ON CHOOSING EFFECTIVE SYMMETRY CLASSES FOR ELASTICITY TENSORS

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Summary

We formulate a method of representing a generally anisotropic elasticity tensor by an elasticity tensor exhibiting a material symmetry: an effective tensor. The method for choosing the effective tensor is based on examining the features of the plot of the monoclinic-distance function of a given tensor, choosing an appropriate symmetry class, and then finding the closest tensor in that class. The concept of the effective tensor is not tantamount to the closest tensor since one always obtains a closer approximation using a monoclinic tensor than a tensor of any other nontrivial symmetry. Hence, we use qualitative features of the plot of the monoclinic-distance function to choose an effective symmetry class within which the closest tensor can be computed.

1. Introduction

The motivation for the present work is a relation between materials studied in seismology and their idealization stated by Hooke’s law. In particular, we formulate a method of representing an elasticity tensor, which might be obtained from the laboratory or seismic measurements (1), by an elasticity tensor exhibiting a particular material symmetry, to which we refer as an effective tensor. Following the work of researchers studying the distance in the space of elasticity tensors (2 to 6), we focus our attention on choosing the effective symmetry class of a given generally anisotropic elasticity tensor. Gazis et al. (2) and Moakher and Norris (4) find the closest tensor for a given symmetry class by taking the projection of the tensor onto a linear subspace of symmetric elasticity tensors in one coordinate system. Kochetov and Slawinski (5) take the projections of a given tensor to the linear subspace of transversely isotropic tensors in all coordinate systems and then find the minimum distance in order to determine the closest transversely isotropic tensor. Kochetov and Slawinski (6) propose a method to find the closest orthotropic elasticity tensor for a given generally anisotropic tensor for all orientations of Cartesian coordinate systems. In this paper, we generalize the problem for any linear symmetric subspace expressed in any coordinate system. No a priori assumption about the symmetry class or orientations of symmetry axes and planes is made.

The concept of the effective tensor is not tantamount to the closest tensor since one always obtains a closer approximation using a monoclinic tensor than a tensor of any other nontrivial symmetry as
illustrated in Fig. 1. Thus, one cannot choose the effective symmetry class by considering only the distance to different symmetry classes. In this paper, we propose a method for choosing the effective tensor that is based on examining the features of the plot of the monoclinic-distance function of a given tensor, choosing an appropriate symmetry class, and then finding the closest tensor in that class. A similar approach with less detail is discussed by François et al. (3).

We begin this paper by stating the notation we use. In section 3, we present the symmetry classes and symmetry groups of elasticity tensors. In section 4, we describe the distance functions associated with the symmetry classes, except isotropy and general anisotropy, since the distance to isotropy does not require any rotation considerations, and the distance to general anisotropy is zero: every elasticity tensor belongs to general anisotropy. Finally, we consider numerical examples to illustrate a choice of the effective symmetry class and the closest tensor within it.

2. Notation

In this section, we describe the notation used in this paper for studying symmetries of an elasticity tensor, which appears in Hooke's law,

\[ \sigma_{ij} = c_{ijkl} \varepsilon_{kl}, \quad i, j \in \{1, 2, 3\}, \]  

where \( \sigma_{ij}, \varepsilon_{kl} \) and \( c_{ijkl} \) are the components of the stress, strain and elasticity tensors, respectively. Note that repeated indices imply summation. The elasticity tensor, which is a fourth-rank tensor in \( \mathbb{R}^3 \), can be represented by a symmetric \( 6 \times 6 \) matrix (7):

\[
C = \begin{bmatrix}
c_{1111} & c_{1122} & c_{1133} & \sqrt{2}c_{1123} & \sqrt{2}c_{1113} & \sqrt{2}c_{1112} \\
c_{1122} & c_{2222} & c_{2233} & \sqrt{2}c_{2223} & \sqrt{2}c_{2213} & \sqrt{2}c_{2212} \\
c_{1133} & c_{1133} & c_{3333} & \sqrt{2}c_{3323} & \sqrt{2}c_{3313} & \sqrt{2}c_{3312} \\
\sqrt{2}c_{1123} & \sqrt{2}c_{2223} & \sqrt{2}c_{2233} & 2c_{2323} & 2c_{2313} & 2c_{2312} \\
\sqrt{2}c_{1113} & \sqrt{2}c_{2213} & \sqrt{2}c_{3313} & 2c_{2313} & 2c_{1313} & 2c_{1312} \\
\sqrt{2}c_{1112} & \sqrt{2}c_{2212} & \sqrt{2}c_{3312} & 2c_{2312} & 2c_{1312} & 2c_{1212} \\
\end{bmatrix}.
\]
For notational convenience, we include factors $\sqrt{2}$ and 2 in the corresponding elasticity parameters; for instance, we write $C_{16} = \sqrt{2}c_{1112}$. Hence,

$$C = [C_{ij}]_{1 \leq i, j \leq 6}$$  \hspace{1cm} (2.3)$$

represents matrix (2.2). An orthogonal transformation in $\mathbb{R}^3$, given by a matrix $A = [A_{ij}] \in O(3)$, results in the following transformation of matrix (2.2):

$$C' = \tilde{A}^T C \tilde{A},$$  \hspace{1cm} (2.4)$$

where $\tilde{A}$ is the following orthogonal $6 \times 6$ matrix (7):

$$\begin{bmatrix}
A^2_{11} & A^2_{12} & A^2_{13} & \sqrt{2}A_{12}A_{13} & \sqrt{2}A_{11}A_{13} & \sqrt{2}A_{11}A_{12} \\
A^2_{21} & A^2_{22} & A^2_{23} & \sqrt{2}A_{22}A_{23} & \sqrt{2}A_{21}A_{23} & \sqrt{2}A_{21}A_{22} \\
A^2_{31} & A^2_{32} & A^2_{33} & \sqrt{2}A_{32}A_{33} & \sqrt{2}A_{31}A_{33} & \sqrt{2}A_{31}A_{32} \\
\sqrt{2}A_{12}A_{31} & \sqrt{2}A_{22}A_{32} & \sqrt{2}A_{23}A_{33} & A_{22}A_{33}+A_{23}A_{32} & A_{21}A_{33}+A_{23}A_{31} & A_{21}A_{32}+A_{22}A_{31} \\
\sqrt{2}A_{11}A_{31} & \sqrt{2}A_{12}A_{32} & \sqrt{2}A_{13}A_{33} & A_{12}A_{33}+A_{13}A_{32} & A_{11}A_{33}+A_{13}A_{31} & A_{11}A_{32}+A_{12}A_{31} \\
\sqrt{2}A_{11}A_{21} & \sqrt{2}A_{12}A_{22} & \sqrt{2}A_{13}A_{23} & A_{12}A_{23}+A_{13}A_{22} & A_{11}A_{23}+A_{13}A_{21} & A_{11}A_{22}+A_{12}A_{21}
\end{bmatrix}.$$

