Objectives for Pattern Parameter Optimization

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We start by seeking an objective function to fit a particular (flattened) elasticity tensor, C, to a target tensor, C^*. We first show the naïve objective penalizing (squared) Frobenius norm distance,

$$J_C = ||C - C^*||_F^2$$

is poorly behaved and then propose a more physically motivated objective function: Frobenius norm distance of the flattened compliance tensors. Finally, we suggest various improvements over this objective, including reformulating the pattern optimization as a direct minimization of the global displacement-fitting objective,

$$\begin{aligned} J_{\mathrm{u}} = \int_\Gamma \|P(u - u^*)\|^2 \,\mathrm{d}A \quad \text{s.t.} \\ -\nabla \cdot [C(x) : \epsilon(u)] = f \text{ in } \Omega \\ \hat{n} \cdot [C(x) : \epsilon(u)] = g \text{ on } \Omega, \end{aligned} \tag{1}$$

that is used for material optimization. Here $\Gamma \subseteq \partial\Omega$ is the portion of the boundary where target displacements u^* are specified, and P is a matrix that projects out unspecified components of u^* (e.g., if we only want to specify the y coordinate of the target displacement).

Throughout this discussion, it is important to keep in mind that this is the over-all goal of our pipeline: to achieve the target displacements, u^*.

1 Problems with J_C

We examine objective J_C in a simplified 2D setting where both C and C^* are isotropic (functions of Young's modulus E and Poisson ratio ν):

$$J_C(E,\nu) = \left\| E \begin{pmatrix} \frac{1}{1-\nu^2} & \frac{\nu}{1-\nu^2} & 0 \\ \frac{\nu}{1-\nu^2} & \frac{1}{1-\nu^2} & 0 \\ 0 & 0 & \frac{1}{2\nu+2} \end{pmatrix} - E^* \begin{pmatrix} \frac{1}{1-\nu^{*2}} & \frac{\nu^*}{1-\nu^{*2}} & 0 \\ \frac{\nu^*}{1-\nu^{*2}} & \frac{1}{1-\nu^{*2}} & 0 \\ 0 & 0 & \frac{1}{2\nu^*+2} \end{pmatrix} \right\|_F^2$$

There are two drawbacks with this objective:

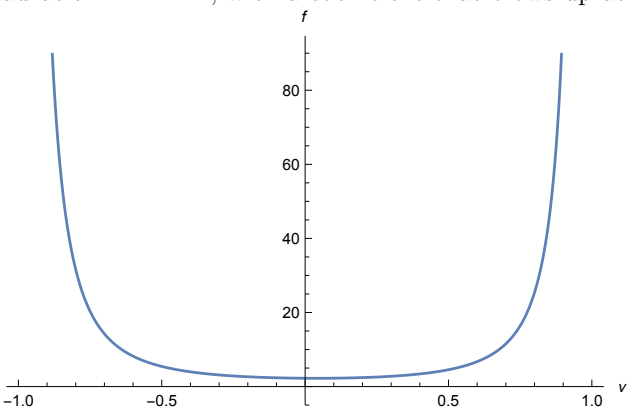
1. Deviations of Young's modulus and Poisson ratios are not penalized in a physically meaningful way.
2. Poisson ratio and Young's modulus effects are not neatly separated.

1.1 Nonphysical penalty on deviations

First, consider the simplified case, $\nu = \nu^*$. Then, the Frobenius norm objective reduces to:

$$J_C(E,\nu) = f(\nu^*)(E - E^*)^2 \quad \text{where } f(\nu) = \frac{9\nu^2 - 2\nu + 9}{4\left(\nu^2 - 1\right)^2}$$

Thus, the penalty is quadratic in $E - E^*$, with a coefficient that blows up at $\nu = \nu^* = \pm 1$:



A penalty proportional to squared absolute distance $(E - E^*)^2$ is bad for two obvious reasons:

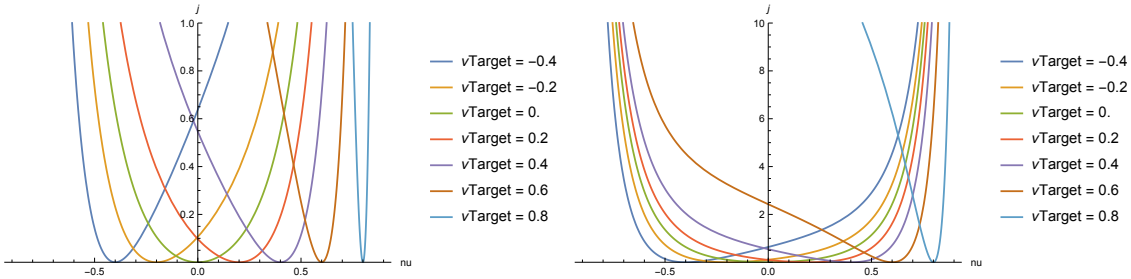
1. An particular absolute difference from $E^* = 1$ is much worse (from a displacements perspective) than the same absolute difference from $E^* = 100$, suggesting that there could be weighting problems in the anisotropic case with differing E_x^* and E_y^*.

