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**THE ISOTROPIC MATERIAL CLOSEST TO A
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The isotropic elastic moduli closest to a given anisotropic elasticity tensor are defined using three definitions of elastic distance: the standard Frobenius (Euclidean) norm, the Riemannian distance for tensors, and the log-Euclidean norm. The closest moduli are unique for the Riemannian and the log-Euclidean norms, independent of whether the difference in stiffness or compliance is considered. Explicit expressions for the closest bulk and shear moduli are presented for cubic materials, and an algorithm is described for finding them for materials with arbitrary anisotropy. The method is illustrated by application to a variety of materials, which are ranked according to their distance from isotropy.

1. Introduction

The objective here is to answer the question: what is the isotropic material closest to a given anisotropic material? In order to attempt an answer one needs a distance or length function which measures the difference between the elastic moduli of two materials. The Euclidean norm provides a natural definition for distance, and using it one can find the elastic tensor of a given symmetry nearest to an anisotropic elastic tensor [Gazis et al. 1963; Arts et al. 1991; Helbig 1996; Cavallini 1999; Gangi 2000; Browaeys and Chevrot 2004]. The Euclidean distance function is, however, not invariant under inversion, that is, considering compliance instead of stiffness, and as such does not lead to a unique answer to the question posed. To see this, let ΔC_{ijkl} and ΔS_{ijkl} be the elements of the fourth order tensors for the differences in elastic stiffness and compliance, respectively. Define the length of a fourth order tensor with elements T_{ijkl} by $(T_{ijkl}T_{ijkl})^{1/2}$. Then it is clear that the length using ΔC_{ijkl} is not simply related to that of ΔS_{ijkl} .

Recently and separately, Moakher [2006] and Arsigny et al. [2005] (see also [Matthies and Humbert 1995]) introduced two distance functions for elasticity tensors which are unchanged whether one uses stiffness or compliance. The two measures of elastic distances, called the Riemannian distance [Moakher 2006] and the log-Euclidean metric [Arsigny et al. 2005], each provide a means to define

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unambiguously the distance between any two elasticity tensors. The focus here is on finding the isotropic material closest to a given arbitrarily anisotropic material.

The distance functions are first reviewed in Section 2 along with the more common Frobenius or Euclidean norm. The theory is developed in terms of matrices, with obvious application to tensors. Preliminary results for elastic materials are presented in Section 4, where closed-form expressions are derived for the isotropic moduli closest to a given material of cubic symmetry. The general problem for materials of arbitrary anisotropy is solved in Section 5, and applications to sample materials are described in Section 6.

2. Matrix distance functions

We begin with $\mathcal{P}(n)$, the vector space of positive definite symmetric matrices in $\mathbb{M}^{n \times n}$, the space of $n \times n$ real matrices. Recall that a matrix \mathbf{P} is symmetric if $\mathbf{x}^T \mathbf{P} \mathbf{y} = \mathbf{y}^T \mathbf{P} \mathbf{x}$ for all \mathbf{x}, \mathbf{y} in \mathbb{R}^n , and positive definite if $\mathbf{x}^T \mathbf{P} \mathbf{x} > 0$ for all nonzero $\mathbf{x} \in \mathbb{R}^n$. The spectral decomposition is

$$\mathbf{P} = \sum_{i=1}^n \lambda_i \mathbf{v}_i \mathbf{v}_i^T, \quad (1)$$

where λ_i are the eigenvalues and $\mathbf{v}_i \in \mathbb{R}^n$ the eigenvectors, which satisfy $\lambda_i > 0$, $\mathbf{v}_i^T \mathbf{v}_j = \delta_{ij}$. Functions of \mathbf{P} can be readily found based on the diagonalized form; in particular, the logarithm of a matrix is defined as

$$\text{Log } \mathbf{P} = \sum_{i=1}^n \ln \lambda_i \mathbf{v}_i \mathbf{v}_i^T. \quad (2)$$

Three distinct metrics for positive definite symmetric matrices are considered: the conventional Euclidean or Frobenius metric d_F , the log-Euclidean distance d_L [Arsigny et al. 2005], and the Riemannian distance d_R [Moakher 2006]. Thus, for any pair $\mathbf{A}, \mathbf{B} \in \mathcal{P}(n)$

$$d_F(\mathbf{A}, \mathbf{B}) = \|\mathbf{A} - \mathbf{B}\|, \quad (3)$$

$$d_L(\mathbf{A}, \mathbf{B}) = \|\text{Log}(\mathbf{A}) - \text{Log}(\mathbf{B})\|, \quad (4)$$

$$d_R(\mathbf{A}, \mathbf{B}) = \|\text{Log}(\mathbf{A}^{-1/2} \mathbf{B} \mathbf{A}^{-1/2})\|, \quad (5)$$

where $\|\mathbf{M}\| \equiv [\text{tr}(\mathbf{M}^T \mathbf{M})]^{1/2}$ for any $\mathbf{M} \in \mathbb{M}^{n \times n}$. The distance function d_R is a consequence of the scalar product

$$\langle \mathbf{M}_1, \mathbf{M}_2 \rangle_{\mathbf{P}} \equiv \text{tr}(\mathbf{P}^{-1} \mathbf{M}_1 \mathbf{P}^{-1} \mathbf{M}_2), \quad (6)$$

for $\mathbf{P} \in \mathcal{P}(n)$ and symmetric $\mathbf{M}_1, \mathbf{M}_2 \in \mathbb{M}^{n \times n}$, and is also related to the exponential map [Lang 1998; Moakher 2006]. The metric d_L is associated with the Lie

group on $\mathcal{P}(n)$ defined by the following multiplication that preserves symmetry and positive definiteness [Arsigny et al. 2005] :

$$\mathbf{P}_1 \odot \mathbf{P}_2 \equiv \exp(\text{Log}(\mathbf{P}_1) + \text{Log}(\mathbf{P}_2)), \quad \mathbf{P}_1, \mathbf{P}_2 \in \mathcal{P}(n). \quad (7)$$

The three distance functions possess the properties expected of a distance function d :

- (i) it is symmetric with respect to its arguments, $d(\mathbf{A}, \mathbf{B}) = d(\mathbf{B}, \mathbf{A})$;
- (ii) it has nonnegative $d(\mathbf{A}, \mathbf{B}) \geq 0$ with equality if and only if $\mathbf{A} = \mathbf{B}$;
- (iii) it is invariant under a change of basis, $d(\mathbf{Q}\mathbf{A}\mathbf{Q}^T, \mathbf{Q}\mathbf{B}\mathbf{Q}^T) = d(\mathbf{A}, \mathbf{B})$ for all orthogonal $\mathbf{Q} \in \mathbb{M}^{n \times n}$, $\mathbf{Q}\mathbf{Q}^T = \mathbf{Q}^T\mathbf{Q} = \mathbf{I}$; and
- (iv) it satisfies the triangle inequality $d(\mathbf{A}, \mathbf{C}) \leq d(\mathbf{A}, \mathbf{B}) + d(\mathbf{B}, \mathbf{C})$ for all $\mathbf{A}, \mathbf{B}, \mathbf{C} \in \mathcal{P}(n)$.