3. Symmetry classes of elasticity tensors

In view of (2.4), an elasticity tensor is invariant under an orthogonal transformation $A \in O(3)$ if and only if

$$C = \tilde{A}^T C \tilde{A}.$$  \hspace{1cm} (3.1)$$

As shown by several researchers (8 to 10), there are eight symmetry classes of elasticity tensor: isotropy, cubic symmetry, transverse isotropy (TI), tetragonal symmetry, trigonal symmetry, orthotropic symmetry, monoclinic symmetry and general anisotropy. In other words, the symmetry group of any elasticity tensor is conjugate to one of the following eight groups:

$$G^{iso} = O(3),$$  \hspace{1cm} (3.2)$$

$$G^{cubic} = \{A \in O(3) | A(e_j) = \pm e_j \text{ for any } i, j \in \{1, 2, 3\}\},$$  \hspace{1cm} (3.3)$$

$$G^{TI} = \{\pm I, \pm R_{\theta,e_1} \pm M_{\vec{v}} | \theta \in [0, 2\pi) \text{ and } \vec{v} \text{ in the } e_1e_2\text{-plane}\},$$  \hspace{1cm} (3.4)$$

$$G^{teta} = \left\{ \pm I, \pm R_{\frac{\pi}{2}, e_3}, \pm R_{\frac{\pi}{2}, e_3}, \pm M_{e_1}, \pm M_{e_2}, \pm M_{e_3}, \pm M_{1,1,0}, \pm M_{1,-1,0} \right\},$$  \hspace{1cm} (3.5)$$

$$G^{trigo} = \left\{ \pm I, \pm R_{\frac{\pi}{2}, e_3}, \pm M_{e_1}, \pm M_{e_2}, \pm M_{e_3}, \pm M_{\left(\cos \frac{\pi}{2}, \sin \frac{\pi}{2}, 0\right)}, \pm M_{\left(\cos \frac{\pi}{2}, -\sin \frac{\pi}{2}, 0\right)} \right\}. $$  \hspace{1cm} (3.6)$$

$$G^{ortho} = \{\pm I, \pm M_{e_1}, \pm M_{e_2}, \pm M_{e_3}\},$$  \hspace{1cm} (3.7)$$

$$G^{mono} = \{\pm I, \pm M_{e_3}\},$$  \hspace{1cm} (3.8)$$

$$G^{aniso} = \{\pm I\},$$  \hspace{1cm} (3.9)$$

where $R_{\theta,\vec{v}}$ denotes the rotation around the vector $\vec{v}$ by angle $\theta$ and $M_{\vec{v}}$ denotes the reflection about the plane whose normal is $\vec{v}$.

The order relation among the symmetry groups is shown in Fig. 1. The dots are connected by a line if, up to conjugation, the symmetry group corresponding to the dot below is contained in
the symmetry group corresponding to the dot above. We have to say ‘up to conjugation’ because the form of $G_{\text{trigo}}$ presented above, and commonly found in the literature, has $e_3$ as a three-fold rotation axis, which is not the normal of any mirror-symmetry plane. Hence, $G^{\text{mono}}$ is not contained in $G^{\text{trigo}}$, but it is contained in the conjugate group, $G^{\text{trigo}'}$, that has $e_1$ as a three-fold rotation axis. With this in mind, the monoclinic symmetry group is a subgroup of all other nontrivial symmetry groups: all except the general anisotropy.

We say that a basis, \{e_1, e_2, e_3\}, is a natural coordinate system for $C$ if the symmetry group of $C$ is $G^{\text{sym}}$ (not just conjugate to $G^{\text{sym}}$), where $G^{\text{sym}}$ is one of the groups listed above. For each symmetry class, one can find the form of matrix (2.2) representing an elasticity tensor in a natural coordinate system (11, 12).

4. Distance function

4.1 Definition

To consider the concept of distance in the space of elasticity tensors, we invoke the Frobenius norm:

$$\|c_{ijkl}\|^2 := c_{ijkl}c_{ijkl}.$$  \hfill (4.1)

For each symmetry class, $\text{sym}$, we define a linear subspace of elasticity tensors, $L^{\text{sym}}$, as the set of all $C$ such that its symmetry group includes $G^{\text{sym}}$. Hence, the distance between $C$ and $L^{\text{sym}}$ is the norm of the difference of $C$ and $C^{\text{sym}}$, the orthogonal projection of $C$ onto $L^{\text{sym}}$; in other words,

$$\min_{C' \in L^{\text{sym}}} \|C - C'\| = \|C - C^{\text{sym}}\|,$$

where, as shown by Gazis et al. (2),

$$C^{\text{sym}} = \frac{1}{\sqrt{|G^{\text{sym}}|}} \sum_{A \in G^{\text{sym}}} A^T C A.$$  \hfill (4.2)

For all classes, except for isotropy and TI, this average involves a finite sum.

Hence, the squared distance from a generic elasticity tensor $C$ to $L^{\text{sym}}$ is

$$d(C, L^{\text{sym}}) = \|C - C^{\text{sym}}\|^2 = \|C\|^2 - \|C^{\text{sym}}\|^2,$$  \hfill (4.3)

where the second equality holds since $C - C^{\text{sym}}$ and $C^{\text{sym}}$ are orthogonal to one another.

4.2 Explicit expressions

In this section, for convenience of the reader, we present explicit expressions for the distance functions for all nontrivial symmetry classes, except isotropy, which is well known. These expressions can be obtained by using (4.2) to calculate the projection of a generic elasticity tensor $C$ to $L^{\text{sym}}$, where $\text{sym}$ is any of the six symmetry classes and then using (4.3) to obtain the distance function for $\text{sym}$. The calculation of projection can be simplified by observing that, since the transformation $-I \in O(3)$ has no effect on $C$, it suffices to take only elements of $G^{\text{sym}} \cap SO(3)$ in (4.2). Moakher and Norris (4) use a different method to obtain these projections.

