Shape Derivatives for Functions of Homogenized Elasticity Tensors

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We compute the shape derivative of a homogenized elasticity tensor and show how it can be used to optimize various objective functions.

Recall from the periodic homogenization writeup that each component of homogenized elasticity tensor for a microstructure ω in unit cell Y can be written as an energy-like integral involving the fluctuation displacements, $\mathbf{w}^{ij}$:

$$C^H_{ijkl} = \frac{1}{|Y|}\int_\omega (e^{ij} + e(\mathbf{w}^{ij})) : C : (e^{kl} + e(\mathbf{w}^{kl}))\,\mathrm{d}\mathbf{y}. \tag{1}$$

where the fluctuation displacements solve the cell problem:

$$\begin{aligned} -\nabla\cdot(C : [e^{ij} + e(\mathbf{w}^{ij})]) &= \mathbf{0} \quad \text{in } \omega \\ \hat{\mathbf{n}}\cdot(C : [e^{ij} + e(\mathbf{w}^{ij})]) &= \mathbf{0} \quad \text{on } \partial\omega \setminus \partial Y \\ \mathbf{w}^{ij}(\mathbf{y})\ &Y\text{-periodic} \\ \int_\omega \mathbf{w}^{ij}(\mathbf{y})\,\mathrm{d}\mathbf{y} &= \mathbf{0} \end{aligned} \tag{2}$$

for each of the 6 (3 in 2D), constant strain basis tensors e^{ij}.

1 Shape Derivative of C^H_{ijkl}

Because energy functionals are self-adjoint, the shape derivative of (1) turns out to be surprisingly simple. We start by computing the change in C^H_{ijkl} caused by an arbitrary boundary perturbation, then give the result for parametrized microstructure boundaries.

1.1 Arbitrary Boundary Perturbations

Consider a perturbation of the shape's boundary, $\delta\omega$, caused by advecting the boundary with an infinitesimal velocity field $\mathbf{v}$. The resulting variation of C^H_{ijkl} for $ij \neq kl$ ($ij = kl$ gets an identical final result by product rule) is:

$$\delta C^H_{ijkl} = \left\langle \frac{\partial C^H_{ijkl}}{\partial\omega}, \delta\omega \right\rangle + \left\langle \frac{\partial C^H_{ijkl}}{\partial\mathbf{w}^{ij}}, \delta\mathbf{w}^{ij} \right\rangle + \left\langle \frac{\partial C^H_{ijkl}}{\partial\mathbf{w}^{kl}}, \delta\mathbf{w}^{kl} \right\rangle.$$

Consider the linear functional $\left\langle \frac{\partial C^H_{ijkl}}{\partial\mathbf{w}^{ij}}, \cdot \right\rangle$ on an arbitrary admissible perturbation of $\mathbf{w}^{ij}$ (i.e. periodic and with no rigid translation component), ϕ:

$$\left\langle \frac{\partial C^H_{ijkl}}{\partial\mathbf{w}^{ij}}, \phi \right\rangle = \lim_{h\to 0} \frac{\mathrm{d}}{\mathrm{d}h}\frac{1}{|Y|}\int_\omega (e^{ij} + e(\mathbf{w}^{ij} + h\phi)) : C : (e^{kl} + e(\mathbf{w}^{kl}))\,\mathrm{d}\mathbf{y}$$

Differentiating under the integral and using the linearity of strain, this is:

$$\left\langle \frac{\partial C^H_{ijkl}}{\partial\mathbf{w}^{ij}}, \phi \right\rangle = \frac{1}{|Y|}\int_\omega e(\phi) : C : (e^{kl} + e(\mathbf{w}^{kl}))\,\mathrm{d}\mathbf{y}$$

