} = \mathbf{R}_p \mathbf{m}_{R-\text{LC}}$$

was used to define $\mathbf{R}_p$ ($\mathbf{R}_p$ is unique, as $\mathbf{R}_p = \mathbf{m}_{R-\text{PA}} \mathbf{m}_{R-\text{LC}}^t$).

Thereby, we see that $\mathbf{m}_{R-\text{PA}}$ is the composition of two rotations, $\mathbf{R}_p$ and $\mathbf{m}_{R-\text{LC}}$. We capture the set of all $\mathbf{m}_{R-\text{PA}}$ matrices by allowing $\mathbf{R}_p$ to vary, where variations in $\mathbf{R}_p$ stem from variations of $\mathbf{Q}_1$, $\mathbf{Q}_2$, and ε .

Further interpretation. In practice, with a view to minimizing the retardance and using results from section D in the appendix, we do not miss any solution if we restrict the variations of $\mathbf{R}_p$ to the case $\mathbf{Q}_1 = \mathbf{Q}_2 (= \mathbf{Q})$. Doing this, $\mathbf{R}_p$ writes

$\mathbf{R}_p = \mathbf{V}^{(p)} \mathbf{Q} [e^{(p)} \varepsilon] \mathbf{Q}^t \mathbf{V}^{(p)t}$. Possible candidates for the diagonal matrix $e^{(p)} \varepsilon$ are (i) the identity, (ii) any matrix among a set of three matrices, comprising one "1" and two "-1"s on its diagonal. In case (i), $\mathbf{R}_p$ is the identity and $\mathbf{m}_{R-\text{PA}} = \mathbf{m}_{R-\text{LC}}$. In case (ii), $\mathbf{R}_p$ is a rotation matrix of angle π , also called a binary rotation [22].

Remark 1. In the standard case $s_1 > s_2 > s_3 > 0$, $\mathbf{Q}_1 = \mathbf{Q}_2 = \text{diag}([\pm 1 \pm 1 \pm 1])$, and the ΔRF set boils down to

$$(\mathbf{V}^{(p)} \varepsilon \mathbf{S} \mathbf{V}^{(p)t}, \mathbf{V}^{(p)} \varepsilon \mathbf{U}^{(p)t}).$$

There are eight possibilities for ε , among which four match the $\det \mathbf{m}_R = 1$ condition. This is in contrast with the LC-GPD, where only one candidate exists, corresponding to $\varepsilon = \text{diag}([1 \ 1 \ 1])$ or to $\varepsilon = -\text{diag}([1 \ 1 \ 1])$.

Those four options for sign flipping may be linked to sign flipping used in the literature (see e.g., [Eq. 12, 23], or [Eq. 8b, 16]). We defer the corresponding discussion to section 3-C.

Remark 2. In general, eight different cases (one standard case, seven non standard cases) should be distinguished, since there are eight possible configurations for the structure of the three eigenvalues s_1, s_2, s_3 , each one yielding a specific structure for $\mathbf{Q}_1$ and $\mathbf{Q}_2$. The complete study is achieved in section D in the appendix. This is in contrast with the three different non standard cases distinguished in [Appendix B, 8]. Some particular cases in [8] encompass several particular cases of the proposed approach. The standard case in [8] encompasses the standard case and several particular cases of the proposed approach.

For the non standard cases (addressed in [Appendix B, 8]) as for the standard case in [8], we bring forth a larger set of admissible GPD candidates. The final GPD will correspond to the minimizer of the retardance R , as in [8]. One consequence is that our methodology may yield a smaller retardance R than the solution from [8].

Remark 3. As already mentioned, we may question whether minimizing the retardance R is the best choice to be made from a physical point of view. For example, in [section 3, 16], the authors make a choice with respect to the orientation of the rotation axis of $\mathbf{m}_R$, and this may be in contradiction with the minimization of R . It should be noted that in this cited reference, the lower retardance (Eq. 20a) as stemming from Eq. 18a is not part of a GPD, since the corresponding $\mathbf{m}_\Delta$ in Eq. 18b is not symmetric. As a consequence, the retardance given in Eq. 20a will not appear in the set of admissible GPD candidates.

B. The $\mathbf{M}_D$ singular case

We address here the case $D = 1$ [Appendix A, 8]. Matrix $\mathbf{M}_D$ being singular, many couples $(\mathbf{M}_\Delta, \mathbf{M}_R)$ will match $\mathbf{M} = \mathbf{M}_\Delta \mathbf{M}_R \mathbf{M}_D$. It is recalled (see section 2 and section A in the appendix) that $\mathbf{M}$ writes

$$\mathbf{M} = m_{00} \begin{bmatrix} 1 \\ \mathbf{P} \end{bmatrix} [1 \quad \mathbf{D}^t] = m_{00} \begin{bmatrix} 1 & \mathbf{D}^t \\ \mathbf{P} & \mathbf{P} \mathbf{D}^t \end{bmatrix}.$$

Thereby, $\mathbf{M}$ maps $\begin{bmatrix} 1 \\ \mathbf{D} \end{bmatrix}$ to $2 m_{00} \begin{bmatrix} 1 \\ \mathbf{P} \end{bmatrix}$.

Besides, considering the SVD of $\mathbf{M}_D$ given in section 2, we notice that the range of $\mathbf{M}_D$ when $D = 1$ is $\text{span}\left(\begin{bmatrix} 1 \\ \mathbf{D} \end{bmatrix}\right)$. Thereby, with $\mathbf{M} = \mathbf{M}' \mathbf{M}_D$, $\mathbf{M}'$ is attacked only along $\text{span}\left(\begin{bmatrix} 1 \\ \mathbf{D} \end{bmatrix}\right)$, and

the image through M' of any vector orthogonal to $\begin{bmatrix} 1 \\ D \end{bmatrix}$ make take any value. This is a degree of freedom in the choice of M' .

Equality $M \begin{bmatrix} 1 \\ D \end{bmatrix} = M' M_D \begin{bmatrix} 1 \\ D \end{bmatrix}$ yields $M' \begin{bmatrix} 1 \\ D \end{bmatrix} = \begin{bmatrix} 1 \\ P \end{bmatrix}$. This last equation is a necessary and sufficient condition on M' , which is equivalent to $P = P_\Delta + m' D$. If we choose $P_\Delta = 0$ as in [8], we get $P = m' D$ as a necessary and sufficient condition. It is necessary and sufficient for matrix m' to map D onto P .

The couple

$$M_\Delta = \begin{bmatrix} 1 & 0^t \\ 0 & P I \end{bmatrix}, \quad M_R = \begin{bmatrix} 1 & 0^t \\ 0 & \mathcal{R}(D, \hat{P}) \end{bmatrix}$$

is selected in [8]. Matrix m_R rotates D onto $\hat{P}$, matrix m_Δ maps $\hat{P}$ onto P . As a consequence, matrix m' maps D onto P .

It should be noticed that if the goal is the minimization of the retardance R , the couple

$$M_\Delta = \begin{bmatrix} 1 & 0^t \\ 0 & -P I \end{bmatrix}, \quad M_R = \begin{bmatrix} 1 & 0^t \\ 0 & \mathcal{R}(D, -\hat{P}) \end{bmatrix}$$

is a better candidate if $\cos(\hat{P}, D) < 0$. In this case, D is rotated onto $-\hat{P}$, and the reflection in m_Δ will ensure that $m' D = P$.

Adhering to the principle of [8], the undeterminacy should be solved by minimizing R . In fact, $R = 0$ and $m_R = I$ are part of an admissible solution, since there exists a reflection matrix m_Δ which maps D onto P .

Let us define vectors z_1, z_2, q_1, q_2, q_3 (the q_i 's are unit-normed), and scalars $\alpha_1 > 0$ and $\alpha_2 > 0$ such that (see Fig. 1)

$$\begin{cases} \hat{P} + \hat{D} = 2 z_1 = \alpha_1 q_1, \\ \hat{P} - \hat{D} = 2 z_2 = \alpha_2 q_2, \end{cases}$$

with $q_3 = q_1 \times q_2$. Thereby $\hat{D} = z_1 - z_2$ and $\hat{P} = z_1 + z_2$. Let us define $Q_\Delta = [q_1 \ q_2 \ q_3]$ and let us consider $m_\Delta = Q_\Delta \text{diag}([P - P P]) Q_\Delta^t = P q_1 q_1^t - P q_2 q_2^t + P q_3 q_3^t$. We derive: $(\hat{P} + \hat{D})^t (\hat{P} - \hat{D}) = 1 - 1 = 0$, which yields $z_1^t z_2 = 0$ and $q_1^t q_2 = 0$.