4.2.1 Monoclinic. Since, as stated in (3.8), $G^{\text{mono}} = \{\pm I, \pm M_{e_3}\}$, the projection of $C$ onto $L^{\text{mono}}$ is

$$C^{\text{mono}} = \frac{1}{2} (C + \tilde{M}_{e_3}^T C \tilde{M}_{e_3}).$$  \hfill (4.4)
Evaluating the right-hand side of (4.4), we obtain
\[
\begin{bmatrix}
C_{11} & C_{12} & C_{13} & 0 & 0 & C_{16} \\
C_{12} & C_{22} & C_{23} & 0 & 0 & C_{26} \\
C_{13} & C_{23} & C_{33} & 0 & 0 & C_{36} \\
0 & 0 & 0 & C_{44} & C_{45} & 0 \\
0 & 0 & 0 & C_{45} & C_{55} & 0 \\
C_{16} & C_{26} & C_{36} & 0 & 0 & C_{66}
\end{bmatrix}
\] (4.5)

The distance of \(C\) to \(L_{\text{mono}}\) is found by substituting matrix (4.5) into expression (4.3),
\[
d(C, L_{\text{mono}}) = 2(C_{14}^2 + C_{15}^2 + C_{24}^2 + C_{25}^2 + C_{34}^2 + C_{35}^2 + C_{46}^2 + C_{56}^2).
\]

4.2.2 Orthotropic. In a similar manner, one can find the projection of \(C\) onto \(L_{\text{ortho}}\),
\[
C_{\text{ortho}} = \frac{1}{4} \left( C + M_{e_1}^T C M_{e_1} + M_{e_2}^T C M_{e_2} + M_{e_3}^T C M_{e_3} \right),
\] (4.6)
since \(G_{\text{ortho}} = \{ \pm I, \pm M_{e_1}, \pm M_{e_2}, \pm M_{e_3} \}\) as stated in expression (3.7). This results in
\[
C_{\text{ortho}} = \begin{bmatrix}
C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\
C_{12} & C_{22} & C_{23} & 0 & 0 & 0 \\
C_{13} & C_{23} & C_{33} & 0 & 0 & 0 \\
0 & 0 & 0 & C_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & C_{55} & 0 \\
0 & 0 & 0 & 0 & 0 & C_{66}
\end{bmatrix}
\] (4.7)

According to expression (4.3), the distance of \(C\) to \(L_{\text{ortho}}\) is
\[
d(C, L_{\text{ortho}}) = 2(C_{14}^2 + C_{15}^2 + C_{24}^2 + C_{25}^2 + C_{34}^2 + C_{35}^2 + C_{46}^2 + C_{56}^2).
\]

4.2.3 Tetragonal. The projection of \(C\) onto \(L_{\text{tetra}}\) is
\[
C_{\text{tetra}} = \begin{bmatrix}
\frac{1}{2}(C_{11}+C_{22}) & C_{12} & \frac{1}{2}(C_{13}+C_{23}) & 0 & 0 & 0 \\
C_{12} & \frac{1}{2}(C_{11}+C_{22}) & \frac{1}{2}(C_{13}+C_{23}) & 0 & 0 & 0 \\
\frac{1}{2}(C_{13}+C_{23}) & \frac{1}{2}(C_{13}+C_{23}) & C_{33} & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{1}{2}(C_{44}+C_{55}) & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{1}{2}(C_{44}+C_{55}) & 0 \\
0 & 0 & 0 & 0 & 0 & C_{66}
\end{bmatrix}
\]

Thus, the distance of \(C\) to \(L_{\text{tetra}}\) is
\[
d(C, L_{\text{tetra}}) = \frac{1}{2}(C_{11} - C_{22})^2 + \frac{1}{2}(C_{44} - C_{55})^2 + (C_{13} - C_{23})^2
\]
\[
+ 2(C_{14}^2 + C_{24}^2 + C_{34}^2 + C_{15}^2 + C_{25}^2 + C_{35}^2 + C_{16}^2 + C_{26}^2 + C_{36}^2 + C_{45}^2 + C_{46}^2 + C_{56}^2).
\]
4.2.4 Trigonal. Similarly, $C^{\text{trigo}}$ is

$$C^{\text{trigo}} = \begin{bmatrix}
C^{\text{trigo}}_{11} & C^{\text{trigo}}_{12} & C^{\text{trigo}}_{13} & C^{\text{trigo}}_{14} & 0 & 0 \\
C^{\text{trigo}}_{12} & C^{\text{trigo}}_{11} & C^{\text{trigo}}_{13} & C^{\text{trigo}}_{24} & 0 & 0 \\
C^{\text{trigo}}_{13} & C^{\text{trigo}}_{12} & C^{\text{trigo}}_{33} & 0 & 0 & 0 \\
C^{\text{trigo}}_{14} & C^{\text{trigo}}_{24} & 0 & C^{\text{trigo}}_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & C^{\text{trigo}}_{44} & C^{\text{trigo}}_{56} \\
0 & 0 & 0 & 0 & C^{\text{trigo}}_{56} & C^{\text{trigo}}_{66}
\end{bmatrix},$$

(4.8)

where

$$C^{\text{trigo}}_{11} = C^{\text{trigo}}_{22} = \frac{1}{8} (3C_{11} + 3C_{22} + 2C_{12} + 2C_{66}),$$

$$C^{\text{trigo}}_{12} = \frac{1}{8} (C_{11} + C_{22} + 6C_{12} - 2C_{66}),$$

$$C^{\text{trigo}}_{13} = C^{\text{trigo}}_{23} = \frac{1}{2} (C_{13} + C_{23}),$$

$$C^{\text{trigo}}_{14} = -C^{\text{trigo}}_{24} = \frac{1}{4} (C_{14} - C_{24} + \sqrt{2}C_{56}),$$

$$C^{\text{trigo}}_{33} = C_{33},$$

$$C^{\text{trigo}}_{44} = C^{\text{trigo}}_{55} = \frac{1}{2} (C_{44} + C_{55}),$$

$$C^{\text{trigo}}_{44} = \frac{\sqrt{2}}{4} (C_{14} - C_{24} + \sqrt{2}C_{56}),$$

$$C^{\text{trigo}}_{66} = \frac{1}{4} (C_{11} + C_{22} - 2C_{12} + 2C_{66}).$$

Following expression (4.3), we get

$$d(C, L^{\text{trigo}}) = 2(C_{16}^2 + C_{26}^2 + C_{15}^2 + C_{25}^2 + C_{34}^2 + C_{35}^2 + C_{36}^2 + C_{45}^2 + C_{46}^2)$$

$$+ \frac{1}{2} (C_{11} - C_{22})^2 + (C_{13} - C_{23})^2 + (C_{14} + C_{24})^2 + \frac{1}{2} (C_{44} - C_{55})^2$$

$$+ \frac{1}{2} \left( \frac{1}{\sqrt{2}} C_{11} + \frac{1}{\sqrt{2}} C_{22} - C_{12} - C_{66} \right)^2 + \left( \frac{1}{\sqrt{2}} C_{14} - \frac{1}{\sqrt{2}} C_{24} - C_{56} \right)^2.$$  

Remark 4.1 It is sometimes more convenient to use an alternative form of projection, $C^{\text{trigo}'}$, which is associated with the form of trigonal symmetry group, $G^{\text{trigo}'}$, that has $e_1$ (rather than $e_3$) as a three-fold rotation axis. $C^{\text{trigo}'}$ is obtained by interchanging 1 and 3 in the subscripts of the components of $C^{\text{trigo}}$ and adjusting matrix (4.8) accordingly. The resulting matrix is consistent with (4.5) in the sense of having zeros in the same places.