Then, integrating by parts to move the strain off ϕ:

$$\left\langle \frac{\partial C^H_{ijkl}}{\partial \mathbf{w}^{ij}}, \phi \right\rangle = -\frac{1}{|Y|}\int_\omega \phi \cdot \left(\nabla \cdot \left[C : (e^{kl} + e(\mathbf{w}^{kl}))\right]\right) \mathrm{d}\mathbf{y} + \frac{1}{|Y|}\int_{\partial\omega} \phi \cdot \left(\hat{\mathbf{n}} \cdot \left[C : (e^{kl} + e(\mathbf{w}^{kl}))\right]\right) \mathrm{d}\mathbf{y}$$

The volume integral vanishes because $\mathbf{w}^{kl}$ solves the kl^{th} cell problem. The $\partial\omega \setminus \partial Y$ portion of the surface integral vanishes for the same reason, and the $\partial\omega \cap \partial Y$ portion vanishes because ϕ, C, e^{kl}, and $e(\mathbf{w}^{kl})$ are all either constant or periodic. The same argument holds for $\left\langle \frac{\partial C^H_{ijkl}}{\partial \mathbf{w}^{kl}}, \phi \right\rangle$, so we have

$$\left\langle \frac{\partial C^H_{ijkl}}{\partial \mathbf{w}^{ij}}, \phi \right\rangle = \left\langle \frac{\partial C^H_{ijkl}}{\partial \mathbf{w}^{kl}}, \phi \right\rangle = 0$$

without solving any adjoint problem! Thus Reynold's transport theorem gives the full shape derivative:

$$\dot{C}^H_{ijkl}[\mathbf{v}] := \delta C^H_{ijkl} = \left\langle \frac{\partial C^H_{ijkl}}{\partial \omega}, \delta\omega \right\rangle = \boxed{\frac{1}{|Y|}\int_{\partial\omega} \left[(e^{ij} + e(\mathbf{w}^{ij})) : C : (e^{kl} + e(\mathbf{w}^{kl}))\right] \mathbf{v} \cdot \hat{\mathbf{n}}\, \mathrm{d}A(\mathbf{y}).}$$

1.2 Parametrized Boundary Perturbations

In our setting, the microstructure boundary $\partial\omega$ is parametrized by a vector $\mathbf{p}$, consisting of e.g. wire mesh node offsets and thicknesses. This parametrization is smooth in the sense that we can define parameter velocity fields $\mathbf{v}_{p_i}(\mathbf{y}, \mathbf{p})$ at almost all points $\mathbf{y} \in \partial\omega(\mathbf{p}) \setminus \partial Y$. These velocity fields give how the point $\mathbf{y}$ moves to stay on the boundary as p_a changes. The derivative of C^H_{ijkl} with respect to parameter p_a is just $\dot{C}^H_{ijkl}$ evaluated on the $\mathbf{v}_{p_a}$ velocity field:

$$\frac{\partial C^H_{ijkl}}{\partial p_a} = \frac{1}{|Y|}\int_{\partial\omega} \left[(e^{ij} + e(\mathbf{w}^{ij})) : C : (e^{kl} + e(\mathbf{w}^{kl}))\right] \mathbf{v}_{p_a} \cdot \hat{\mathbf{n}}\, \mathrm{d}A(\mathbf{y}). \tag{3}$$

Thus, we can compute the derivative of each homogenized coefficient with respect to each parameter p_a provided that we know the normal velocity scalar field induced by changing p_a, $\hat{\mathbf{n}} \cdot \mathbf{v}_{p_a}$.

1.3 Discretization

If linear finite elements are used, (3) is particularly easy to compute; the energy density term $(e^{ij} + e(\mathbf{w}^{ij})) : C : (e^{kl} + e(\mathbf{w}^{kl}))$ is constant on each boundary element and can be stored as a per-boundary-element tensor C^e_{ijkl}. Then the integral can be computed as:

$$\frac{\partial C^H_{ijkl}}{\partial p_a} = \sum_e \frac{1}{|Y|} C^e_{ijkl} \int_e \mathbf{v}_{p_a} \cdot \hat{\mathbf{n}}\, \mathrm{d}A(\mathbf{y}) := \frac{1}{|Y|} C^e_{ijkl} v^e,$$

where v^e is the integral of parameter p_a's (linear) normal velocity field over boundary element e. In other words, computing how a particular C_{ijkl} changes with respect to p_a is just a dot product.