This gives

$$\begin{cases} q_1 q_1^t \hat{D} = q_1 q_1^t (z_1 - z_2) = z_1, \\ q_2 q_2^t \hat{D} = q_2 q_2^t (z_1 - z_2) = -z_2. \end{cases}$$

Finally, $m_\Delta D = P z_1 + P z_2 = P \hat{P} = P$ and this particular m_Δ maps D onto P . Matrix m_Δ takes the form

$$m_\Delta = P (q_1 q_1^t - q_2 q_2^t + q_3 q_3^t) = P (I - 2 q_2 q_2^t),$$

which is the composition of a uniform scaling and of a Householder reflection of vector q_2 .

C. Accounting for physical constraints

The choice of ϵ may sometimes be achieved under physical considerations. Work has been devoted to this topic in the case of Mueller matrices with negative determinants (see e.g., [16] and the references therein). For example, for scattering media, the common choice is $\epsilon = \text{diag}([1 \ 1 \ -1])$ [16]. Such constraints are naturally accounted for in the proposed methodology.

The methodology in [16] can straightforwardly be linked to the present work. With the notations of the present article, Eq. 10 in [16] reads $m' = V^{(p)} S U^{(p)'}$, Eq. 15a reads $m_R = V^{(p)} \epsilon U^{(p)t}$, Eq. 15b reads $m_\Delta = V^{(p)} S \epsilon V^{(p)t}$. It should be noticed that the derivations in [16] are different from ours, and do not address cases different than the case labeled (a) in the present work. In the case of matrix M considered in [16] (see Eq. 16), both solutions coincide: our (unconstrained) approach yields a GPD where $\epsilon = \text{diag}([1 \ 1 \ -1])$ and yields M_R and M_Δ found in Eqs. 19a and 19b. The LC-GPD, which selects $\epsilon = -I$, yields $R = 165$ degrees, instead of $R = 79$ degrees with [16] and with the present approach. Nevertheless, imposing ϵ on physical grounds does not always give the lowest possible retardance, as will be seen in section 4.

We propose here a unified framework, where positive-determinant Mueller matrices are decomposed with the same approach as negative-determinant ones, for diagonal as well as non diagonal depolarizers, as opposed to previous works where those cases were distinguished (see e.g., [16] and the references therein).

D. Application on synthetic Mueller matrices

To supplement the preceding derivations, we propose two applications. The first application addresses the standard case (M_D invertible, $s_1 > s_2 > s_3 > 0$ (case (a))), the second application addresses comparisons with [Appendix B, 8].

First application. We draw random matrices m_Δ and m_R as part of the process of generating a Mueller matrix from elementary components, and devise $m' = m_\Delta m_R$ (see section E in the appendix for the algorithm used to generate random Mueller matrices). Minimizing the retardance R amounts to maximizing the trace of m_R , since $\text{Tr}(m_R) = 1 + 2 \cos R$ (see [Eq. 15, 8]). The only degree of freedom for the maximization of the trace is the choice of ϵ . We get three different such ϵ : ϵ_{GT} , corresponding to the ground truth, stemming from the underlying generated data; ϵ_{LC} , corresponding to the Lu and Chipman solution; and ϵ_{PA} , corresponding to the proposed approach.

Examining the simulation outcomes, we see that all possibilities of binary vectors appear for ϵ_{GT} and for ϵ_{PA} . This shows that all binary vectors are physically admissible, since all possible binary vectors appear in ϵ_{GT} .

In section F in the appendix, we show that all possibilities of binary vectors may effectively appear for ϵ_{GT} . Therefore, for a given matrix m' , there are four possible binary vectors, among which anyone may be the ground truth. From a purely numerical perspective, nothing allows to distinguish the ground truth for the other binary vectors. Selecting the ground truth among the possibilities should therefore be achieved using physical arguments.

We see that the ground truth ϵ_{GT} does not always minimize the retardance R , and that the retardance from [8] is never smaller than the retardance from the proposed approach (see Fig. 2). Vector ϵ_{GT} reaches the minimal retardance in about 55 % of all cases, whereas vector ϵ_{LC} reaches the minimal retardance in about 27 % of all cases. Of course, those rates depend on the probability laws used to generate the data.

Second application. The goal here is to assess [Appendix B, 8]. We draw random matrices m_Δ and m_R as above, but enforce the conditions corresponding to cases (b) to (h). Cases (b) to (d) correspond to the standard case in [8]. Cases (e) and (f) correspond to the case $s_1 \neq 0, s_2 \neq 0, s_3 = 0$ in [8]. Case (g)

Fig. 1. Mapping of vector D onto vector $\hat{P}$ by a Householder reflection of vector q_2 . Represented here is the plane defined by vectors D and $\hat{P}$. The ambient space is $\mathbb{R}^3$. Vectors q_1 and q_2 are not represented at the right scale (they are unit norm vectors, as D and $\hat{P}$ are). Vector q_3 comes out of the figure, as $q_3 = q_1 \times q_2$, and is not represented.

Fig. 2. Comparison of retardances (in degrees), for 100 randomly simulated matrices m' , in case (a): $s_1 > s_2 > s_3 > 0$. One realization of matrix m' appears twice, once in each subplot. (A): retardance R_{GT} of the ground truth *versus* retardance R_{PA} of the proposed approach, (B): retardance R_{LC} of the Lu and Chipman solution *versus* retardance R_{PA} of the proposed approach.

corresponds to the case $s_1 \neq 0, s_2 = s_3 = 0$ in [8]. It appears (see Fig. 3) that the solution from [8] does not always yield the minimal retardance, for any of the last two cases addressed in [Appendix B, 8]. The first case of [Appendix B, 8], where $m' = 0$, is not assessed here, its solution being trivial.

Comments on Fig. 2 and on Fig. 3. Let m_{R-LC} be the Lu and Chipman solution, and m_{R-PA} be the proposed approach solution. Let R_{LC} and R_{PA} be the corresponding rotation angles.

- as expected, we always have $R_{LC} \geq R_{PA}$, and for each case there are samples such that $R_{LC} > R_{PA}$;

- we always have $R_{PA} \leq 120$ degrees.

This may be justified as follows. Rotation m_{R-PA} writes $m_{R-PA} = V^{(p)} \hat{Q}_1 \hat{\varepsilon} \hat{Q}_2^t U^{(p)t}$, which we rewrite $\hat{V} \hat{\varepsilon} \hat{U}^t$, with $\hat{V} = V^{(p)} \hat{Q}_1$ and $\hat{U} = U^{(p)} \hat{Q}_2$. The hat notation recalls that $(\hat{Q}_1, \hat{Q}_2, \hat{\varepsilon})$ are resulting from an optimization procedure.

Defining indices $a, b, c \in \{1, 2, 3\}$ such that

$$|\langle v_a, u_a \rangle| \geq |\langle v_b, u_b \rangle| \geq |\langle v_c, u_c \rangle|,$$

we have, as a consequence of $\hat{\varepsilon}$ being the maximizer,

$$\begin{aligned} \text{Tr } m_{R-PA} &= \hat{\varepsilon}_a \langle v_a, u_a \rangle + \hat{\varepsilon}_b \langle v_b, u_b \rangle + \hat{\varepsilon}_c \langle v_c, u_c \rangle \\ &= |\langle v_a, u_a \rangle| + |\langle v_b, u_b \rangle| + \hat{\varepsilon}_c \langle v_c, u_c \rangle. \end{aligned}$$

Since

$$|\langle v_b, u_b \rangle| + \varepsilon_c \langle v_c, u_c \rangle \geq |\langle v_b, u_b \rangle| - |\langle v_c, u_c \rangle| \geq 0,$$

we have $\text{Tr } m_{R-PA} \geq 0$, and since $\text{Tr } m_{R-PA} = 1 + 2 \cos R_{PA}$, we get $R_{PA} \leq 120$ degrees;

- for each case, there is an exclusion zone defined by the three points $\{(0, 0), (90, 90), (0, 180)\}$: no sample lies inside this triangle. In others words, if $m_{R-LC} \neq m_{R-PA}$, then $R_{LC} \geq 180 - R_{PA}$.