4.2.5 Cubic. The projection of $C$ onto $L^{\text{cubic}}$ is

$$C^{\text{cubic}} = \begin{bmatrix}
C^{\text{cubic}}_{11} & C^{\text{cubic}}_{12} & C^{\text{cubic}}_{12} & C^{\text{cubic}}_{12} & 0 & 0 & 0 \\
C^{\text{cubic}}_{12} & C^{\text{cubic}}_{11} & C^{\text{cubic}}_{11} & C^{\text{cubic}}_{11} & 0 & 0 & 0 \\
C^{\text{cubic}}_{12} & C^{\text{cubic}}_{12} & C^{\text{cubic}}_{11} & C^{\text{cubic}}_{11} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & C^{\text{cubic}}_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & C^{\text{cubic}}_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & C^{\text{cubic}}_{44} & 0
\end{bmatrix},$$

(4.9)
where
\[ C_{11}^{\text{cubic}} = \frac{1}{3}(C_{11} + C_{22} + C_{33}), \quad C_{12}^{\text{cubic}} = \frac{1}{3}(C_{12} + C_{13} + C_{23}), \quad C_{44}^{\text{cubic}} = \frac{1}{3}(C_{44} + C_{55} + C_{66}) \]

Hence, by expression (4.3), we get
\[
d(C, L^{\text{cubic}}) = 2(C_{14}^2 + C_{15}^2 + C_{16}^2 + C_{24}^2 + C_{25}^2 + C_{26}^2 + C_{34}^2 + C_{35}^2 + C_{36}^2 + C_{45}^2 + C_{46}^2 + C_{56}^2)
+ \frac{1}{3}((C_{11} - C_{22})^2 + (C_{12} - C_{33})^2 + (C_{22} - C_{33})^2 + (C_{44} - C_{55})^2 + (C_{44} - C_{66})^2
+ (C_{55} - C_{66})^2 + \frac{2}{3} ((C_{12} - C_{13})^2 + (C_{12} - C_{23})^2 + (C_{13} - C_{23})^2).
\]

4.2.6 Transversely isotropic. The projection of \( C \) onto \( L^{\text{TI}} \) is
\[
C^{\text{TI}} = \begin{bmatrix}
C_{11}^{\text{TI}} & C_{12}^{\text{TI}} & C_{13}^{\text{TI}} & 0 & 0 & 0 \\
C_{12}^{\text{TI}} & C_{11}^{\text{TI}} & C_{13}^{\text{TI}} & 0 & 0 & 0 \\
C_{13}^{\text{TI}} & C_{12}^{\text{TI}} & C_{11}^{\text{TI}} & 0 & 0 & 0 \\
0 & 0 & 0 & C_{44}^{\text{TI}} & 0 & 0 \\
0 & 0 & 0 & 0 & C_{44}^{\text{TI}} & 0 \\
0 & 0 & 0 & 0 & 0 & C_{11}^{\text{TI}} - C_{12}^{\text{TI}}
\end{bmatrix},
\]

where
\[
C_{11}^{\text{TI}} = \frac{1}{8}(3C_{11} + 3C_{22} + 2C_{12} + 4C_{66}), \quad C_{12}^{\text{TI}} = \frac{1}{8}(C_{11} + C_{22} + 6C_{12} - 4C_{66}),
\]
\[
C_{13}^{\text{TI}} = \frac{1}{2}(C_{13} + C_{23}), \quad C_{33}^{\text{TI}} = C_{33}, \quad C_{44}^{\text{TI}} = \frac{1}{4}(C_{44} + C_{55}).
\]

Substituting \( C^{\text{TI}} \) into expression (4.3), we get
\[
d(C, L^{\text{TI}}) = 2(C_{14}^2 + C_{15}^2 + C_{16}^2 + C_{24}^2 + C_{25}^2 + C_{26}^2 + C_{34}^2 + C_{35}^2 + C_{36}^2 + C_{45}^2 + C_{46}^2 + C_{56}^2)
+ \frac{1}{2}(C_{11} - C_{22})^2 + (C_{12} - C_{33})^2 + \frac{1}{2}(C_{44} - C_{55})^2 + \frac{1}{2} \left( C_{66} - \frac{C_{11} + C_{22}}{2} + C_{12} \right)^2.
\]

4.3 Orientation

For the cases considered above, \( L^{\text{sym}} \) is a space that includes only those tensors whose natural coordinate system is \( \{e_1, e_2, e_3\} \). If \( C \) belongs to \( \text{sym} \) but is expressed in a coordinate system different from its natural one, then the distance from \( C \) to \( L^{\text{sym}} \) is not zero. To address this issue, we consider the projections of \( C \) on a rotated space, \( L^{\text{sym}} \), for all orientations of the coordinate system. Hence, we define the distance function as the function of a rotation matrix, \( X \in SO(3) \),
\[
d(C, X) = d(C, X) = \|X^T C X \|^2 - \|X^T C X \|^2 \text{sym} \]
\[
= \|C\|^2 - \|X^T C X \|^2 \text{sym}.\]
Thus, the squared distance from \( C \) to the symmetry class \( sym \) is the minimum value of the distance function over all \( X \in SO(3) \). Any rotation matrix \( X \in SO(3) \) that rotates the coordinate system \( \{ e_1, e_2, e_3 \} \) to the coordinate system \( \{ e'_1, e'_2, e'_3 \} \), namely \( X(e_i) = e'_i \) for \( i \in \{1, 2, 3\} \), can be obtained by multiplying three elementary rotations, namely \( Z_1, Z_2 \) and \( Z_3 \):

\[
X = Z_1Z_2Z_3
\]

\[
= \begin{bmatrix}
\cos \psi \cos \theta - \sin \psi \cos \phi \sin \theta & -\cos \psi \sin \theta - \sin \psi \cos \phi \cos \theta & \sin \psi \sin \phi \\
\sin \psi \cos \theta + \cos \psi \cos \phi \sin \theta & -\sin \psi \sin \theta + \cos \psi \cos \phi \cos \theta & -\cos \psi \sin \phi \\
\sin \phi \cos \theta & \sin \phi \sin \theta & \cos \phi 
\end{bmatrix},
\]

where \( Z_1 \) is the rotation around \( e_3 \) by angle \( \phi \), \( Z_2 \) around \( e_1 \) by \( \psi \) and \( Z_3 \) around \( e_3 \) by \( \theta \); \( \phi, \psi \) and \( \theta \) are the Euler angles. The \( z \)-axis of the coordinate system in which the tensor is expressed after rotation is

\[
X(e_3) = \left( \cos \left( \psi - \frac{\pi}{2} \right) \sin \phi, \sin \left( \psi - \frac{\pi}{2} \right) \sin \phi, \cos \phi \right).
\]

For monoclinic and transversely isotropic symmetry classes, the distance function depends only on \( \phi \) and \( \psi \), that is, \( Z_3 \) in \( X \) does not change the value of the function. In other words, the values of \( d(X^T C \bar{X}, L^{\text{mono}}) \) and \( d(X^T \bar{C} \bar{X}, L^{\text{TI}}) \) are determined by \( X(e_3) \) (14). Hence, we can plot these two functions on the surface of the unit sphere in \( \mathbb{R}^3 \). A code for plotting the distance functions can be found in (14).