If higher order elements are used, we can still use this trick if we approximate either the energy density term or the normal velocity field as piecewise constant. However, to compute the integral exactly requires quadrature over each boundary element.

2 Objective Functions

2.1 Elasticity Tensor Fit

The simplest objective function is the squared Frobenius norm distance to a target tensor C^*:

$$J_C = \frac{1}{2}||C^H - C^*||_F^2 = \frac{1}{2}\left[C^H - C^*\right]_{ijkl}\left[C^H - C^*\right]_{ijkl}$$

Then

$$\frac{\partial J_C}{\partial p_a} = \left[C^H - C^*\right]_{ijkl} \frac{\partial C^H_{ijkl}}{\partial p_a}.$$

Unfortunately, as discussed in the "Objectives for Pattern Parameter Optimization" writeup, this objective is poorly behaved. A better one uses the compliance tensor, $S = C^{-1}$, or some function of it's entries (e.g. Young's modulus, Poisson ratio).

2.2 Compliance Tensor Fit

Inverting rank 4 tensors requires a bit more than just inverting the flattened tensor representation; see the "Tensor Flattening" writeup for the details. But following the formula there, we can differentiate the inverted tensor $S = C^{-1}$:

$$\begin{aligned}
F(C:S) = F(I) \quad &\Longrightarrow \\
F(C)\mathscr{D}F(S) = \mathscr{D}^{-1} \quad &\Longrightarrow \\
\frac{\partial}{\partial p_a}\left[F(C)\mathscr{D}F(S)\right] = \frac{\partial F(C)}{\partial p_a}\mathscr{D}F(S) + F(C)\mathscr{D}\frac{\partial F(S)}{\partial p_a} &= 0 \Longrightarrow \\
\frac{\partial F(S)}{\partial p_a} = -\mathscr{D}^{-1}F(C)^{-1}\frac{\partial F(C)}{\partial p_a}\mathscr{D}F(S) = -F(S)\mathscr{D}\frac{\partial F(C)}{\partial p_a}\mathscr{D}F(S) &= -F\left(S : \frac{\partial F(C)}{\partial p_a} : S\right),
\end{aligned}$$

where we used $F(C)^{-1} = \mathscr{D}F(S)\mathscr{D}$, which follows directly from the inversion formula in the tensor flattening writeup. The derivative of the compliance tensor, $\frac{\partial S^H}{\partial p_a}$, can then be read off by unflattening $\frac{\partial F(S)}{\partial p_a}$.

Now the squared Frobenius norm distance to a target compliance tensor S^* can be differentiated:

$$\begin{aligned}
J_S &= \frac{1}{2}||S^H - S^*||_F^2 \\
\frac{\partial J_S}{\partial p_a} &= \left[S^H - S^*\right]_{ijkl} \frac{\partial S^H_{ijkl}}{\partial p_a}.
\end{aligned}$$

As mentioned in the objectives writeup, it may instead be desirable to use some other weighting of the Frobenius norm terms. For example, we could use Frobenius norm distance in flattened form:

$$\begin{aligned}
J_{F(S)} &= \frac{1}{2}\|F(S) - F(S^*)\|_F^2 = \frac{1}{2}\left[F(S) - F(S^*)\right]_{ij}\left[F(S) - F(S^*)\right]_{ij} \\
\frac{\partial J_{D^{-1}}}{\partial p_a} &= \left[D^{-1} - D^{*-1}\right]_{ij}\left[\frac{\partial D^{-1}}{\partial p_a}\right]_{ij} = \frac{\partial J_{F(S)}}{\partial p_a} = \left[F(S) - F(S^*)\right]_{ij}\left[\frac{\partial F(S)}{\partial p_a}\right]_{ij}.
\end{aligned}$$

2.3 Elastic Moduli Fit

For objectives that can be written as functions of the Elastic moduli (or for finding extremal moduli), it's also useful to differentiate the moduli. To simplify notation for the following, we are going to overload S to be the flattened homogenized compliance tensor.