This may be justified as follows. The analysis boils down to the case $Q_1 = Q_2 (= Q)$: for cases (a)–(d), $Q_1 = Q_2$ stems from the SVD; for cases (e)–(h), $Q_1 = Q_2$ is a consequence of the optimization procedure (see section D in the appendix). We write $m_{R-PA} = V^{(p)} \hat{Q} \hat{\varepsilon} \hat{Q}^t U^{(p)t}$.

Cases (a)–(d) correspond to the standard case in [8], where $m_{R-LC} = e^{(p)} V^{(p)} U^{(p)t} = e^{(p)} V^{(p)} \hat{Q} \hat{Q}^t U^{(p)t} = V^{(p)} \hat{Q} \varepsilon_{LC} \hat{Q}^t U^{(p)t}$, with $\varepsilon_{LC} = e^{(p)} I$.

Cases (e)–(f) correspond to the third case in [Appendix B, 8], where $m_{R-LC} = V^{(p)} \varepsilon_{LC} U^{(p)t}$, with $\varepsilon_{LC} = \text{diag}([1 \ 1 \ \pm 1])$, ε_{LC} being fixed by the condition $\det m_{R-LC} = 1$. More precisely, for case (e), $\hat{Q} = \mathcal{R}(e_z, \hat{\alpha})$ and $\hat{Q} \varepsilon_{LC} \hat{Q}^t = \varepsilon_{LC}$ whereas for case (f), $\hat{Q}$ is diagonal and matches $\hat{Q} \varepsilon_{LC} \hat{Q}^t = \varepsilon_{LC}$. Finally, we get $m_{R-LC} = V^{(p)} \hat{Q} \varepsilon_{LC} \hat{Q}^t U^{(p)t}$.

See the *Remark* below for case (g).

For cases (a)–(f), we may then write

$$\begin{cases} m_{R-LC} &= V^{(p)} \hat{Q} \varepsilon_{LC} \hat{Q}^t U^{(p)t}, \\ m_{R-PA} &= V^{(p)} \hat{Q} \varepsilon_{PA} \hat{Q}^t U^{(p)t}. \end{cases}$$

Let us define ε_m such that $\varepsilon_{LC} = \varepsilon_m \varepsilon_{PA}$. Thereby, we may write

$$\begin{aligned} \mathbf{m}_{R-LC} &= \begin{bmatrix} V^{(p)} \hat{Q} \varepsilon_m \hat{Q}^t V^{(p)t} \\ V^{(p)} \hat{Q} \varepsilon_m \hat{Q}^t V^{(p)t} \end{bmatrix} \begin{bmatrix} V^{(p)} \hat{Q} \varepsilon_{PA} \hat{Q}^t U^{(p)t} \\ \mathbf{m}_{R-PA} \end{bmatrix} \\ &= \begin{bmatrix} V^{(p)} \hat{Q} \varepsilon_m \hat{Q}^t V^{(p)t} \\ V^{(p)} \hat{Q} \varepsilon_m \hat{Q}^t V^{(p)t} \end{bmatrix} \mathbf{m}_{R-PA}, \end{aligned}$$

which reads $\mathbf{R}_3 = \mathbf{R}_2 \mathbf{R}_1$. Let (w_i, θ_i) be the parameters associated to rotation $\mathbf{R}_i$. If $\mathbf{m}_{R-LC} \neq \mathbf{m}_{R-PA}$, then $\varepsilon_m \neq \mathbf{I}$, and since $\det \mathbf{R}_2 = \det \varepsilon_m = 1$, $\text{Tr} \varepsilon_m = -1$. Thereby, $\theta_2 = \pi$ and as a consequence (see section C in the appendix):

$$\cos \frac{\theta_3}{2} = \left| \sin \frac{\theta_1}{2} \langle w_1, w_2 \rangle \right|.$$

This yields $\cos \frac{\theta_3}{2} \leq \left| \sin \frac{\theta_1}{2} \right|$, which gives

$$\cos \frac{\theta_3}{2} \leq \sin \frac{\theta_1}{2} \left(= \cos \left(\frac{\pi}{2} - \frac{\theta_1}{2} \right) \right).$$

It is recalled that $\theta_1 \in [0, \pi]$ and $\theta_3 \in [0, \pi]$, since θ_1 and θ_3 are rotation angles. Thereby, $\theta_3 \geq \pi - \theta_1$. QED.

Remark: the analysis above does not apply to case (g), since in this case, and only in this case, $V^{(p)}$ and $U^{(p)}$ in $\mathbf{m}_{R-PA}$ are user-chosen and therefore may not correspond to the matrices $V^{(p)}$ and $U^{(p)}$ used in $\mathbf{m}_{R-LC}$. The particular structure of Fig. 3-(g) is justified in section D in the appendix;

- the particular structure of Fig. 3-(d) is justified in section D in the appendix.

4. THE GENERALIZED POLAR DECOMPOSITION IN PRACTICE – ANALYSIS OF A BIOLOGICAL SAMPLE

In practice, no singular value will ever vanish, and two singular values will never be strictly equal due to roundoff errors. We let the user define a threshold τ under which a singular value will be considered vanishing. If the absolute difference between two singular values lies under the same threshold τ , those singular values will be considered equal. Matrix $\mathbf{M}_D$ will be considered invertible if and only if $1 - D > \tau$.

This procedure is used for three decompositions (LC-GPD, OV-GPD (Ossikovski and Vizet, [16]), and PA-GPD), to analyze a biological sample (see Fig. 4). The sample corresponds to mouse skin measured *in vivo* at 810 nm. This measurement has been acquired as part of a larger study for the monitoring with multi-spectral polarimetric imaging of grafted tumors [24]. As in [16], the chosen sample contains a zone of pixels with negative-determinant Mueller matrices. Fig. 4-(d) shows the m_{00} map of the imaged area, the region of interest being delimited by a black box. The results in terms of retardance maps of the region of interest are given Fig. 4-(a-c). We used $\tau = 10^{-8}$.

Negative-determinant pixels are easily spotted in the LC-GPD retardance map (see Fig. 4-(a)) as they are characterized by very high values (close to 180 degrees) in contrast with the low retardance values normally observed with mouse skin. As expected, at these locations on the sample the retardance is significantly reduced in OV-GPD and PA-GPD, as compared to LC-GPD. For a more quantitative comparison, a profile of the retardance values along the red line in Fig. 4-(d) is shown for all three decomposition methods in Fig. 4-(e). While in many cases the OV-GPD (i.e., taking $\varepsilon_{OV} = \text{diag}[1 \ 1 \ -1]$) yields results similar to those of the proposed approach, it gives even larger

values of retardance than LC-GPD in some cases. Hence, a reduction in retardance is gained from OV-GPD to PA-GPD.

Besides, the R_{PA} retardance map is smoother than the R_{LC} map, and also smoother than the R_{OV} map (see Fig. 4). Smoothness and continuity arguments may be at stake to select a decomposition (see e.g., [16], for the particular case of negative-determinant Mueller matrices).

As already stated (see section 3-A), the PA-GPD aims at minimizing the retardance. This goal is reached. Other goals may be aimed at, such as considerations on the orientation of the rotation axis, or continuity considerations on given parameters, such as M_Δ [16]. Effectively, abrupt transitions will probably not correspond to any underlying biological reality, and exhibiting non smooth parameter maps is an issue in this context. Generally speaking, smoother maps will probably correspond to more pertinent descriptions of biological tissues. Abrupt changes could therefore be attributed to modeling artifacts or issues, such as minimizing the retardance on a reduced set of candidates. If avoiding discontinuities should undoubtedly be aimed at, perfect smoothness (i.e., constant maps) should definitely be avoided, since we aim at being sensitive to the underlying scene. Indeed, one goal is to use the extracted GPD as features for classification algorithms, with a view to early diagnosis on biological tissues (see e.g., [15]). As a consequence, reducing the roughness of given parameter maps beyond some degree should be carried out only in the light of classification performances. Besides, roughness reduction should also be handled along with the estimation of Mueller matrices from raw measurement images, where noise disturbs the estimates: reducing roughness also comes partly from the estimation procedures retained.