5. Determining effective elasticity tensor

5.1 Formulation

In this section, we propose a method of choosing the symmetry class to approximate a given generally anisotropic elasticity tensor. Then, we evaluate the closest tensor that belongs to that class among all orientations of the coordinate systems. Hence, the orientation of the closest tensor is found.

The choice of the effective symmetry class of a given \( C \) is guided by the plot of the monoclinic-distance function of \( C \). Diner (13) and Diner et al. (14) discuss features of monoclinic-distance plots and TI-distance plots of elasticity tensors that belong to nontrivial symmetry classes. Apart from the fact that the monoclinic-distance function can be plotted on a sphere, it has two important properties. First, it vanishes in the directions of the normals of the mirror planes of a given elasticity tensor. Second, the distance function is symmetric with respect to the symmetry group of the tensor. Hence, if a tensor is symmetric with respect to an orthogonal transformation so is the plot of the distance function as illustrated by Diner et al. (14).

Herein, we consider \( C \) to be a small perturbation of such a tensor. Thus, the monoclinic-distance function of \( C \) is also a slight perturbation of the monoclinic-distance function of the symmetric tensor. Moreover, we prove that, for a generally anisotropic elasticity tensor that is a small perturbation of an orthotropic, tetragonal, trigonal or cubic symmetry, the near-zero minima of the monoclinic-distance function are in the neighbourhood of the mirror plane normals of the symmetric tensor. Hence, the pattern of near-zero minima of the monoclinic-distance function can be used to recognize the appropriate symmetry class and to determine the orientation of a natural coordinate system.

**Theorem 5.1.** Let \( C^0 \) be a tensor that belongs to one of the following symmetry classes: orthotropic, tetragonal, trigonal or cubic. Let \( n \) be a normal to a mirror plane of symmetry for
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$C^0$. Then, for a sufficiently small perturbation of $C^0$, which we denote by $C$, there is a unique near-zero minimum of $d(\tilde{\mathbf{X}}^T C \tilde{\mathbf{X}}, \mathbf{L}^{\text{mono}})$ in a neighbourhood of $\mathbf{n}$.

**Proof.** Referring to Fig. 1, we see that, to prove the theorem, it suffices to consider two cases: 1. $C^0$ has at least orthotropic but not transversely isotropic symmetry and 2. $C^0$ has at least trigonal but not transversely isotropic symmetry.

Let $f(u, v, w; C) = d(\tilde{\mathbf{X}}^T C \tilde{\mathbf{X}}, \mathbf{L}^{\text{mono}})$, where $X(e_3) = (u, v, w)$. Then $f(u, v, w; C^0)$ attains its absolute minimum of zero on the unit sphere, $u^2 + v^2 + w^2 = 1$, at the points corresponding to the normals to mirror planes of $C^0$. Taking $\{e_1, e_2, e_3\}$ to be a natural coordinate system of $C^0$ (regarded as orthotropic or trigonal tensor, disregarding higher symmetry, if any, and using the alternative form of the trigonal symmetry class as in Remark 4.1), we may assume $\mathbf{n} = (0, 0, 1)$ and use $(u, v)$ as local coordinates on the sphere, with $w = \sqrt{1 - u^2 - v^2}$; note that in the case of a cubic $C^0$ some of the normals are covered by Case 1 and others by Case 2. The critical points of $f(u, v, \sqrt{1 - u^2 - v^2}; C)$ are determined by $\frac{\partial f}{\partial u} = 0$ and $\frac{\partial f}{\partial v} = 0$. If $C$ is in a small neighbourhood of $C^0$, then there exists a neighbourhood of $(0, 0, 1)$ where this system of equations has a unique solution, provided we can show that the Jacobian of the system, which herein is the Hessian of $f$,

$$H = \frac{\partial^2 f}{\partial u^2} \frac{\partial^2 f}{\partial v^2} - \left( \frac{\partial^2 f}{\partial u \partial v} \right)^2,$$

does not vanish at $(0, 0, 1)$ and $C = C^0$.

Case 1 was shown by Kochetov and Slawinski (6, p. 158). In fact, the Hessian was seen to be positive, which implies that the critical point in question is a minimum.

We consider Case 2. Using Maple to evaluate the partial derivatives at $(0, 0, 1)$ and $C = C^0$, we obtain

$$\frac{\partial^2 f}{\partial u^2} = 144(C_{14}^0)^2, \quad \frac{\partial^2 f}{\partial u \partial v} = 0, \quad \frac{\partial^2 f}{\partial v^2} = 4(22(C_{14}^0)^2 + P^T MP),$$

where

$$M = \begin{bmatrix}
3 & 0 & -1 & -2 & -3 \\
0 & 2 & 0 & -2 & -2 \\
-1 & 0 & 3 & -2 & 1 \\
-2 & -2 & -2 & 6 & 4 \\
-3 & -2 & 1 & 4 & 5
\end{bmatrix}, \quad (5.1)$$

and $P = [C_{11}^0 \ C_{33}^0 \ C_{12}^0 \ C_{13}^0 \ C_{44}^0]^T$. Therefore, the Hessian is

$$H = 576(C_{14}^0)^2(22(C_{14}^0)^2 + P^T MP).$$

Since matrix (5.1) is positive semidefinite, we have $H \geq 0$ and the vanishing of the Hessian requires $C_{14}^0 = 0$, which implies that $C^0$ is transversely isotropic with rotation axis $e_2$, a contradiction. Hence, $H > 0$, and the proof is complete.

**Remark 5.2** Theorem 5.1 holds if $C^0$ is a transversely isotropic tensor and $\mathbf{n}$ coincides with the rotation axis of $C^0$.  


5.2 Trigonal tensor

In this section, we discuss the problem of choosing the trigonal symmetry class as an effective symmetry class of a generally anisotropic elasticity tensor. Consider

$$C = \begin{bmatrix}
\end{bmatrix} \quad (5.2)$$

Figures 2 and 3 are plots of the monoclinic-distance function of $C$.