The Riemannian and log-Euclidean distances have additional properties not shared with d_F :

$$d_{L,R}(a\mathbf{A}, a\mathbf{B}) = d_{L,R}(\mathbf{A}, \mathbf{B}), \quad a \in \mathbb{R}_+, \quad (8)$$

$$d_{L,R}(\mathbf{A}^b, \mathbf{B}^b) = |b| d_{L,R}(\mathbf{A}, \mathbf{B}), \quad b \in \mathbb{R}, \quad (9)$$

where $d_{L,R}$ signifies either d_L or d_R . Thus d_L and d_R are bi-invariant metrics, that is, distances are invariant under multiplication and inversion. This property makes them consistent and unambiguous metrics for elasticity tensors. Moakher [2006] introduced another bi-invariant distance function, the Kullback–Leibler metric, but it does not satisfy the triangle inequality, and we do not consider it here.

The distance function d_R can be expressed in alternative forms by using the property $\mathbf{B}(\text{Log } \mathbf{A})\mathbf{B}^{-1} = \text{Log}(\mathbf{B}\mathbf{A}\mathbf{B}^{-1})$, for example,

$$d_R(\mathbf{A}, \mathbf{B}) = [\text{tr } \text{Log}^2(\mathbf{A}^{-1}\mathbf{B})]^{1/2} = [\text{tr } \text{Log}^2(\mathbf{B}^{-1}\mathbf{A})]^{1/2}, \quad (10)$$

or in terms of eigenvalues, using Equations (2) and (5),

$$d_R(\mathbf{A}, \mathbf{B}) = \left[\sum_{i=1}^n (\ln \lambda_i)^2 \right]^{1/2}, \quad (11)$$

where $\lambda_i, i = 1, 2, \dots, n$ are the eigenvalues of $\mathbf{P} = \mathbf{A}^{-1/2}\mathbf{B}\mathbf{A}^{-1/2}$, or equivalently, of the matrices $\mathbf{A}^{-1}\mathbf{B}, \mathbf{B}^{-1}\mathbf{A}, \mathbf{A}\mathbf{B}^{-1}$, etc. Note that d_R also satisfies

$$d_R(\mathbf{S}\mathbf{A}\mathbf{S}^T, \mathbf{S}\mathbf{B}\mathbf{S}^T) = d_R(\mathbf{A}, \mathbf{B}), \quad \text{for all invertible } \mathbf{S} \in \mathbb{M}^{n \times n}. \quad (12)$$

3. Preliminary examples

The remainder of the paper is concerned with applications to elasticity, with $n = 6$.

3.1. Definition of elastic moduli. 6×6 symmetric matrices are used to describe elastic moduli, whether of stiffness or compliance. The matrix representation is based on Kelvin's [Thomson 1856] observation in 1856 that the twenty one coefficients of elasticity define a quadratic form (the energy) in the six strains, and therefore possess six "principal strains". Although Kelvin did not write the elasticity tensor explicitly as a symmetric positive definite matrix, the idea has proved useful and has been developed extensively, notably by Rychlewski [1984] and Mehrabadi and Cowin [1990]. The notation of Mehrabadi and Cowin is employed here. Thus, the matrix $\widehat{\mathbf{C}} \in \mathcal{P}(6)$ represents the elastic stiffness, and its inverse is the elastic compliance, $\widehat{\mathbf{S}}$, satisfying

$$\widehat{\mathbf{S}}\widehat{\mathbf{C}} = \widehat{\mathbf{C}}\widehat{\mathbf{S}} = \widehat{\mathbf{I}}, \quad \text{where } \widehat{\mathbf{I}} = \text{diag}(1, 1, 1, 1, 1, 1). \quad (13)$$

The elements of the elastic stiffness matrix are

$$\widehat{\mathbf{C}} = \begin{pmatrix} \hat{c}_{11} & \hat{c}_{12} & \hat{c}_{13} & \hat{c}_{14} & \hat{c}_{15} & \hat{c}_{16} \\ \hat{c}_{12} & \hat{c}_{22} & \hat{c}_{23} & \hat{c}_{24} & \hat{c}_{25} & \hat{c}_{26} \\ \hat{c}_{13} & \hat{c}_{23} & \hat{c}_{33} & \hat{c}_{34} & \hat{c}_{35} & \hat{c}_{36} \\ \hat{c}_{14} & \hat{c}_{24} & \hat{c}_{34} & \hat{c}_{44} & \hat{c}_{45} & \hat{c}_{46} \\ \hat{c}_{15} & \hat{c}_{25} & \hat{c}_{35} & \hat{c}_{45} & \hat{c}_{55} & \hat{c}_{56} \\ \hat{c}_{16} & \hat{c}_{26} & \hat{c}_{36} & \hat{c}_{46} & \hat{c}_{56} & \hat{c}_{66} \end{pmatrix} = \begin{pmatrix} c_{11} & c_{12} & c_{13} & \sqrt{2}c_{14} & \sqrt{2}c_{15} & \sqrt{2}c_{16} \\ c_{12} & c_{22} & c_{23} & \sqrt{2}c_{24} & \sqrt{2}c_{25} & \sqrt{2}c_{26} \\ c_{13} & c_{23} & c_{33} & \sqrt{2}c_{34} & \sqrt{2}c_{35} & \sqrt{2}c_{36} \\ \sqrt{2}c_{14} & \sqrt{2}c_{24} & \sqrt{2}c_{34} & 2c_{44} & 2c_{45} & 2c_{46} \\ \sqrt{2}c_{15} & \sqrt{2}c_{25} & \sqrt{2}c_{35} & 2c_{45} & 2c_{55} & 2c_{56} \\ \sqrt{2}c_{16} & \sqrt{2}c_{26} & \sqrt{2}c_{36} & 2c_{46} & 2c_{56} & 2c_{66} \end{pmatrix}, \quad (14)$$

where c_{ij} , $i, j = 1, 2, \dots, 6$ are the coefficients in the Voigt notation.