5. CONCLUSION

In this article, we revisit the classical Lu and Chipman GPD of Mueller matrices [8]. We devise the entire set of GPD candidates attached to a Mueller matrix. We show that the effective set of GPD candidates is richer than the set considered in the original work [8], and recover the decomposition selected in the literature on physical grounds for negative-determinant Mueller matrices [16].

In [8], the choice among different GPD candidates is achieved by minimizing the retardance. We applied the same principle, and as a result, achieved a better minimization of the retardance. This is illustrated on synthetic Mueller matrices, as well as on a biological sample. On the biological sample, the proposed retardance map proved to be smoother, which is a desirable property in the context of analyzing biological tissues.

Other criteria than the minimization of the retardance on the set of GPD candidates may also be considered. This is left for future work.

APPENDIX

A. Derivation of M in the $D = 1$ case

If $\mathbf{M}_D$ is singular ($D = 1$), then $M = m_{00} \begin{bmatrix} 1 & D^t \\ P & P D^t \end{bmatrix}$. This expression may be found in [Eq. A3, 8] and in [Eq. 234, 9]. We propose to derive it here, with an algebraic approach, because of the insight given. This derivation is not given in the cited references.

We use the SVD $(V_D, \text{diag}(S_D), V_D)$ of $\mathbf{M}_D$ (see section 2). With $M = M_\Delta M_R M_D$, and $M = m_{00} \begin{bmatrix} 1 & D^t \\ P & P D^t \end{bmatrix}$, $M_D \begin{bmatrix} 1 \\ -\hat{D} \end{bmatrix} = 0$

Fig. 3. Comparison of retardances (in degrees), for randomly simulated matrices m' . Cases (b), (c), (d), (e), (f), and (g), 100 samples for each case. The retardance R_{LC} from the Lu and Chipman approach is plotted against the retardance R_{PA} from the proposed approach. It may be noticed that, as expected, R_{PA} is lower than R_{LC} across all cases, for all samples. The particular structure of (d) and (g) is justified in the appendix (section D). Generally speaking, the structure of all subfigures is justified in the *Comments on figures* part, in section 3-D.

Fig. 4. Analysis of mouse skin. (d): m_{00} map of the imaged area. The region of interest is delimited by the black box; (a), (b), (c): retardance maps in the region of interest, using the three different approaches (R_{LC} : retardance stemming from the Lu and Chipman approach, R_{OV} : retardance stemming from the Ossikovski and Vizet approach, R_{PA} : retardance stemming from the proposed approach); (e): the three retardances plotted against the pixel number, from top (pixel number 1) to bottom (pixel number 100) along the yellow segment appearing in subplots (a)–(d); (f): scatterplot of R_{OV} against R_{PA} , for negative-determinant pixels in the region of interest.

yields $M \begin{bmatrix} 1 \\ -\hat{D} \end{bmatrix} = 0$, which in turn yields $P = m \hat{D}$ (see also Eq. 1, with $D = 1$). Finally, we obtain

$$M \begin{bmatrix} 1 \\ \hat{D} \end{bmatrix} = m_{00} \begin{bmatrix} 1 + D^t \hat{D} \\ P + m \hat{D} \end{bmatrix} = 2 m_{00} \begin{bmatrix} 1 \\ P \end{bmatrix}. \quad (4)$$

Since M_D is a rank-1 matrix, M is also a rank-1 matrix, and using Eq. 4, we conclude that M writes

$$M = m_{00} \begin{bmatrix} 1 \\ P \end{bmatrix} \begin{bmatrix} 1 & \hat{D}^t \end{bmatrix} = m_{00} \begin{bmatrix} 1 & D^t \\ P & P D^t \end{bmatrix}.$$

More generally, if $D = 1$ and/or $P = 1$, M writes $m_{00} \begin{bmatrix} 1 & D^t \\ P & P D^t \end{bmatrix}$ (see [25]).

B. The non unicity of the singular value decomposition

We address here the non unicity of the SVD. We give theorems 3.1.1 and 3.1.1' of [26]. The reader may also refer to [20] and the references therein.

Theorem 3.1.1 Let $A \in M_{m,n}$ be given, and let $q = \min\{m, n\}$. There is a matrix $\Sigma = [\sigma_{ij}] \in M_{m,n}$ with $\sigma_{ij} = 0$ for all $i \neq j$, and $\sigma_{11} \geq \sigma_{22} \geq \dots \geq \sigma_{qq} \geq 0$, and there are two unitary matrices $V \in M_m$ and $W \in M_n$ such that $A = V \Sigma W^*$. If $A \in M_{m,n}(\mathbb{R})$, matrices V and W may be taken to be real orthogonal matrices.

Theorem 3.1.1' Under the assumptions of Theorem (3.1.1), suppose that the distinct nonzero singular values of A are $s_1 > \dots > s_k > 0$, with respective multiplicities $\mu_1, \dots, \mu_k \geq 1$. Let $\mu_1 + \dots + \mu_k = r$ and let $A = V \Sigma W^*$ be a given singular value decomposition with $\Sigma = \text{diag}(s_1 \mathbf{I}_{\mu_1}, \dots, s_k \mathbf{I}_{\mu_k}, \mathbf{0}_{q-r}) \in M_{m,n}$. Let $\hat{V} \in M_m$ and $\hat{W} \in M_n$ be given unitary matrices. Then $A = \hat{V} \Sigma \hat{W}^*$ if and only if there are unitary matrices $U_i \in M_{\mu_i}$, $i = 1, \dots, k$, $\tilde{V} \in M_{m-r}$, and $\tilde{W} \in M_{n-r}$ such that

$$\hat{V} = V [U_1 \oplus \dots \oplus U_k \oplus \tilde{V}] \quad (5)$$

and

$$\hat{W} = W [U_1 \oplus \dots \oplus U_k \oplus \tilde{W}]. \quad (6)$$

Notations: $M_{m,n}$ denotes m -by- n complex matrices, M_n denotes n -by- n complex matrices, $M_{m,n}(\mathbb{F})$ denotes m -by- n matrices with entries from $\mathbb{F}$. Matrix $B \oplus C$ is the direct sum (i.e., the blockdiagonal matrix) $\begin{bmatrix} B & 0 \\ 0 & C \end{bmatrix}$. Matrix A^* is the Hermitian adjoint of $A \in M_{m,n}(\mathbb{C})$. Matrix $\mathbf{I}_n$ is the identity matrix in M_n .

C. The composition of 3D rotations

The composition of two 3D rotations is a 3D rotation. We recall here some relations at stake (see e.g., [section 9.4, 22], from which this section is taken).

Let $R_3 = R_2 R_1$, with the parameters $R_i = \mathcal{R}(u_i, \theta_i)$ for the rotation of angle θ_i around unit vector u_i . Let $\lambda_i = \cos \frac{\theta_i}{2}$, $\Lambda_i = \sin \frac{\theta_i}{2} u_i$.

Parameters (λ_i, Λ_i) are called the Euler-Rodrigues parameters, and correspond to quaternion components. The parameters combine as

$$\begin{cases} \lambda_3 &= \lambda_1 \lambda_2 - \langle \Lambda_1, \Lambda_2 \rangle, \\ \Lambda_3 &= \lambda_1 \Lambda_2 + \lambda_2 \Lambda_1 + \Lambda_2 \times \Lambda_1. \end{cases}$$

Remark: using the previous expressions, λ_3 may take negative values, corresponding to θ_3 out of the range $[0, \pi]$ (i.e., $\theta_3 > \pi$). This is useful in some cases. In the present case, if we want to come out with a rotation parameter in $[0, \pi]$, we may proceed as follows if $\lambda_3 < 0$.

We have $\mathcal{R}(u_3, \theta_3) = \mathcal{R}(-u_3, -\theta_3) = \mathcal{R}(-u_3, 2\pi - \theta_3) = \mathcal{R}(-u_3, \theta'_3)$, with $\theta'_3 = 2\pi - \theta_3 \in [0, \pi]$.

If (λ'_3, Λ'_3) are the parameters of $\mathcal{R}(-u_3, \theta'_3)$, we get:

$$\begin{cases} \lambda'_3 &= \cos \frac{\theta'_3}{2} = -\cos \frac{\theta_3}{2} = -\lambda_3, \\ \Lambda'_3 &= -\sin \frac{\theta'_3}{2} u_3 = -\sin \frac{\theta_3}{2} u_3 = -\Lambda_3. \end{cases}$$

Finally, in the case $\lambda_3 < 0$, $(-\lambda_3, -\Lambda_3)$ are parameters of a rotation with angle in the range $[0, \pi]$.