One can observe that the plot in Fig. 2 is close to a three-fold symmetry. Moreover, Fig. 3 contains three near-zero minima that are close to the plane that is perpendicular to what would be the three-fold symmetry axis. Moreover, unit vectors pointing to these minima are roughly 60° apart. In view of Theorem 5.1, these features suggest that the effective symmetry class of $C$ can be chosen as the trigonal symmetry. The orientations of the minima shown in Fig. 3 and the values of the monoclinic-distance function along those directions can be found using the code presented in (14). One seeks the minimum of the distance function in the neighbourhood of dark regions shown in Fig. 3 to get

$$v_1 = \left( \sin \frac{117.80238\pi}{180}, \cos \frac{102.09231\pi}{180}, \sin \frac{117.80238\pi}{180}, \sin \frac{102.09231\pi}{180}, \cos \frac{117.80238\pi}{180} \right),$$
$$v_2 = \left( \sin \frac{88.86122\pi}{180}, \cos \frac{157.12134\pi}{180}, \sin \frac{88.86122\pi}{180}, \sin \frac{157.12134\pi}{180}, \cos \frac{88.86122\pi}{180} \right),$$
$$v_3 = \left( \sin \frac{119.08658\pi}{180}, \cos \frac{33.08494\pi}{180}, \sin \frac{119.08658\pi}{180}, \sin \frac{33.08494\pi}{180}, \cos \frac{119.08658\pi}{180} \right).$$
where $v_1$ is in the middle of Fig. 3, $v_2$ is to the right of $v_1$ and $v_3$ is to the left of $v_1$. The angle between $v_1$ and $v_2$ is $58.285^\circ$ and between $v_1$ and $v_3$ is $69.015^\circ$. The values of the monoclinic-distance function in those directions are

$$d(\tilde{X}_1^T C \tilde{X}_1, \mathcal{L}_{\text{mono}}) = 24.53272,$$

where $X_1(e_3) = v_1$,

$$d(\tilde{X}_2^T C \tilde{X}_2, \mathcal{L}_{\text{mono}}) = 47.10467,$$

where $X_2(e_3) = v_2$,

$$d(\tilde{X}_3^T C \tilde{X}_3, \mathcal{L}_{\text{mono}}) = 74.03831,$$

where $X_3(e_3) = v_3$.

One can search for the absolute minimum of the trigonal distance function, $d(\tilde{X}_0^T C \tilde{X}_0, \mathcal{L}_{\text{trigo}})$, with $X$ such that $X(e_1)$ is close to $v_1$ and $X(e_3)$ is close to being normal to the plane spanned by $v_2$ and $v_3$. (Unlike the rotation axes of tetragonal, cubic and TI tensors, the rotation axis of the trigonal rotation tensor is not aligned with a normal of a mirror plane. Thus, there is no extremum along the would be three-fold rotation axis of $C$ in Fig. 2.) The search for the absolute minimum is done by the code shown in the Appendix, and results in $d(\tilde{X}_0^T C \tilde{X}_0, \mathcal{L}_{\text{trigo}}) = 97.18723$, where the Euler angles of $X_0$ are $\phi = 33.34485^\circ$, $\psi = 65.38897^\circ + 90^\circ$ and $\theta = 122.05007^\circ$. Hence, the effective trigonal elasticity tensor expressed in its natural coordinates can be found by, first, rotating the tensor $C$ to a coordinate system where its minimum is achieved, namely the Euler angles of $X_0$, and evaluating the closest trigonal tensor, by (4.8), in that coordinate system. We get

$$(X_0^T C X_0)^{\text{trigo}} = \begin{bmatrix}
58.00539 & 13.83418 & 3.00375 & 12.62102 & 0 & 0 \\
13.83418 & 58.00539 & 3.00375 & -12.62102 & 0 & 0 \\
3.00375 & 3.00375 & 24.30584 & 0 & 0 & 0 \\
12.62102 & -12.62102 & 0 & 8.75607 & 0 & 0 \\
0 & 0 & 0 & 0 & 8.75607 & 17.84882 \\
0 & 0 & 0 & 0 & 17.84882 & 44.17122
\end{bmatrix}.$$
5.3 Transversely isotropic and orthotropic tensors

In this section, we discuss the problem of choosing either the transversely isotropic symmetry class or the orthotropic symmetry class as the effective class of a given generally anisotropic elasticity tensor. The distinction between the two effective classes might depend on the required accuracy. Since the orthotropic group is a subgroup of the transversely isotropic group, we can view the effective TI tensor as a less accurate representation of the effective orthotropic tensor.

The symmetry group of a transversely isotropic tensor has one mirror plane whose normal is aligned with the rotation axis and infinitely many mirror planes whose normals are perpendicular to the rotation axis. Since the value of the monoclinic-distance function is zero along the normal of a mirror plane, the monoclinic-distance function plot for a TI tensor exhibits an equatorial plane, so that the distance to $L^{\text{mono}}$ is zero for any direction in that plane and along its normal. Thus, for a generally anisotropic elasticity tensor that is a small perturbation of a TI tensor, the plot of a monoclinic-distance function has an equatorial plane with values close to zero and a near-zero minimum close to the normal of that plane (Remark 5.2).

Consider

\[
C = \begin{bmatrix}
185.8183 & 59.8984 & 67.5846 & 0.4290 & 0.0272 & 0.0268 \\
59.8984 & 191.5953 & 64.2541 & -0.2710 & 0.8688 & -1.5136 \\
67.5846 & 64.2541 & 161.5560 & -0.2707 & -1.5353 & 0.8571 \\
0.4290 & -0.2710 & -0.2707 & 106.9964 & -1.6032 & -1.6301 \\
0.0272 & 0.8688 & -1.5353 & -1.6032 & 98.1860 & 0.1026 \\
0.0268 & -1.5136 & 0.8571 & -1.6301 & 0.1026 & 126.1984
\end{bmatrix}.
\]

(5.3)

Figure 4 contains the plot of the monoclinic-distance function of $C$, with an equatorial plane. Since the equatorial plane is between two contours, the distance function along that plane can take only values in a small, near-zero range.

Fig. 4  Plot of the monoclinic-distance function of $C$ given in matrix (5.3). Note the equatorial plane and the direction perpendicular to that plane. Dark shades of grey mean that the values are close to zero.
If we choose the TI symmetry class to approximate $C$, then the search for the absolute minimum of the TI-distance function among all orientations in $\mathbb{R}^3$ gives the closest TI tensor to $C$. One can plot the TI-distance function and make a search for the minimum guided by its plot. A code for plotting this distance function and searching for the minimum is given in (14). Figure 5 shows the plot of the distance function. The search results in the rotation axis $v = \left( \sin \frac{2.6915\pi}{180}, \cos \frac{10.000\pi}{180}, \sin \frac{2.6915\pi}{180}, \sin \frac{10.000\pi}{180}, \cos \frac{2.6915\pi}{180} \right)$.