Recall that for orthotropic, axis-aligned materials, the flattened compliance tensor looks like:

$$F(S) = \begin{pmatrix}
\frac{1}{E_x} & -\frac{\nu_{yx}}{E_y} & -\frac{\nu_{zx}}{E_z} & 0 & 0 & 0 \\
-\frac{\nu_{yx}}{E_y} & \frac{1}{E_y} & -\frac{\nu_{zy}}{E_z} & 0 & 0 & 0 \\
-\frac{\nu_{zx}}{E_z} & -\frac{\nu_{zy}}{E_z} & \frac{1}{E_z} & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{1}{4\mu_{yz}} & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{1}{4\mu_{zx}} & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{4\mu_{xy}}
\end{pmatrix}.$$

The orthotropic moduli can therefore be written as simple functions of the compliance tensor entries. For clarity, we overload S and C to mean their flattened counterparts when indexed with only 2 indices (i.e. $S_{ij} := F(S)_{ij}$, $C_{ij} := F(C)_{ij}$):

$$E_x = \frac{1}{S_{00}}, \quad E_y = \frac{1}{S_{11}}, \quad E_z = \frac{1}{S_{22}},$$
$$\nu_{yx} = -E_y S_{01}, \quad \nu_{zx} = -E_z S_{02}, \quad \nu_{zy} = -E_z S_{12},$$
$$\mu_{yz} = \frac{1}{4S_{33}}, \quad \mu_{zx} = \frac{1}{4S_{44}}, \quad \mu_{xy} = \frac{1}{4S_{55}}.$$

Thus:

$$\frac{\partial E_x}{\partial p_a} = -\frac{1}{S_{00}^2}\frac{\partial S_{00}}{\partial p_a}, \quad \frac{\partial E_y}{\partial p_a} = -\frac{1}{S_{11}^2}\frac{\partial S_{11}}{\partial p_a}, \quad \frac{\partial E_z}{\partial p_a} = -\frac{1}{S_{22}^2}\frac{\partial S_{22}}{\partial p_a},$$
$$\frac{\partial \nu_{yx}}{\partial p_a} = \frac{S_{01}}{S_{11}^2}\frac{\partial S_{11}}{\partial p_a} - E_y\frac{\partial S_{01}}{\partial p_a}, \quad \frac{\partial \nu_{zx}}{\partial p_a} = \frac{S_{02}}{S_{22}^2}\frac{\partial S_{22}}{\partial p_a} - E_y\frac{\partial S_{02}}{\partial p_a}, \quad \frac{\partial \nu_{zy}}{\partial p_a} = \frac{S_{12}}{S_{22}^2}\frac{\partial S_{22}}{\partial p_a} - E_y\frac{\partial S_{12}}{\partial p_a},$$
$$\frac{\partial \mu_{yx}}{\partial p_a} = -\frac{1}{4S_{33}^2}\frac{\partial S_{33}}{\partial p_a}, \quad \frac{\partial \mu_{zx}}{\partial p_a} = -\frac{1}{4S_{44}^2}\frac{\partial S_{44}}{\partial p_a}, \quad \frac{\partial \mu_{xy}}{\partial p_a} = -\frac{1}{4S_{55}^2}\frac{\partial S_{55}}{\partial p_a}.$$

Since shear moduli also appear on the lower diagonal of $F(C)$, we can express their shape derivatives more simply as:

$$\frac{\partial \mu_{yx}}{\partial p_a} = \frac{\partial C_{33}}{\partial p_a}, \quad \frac{\partial \mu_{zx}}{\partial p_a} = \frac{\partial C_{44}}{\partial p_a}, \quad \frac{\partial \mu_{xy}}{\partial p_a} = \frac{\partial C_{55}}{\partial p_a}.$$