In any case, whatever the sign of λ_3 , we will consider a rotation for which the cosine of the half-angle will read $|\lambda_1 \lambda_2 - \langle \Lambda_1, \Lambda_2 \rangle|$. This latter relation will be used in the present article, with a view of minimizing a rotation angle, or of maximizing the cosine of its half.

D. Exhaustive analysis of the ΔR_F , when $D < 1$

We address the case where $D < 1$: m' is uniquely defined, and we aim at computing its ΔR_F . Eight cases should be considered, each one corresponding to a particular structuration of the eigenvalues, and yielding a particular structure for Q_1 and Q_2 , where Q_1 and Q_2 are such that $m' = V^{(p)} Q_1 \varepsilon S Q_2^t U^{(p)t}$:

- case (a): $s_1 > s_2 > s_3 > 0 (\Rightarrow Q_1 = Q_2)$;
- case (b): $s_1 = s_2 > s_3 > 0 (\Rightarrow Q_1 = Q_2)$;
- case (c): $s_1 > s_2 = s_3 > 0 (\Rightarrow Q_1 = Q_2)$;
- case (d): $s_1 = s_2 = s_3 > 0 (\Rightarrow Q_1 = Q_2)$;
- case (e): $s_1 = s_2 > s_3 = 0$;
- case (f): $s_1 > s_2 > s_3 = 0$;
- case (g): $s_1 > s_2 = s_3 = 0$;
- case (h): $s_1 = s_2 = s_3 = 0$.

For each of these cases, the goal is to identify the triple $(\hat{Q}_1, \hat{Q}_2, \hat{\varepsilon})$, which minimizes the retardance R among all admissible candidates (Q_1, Q_2, ε) . Since $\text{Tr}(m_R) = 1 + 2 \cos R$ (see [Eq. 15, 8]), minimizing the retardance amounts to maximizing the trace of m_R . To save space, we will not go into details of the resolution of each of those subproblems. Only the main lines will be given.

Once the solution $m_R = V^{(p)} \hat{Q}_1 \hat{\varepsilon} \hat{Q}_2^t U^{(p)t}$ is determined, we derive m_Δ from $m_\Delta = m' m_R^t$.

In the sequel, all ε 's, whatever their subscript, are taken in $\{-1, 1\}$. Vectors e_x, e_y , and e_z denote the unit vectors of the canonical basis of $\mathbb{R}^3$. As in [8], let u_1, u_2, u_3 be the column vectors of $U^{(p)}$, and let v_1, v_2, v_3 be the column vectors of $V^{(p)}$.

We use a routine which yields

$$\hat{a} = \arg \min_a \cos(2a) + b \sin(2a)$$

in closed form, where $a, b \in \mathbb{R}$ are given. Its usefulness appears in the sequel.

Algorithmically, we successively consider the four possibilities in $(\varepsilon_1, \varepsilon_2) \in \{-1, 1\}^2$. The third component ε_3 is then fixed by the $\det \mathbf{m}_R = 1$ constraint, as: $\varepsilon_3 = \varepsilon_1 \varepsilon_2 \det \left(\mathbf{V}^{(p)} \mathbf{Q}_1 \mathbf{Q}_2 \mathbf{U}^{(p)t} \right)$.

- case (a): $\mathbf{Q}_1 = \mathbf{Q}_2$, and both matrices are diagonal ($\text{diag}([\pm 1 \pm 1 \pm 1])$). They cancel out. The Δ RF writes

$$\left(\mathbf{V}^{(p)} \varepsilon \mathbf{S} \mathbf{V}^{(p)t}, \mathbf{V}^{(p)} \varepsilon \mathbf{U}^{(p)t} \right).$$

Among all four candidates for ε , we select the one maximizing the trace of $\mathbf{m}_R$.

In practice, with a view to reducing the computational cost, we need not examine all four possibilities. Defining indices $a, b, c \in \{1, 2, 3\}$ such that

$$|\langle \mathbf{v}_a, \mathbf{u}_a \rangle| \geq |\langle \mathbf{v}_b, \mathbf{u}_b \rangle| \geq |\langle \mathbf{v}_c, \mathbf{u}_c \rangle|,$$

the trace of $\mathbf{V}^{(p)} \varepsilon \mathbf{U}^{(p)t}$, which writes

$$\varepsilon_a \langle \mathbf{v}_a, \mathbf{u}_a \rangle + \varepsilon_b \langle \mathbf{v}_b, \mathbf{u}_b \rangle + \varepsilon_c \langle \mathbf{v}_c, \mathbf{u}_c \rangle,$$

is maximized for

$$\begin{cases} \varepsilon_a &= \text{sign}(\langle \mathbf{v}_a, \mathbf{u}_a \rangle), \\ \varepsilon_b &= \text{sign}(\langle \mathbf{v}_b, \mathbf{u}_b \rangle), \\ \varepsilon_c &\text{ such that } \det \left(\mathbf{V}^{(p)} \varepsilon \mathbf{U}^{(p)t} \right) = 1. \end{cases}$$

In other words, the optimal trace writes

$$|\langle \mathbf{v}_a, \mathbf{u}_a \rangle| + |\langle \mathbf{v}_b, \mathbf{u}_b \rangle| + \varepsilon_c \langle \mathbf{v}_c, \mathbf{u}_c \rangle;$$

- case (b): $\mathbf{Q}_1 = \mathbf{Q}_2 = \mathbf{Q} = \begin{bmatrix} \cos \alpha & -\varepsilon_\alpha \sin \alpha & 0 \\ \sin \alpha & \varepsilon_\alpha \cos \alpha & 0 \\ 0 & 0 & \varepsilon_0 \end{bmatrix}$.

Thereby, $\mathbf{Q}$ writes $\begin{bmatrix} \cos \alpha & -\sin \alpha & 0 \\ \sin \alpha & \cos \alpha & 0 \\ 0 & 0 & 1 \end{bmatrix} \text{diag}([1 \ \varepsilon_\alpha \ \varepsilon_0])$,

and $\mathbf{Q} = \mathcal{R}(e_z, \alpha) \text{diag}([1 \ \varepsilon_\alpha \ \varepsilon_0])$.

Moreover: $\mathbf{Q} \varepsilon \mathbf{Q}^t = \mathcal{R}(e_z, \alpha) \varepsilon \mathcal{R}(e_z, -\alpha)$ (the $\text{diag}([1 \ \varepsilon_\alpha \ \varepsilon_0])$ part appears twice and cancels out).

- for $\varepsilon_1 = 1, \varepsilon_2 = 1$: $\mathbf{Q} \varepsilon \mathbf{Q}^t = \text{diag}([1 \ 1 \ \varepsilon_3])$ and $\text{Tr } \mathbf{m}_R = \langle \mathbf{u}_1, \mathbf{v}_1 \rangle + \langle \mathbf{u}_2, \mathbf{v}_2 \rangle + \varepsilon_3 \langle \mathbf{u}_3, \mathbf{v}_3 \rangle$;
- for $\varepsilon_1 = -1, \varepsilon_2 = -1$: $\text{Tr } \mathbf{m}_R = -\langle \mathbf{u}_1, \mathbf{v}_1 \rangle - \langle \mathbf{u}_2, \mathbf{v}_2 \rangle + \varepsilon_3 \langle \mathbf{u}_3, \mathbf{v}_3 \rangle$;
- for $\varepsilon_1 = 1, \varepsilon_2 = -1$:

$$\begin{aligned} \text{Tr } \mathbf{m}_R &= \cos(2\alpha) (\langle \mathbf{u}_1, \mathbf{v}_1 \rangle - \langle \mathbf{u}_2, \mathbf{v}_2 \rangle) \\ &+ \sin(2\alpha) (\langle \mathbf{u}_2, \mathbf{v}_1 \rangle + \langle \mathbf{u}_1, \mathbf{v}_2 \rangle) \\ &+ \varepsilon_3 \langle \mathbf{u}_3, \mathbf{v}_3 \rangle. \end{aligned}$$

Using the aforementioned routine, $\hat{\alpha}$ is computed and plugged into the expression of the trace;

- for $\varepsilon_1 = -1, \varepsilon_2 = 1$: $\text{Tr } \mathbf{m}_R = \cos(2\alpha) (-\langle \mathbf{u}_1, \mathbf{v}_1 \rangle + \langle \mathbf{u}_2, \mathbf{v}_2 \rangle) + \sin(2\alpha) (-\langle \mathbf{u}_2, \mathbf{v}_1 \rangle - \langle \mathbf{u}_1, \mathbf{v}_2 \rangle) + \varepsilon_3 \langle \mathbf{u}_3, \mathbf{v}_3 \rangle$;

- case (c): this case is very close to case (b), with $\mathbf{Q}_1 = \mathbf{Q}_2 = \mathbf{Q} = \begin{bmatrix} \varepsilon_0 & 0 & 0 \\ 0 & \cos \alpha & -\varepsilon_\alpha \sin \alpha \\ 0 & \sin \alpha & \varepsilon_\alpha \cos \alpha \end{bmatrix}$.