Then, the orthogonal transformation matrix, $X_0$, that maps $e_3$ to $v$ has the Euler angles, $\phi = 2.6915^\circ$, $\psi = 10.000^\circ + 90^\circ$; $\theta$ can be set to zero since the TI-distance function does not depend on it. Hence, the effective TI tensor evaluated in that coordinate system can be found using (4.10) to get

$$ (X_0^T C X_0)^{\text{TI}} = \begin{bmatrix}
219.5173 & 28.9930 & 66.0139 & 0.0000 & 0.0000 & 0.0000 \\
28.9930 & 219.5173 & 66.0139 & 0.0000 & 0.0000 & 0.0000 \\
66.0139 & 66.0139 & 161.3675 & 0.0000 & 0.0000 & 0.0000 \\
0.0000 & 0.0000 & 0.0000 & 51.3374 & 0.0000 & 0.0000 \\
0.0000 & 0.0000 & 0.0000 & 0.0000 & 51.3374 & 0.0000 \\
0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 190.5243
\end{bmatrix}. $$

The squared distance of the elasticity tensor $\tilde{X}_0^T C \tilde{X}_0$ to $L^{\text{TI}}$ is $d(\tilde{X}_0^T C \tilde{X}_0, L^{\text{TI}}) = 87.5430$, which is the absolute minimum of the distance of $\tilde{X}_0^T C \tilde{X}$ to $L^{\text{TI}}$ among all $X \in SO(3)$.

The existence of an equatorial plane and a near-zero minimum close to the normal of that plane suggested the effective symmetry class to be TI. However, depending on the accuracy with which $C$ is known, one may choose a less symmetric class to approximate $C$.

Consider Fig. 6, which is the monoclinic plot of $C$ drawn with more contours than shown in Fig. 4. One of the features of the plot is the existence of three near-zero minima that are almost
perpendicular to each other. In view of Theorem 5.1, this suggests orthotropic symmetry. To facilitate the search for the orientation of the coordinate system where the orthotropic distance function achieves its absolute minimum, we may use the following theorem due to Diner (13).

**Theorem 5.3.** Let $C$ be an elasticity tensor. Let $R_{\frac{\pi}{2}, e_2}$ and $R_{\frac{\pi}{2}, e_1}$ denote the matrices of rotations by $\frac{\pi}{2}$ around $e_1$ and $e_2$. Then, the following equation holds:

$$d(C, L^{\text{ortho}}) = \frac{1}{2} \left( d(C, L^{\text{mono}}) + d \left( \tilde{R}_{\frac{\pi}{2}, e_1} C \tilde{R}_{\frac{\pi}{2}, e_1}, L^{\text{mono}} \right) + d \left( \tilde{R}_{\frac{\pi}{2}, e_2} C \tilde{R}_{\frac{\pi}{2}, e_2}, L^{\text{mono}} \right) \right).$$

The theorem states that the distance to orthotropic symmetry class is equal to the sum of the monoclinic-distances along the three perpendicular directions. Hence, in order to find the absolute minimum of the orthotropic distance function, $d(\tilde{X}^T C \tilde{X}, L^{\text{ortho}})$, one may restrict the search to $X$ that maps $e_1$, $e_2$ and $e_3$ to the neighbourhoods of the three minima of the monoclinic-distance function, namely, $v_1$, $v_2$ and $v_3$. A search guided by Fig. 6 results in

$$v_1 = \left( \frac{\sin 92.1252 \pi}{180}, \frac{\cos 9.9907 \pi}{180}, \frac{\sin 92.1252 \pi}{180}, \frac{\sin 9.9907 \pi}{180}, \frac{\cos 92.1252 \pi}{180} \right),$$
$$v_2 = \left( \frac{\sin 90.0003 \pi}{180}, \frac{\cos 99.9915 \pi}{180}, \frac{\sin 90.0003 \pi}{180}, \frac{\sin 99.9915 \pi}{180}, \frac{\cos 90.0003 \pi}{180} \right),$$
$$v_3 = \left( \frac{\sin 2.1252 \pi}{180}, \frac{\cos 10.0048 \pi}{180}, \frac{\sin 2.1252 \pi}{180}, \frac{\sin 10.0048 \pi}{180}, \frac{\cos 2.1252 \pi}{180} \right).$$

The values of the monoclinic-distance function in these directions are

$$d(\tilde{X}_1^T C \tilde{X}_1, L^{\text{mono}}) = 8.98037, \quad \text{where } X_1(e_3) = v_1,$$
$$d(\tilde{X}_2^T C \tilde{X}_2, L^{\text{mono}}) = 0.00000, \quad \text{where } X_2(e_3) = v_2,$$
$$d(\tilde{X}_3^T C \tilde{X}_3, L^{\text{mono}}) = 8.98034, \quad \text{where } X_3(e_3) = v_3.$$
The restricted search for the minimum of the orthotropic distance function results in \( d(\tilde{X}_0^TC\tilde{X}_0, L^{\text{ortho}}) = 8.9804 \), where the Euler angles of \( X_0 \) are \( \phi = 2.1252^\circ, \psi = 100.0028^\circ \) and \( \theta = -0.0117^\circ \). Hence, the effective orthotropic tensor expressed in its natural coordinates is

\[
(\tilde{X}_0^TC\tilde{X}_0)^{\text{ortho}} = \begin{bmatrix}
191.9780 & 59.6635 & 64.1847 & 0 & 0 & 0 \\
59.6635 & 185.7667 & 67.7993 & 0 & 0 & 0 \\
64.1847 & 67.7993 & 161.4039 & 0 & 0 & 0 \\
0 & 0 & 0 & 98.1199 & 0 & 0 \\
0 & 0 & 0 & 0 & 107.1766 & 0 \\
0 & 0 & 0 & 0 & 0 & 125.9062 
\end{bmatrix}.
\]

As expected, the absolute minimum of \( d(\tilde{X}^TC\tilde{X}, L^{\text{ortho}}) \) is less than the absolute minimum of \( d(\tilde{X}_2^TC\tilde{X}_2, L^{\text{TI}}) \). The vanishing of \( d(\tilde{X}_2^TC\tilde{X}_2, L^{\text{mono}}) \) means that \( C \) is, in fact, monoclinic.

6. Conclusions

Since Hookean solids exist only in mathematical formulations, their relation to seismic measurements can be achieved only as an approximation. Hence, no real material belongs to a given symmetry class of a Hookean solid, it can only be approximated by such a solid. The concept of distance in the space of elasticity tensors allows us to quantify this approximation.

The importance of considering a material symmetry is at least two-fold. First, these symmetries provide us with an insight into the materials, such as their laminations, layering or fractures. Secondly, we might be able to describe the material using simpler expressions without loss of accuracy. In many cases, the assumption of isotropy, whose description requires only 2 parameters, is sufficient, without invoking the 21 parameters of a generally anisotropic Hookean solid. The choice of a more or less symmetric tensor to represent the given material depends on accuracy available and required.