Before considering materials of arbitrary anisotropy, it is instructive to examine the distance functions for materials possessing the simplest type of anisotropy: cubic symmetry. Materials of cubic symmetry are described by three independent moduli: $c_{11} = c_{22} = c_{33}$, $c_{12} = c_{23} = c_{13}$, $c_{44} = c_{55} = c_{66}$, with the rest equal to zero. The three moduli commonly used are the bulk modulus κ and the two distinct shear moduli μ and η , which are related to the matrix elements by

$$3\kappa = \hat{c}_{11} + 2\hat{c}_{12}, \quad 2\mu = \hat{c}_{44}, \quad 2\eta = \hat{c}_{11} - \hat{c}_{12}. \quad (15)$$

Isotropic materials have only two independent moduli, κ , μ , and are of the same form as for cubic materials with the restriction $\hat{c}_{11} - \hat{c}_{12} - \hat{c}_{44} = 0$, or equivalently, $\eta = \mu$.

A concise notation is used for isotropic and cubic matrices, based upon Walpole's [Walpole 1984] general scheme for performing algebra with elasticity tensors. Define the matrices $\widehat{\mathbf{J}}$, $\widehat{\mathbf{K}}$, $\widehat{\mathbf{L}}$ and $\widehat{\mathbf{M}}$ by

$$\widehat{\mathbf{K}} = \widehat{\mathbf{I}} - \widehat{\mathbf{J}}, \quad \widehat{\mathbf{J}} = \mathbf{u}\mathbf{u}^T, \quad \text{where } \mathbf{u} = \left(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, 0, 0, 0 \right)^T, \quad (16)$$

$$\widehat{\mathbf{M}} = \widehat{\mathbf{K}} - \widehat{\mathbf{L}}, \quad \widehat{\mathbf{L}} = \text{diag}(0, 0, 0, 1, 1, 1). \quad (17)$$

Note that $\widehat{\mathbf{I}}$ and $\widehat{\mathbf{J}}$ correspond, respectively, to the fourth order isotropic symmetric tensors with components $I_{ijkl} = (\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})/2$ and $J_{ijkl} = (1/3)\delta_{ij}\delta_{kl}$. Elastic moduli of isotropic and cubic materials are of the generic form

$$\widehat{\mathbf{C}}_{\text{iso}}(3\kappa, 2\mu) \equiv 3\kappa \widehat{\mathbf{J}} + 2\mu \widehat{\mathbf{K}}, \quad \kappa, \mu > 0, \quad (18)$$

$$\widehat{\mathbf{C}}_{\text{cub}}(3\kappa, 2\mu, 2\eta) \equiv 3\kappa \widehat{\mathbf{J}} + 2\mu \widehat{\mathbf{L}} + 2\eta \widehat{\mathbf{M}}, \quad \kappa, \mu, \eta > 0. \quad (19)$$

The isotropic matrices $\{\widehat{\mathbf{J}}, \widehat{\mathbf{K}}\}$ are idempotent and their matrix product vanishes: $\widehat{\mathbf{J}}^2 = \widehat{\mathbf{J}}$, $\widehat{\mathbf{K}}^2 = \widehat{\mathbf{K}}$, $\widehat{\mathbf{J}}\widehat{\mathbf{K}} = \widehat{\mathbf{K}}\widehat{\mathbf{J}} = 0$. Similarly, it may be checked that the three basis matrices for cubic materials $\{\widehat{\mathbf{J}}, \widehat{\mathbf{L}}, \widehat{\mathbf{M}}\}$ are idempotent and have zero mutual products. The algebra of matrix multiplication for isotropic and cubic materials follows from these basic multiplication tables:

$$\begin{array}{c|cc} & \widehat{\mathbf{J}} & \widehat{\mathbf{K}} \\ \hline \widehat{\mathbf{J}} & \widehat{\mathbf{J}} & 0 \\ \widehat{\mathbf{K}} & 0 & \widehat{\mathbf{K}} \end{array} \quad \begin{array}{c|ccc} & \widehat{\mathbf{J}} & \widehat{\mathbf{L}} & \widehat{\mathbf{M}} \\ \hline \widehat{\mathbf{J}} & \widehat{\mathbf{J}} & 0 & 0 \\ \widehat{\mathbf{L}} & 0 & \widehat{\mathbf{L}} & 0 \\ \widehat{\mathbf{M}} & 0 & 0 & \widehat{\mathbf{M}} \end{array}.$$

Thus, the inverses are

$$\widehat{\mathbf{S}}_{\text{cub}} = \widehat{\mathbf{C}}_{\text{cub}}^{-1} = \widehat{\mathbf{C}}_{\text{cub}} \left(\frac{1}{3\kappa}, \frac{1}{2\mu}, \frac{1}{2\eta} \right), \quad \widehat{\mathbf{S}}_{\text{iso}} = \widehat{\mathbf{C}}_{\text{iso}} \left(\frac{1}{3\kappa}, \frac{1}{2\mu} \right),$$

and the products are

$$\widehat{\mathbf{C}}_{\text{iso}}^{-1}(3\kappa_1, 2\mu_1) \widehat{\mathbf{C}}_{\text{iso}}(3\kappa_2, 2\mu_2) \equiv \frac{\kappa_2}{\kappa_1} \widehat{\mathbf{J}} + \frac{\mu_2}{\mu_1} \widehat{\mathbf{K}}, \quad (20)$$

$$\widehat{\mathbf{C}}_{\text{cub}}^{-1}(3\kappa_1, 2\mu_1, 2\eta_1) \widehat{\mathbf{C}}_{\text{cub}}(3\kappa_2, 2\mu_2, 2\eta_2) \equiv \frac{\kappa_2}{\kappa_1} \widehat{\mathbf{J}} + \frac{\mu_2}{\mu_1} \widehat{\mathbf{L}} + \frac{\eta_2}{\eta_1} \widehat{\mathbf{M}}. \quad (21)$$

Results for isotropic materials follow from those for cubic with $\eta = \mu$. For the sake of simplicity and brevity we therefore focus on properties for cubic materials in the next subsection.