- for $\varepsilon_2 = 1, \varepsilon_3 = 1$: $\text{Tr } \mathbf{m}_R = \varepsilon_1 \langle \mathbf{u}_1, \mathbf{v}_1 \rangle + \langle \mathbf{u}_2, \mathbf{v}_2 \rangle + \langle \mathbf{u}_3, \mathbf{v}_3 \rangle$;
- for $\varepsilon_2 = -1, \varepsilon_3 = -1$: $\text{Tr } \mathbf{m}_R = \varepsilon_1 \langle \mathbf{u}_1, \mathbf{v}_1 \rangle - \langle \mathbf{u}_2, \mathbf{v}_2 \rangle - \langle \mathbf{u}_3, \mathbf{v}_3 \rangle$;
- for $\varepsilon_2 = 1, \varepsilon_3 = -1$: $\text{Tr } \mathbf{m}_R = \cos(2\alpha) (\langle \mathbf{u}_2, \mathbf{v}_2 \rangle - \langle \mathbf{u}_3, \mathbf{v}_3 \rangle) + \sin(2\alpha) (\langle \mathbf{u}_3, \mathbf{v}_2 \rangle + \langle \mathbf{u}_2, \mathbf{v}_3 \rangle) + \varepsilon_1 \langle \mathbf{u}_1, \mathbf{v}_1 \rangle$;
- for $\varepsilon_2 = -1, \varepsilon_3 = 1$: $\text{Tr } \mathbf{m}_R = \cos(2\alpha) (-\langle \mathbf{u}_2, \mathbf{v}_2 \rangle + \langle \mathbf{u}_3, \mathbf{v}_3 \rangle) - \sin(2\alpha) (\langle \mathbf{u}_3, \mathbf{v}_2 \rangle + \langle \mathbf{u}_2, \mathbf{v}_3 \rangle) + \varepsilon_1 \langle \mathbf{u}_1, \mathbf{v}_1 \rangle$;

- case (d): we have $\mathbf{S} = s \mathbf{I}$, $s > 0$, $\mathbf{m}' = s \mathbf{V}^{(p)} \mathbf{U}^{(p)t}$, $\mathbf{Q}_1 = \mathbf{Q}_2 = \mathbf{Q}$, $\mathbf{m}_R = \mathbf{V}^{(p)} \mathbf{Q} \varepsilon \mathbf{Q}^t \mathbf{U}^{(p)t}$, $\mathbf{m}_\Delta = s \mathbf{V}^{(p)} \mathbf{Q} \varepsilon \mathbf{Q}^t \mathbf{V}^{(p)t}$. The trace of $\mathbf{m}_R$ must be optimized with respect to $\mathbf{Q}$ and ε .

Let $e^{(p)} = \det \left(\mathbf{V}^{(p)} \mathbf{U}^{(p)t} \right)$. The LC-GPD writes

$$\left(s e^{(p)} \mathbf{I}, e^{(p)} \mathbf{V}^{(p)} \mathbf{U}^{(p)t} \right).$$

Rotation matrix $\mathbf{m}_R$ may be linked to the Lu and Chipman rotation matrix $\mathbf{m}_{R-LC} = e^{(p)} \mathbf{V}^{(p)} \mathbf{U}^{(p)t}$ as

$$\begin{aligned} \mathbf{m}_R &= \mathbf{V}^{(p)} \mathbf{Q} \varepsilon \mathbf{Q}^t \mathbf{U}^{(p)t} \\ &= \begin{bmatrix} e^{(p)} \mathbf{V}^{(p)} \mathbf{Q} \varepsilon \mathbf{Q}^t \mathbf{V}^{(p)t} \end{bmatrix} \begin{bmatrix} e^{(p)} \mathbf{V}^{(p)} \mathbf{U}^{(p)t} \end{bmatrix} \\ &= \begin{bmatrix} e^{(p)} \mathbf{V}^{(p)} \mathbf{Q} \varepsilon \mathbf{Q}^t \mathbf{V}^{(p)t} \end{bmatrix} \mathbf{m}_{R-LC}. \end{aligned}$$

Matrix $e^{(p)} \mathbf{V}^{(p)} \mathbf{Q} \varepsilon \mathbf{Q}^t \mathbf{V}^{(p)t}$ corresponds to a rotation, and the previous equation reads $\mathbf{R}_3 = \mathbf{R}_2 \mathbf{R}_1$, with parameters (w_i, θ_i) associated to rotation $\mathbf{R}_i$.

The goal is now to adjust $\mathbf{R}_2$, i.e., to find matrix $\mathbf{Q}$ and vector ε satisfying $\det \mathbf{m}_R = 1$, i.e., $\det(\varepsilon) = \det \left(\mathbf{V}^{(p)} \mathbf{U}^{(p)t} \right) = e^{(p)}$, such that θ_3 is minimized.

We notice that $e^{(p)} \varepsilon$ is a diagonal matrix, which is either (i) the identity matrix, or (ii) composed of one "1" and two "-1"s.

In case (i), $\mathbf{Q} \varepsilon \mathbf{Q}^t = e^{(p)} \mathbf{I}$, and $\mathbf{m}_R = e^{(p)} \mathbf{V}^{(p)} \mathbf{U}^{(p)t}$. Therefore, the PA-GPD is identical to the LC-GPD.

In case (ii), $\text{Tr } \mathbf{R}_2 = 1 + 2 \cos \theta_2 = e^{(p)} \text{Tr } \varepsilon = -1$ (this stems from the property $\text{Tr}(\mathbf{AB}) = \text{Tr}(\mathbf{BA})$). As a consequence, $\theta_2 = \pi$, which gives (see section C in the appendix):

$$\cos \frac{\theta_3}{2} = \left| \sin \frac{\theta_1}{2} \langle \mathbf{w}_1, \mathbf{w}_2 \rangle \right| = \sin \frac{\theta_1}{2} |\langle \mathbf{w}_1, \mathbf{w}_2 \rangle|.$$

We aim at maximizing $\cos \frac{\theta_3}{2}$, which amounts to maximizing $|\langle \mathbf{w}_1, \mathbf{w}_2 \rangle|$. This yields $\mathbf{w}_2 = \pm \mathbf{w}_1$. It may be noticed that both possibilities for $\mathbf{w}_2$ correspond to the same rotation. In the sequel, we will consider $\mathbf{w}_2 = \mathbf{w}_1$. Thereby $\mathbf{R}_2$, and $\mathbf{R}_3$ as a consequence, are completely defined. In this case, $\cos \frac{\theta_3}{2} = \sin \frac{\theta_1}{2}$, and $\theta_3 = \pi - \theta_1$.

It remains to be checked whether $\mathbf{w}_2 = \mathbf{w}_1$, where $\mathbf{w}_1$ given, is accessible, and to compute $\mathbf{Q} \varepsilon \mathbf{Q}^t$. Vector $\mathbf{w}_1$ being unconstrained, the problem boils down to: given any

w_2 , find Q and ε such that the rotation $e^{(p)} V^{(p)} Q \varepsilon Q^t V^{(p)t}$ has axis w_2 (i.e., w_2 is a vector associated to the eigenvalue 1 of this rotation matrix) and angle $\theta_2 = \pi$.