2. More seriously, consider $E^* = 1$ and compare the behavior with $E = .5$ and $E = 1.5$ (both with the same relative and absolute difference from E^*). The Frobenius norm objective assigns the same penalty to both, but the former will deform twice as much with a particular load (a 100% displacement difference), while the latter deforms 2/3 as much (only a 33% difference). We clearly want our objective to penalize the former more.

Now, consider the case $E = E^*$, where the objective reduces to:

$$J_C(E, \nu) = j(\nu)E^2 \quad \text{where } j = 2\left(\frac{1}{1-\nu^2} - \frac{1}{1-\nu^{*2}}\right)^2 + 2\left(\frac{\nu}{1-\nu^2} - \frac{\nu^*}{1-\nu^{*2}}\right)^2 + \left(\frac{1}{2\nu+2} - \frac{1}{2\nu^*+2}\right)^2$$

$J_C(1, \nu)$ is plotted below with various target Poisson ratios, ν^* in the range -0.4 to 0.8, with a zoomed out view on the right.

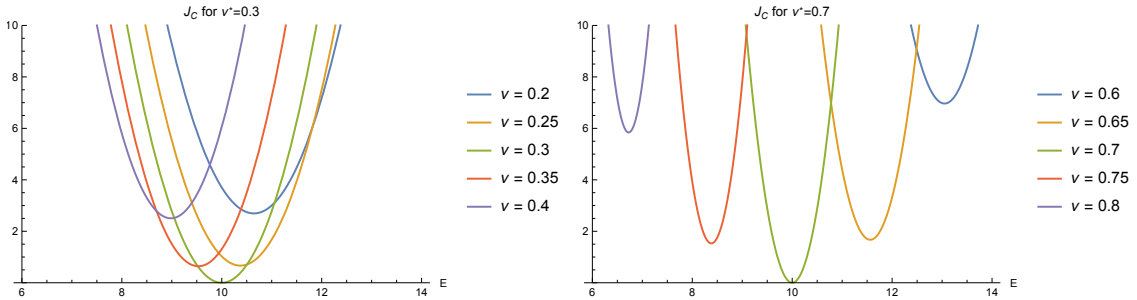


Small deviations from ν^* are penalized much more severely at higher values of $|\nu^*|$, which is the opposite of what we want from a relative-displacement-error perspective.

1.2 Interplay of E and ν

When either E or ν differs from its target value, the elasticity-tensor-based objective, J_C, does a poor job of fitting the other parameter.

For example, consider a target isotropic tensor $E^* = 5, \nu^* = 0.3$. When ν deviates from ν^*, the optimal E according to J_C drifts away from E^*. As ν^* becomes larger, this effect becomes more pronounced:



In practice, this has caused bad Young's moduli to be chosen by the lookup table projection when Poisson ratio cannot be matched closely.

2 Better objectives

We consider better-behaved objectives than J_C, first ignoring the greater goal of minimizing J_u.

2.1 J_S: Compliance-based, "absolute displacements" objective

Most of the problems mentioned above can be fixed by instead penalizing the Frobenius norm distance of the (flattened) compliance tensors S and S^*:

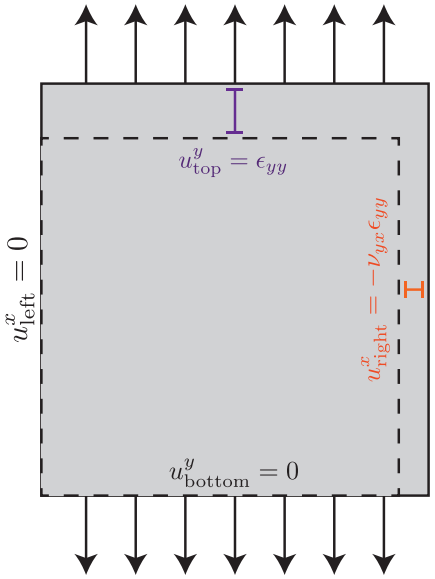
$$J_S = ||S - S^*||_F^2.$$

In the 2D orthotropic case using the flattening conventions from the tensor flattening writeup, this can be written as:

$$J_S(E_x, E_y, \nu_{yx}, \mu) = \left(\frac{1}{E_x} - \frac{1}{E_x^*}\right)^2 + \left(\frac{1}{E_y} - \frac{1}{E_y^*}\right)^2 + 2\left(\frac{\nu_{yx}}{E_y} - \frac{\nu_{yx}^*}{E_y^*}\right)^2 + \frac{1}{16}\left(\frac{1}{\mu} - \frac{1}{\mu^*}\right)^2 \tag{2}$$