3.2. Elastic distance for cubic and isotropic materials. Consider two cubic materials with moduli $\widehat{\mathbf{C}}_1 = \widehat{\mathbf{C}}_{\text{cub}}(3\kappa_1, 2\mu_1, 2\eta_1)$ and $\widehat{\mathbf{C}}_2 = \widehat{\mathbf{C}}_{\text{cub}}(3\kappa_2, 2\mu_2, 2\eta_2)$. The Euclidean distance function of Equation (3) follows from the above properties

and the relations $\text{tr } \widehat{\mathbf{J}} = 1$, $\text{tr } \widehat{\mathbf{L}} = 3$, $\text{tr } \widehat{\mathbf{M}} = 2$. Similarly, the Riemannian and log-Euclidean distances follow from the identities

$$\text{Log}(\widehat{\mathbf{C}}_2) - \text{Log}(\widehat{\mathbf{C}}_1) = \text{Log} \widehat{\mathbf{C}}_1^{-1} \widehat{\mathbf{C}}_2 = \ln\left(\frac{\kappa_2}{\kappa_1}\right) \widehat{\mathbf{J}} + \ln\left(\frac{\mu_2}{\mu_1}\right) \widehat{\mathbf{L}} + \ln\left(\frac{\eta_2}{\eta_1}\right) \widehat{\mathbf{M}}. \quad (22)$$

Thus, the distances functions are

$$d_F(\widehat{\mathbf{C}}_1, \widehat{\mathbf{C}}_2) = [(3\kappa_1 - 3\kappa_2)^2 + 3(2\mu_1 - 2\mu_2)^2 + 2(2\eta_1 - 2\eta_2)^2]^{1/2}, \quad (23)$$

$$d_{L,R}(\widehat{\mathbf{C}}_1, \widehat{\mathbf{C}}_2) = \left[\left(\ln \frac{\kappa_2}{\kappa_1} \right)^2 + 3 \left(\ln \frac{\mu_2}{\mu_1} \right)^2 + 2 \left(\ln \frac{\eta_2}{\eta_1} \right)^2 \right]^{1/2}. \quad (24)$$

It is clear that d_L and d_R are invariant under inversion,

$$d_{L,R}(\widehat{\mathbf{S}}_1, \widehat{\mathbf{S}}_2) = d_{L,R}(\widehat{\mathbf{C}}_1, \widehat{\mathbf{C}}_2).$$

Note that the first identity in (22) is a consequence of the fact that $\widehat{\mathbf{C}}_1$ and $\widehat{\mathbf{C}}_2$ commute, which is not true in general for material symmetries lower than cubic.

What is the isotropic material closest to a given cubic material? The answer may be found by considering the distance functions between an arbitrary cubic stiffness $\widehat{\mathbf{C}}_{\text{cub}}(3\kappa, 2\mu, 2\eta)$ and the isotropic stiffness $\widehat{\mathbf{C}}_{\text{iso}}(3\kappa_*, 2\mu_*)$. The same question will also be considered for the compliances. Minimizing with respect to the isotropic moduli κ_* , μ_* yields

$$\min_{\kappa_*, \mu_*} d_{L,R}(\widehat{\mathbf{C}}_{\text{cub}}, \widehat{\mathbf{C}}_{\text{iso}}(3\kappa_*, 2\mu_*)) = \min_{\kappa_*, \mu_*} d_{L,R}(\widehat{\mathbf{S}}_{\text{cub}}, \widehat{\mathbf{S}}_{\text{iso}}) = \sqrt{\frac{6}{5}} \left| \ln \frac{\mu}{\eta} \right|, \quad (25)$$

$$\min_{\kappa_*, \mu_*} d_F(\widehat{\mathbf{C}}_{\text{cub}}, \widehat{\mathbf{C}}_{\text{iso}}(3\kappa_*, 2\mu_*)) = \sqrt{\frac{6}{5}} |2\mu - 2\eta|, \quad (26)$$

$$\min_{\kappa_*, \mu_*} d_F(\widehat{\mathbf{C}}_{\text{cub}}^{-1}, \widehat{\mathbf{C}}_{\text{iso}}^{-1}(3\kappa_*, 2\mu_*)) = \sqrt{\frac{6}{5}} \left| \frac{1}{2\mu} - \frac{1}{2\eta} \right|. \quad (27)$$

Denote the values of the closest isotropic moduli by (κ_L, μ_L) , (κ_R, μ_R) for d_L , d_R , and (κ_A, μ_A) or (κ_H, μ_H) for d_F depending on whether the stiffness (A) or its inverse (H) is used. Thus,

$$\kappa_{L,R,A,H} = \kappa, \quad \mu_{L,R} = (\mu^3 \eta^2)^{1/5}, \quad \mu_A = \frac{3}{5}\mu + \frac{2}{5}\eta, \quad \frac{1}{\mu_H} = \frac{3}{5\mu} + \frac{2}{5\eta}. \quad (28)$$

Equations (25) and (28) show clearly that the “closest” isotropic material using the Frobenius metric is ambiguous because it depends on whether one uses stiffness or compliance. Each gives a different isotropic material since $\mu_H < \mu_{L,R} < \mu_A$ for $\mu - \eta \neq 0$. The Riemannian and log-Euclidean metrics give the same unique “closest” isotropic material, regardless of whether the stiffness or the compliance is used. The fact that they agree is particular to the case of cubic symmetry, as noted above, and is not true in general.

In summary, the closest isotropic material to a given cubic material, in the sense of d_R and d_L , is defined by moduli

$$\kappa_R = \kappa_L = \frac{1}{3} (\hat{c}_{11} + 2\hat{c}_{12})$$

and

$$\mu_R = \mu_L = \frac{1}{2} [\hat{c}_{44}^3 (\hat{c}_{11} - \hat{c}_{12})^2]^{1/5},$$

and the distance from isotropy is

$$d_{L,R} = \sqrt{\frac{6}{5}} \left| \ln \frac{\hat{c}_{11} - \hat{c}_{12}}{\hat{c}_{44}} \right|.$$

These results will be generalized to materials of arbitrary anisotropy next.

4. Closest isotropic moduli

We now turn to the more general question of finding the isotropic material closest to a given anisotropic material characterized by $\hat{\mathbf{C}}$ or its inverse $\hat{\mathbf{S}}$. The solution using the Euclidean metric is relatively simple, and is considered first.

4.1. Minimum Frobenius distances. The closest isotropic elastic moduli are assumed to be of general isotropic form $\hat{\mathbf{C}}_{\text{iso}}(3\kappa, 2\mu)$; see Equations (18)–(19). The bulk and shear moduli are found by minimizing $d_F(\hat{\mathbf{C}}_{\text{iso}}, \hat{\mathbf{C}})$, which implies

$$3\kappa \operatorname{tr} \hat{\mathbf{J}} = \operatorname{tr} \hat{\mathbf{J}} \hat{\mathbf{C}}, \quad 2\mu \operatorname{tr} \hat{\mathbf{K}} = \operatorname{tr} \hat{\mathbf{K}} \hat{\mathbf{C}}. \quad (29)$$