Let $z_a = V^{(p)t} w_2$. The goal is to compute Q and ε such that $e^{(p)} V^{(p)} Q \varepsilon Q^t V^{(p)t} w_2 = w_2$ ($\Leftrightarrow e^{(p)} Q \varepsilon Q^t z_a = z_a$). Let $q_a = z_a$, and (q_b, q_c) be an orthonormal basis of $(\text{span}(q_a))^\perp$. We notice that

$$\begin{cases} Q &= [q_a \ q_b \ q_c], \\ \varepsilon &= e^{(p)} \text{diag}([1 \ -1 \ -1]), \end{cases} \quad (7)$$

meets all conditions. With this choice, we get

$$Q \varepsilon Q^t = e^{(p)} (q_a q_a^t - q_b q_b^t - q_c q_c^t),$$

which gives

$$\begin{aligned} R_2 w_2 &= e^{(p)} V^{(p)} Q \varepsilon Q^t V^{(p)t} w_2 \\ &= V^{(p)} (q_a q_a^t - q_b q_b^t - q_c q_c^t) q_a \\ &= V^{(p)} q_a = V^{(p)} z_a = w_2, \end{aligned}$$

and any vector y orthogonal to w_2 is inverted, i.e., π -rotated:

$$e^{(p)} V^{(p)} Q \varepsilon Q^t V^{(p)t} y = -y.$$

Final algorithm: let $m_{R-LC} = e^{(p)} V^{(p)} U^{(p)t}$ be the Lu and Chipman rotation, parameterized as $\mathcal{R}(w_1, \theta_1)$.

If $\theta_3 (i) \leq \theta_3 (ii)$, i.e., if $\theta_1 \leq \pi - \theta_1 \Leftrightarrow \theta_1 \leq \pi/2$:

$$m_R = m_{R-LC}.$$

Otherwise, the solution is given by $q_a = V^{(p)t} w_1$, Eqs. (7), and

$$m_R = V^{(p)} Q \varepsilon Q^t U^{(p)t};$$

- case (e): this case is close to case (b), with

$$\begin{aligned} Q_1 &= \begin{bmatrix} \cos \alpha & -\sin \alpha & 0 \\ \sin \alpha & \cos \alpha & 0 \\ 0 & 0 & 1 \end{bmatrix} \text{diag}([1 \ \varepsilon_\alpha \ \varepsilon_{01}]), \\ Q_2 &= \begin{bmatrix} \cos \alpha & -\sin \alpha & 0 \\ \sin \alpha & \cos \alpha & 0 \\ 0 & 0 & 1 \end{bmatrix} \text{diag}([1 \ \varepsilon_\alpha \ \varepsilon_{02}]). \end{aligned}$$

It may be shown that $\det m_R = 1$ yields the condition $\varepsilon_{01} \varepsilon_{02} \varepsilon_3 = \varepsilon_1 \varepsilon_2 \det(V) \det(U)$. Once ε_1 and ε_2 are chosen, the product $\varepsilon_{01} \varepsilon_{02} \varepsilon_3$ is fixed. The individual choices for $\varepsilon_{01}, \varepsilon_{02}, \varepsilon_3$ do not matter, and ε_α cancels out.

Therefore, we do not miss any solution if we fix $\varepsilon_{01} = \varepsilon_{02} = 1$, and let ε_3 be imposed by the choices of ε_1 and ε_2 . We are then in the same configuration as the one of case (b): $Q_1 = Q_2 = \mathcal{R}(e_z, \hat{\alpha})$;

- case (f): this case is close to case (a). We have:

$$Q_1 = \text{diag}([\varepsilon_a \ \varepsilon_b \ \varepsilon_c]) \text{ and } Q_2 = \text{diag}([\varepsilon_a \ \varepsilon_b \ \varepsilon_d]).$$

The condition $\det m_R = 1$ yields $\varepsilon_c \varepsilon_d \varepsilon_3 = \varepsilon_1 \varepsilon_2 \det(V) \det(U)$.

Once ε_1 and ε_2 are chosen, the product $\varepsilon_c \varepsilon_d \varepsilon_3$ is fixed. The individual choices for $\varepsilon_c, \varepsilon_d, \varepsilon_3$ do not matter. We may fix $\varepsilon_c = \varepsilon_d = 1$, and let ε_3 be imposed by the choices of ε_1 and ε_2 . We are then in the same configuration as the one of case (a): $Q_1 = Q_2 = Q$, which is a diagonal matrix;

- case (g): $m' = s_1 v_1 u_1^t$. We choose $u_2 = \frac{1}{\|u_1 \times v_1\|} u_1 \times v_1$, $v_2 = u_2$, $u_3 = u_1 \times u_2$, $v_3 = v_1 \times v_2$.

In the case where $\|u_1 \times v_1\| = 0$, i.e., $u_1 = \pm v_1$, we choose u_2 as any vector orthonormal to v_1 and the sequel still applies.

We now have a particular $V^{(p)}$ and a particular $U^{(p)}$.

We have to optimize the trace of $m_R = V^{(p)} Q_1 \varepsilon Q_2^t U^{(p)t}$ with respect to Q_1, Q_2, ε . This trace is also $\text{Tr}((Q_1 \varepsilon Q_2^t) \times (U^{(p)t} V^{(p)}))$.

Let $\cos \theta = \langle u_1, v_1 \rangle$. We get:

$$U^{(p)t} V^{(p)} = \begin{bmatrix} \cos \theta & 0 & -\sin \theta \\ 0 & 1 & 0 \\ \sin \theta & 0 & \cos \theta \end{bmatrix}.$$

$$\text{We write } Q_1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos \alpha_1 & -\sin \alpha_1 \\ 0 & \sin \alpha_1 & \cos \alpha_1 \end{bmatrix} \text{diag}([\varepsilon_0 \ 1 \ \varepsilon_{\alpha_1}]),$$

$$\text{and } Q_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos \alpha_2 & -\sin \alpha_2 \\ 0 & \sin \alpha_2 & \cos \alpha_2 \end{bmatrix} \text{diag}([\varepsilon_0 \ 1 \ \varepsilon_{\alpha_2}]).$$

As seen above, it appears that we can choose $\varepsilon_{\alpha_1} = \varepsilon_{\alpha_2} = 1$ without missing anything. Moreover, variable ε_0 cancels out. Since

$$\det(U^{(p)t} V^{(p)}) = \det(U^{(p)}) \det(V^{(p)}) = 1 \times 1 = 1,$$

the constraint $\det m_R = 1$ yields $\det \varepsilon = \prod_i \varepsilon_i = 1$.

We distinguish two possibilities:

1. $\varepsilon_2 = \varepsilon_3, \varepsilon_1 = 1$. We get

$$\text{Tr } m_R = \varepsilon_3 \cos(\alpha_1 - \alpha_2) (1 + \cos \theta) + \cos \theta.$$

This trace may be maximized with $\varepsilon_3 = 1, \alpha_1 = \alpha_2 = 0$.

Finally $Q_1 = Q_2 = I, \varepsilon = I, m_R = V^{(p)} U^{(p)t}$, and $\text{Tr } m_R = 1 + 2 \cos \theta$;

2. $\varepsilon_2 = -\varepsilon_3, \varepsilon_1 = -1$. We get

$$\text{Tr } m_R = -\varepsilon_3 \cos(\alpha_1 + \alpha_2) (1 - \cos \theta) - \cos \theta.$$

This trace may be maximized with $\varepsilon_2 = 1, \varepsilon_3 = -1, \alpha_1 = \alpha_2 = 0$. Finally $Q_1 = Q_2 = I, \varepsilon = \text{diag}([-1 \ 1 \ -1])$, $m_R = V^{(p)} \varepsilon U^{(p)t}$, and $\text{Tr } m_R = 1 - 2 \cos \theta$.

The algorithm boils down to:

- if $\cos \theta \geq 0$, the solution is $Q_1 = Q_2 = I, \varepsilon = I, m_R = V^{(p)} U^{(p)t}$, $\text{Tr } m_R = 1 + 2 \cos \theta$;
- if $\cos \theta < 0$, the solution is $Q_1 = Q_2 = I, \varepsilon = \text{diag}([-1 \ 1 \ -1])$, $m_R = V^{(p)} \varepsilon U^{(p)t}$, $\text{Tr } m_R = 1 - 2 \cos \theta$.