Prior to a quantitative analysis of finding the closest tensor, we qualitatively examine the plot of the monoclinic-distance function to choose the effective symmetry class. Notably, the example in section 5.3 was obtained by combining two transversely isotropic tensors whose rotation axes are oriented at \( 80^\circ \) to one another. Since the combination of two such tensors whose rotation axes are \( 90^\circ \) apart results in an orthotropic tensor, we expect our example to be close to orthotropic symmetry as indeed revealed by Fig. 6. In our example, one of the transversely isotropic summands was much greater in norm than the other one. For this reason, our tensor admits also a good TI approximation. Such a tensor could represent a structure of the subsurface; for instance, one TI summand could be due to layering and the other to fractures.

Once the effective symmetry class of a given tensor is chosen, the plot of the monoclinic-distance function allows us to guide the numerical search for the elasticity parameters of the effective tensor and the orientation of its natural coordinates, by virtue of Theorem 5.1 and, for the orthotropic symmetry, also Theorem 5.3, which does not require that the given tensor be a small perturbation of the orthotropic one.

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References

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APPENDIX A

Maple Codes: Finding the Minimum of Distance Functions

We introduce the Maple packages to be used in the code.

restart;
with(LinearAlgebra);
with(Optimization);

The rotation matrix that transforms e_3 to the new z-axis:

X(e_3) := Matrix([[cos(psi), -sin(psi), 0], [sin(psi), cos(psi), 0], [0, 0, 1]]).
Matrix([[1, 0, 0], [0, cos(phi), -sin(phi)], [0, sin(phi), cos(phi)]]);
The rotation matrix that transforms $e_1$ to the new $x$-axis:

$$X(e_1) := \text{Matrix}([[\cos(\theta), -\sin(\theta), 0], [\sin(\theta), 
\cos(\theta), 0], [0, 0, 1]]);$$

The rotation matrix that transforms the coordinate system:

$$X := X(e_3) \ast X(e_1)$$

Finding $\tilde{X} \in SO(6)$ from $X \in SO(3)$ that is going to act on elasticity tensor. Note that $\tilde{X}$ in the article is represented as $X_{\text{tilde}}$ in the code.

$$X_{\text{tilde}} := \text{simplify}(\text{Matrix}([[X[1, 1]^2, X[1, 2]^2, X[1, 3]^2, 
\sqrt{2} \ast X[1, 2] \ast X[1, 3], 
\sqrt{2} \ast X[1, 1] \ast X[1, 3], 
\sqrt{2} \ast X[1, 1] \ast X[1, 2]], 
[X[2, 1]^2, X[2, 2]^2, X[2, 3]^2, 
\sqrt{2} \ast X[2, 2] \ast X[2, 3], 
\sqrt{2} \ast X[2, 1] \ast X[2, 3], 
\sqrt{2} \ast X[2, 1] \ast X[2, 2]], 
[X[3, 1]^2, X[3, 2]^2, X[3, 3]^2, 
\sqrt{2} \ast X[3, 2] \ast X[3, 3], 
\sqrt{2} \ast X[3, 1] \ast X[3, 3], 
\sqrt{2} \ast X[3, 1] \ast X[3, 2]], 
[X[1, 2] \ast X[2, 1], X[1, 2] \ast X[2, 2], X[1, 2] \ast X[2, 3], X[1, 1] \ast X[2, 2], X[1, 1] \ast X[2, 3], X[1, 1] \ast X[2, 1]])\).$$

Introducing the elasticity matrix $C$ in its general form.

$$C := \text{Matrix}(6, \text{symbol} = c, \text{shape} = \text{symmetric});$$

This line is for changing the Voigt notation to the Kelvin notation. Herein, the entries of $C$ is expressed already in the Kelvin notation thus, we do not change anything. Otherwise, the first line should be multiplied by $\sqrt{2}$ and the second line by 2.

$$C[1 .. 3, 4 .. 6] := C[1 .. 3, 4 .. 6];$$
$$C[4 .. 6, 4 .. 6] := C[4 .. 6, 4 .. 6];$$

Introducing the parameters of elasticity matrix.

$$c := \text{Matrix}(6, 6, (1, 1) = 42.03357978, (1, 2) = 32.49305220, (1, 3) = 26.42291512, (1, 4) = 5.79953100, (1, 5) = 9.93816042, (1, 6) = 21.33549018, (2, 1) = 32.49305219, (2, 2) = 36.72218489, (2, 3) = 34.84774953, (2, 4) = -5.22166742, (2, 5) = -35.36967653, (2, 6) = -23.60019509, (3, 1) = 26.42291511, (3, 2) = 34.84774954, (3, 3) = 31.71680164, (3, 4) = 12.16688779, (3, 5) = 3.767088965,}$$
(3, 6) = 10.24209672, (4, 1) = 5.799531000, (4, 2) = -5.221667442,
(4, 3) = 12.84181099, (4, 4) = 20.98631307, (4, 5) = 20.98631307,
(4, 6) = 2.36291613, (5, 1) = 9.938160440, (5, 2) = -35.36967653,
(5, 3) = 3.767088965, (5, 4) = 20.98631308, (5, 5) = -22.64105584,
(5, 6) = -9.709913499, (6, 1) = 21.33549018, (6, 2) = -23.60019510,
(6, 3) = 10.24209672, (6, 4) = 2.36291613, (6, 5) = -9.709913499,
(6, 6) = 11.32667859).

Expressing the elasticity matrix $C$ in any coordinate system by rotating it with a generic orthogonal transformation that is introduced in the above lines.

$$R := \text{evalf}((\text{Transpose}(Xtilde).C.Xtilde);$$

Evaluating the trigonal-distance function, namely $d(\tilde{X}^T C \tilde{X}, L^{\text{trigo}})$. Note that in the code, we denote the trigonal distance function $d(\tilde{X}^T C \tilde{X}, L^{\text{mono}})$ by $\text{Dist-trigo}$.

$$\text{Dist-trigo} := \text{simplify}(2*(R_{16}^2+R_{26}^2+R_{15}^2+R_{25}^2+R_{34}^2+R_{36}^2+R_{45}^2+R_{46}^2+1/2(R_{11}-R_{22})^2+(R_{13}-R_{23})^2+(R_{14}+R_{24})^2+1/2(R_{44}-R_{55})^2+1/2(1/2R_{11}+1/2R_{12}-R_{12}-R_{66})^2+(1/\sqrt{2})R_{14}-(1/\sqrt{2})R_{24}-R_{56})^2);$$

To find a local minimum of the trigonal-distance function, observe dark regions on the plot. Read its orientation from the locator bar of the plot that gives the location of the minimum approximately. To find its exact location, search for the minimum in the neighbourhood of the approximate location:

$$\text{Min_data} := \text{Minimize}(\text{Dist-trigo},$$

phi = (40-20)*(1/180)*Pi .. (40+20)*(1/180)*Pi,
psi = (1/180)*(90-34-20)*Pi .. (1/180)*(90-34+20)*Pi,
theta = (1/180)*(128-20)*Pi .. (1/180)*(128+20)*Pi;