Using suffix A to indicate that the minimization is in the arithmetic sense (in line with [Moakher 2006]),

$$\begin{aligned} 9\kappa_A &= \hat{c}_{11} + \hat{c}_{22} + \hat{c}_{33} + 2(\hat{c}_{23} + \hat{c}_{31} + \hat{c}_{12}), \\ 30\mu_A &= 2(\hat{c}_{11} + \hat{c}_{22} + \hat{c}_{33} - \hat{c}_{23} - \hat{c}_{31} - \hat{c}_{12}) + 3(\hat{c}_{44} + \hat{c}_{55} + \hat{c}_{66}), \end{aligned} \quad (30)$$

which are well known; see, for example, [Fedorov 1968]. Similarly, the closest isotropic elastic compliance can be determined by minimizing

$$d_F(\hat{\mathbf{C}}_{\text{iso}}^{-1}, \hat{\mathbf{C}}^{-1}).$$

Denoting the isotropic moduli with the suffix H for harmonic,

$$\begin{aligned} 1/\kappa_H &= \hat{s}_{11} + \hat{s}_{22} + \hat{s}_{33} + 2(\hat{s}_{23} + \hat{s}_{31} + \hat{s}_{12}), \\ 15/(2\mu_H) &= 2(\hat{s}_{11} + \hat{s}_{22} + \hat{s}_{33} - \hat{s}_{23} - \hat{s}_{31} - \hat{s}_{12}) + 3(\hat{s}_{44} + \hat{s}_{55} + \hat{s}_{66}). \end{aligned} \quad (31)$$

The Euclidean distance does not provide a unique closest isotropic material, although the values in Equations (30) and (31) are sometimes considered as bounds. Equations (29) and (30) also agree with the special case discussed above for cubic materials, Equation (28).

4.2. Minimum log-Euclidean distance. The isotropic elasticity $\widehat{\mathbf{C}}_{\text{iso}}(3\kappa_L, 2\mu_L)$ is found using the same methods as above by replacing $\widehat{\mathbf{C}}_{\text{iso}}$ and $\widehat{\mathbf{C}}$ with $\text{Log}(\widehat{\mathbf{C}}_{\text{iso}})$ and $\text{Log}(\widehat{\mathbf{C}})$, respectively. Thus,

$$\log(3\kappa_L) = \text{tr } \widehat{\mathbf{J}} \text{Log}(\widehat{\mathbf{C}}), \quad 5 \log(2\mu_L) = \text{tr } \widehat{\mathbf{K}} \text{Log}(\widehat{\mathbf{C}}). \quad (32)$$

Adding the two equations and using $\widehat{\mathbf{J}} + \widehat{\mathbf{K}} = \widehat{\mathbf{I}}$, implies the identity

$$\det(\widehat{\mathbf{C}}_{\text{iso}}) = \det(\widehat{\mathbf{C}}). \quad (33)$$

Thus, we have explicit formulae for the closest moduli,

$$\kappa_L = \frac{1}{3} \exp(\text{tr } \widehat{\mathbf{J}} \text{Log}(\widehat{\mathbf{C}})), \quad \mu_L = \frac{1}{2} \exp\left(\frac{1}{5} \text{tr } \widehat{\mathbf{K}} \text{Log}(\widehat{\mathbf{C}})\right). \quad (34)$$

4.3. The minimum Riemannian distance. We look for moduli of the form

$$\widehat{\mathbf{C}}_{\text{iso}}(3\kappa_R, 2\mu_R) = 3\kappa_R \widehat{\mathbf{J}} + 2\mu_R \widehat{\mathbf{K}}, \quad (35)$$

which minimize

$$d_R^2(\widehat{\mathbf{C}}_{\text{iso}}, \widehat{\mathbf{C}}) = \text{tr} [\text{Log}^2(\widehat{\mathbf{C}}_{\text{iso}}^{-1} \widehat{\mathbf{C}})]. \quad (36)$$

This is achieved using the following result (Proposition 2.1 of [Moakher 2005]) for any invertible matrix $\mathbf{X}(t)$ that does not have negative real-valued eigenvalues,

$$\frac{d}{dt} \text{tr} [\text{Log}^2 \mathbf{X}(t)] = 2 \text{tr} [\text{Log} \mathbf{X}(t) \mathbf{X}^{-1}(t) \frac{d}{dt} \mathbf{X}(t)]. \quad (37)$$

Differentiating (36) with respect to κ_R and μ_R separately, implies respectively

$$\text{tr} [\widehat{\mathbf{C}}_{\text{iso}}^{-1} \widehat{\mathbf{J}} \text{Log}(\widehat{\mathbf{C}}_{\text{iso}}^{-1} \widehat{\mathbf{C}})] = 0, \quad \text{tr} [\widehat{\mathbf{C}}_{\text{iso}}^{-1} \widehat{\mathbf{K}} \text{Log}(\widehat{\mathbf{C}}_{\text{iso}}^{-1} \widehat{\mathbf{C}})] = 0. \quad (38)$$

Further simplification yields

$$\text{tr} [\widehat{\mathbf{J}} \text{Log}(\widehat{\mathbf{C}}_{\text{iso}}^{-1} \widehat{\mathbf{C}})] = 0, \quad \text{tr} [\widehat{\mathbf{K}} \text{Log}(\widehat{\mathbf{C}}_{\text{iso}}^{-1} \widehat{\mathbf{C}})] = 0. \quad (39)$$

These conditions, which are necessary for a minimum, can be simplified as follows. Define the eigenvalues and associated eigenvectors by the diagonalization

$$\widehat{\mathbf{C}}_{\text{iso}}^{-1/2} \widehat{\mathbf{C}} \widehat{\mathbf{C}}_{\text{iso}}^{-1/2} = \sum_{i=1}^n \lambda_i \mathbf{v}_i \mathbf{v}_i^T. \quad (40)$$

Adding the two conditions (39) using the identity $\widehat{\mathbf{I}} = \widehat{\mathbf{J}} + \widehat{\mathbf{K}}$, along with the expression (2) for the logarithm of a matrix, yields

$$\prod_{i=1}^n \lambda_i = 1. \quad (41)$$

A second condition follows by direct substitution from (40) into the first of (39), giving

$$\prod_{i=1}^n \lambda_i^{\alpha_i} = 1, \quad \alpha_i \equiv \mathbf{v}_i^T \widehat{\mathbf{J}} \mathbf{v}_i, \quad i = 1, 2, \dots, n. \quad (42)$$

Note that $0 \leq \alpha_i \leq 1$ and α_i form a partition of unity,

$$\sum_{i=1}^n \alpha_i = 1. \quad (43)$$

This follows from the representation $\widehat{\mathbf{J}} = \mathbf{u}\mathbf{u}^T$ where the unit 6 vector \mathbf{u} is defined in Equation (16). Thus, the minimal isotropic moduli are found by satisfying the two simultaneous Equations (41) and (42). We now show how the first of these two conditions can be met, leaving one condition to satisfy.