In other words, if $\cos \theta \geq 0$, m_R is the smallest angle rotation that transfers u_1 to v_1 , whereas if $\cos \theta < 0$, m_R is the smallest angle rotation that transfers u_1 to $-v_1$;

- case (h): $m' = 0$, minimizing R yields $R = 0, m_R = I$.

It should be noticed that cases (e) and (f) are addressed under the same case in [8] (but differently than is done here, and with sometimes a larger R as a result). See [Appendix B, 8], case $s_1 \neq 0, s_2 \neq 0, s_3 = 0$.

Case (g) is addressed by [8] (Appendix B, case $s_1 \neq 0, s_2 = 0, s_3 = 0$). In the original article, u_1 is always transferred to v_1 . We showed that this is appropriate if $\langle u_1, v_1 \rangle > 0$, but if $\langle u_1, v_1 \rangle < 0$, then u_1 should be transferred to $-v_1$ (this is seen in our solution, where $\varepsilon_1 = -1$).

E. Generation of synthetic random Mueller matrices

In this section, we detail the algorithm used to generate random synthetic Mueller matrices. Those sample matrices are used to enlighten the proposed GPD. Therefore, our Mueller matrix synthesis algorithm mimics the GPD: Mueller matrices are devised starting from elementary components (e.g., D , m_D , m_Δ , etc.). The proposed algorithm allows to reach any particular case (e.g., M_D invertible or non invertible, any particular structure (a)–(h), etc.). Besides, any generated sample Mueller matrix is physically admissible, and any physically admissible Mueller matrix may be reached by our generation algorithm (i.e., there is no blind spot in the Mueller matrix space).

Other random Mueller matrix generation algorithms may be found in the literature (see e.g., [section 7, 27]: brute force generation, [section 5.1.1, 28]: generation based on the coherency matrix). But we found none mimicking the GPD, which motivated the development of our own method.

Nine different possibilities stem from P and D : there are three possibilities for D ($D = 0$, $D \in]0, 1[$, $D = 1$) and three possibilities for P ($P = 0$, $P \in]0, 1[$, $P = 1$), to be combined (see [p. 38, 9]). Besides, there are eight different configurations for the singular values of m' ((a) to (h)). Globally, there are $9 \times 8 = 72$ particular cases, structuring the generation of random Mueller matrices.

For a finer analysis, one could want to distinguish three sub-cases: $\hat{P} \neq \pm \hat{D}$, $\hat{P} = \hat{D}$, $\hat{P} = -\hat{D}$. Such a refinement might be of interest in some configurations (see e.g., Fig. 1).

For any particular case taken from the set of 72 possibilities, a candidate Mueller matrix is drawn using the following procedure:

- draw P , D , $\hat{P}$, and $\hat{D}$;
- draw m_{00} , which must meet $m_{00} (1 + D) \leq 1$ and $m_{00} (1 + P) \leq 1$ (see [eq. 225, 9]);
- devise M_R by drawing m_R (draw the angle and the axis of this 3×3 rotation matrix);
- compute M_D using m_{00} and D ;
- draw M_Δ (see below);
- compute the candidate Mueller matrix as the product $M_\Delta M_R M_D$;
- accept the candidate if the physical admissibility conditions $\mathcal{C}$ (see below) are met, otherwise restart the procedure.

Matrix M_Δ is drawn as follows (see [section 6, 8]):

- draw a, b, c in $[0, 1]$. Redefine a, b, c by sorting the previous values in decreasing order. Modify a, b, c by enforcing the condition on the eigenvalues ((a) to (h)) if necessary. Update a, b, c by randomly flipping their signs and randomly swapping their positions;

- draw a 3×3 unitary matrix Q ;
- compute m_Δ as $m_\Delta = Q \text{diag}([a \ b \ c]) Q^t$;
- compute P_Δ using $P = P_\Delta + m_\Delta m_R D$;
- compute M_Δ .

It is reminded that $m' m'^t = m_\Delta m_\Delta^t$ (see section 3–A). Besides, from m_Δ written $m_\Delta = Q \text{diag}([a \ b \ c]) Q^t$, it appears that the singular values of m_Δ are $|a|, |b|, |c|$ (to be taken in decreasing order), and the singular values of m' are s_1, s_2, s_3 . As a consequence, the sets $\{|a|, |b|, |c|\}$ and $\{s_1, s_2, s_3\}$ are equal, and enforcing a condition on the s_i 's amounts to enforcing the same condition on $|a|, |b|, |c|$, which is what is done in the algorithm.

Necessary and sufficient conditions for a 4×4 real matrix to be a physically admissible Mueller matrix are (see e.g., [9]: see Eqs. 171 and 225 in [9], see [p. 29, (4), 9]):

$$(C) \begin{cases} (C_1) & m_{00} + \| [m_{01} \ m_{02} \ m_{03}] \| \leq 1, \\ (C_2) & m_{00} + \| [m_{10} \ m_{20} \ m_{30}] \| \leq 1, \\ (C_3) & \text{the eigenvalues of } H \text{ must be positive,} \end{cases}$$

where H is the corresponding coherency matrix. Conditions C_1 and C_2 respectively read $m_{00} (1 + D) \leq 1$ and $m_{00} (1 + P) \leq 1$.

It may be noticed that the condition $D \leq 1$, which is used in the algorithm, stems from conditions on the gain (minimum and maximum transmittance, see e.g., [Eq. 27, 8], [Eqs. 3.9 and 3.10, 29]). Besides, condition $P \leq 1$ stems from considering the degree of polarization, which must be lower than 1, in particular in the case of an non polarized incoming light (see e.g., [Eq. 31, 8]).

The proposed algorithm enforces only necessary conditions, and checks whether the candidate results meets conditions $\mathcal{C}$. Any physically admissible Mueller matrix may be reached by our procedure.

F. Identifiability issues

We consider here being in case (a), M_D being therefore invertible. We show that by flipping two ε 's, we still get a couple (m_Δ, m_R) which might have been drawn by the procedure described in section E just above. The present section is referred to in section 3–D.

Let $(m_{\Delta i}, m_{Ri})$ be an initial draw with $m' = m_{\Delta i} m_{Ri}$. Matrix $m_{\Delta i}$ is supposed to stem from (Q_i, a_i, b_i, c_i) as $m_{\Delta i} = Q_i \text{diag}([a_i \ b_i \ c_i]) Q_i^t$. We write

$$\text{diag}([a_i \ b_i \ c_i]) = \text{diag}([\text{sign}(a_i) \ \text{sign}(b_i) \ \text{sign}(c_i)]) \\ \times \text{diag}([|a_i| \ |b_i| \ |c_i|]).$$

Defining the permutation matrix Π such that the values of $\Pi^t \text{diag}([|a_i| \ |b_i| \ |c_i|]) \Pi$ appear in decreasing order along the diagonal, we may write

$$m_{\Delta i} = Q_i \Pi [\Pi^t \text{diag}([\text{sign}(a_i) \ \text{sign}(b_i) \ \text{sign}(c_i)]) \Pi] \\ \times [\Pi^t \text{diag}([|a_i| \ |b_i| \ |c_i|]) \Pi] \Pi^t Q_i^t.$$

This expression reads as a SVD of $m_{\Delta i}$, in the form $m_{\Delta i} = V^{(p)} \varepsilon S V^{(p)t}$, with

$$\begin{cases} V^{(p)} &= Q_i \Pi, \\ \varepsilon &= \Pi^t \text{diag}([\text{sign}(a_i) \ \text{sign}(b_i) \ \text{sign}(c_i)]) \Pi, \\ S &= \Pi^t \text{diag}([|a_i| \ |b_i| \ |c_i|]) \Pi. \end{cases}$$

The objective is to show that flipping the sign of two ϵ 's will yield a matrix that may have been drawn from scratch by the general procedure. We flip two ϵ 's (as opposed to one or three) as the resulting associated rotation matrix must have a positive determinant. Flipping two ϵ 's amounts to flipping the sign of two components of $[a_i \ b_i \ c_i]$. Such a flipped vector can be reached by the procedure, and will yield and admissible m_Δ (i.e., symmetrical, with $|a|, |b|, |c| \leq 1$). The rotation matrix m_R would be modified, but would still be an admissible rotation matrix, which as a consequence could be reached by the procedure, since the procedure may reach any rotation matrix.

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The authors declare no conflicts of interest.

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