Let

$$\widehat{\mathbf{C}}_{\text{iso}} = 3\kappa_R (\widehat{\mathbf{J}} + \rho^{-2} \widehat{\mathbf{K}}), \quad (44)$$

where $\rho \geq 0$ is defined by

$$\rho^2 = \frac{3\kappa_R}{2\mu_R} = \frac{1 + \nu_R}{1 - 2\nu_R}, \quad (45)$$

and ν_R is the Poisson's ratio of the minimizer. We choose this form for $\widehat{\mathbf{C}}_{\text{iso}}$ so that $\widehat{\mathbf{C}}_{\text{iso}}^{-1/2} = (3\kappa_R)^{-1/2} (\widehat{\mathbf{J}} + \rho \widehat{\mathbf{K}})$. Hence, the eigenvalues of (40) are of the form

$$\lambda_i = \frac{\bar{\lambda}_i(\rho)}{3\kappa_R}, \quad (46)$$

where the normalized eigenvectors $\bar{\lambda}_i = \bar{\lambda}_i(\rho)$ and the (unchanged) eigenvectors \mathbf{v}_i , $i = 1, 2, \dots, n = 6$ are defined by

$$3\kappa_R \widehat{\mathbf{C}}_{\text{iso}}^{-1/2} \widehat{\mathbf{C}} \widehat{\mathbf{C}}_{\text{iso}}^{-1/2} = (\widehat{\mathbf{J}} + \rho \widehat{\mathbf{K}}) \widehat{\mathbf{C}} (\widehat{\mathbf{J}} + \rho \widehat{\mathbf{K}}) = \sum_{i=1}^n \bar{\lambda}_i \mathbf{v}_i \mathbf{v}_i^T. \quad (47)$$

Turning to the first condition, (41), it is automatically satisfied if the bulk modulus is given by

$$3\kappa_R = \left(\prod_{i=1}^n \bar{\lambda}_i \right)^{1/n}. \quad (48)$$

It remains to determine ρ from the second stationary condition, Equation (42), which can be expressed in terms of the modified eigenvalues as

$$\prod_{i=1}^n \bar{\lambda}_i^{(\alpha_i - 1/n)} = 1. \quad (49)$$

Equation (49) involves the eigenvectors \mathbf{v} through the inner products α_i . However, α_i vanishes identically for eigenvectors of *deviatoric* form—in fact the definition of a deviatoric eigenvector is $\alpha_i = 0$ [Mehrabadi and Cowin 1990]. Conversely, $\alpha_i = 1$ for purely *dilatational* eigenvectors [Mehrabadi and Cowin 1990], that is, eigenvectors parallel to \mathbf{u} of Equation (16).

The solution to Equation (49) may be found numerically by searching for the zero over the permissible range for the Poisson's ratio: $-1 < \nu_R < 1/2$. The minimizing moduli κ_R and μ_R then follow from Equations (48) and (45), or more directly,

$$3\kappa_R = \rho^{5/3} (\det \widehat{\mathbf{C}})^{1/6}, \quad 2\mu_R = \rho^{-1/3} (\det \widehat{\mathbf{C}})^{1/6}, \quad (50)$$

and the minimal distance between $\widehat{\mathbf{C}}_{\text{iso}}$ and $\widehat{\mathbf{C}}$ is given by

$$d_R(\widehat{\mathbf{C}}_{\text{iso}}, \widehat{\mathbf{C}}) = \frac{1}{n} \left[\sum_{i=1}^n \ln^2 \left((\bar{\lambda}_i)^{-n} \prod_{j=1}^n \bar{\lambda}_j \right) \right]^{1/2} \quad (n = 6). \quad (51)$$

We next demonstrate the application of the above procedure to the case of a given elasticity matrix of cubic symmetry.

4.4. Example: cubic materials. By substituting the assumed form $\widehat{\mathbf{C}} = \widehat{\mathbf{C}}_{\text{cub}}$ from Equation (19) into the explicit formulae of Equation (34) for the closest moduli in the log-Euclidean sense, it is a straightforward matter to show that the latter reproduce the results determined directly, in Equation (28). Regarding the closest moduli using the Riemannian distance, the matrix in Equation (47) follows by using the algebra for cubic matrices,

$$(\widehat{\mathbf{J}} + \rho \widehat{\mathbf{K}}) \widehat{\mathbf{C}} (\rho \widehat{\mathbf{J}} + \widehat{\mathbf{K}}) = 3\kappa \widehat{\mathbf{J}} + 2\mu\rho^2 \widehat{\mathbf{L}} + 2\eta\rho^2 \widehat{\mathbf{M}}. \quad (52)$$

Thus, $\bar{\lambda}_1 = 3\kappa$, $\bar{\lambda}_2 = \bar{\lambda}_3 = \bar{\lambda}_4 = 2\mu\rho^2$, $\bar{\lambda}_5 = \bar{\lambda}_6 = 2\eta\rho^2$, and the eigenvectors are either pure dilatational ($\alpha_1 = 1$) or deviatoric ($\alpha_i = 0$, $i = 2, 3, \dots, 6$). Therefore, Equation (49) becomes

$$(3\kappa)^{5/6} (2\mu)^{-1/2} (2\eta)^{-1/3} \rho^{-5/3} = 1. \quad (53)$$

Solving for the intermediate variable ρ , and evaluating μ_R and κ_R from Equations (48) and (45), respectively, gives $\kappa_R = \kappa$ and $\mu_R = (\mu^3 \eta^2)^{1/5}$, again in agreement with Equation (28).

5. Applications and discussion

Table 1 lists the computed distance from isotropy of various anisotropic materials, using data from Musgrave [2003]. Materials of cubic (cub), hexagonal (hex), tetragonal (tet) and orthotropic (ort) symmetry are considered. In each case the

moduli of the closest isotropic material were found using the algorithm described above. The resulting bulk modulus κ_R and Poisson’s ratio ν_R are tabulated.

Table 1 ranks the materials in terms of the Riemannian distance d_R of the original anisotropic moduli from the closest isotropic material. The second column of numbers lists the distance between the closest isotropic materials found using the Riemannian and log-Euclidean distances. That is,

$$\begin{aligned}
 d_{LR} &\equiv d_{L,R}(\widehat{\mathbf{C}}_{\text{iso}}(3\kappa_R, 2\mu_R), \widehat{\mathbf{C}}_{\text{iso}}(3\kappa_L, 2\mu_L)) \\
 &= \left[\left(\ln \frac{\kappa_L}{\kappa_R} \right)^2 + 5 \left(\ln \frac{\mu_L}{\mu_R} \right)^2 \right]^{1/2}, \tag{54}
 \end{aligned}$$

which is identically zero for cubic materials. The arithmetic (κ_A, μ_A) and harmonic (κ_H, μ_H) moduli minimizing the Euclidean distances were also computed, and the Riemannian distance between these two is denoted d_{HA} . The distances d_{RA} and d_{RH} are the distances between the closest isotropic material (κ_R, μ_R) and the arithmetic and harmonic isotropic approximants, respectively. All distances listed in Table 1 are based on the Riemannian metric.

Note that the distance between the closest materials using d_R and d_L is less than 0.05 except for the extremely anisotropic spruce. In order to gain some appreciation for the magnitude of the nondimensional distances in Table 1, consider the distance of any $\mathbf{P} \in \mathcal{P}(n)$ from a multiple of itself:

$$d_R(\mathbf{P}, a\mathbf{P}) = d_L(\mathbf{P}, a\mathbf{P}) = \sqrt{n} |\log a|, \quad a \in \mathbb{R}_+. \tag{55}$$

Small values of the elastic distance can be identified with values of a close to unity, specifically

$$a = 1 \pm \frac{1}{\sqrt{6}} d_{L,R} + O(d_{L,R}^2) \approx 1 \pm 0.4 d_{L,R}. \tag{56}$$

Note that the distance d_{HA} between the arithmetic and harmonic approximations is generally less than the distance from isotropy d_R . This is more so for those materials that are closer to isotropy—at the top of Table 1. As the material gets further from isotropy - the lower half of Table 1—the magnitude of d_{HA} relative to d_R grows as the latter increases. The two distances are of comparable magnitude for the highly anisotropic materials at the very bottom of the table, such as oak and spruce.

As a numerical check on the computations, the triangle inequality

$$d_{HA} \leq d_{RA} + d_{RH} \tag{57}$$

Material	Symm	d_R	$100d_{LR}$	d_{RA}	d_{RH}	d_{HA}	ν_R	κ_R
magnesium	hex	0.18	0.00	0.01	0.01	0.02	0.29	3.53
diamond	cub	0.21	0	0.01	0.01	0.02	0.07	44.20
aluminum	cub	0.21	0	0.01	0.01	0.02	0.35	7.69
beryllium	hex	0.22	0.01	0.01	0.01	0.02	0.05	11.44
sodium fluoride	cub	0.29	0	0.02	0.02	0.04	0.24	4.86
ice (H ₂ O) 257°K	hex	0.31	0.00	0.02	0.02	0.04	0.33	0.89
β -quartz (SiO ₂)	hex	0.35	0.02	0.03	0.03	0.05	0.21	5.64
beryllium	hex	0.37	0.23	0.03	0.03	0.06	0.26	14.41
caesium iodide	cub	0.37	0	0.03	0.03	0.06	0.27	1.29
sodium chloride	cub	0.40	0	0.04	0.03	0.07	0.25	2.45
sodium iodide	cub	0.43	0	0.04	0.04	0.08	0.25	1.46
sodium bromide	cub	0.44	0	0.04	0.04	0.09	0.25	1.94
caesium bromide	cub	0.45	0	0.05	0.04	0.09	0.27	1.59
silicon	cub	0.49	0	0.05	0.05	0.11	0.22	9.78
cobalt	hex	0.51	0.00	0.07	0.05	0.12	0.31	19.03
silver bromide	cub	0.52	0	0.06	0.06	0.12	0.40	4.06
germanium	cub	0.56	0	0.07	0.07	0.14	0.21	7.52
caesium chloride	cub	0.58	0	0.08	0.07	0.15	0.27	1.83
gallium antimonide	cub	0.64	0	0.09	0.10	0.18	0.25	5.64
α -uranium	ort	0.68	0.37	0.10	0.10	0.20	0.20	11.28
silver chloride	cub	0.70	0	0.11	0.10	0.22	0.41	4.42
apatite	hex	0.72	0.11	0.10	0.13	0.22	0.21	8.43
indium antimonide	cub	0.75	0	0.12	0.13	0.25	0.29	4.69
potassium fluoride	cub	0.75	0	0.13	0.12	0.25	0.28	3.19
benzophenone	ort	0.85	1.92	0.15	0.14	0.29	0.30	5.14
zircon	tet	0.98	0.74	0.21	0.18	0.39	0.13	1.99
sulphur	ort	0.98	4.13	0.20	0.18	0.39	0.34	1.88
iron	cub	0.99	0	0.20	0.23	0.43	0.30	17.05
nickel	cub	1.01	0	0.21	0.23	0.44	0.29	18.04
cadmium	hex	1.04	3.43	0.20	0.24	0.44	0.30	5.40
rutile (TiO ₂)	tet	1.07	0.79	0.21	0.28	0.49	0.27	21.49
potassium chloride	cub	1.08	0	0.27	0.24	0.50	0.28	1.78
barium titanate	tet	1.13	3.20	0.26	0.27	0.52	0.36	17.67
potassium bromide	cub	1.14	0	0.30	0.26	0.56	0.29	1.58
gold	cub	1.16	0	0.27	0.31	0.58	0.42	17.28
Rochelle salt	ort	1.17	0.97	0.24	0.34	0.59	0.31	1.97
zinc	hex	1.18	2.58	0.24	0.34	0.57	0.24	6.61
white tin	tet	1.18	0.04	0.24	0.38	0.62	0.35	5.50
ammon. dihyd. phos.	tet	1.19	0.95	0.36	0.25	0.61	0.33	2.70
silver	cub	1.21	0	0.29	0.33	0.63	0.37	10.36
potassium iodide	cub	1.25	0	0.36	0.31	0.67	0.30	1.20
copper	cub	1.28	0	0.32	0.37	0.70	0.35	13.71
potass. dihyd. phos.	tet	1.34	0.01	0.40	0.38	0.78	0.26	2.67
α -brass	cub	1.46	0	0.41	0.48	0.90	0.34	11.96
indium	tet	1.57	0.01	0.50	0.54	1.04	0.44	4.16
oak	ort	2.30	1.75	0.96	1.09	2.05	0.08	0.17
β -brass	cub	2.34	0	0.94	1.19	2.13	0.36	11.62
spruce	ort	5.66	59.5	7.16	3.33	10.45	0.23	0.09

Table 1. Distance from isotropy for some materials - data from [Musgrave 2003]. κ_R units 10^{10} N/m².

was confirmed for each material in Table 1. Since the three vertices of the triangle are isotropic materials, the inequality may be written, using (24), as

$$\begin{aligned} & \left[\left(\ln \frac{\kappa_A}{\kappa_H} \right)^2 + 5 \left(\ln \frac{\mu_A}{\mu_H} \right)^2 \right]^{1/2} \\ & \leq \left[\left(\ln \frac{\kappa_A}{\kappa_R} \right)^2 + 5 \left(\ln \frac{\mu_A}{\mu_R} \right)^2 \right]^{1/2} + \left[\left(\ln \frac{\kappa_R}{\kappa_H} \right)^2 + 5 \left(\ln \frac{\mu_R}{\mu_H} \right)^2 \right]^{1/2}. \end{aligned} \quad (58)$$

For cubic materials $\kappa_A = \kappa_H = \kappa_R$, and consequently the triangle is a straight line:

$$d_{HA} = d_{RA} + d_{RH} \quad \text{for cubic materials only.} \quad (59)$$

The quantity $(d_{RA} + d_{RH} - d_{HA})/d_{HA}$ was found to be very small for all the cases considered (and numerically zero for the cubic examples), less than 10^{-3} for all materials considered except barium titanate (1.2×10^{-3}) and spruce (2.8×10^{-3}). The “triangle” is almost flat, indicating that the closest moduli (κ_R, μ_R) are in some sense optimally centered between the arithmetic and harmonic approximations. Note however, that κ_R, μ_R are not equal to the Riemannian mean [Moakher 2006] of the arithmetic and harmonic approximations, denoted as κ_{AH}, μ_{AH} . The Riemannian mean of two elasticity matrices \widehat{C}_1 and \widehat{C}_2 is $\widehat{C}_1 (\widehat{C}_1^{-1} \widehat{C}_2)^{1/2}$ [Moakher 2006], and consequently the means of the arithmetic and harmonic moduli are $\kappa_{AH} = (\kappa_A \kappa_H)^{1/2}$, $\mu_{AH} = (\mu_A \mu_H)^{1/2}$. By considering the case of cubic materials, for which all these quantities have explicit expressions, it may be shown that $(\mu_R - \mu_{AH})(\eta - \mu) > 0$ for $\eta - \mu \neq 0$.

6. Conclusions

We have presented a method for finding the isotropic elastic moduli closest to a given material of arbitrary symmetry based on three different metrics. Unlike the Frobenius (Euclidean) distance, the Riemannian and log-Euclidean metrics provide unique isotropic moduli. The values obtained according to these two metrics are identical if the comparison medium has cubic symmetry, and are otherwise relatively close. The procedures developed here for finding the closest isotropic moduli can be generalized to find the closest material of lower symmetry. The solution for cubic symmetry with the cube axes given is presented in the Appendix, and other, lower symmetries will be considered elsewhere. Another generalization of the present problem is that of determining the closest material of cubic or lower symmetry where the symmetry axes are unrestrained. These and other challenging questions make this an interesting topic for some time to come.

Appendix: The closest cubic material

The cubic stiffness (compliance) closest to $\widehat{\mathbf{C}}(\widehat{\mathbf{S}})$ in the Euclidean metric d_F has moduli κ_A, μ_A, η_A (κ_H, μ_H and η_H), where κ_A and κ_H are given by Equations (30) and (31), and

$$6\mu_A = \hat{c}_{44} + \hat{c}_{55} + \hat{c}_{66}, \quad 6\eta_A = \hat{c}_{11} + \hat{c}_{22} + \hat{c}_{33} - \hat{c}_{23} - \hat{c}_{31} - \hat{c}_{12}, \quad (\text{A.1})$$

$$\frac{3}{2\mu_H} = \hat{s}_{44} + \hat{s}_{55} + \hat{s}_{66}, \quad \frac{3}{2\eta_H} = \hat{s}_{11} + \hat{s}_{22} + \hat{s}_{33} - \hat{s}_{23} - \hat{s}_{31} - \hat{s}_{12}. \quad (\text{A.2})$$

Using the method for deriving Equation (34), we find the following for the log-Euclidean distance,

$$\begin{aligned} \kappa_L &= \frac{1}{3} \exp(\text{tr } \widehat{\mathbf{J}} \text{Log}(\widehat{\mathbf{C}})), \\ \mu_L &= \frac{1}{2} \exp\left(\frac{1}{3} \text{tr } \widehat{\mathbf{L}} \text{Log}(\widehat{\mathbf{C}})\right), \\ \eta_L &= \frac{1}{2} \exp\left(\frac{1}{2} \text{tr } \widehat{\mathbf{M}} \text{Log}(\widehat{\mathbf{C}})\right). \end{aligned} \quad (\text{A.3})$$

Note the identity, similar to Equation (33),

$$\det(\widehat{\mathbf{C}}_{\text{cub}}) = \det(\widehat{\mathbf{C}}). \quad (\text{A.4})$$

For the Riemannian distance d_R we find that the closest cubic material $\widehat{\mathbf{C}}_{\text{cub}}$ of the form Equation (19) is determined by three equations:

$$\prod_{i=1}^n \lambda_i = 1, \quad \prod_{i=1}^n \lambda_i^{\alpha_i} = 1, \quad \prod_{i=1}^n \lambda_i^{\beta_i} = 1, \quad (\text{A.5})$$

where

$$\alpha_i \equiv \mathbf{v}_i^T \widehat{\mathbf{J}} \mathbf{v}_i, \quad \beta_i \equiv \mathbf{v}_i^T \widehat{\mathbf{L}} \mathbf{v}_i, \quad i = 1, 2, \dots, n, \quad (\text{A.6})$$

and $\{\lambda_i, \mathbf{v}_i\}$ are the eigenvalues and eigenvectors of

$$\widehat{\mathbf{C}}_{\text{cub}}^{-1/2} \widehat{\mathbf{C}} \widehat{\mathbf{C}}_{\text{cub}}^{-1/2}.$$

The parameters α_i satisfy the same properties as before, including the fact that they sum to unity. Since $\{\mathbf{v}_i\}$ form an orthonormal basis, it follows that

$$\sum_{i=1}^n \beta_i = \dim \widehat{\mathbf{L}} = 3.$$

Furthermore, $\beta_i = 0$ if the eigenvector is dilatational. The three equations (A.5) may be reduced to two by assuming the unknown moduli are of the form

$$\widehat{\mathbf{C}}_{\text{cub}} = 3\kappa_R (\widehat{\mathbf{J}} + \rho_1^{-2} \widehat{\mathbf{L}} + \rho_2^{-2} \widehat{\mathbf{M}}).$$

Define the modified eigenvalues $\bar{\lambda}_i = \bar{\lambda}_i(\rho_1, \rho_2)$ to be the eigenvalues of

$$(\hat{\mathbf{J}} + \rho_1 \hat{\mathbf{L}} + \rho_2 \hat{\mathbf{M}}) \hat{\mathbf{C}} (\hat{\mathbf{J}} + \rho_1 \hat{\mathbf{L}} + \rho_2 \hat{\mathbf{M}}),$$

then κ_R is given by the formula (48), while ρ_1, ρ_1 solve the simultaneous equations

$$\prod_{i=1}^n \bar{\lambda}_i^{(\alpha_i-1/n)} = 1, \quad \prod_{i=1}^n \bar{\lambda}_i^{(\beta_i-1/n)} = 1. \quad (\text{A.7})$$

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