Each term has a nice physical interpretation: consider two squares with edge length l, one filled with material $(E_x, E_y, \nu_{yx}, \mu)$ and the other with target material $(E_x^*, E_y^*, \nu_{yx}^*, \mu^*)$. Each term of J_S measures how the two squares' displacements differ when probed with a particular load.

For example, consider a vertical load that stretches the squares, causing a constant strain and stress displacement:



Choosing coordinates so that the bottom and left edges do not displace (or applying Dirichlet conditions), the displacements of the squares' tops are:

$$u^y_{\text{top}} = l\epsilon_{yy} = \frac{l\sigma_{yy}}{E_y}, \quad {u^y_{\text{top}}}^* = l\epsilon^*_{yy} = \frac{l\sigma_{yy}}{E^*_y},$$

and the displacements of their right edges are:

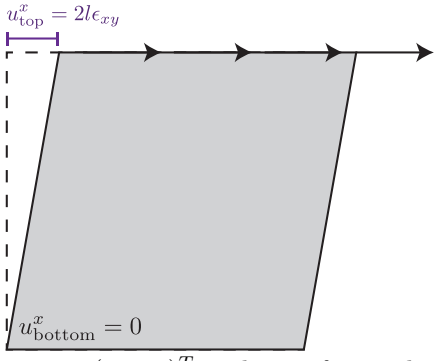
$$u^x_{\text{right}} = l\epsilon_{xx} = -l\nu_{yx}\epsilon_{yy} = -\frac{l\sigma_{yy}\nu_{yx}}{E_y}, \quad {u^x_{\text{right}}}^* = l\epsilon^*_{xx} = l\nu^*_{yx}\epsilon^*_{yy} = -\frac{l\sigma_{yy}\nu^*_{yx}}{E^*_y}.$$

Choosing a vertical load such that $\sigma_{yy} = \frac{1}{l}$ (i.e. total force 1N),

$$u^y_{\text{top}} = \frac{1}{E_y}, \quad {u^y_{\text{top}}}^* = \frac{1}{E^*_y}, \quad u^x_{\text{right}} = -\frac{\nu_{yx}}{E_y}, \quad {u^x_{\text{right}}}^* = -\frac{\nu^*_{yx}}{E^*_y},$$

and the second and third terms of J_S in (2) clearly penalize the (squared) difference in resulting top and left displacements. Similarly, the first and third terms can be interpreted as penalizing the (squared) difference in left and top displacements under a horizontal load causing $\sigma_{xx} = \frac{1}{l}$.

Now, consider applying a constant-strain shearing displacement:



This is done by prescribing normal traction $(\sigma_{xy}, 0)^T$ at the top face and a $u = 0$ Dirichlet boundary condition on the bottom face. In this case,

$$u^x_{\text{top}} = 2l\epsilon_{xy} = 2l\frac{\sigma_{xy}}{2\mu} = \frac{l\sigma_{xy}}{\mu}, \quad {u^x_{\text{top}}}^* = \frac{l\sigma_{xy}}{\mu^*}.$$

Choosing $\sigma_{xy} = \frac{1}{l}$ (total force 1N) gives x displacements of the top whose squared difference is measured by the fourth term in (2).

Thus, minimizing J_S can be viewed as a multi-objective optimization—trying to simultaneously fit five 1N displacements—that has been "linearly scalarized" with particular weights (the third term in (2) actually penalizes two different displacement quantities that equal). This scalarization is guaranteed to give us a Pareto optimal solution to the multi-objective problem, but not necessarily the Pareto optimum we want. For example, the shear term is probably weighted much less than it should be. Ideally we would choose weights based on how sensitive the over-all objective (1) is to an error in each of the sub-objectives.

2.2 Full vs. flattened tensor norms

There is a question whether we should be using the matrix Frobenius norm on the flattened tensors, as done in (2), or the full rank four tensor Frobenius norm. As shown in the Tensor Flattening writeup, the difference is in the scaling of the shear term only. The symmetric rank 4 tensor version is:

$$J_{S4}(E_x, E_y, \nu_{yx}, \mu) = \left(\frac{1}{E_x} - \frac{1}{E^*_x}\right)^2 + \left(\frac{1}{E_y} - \frac{1}{E^*_y}\right)^2 + 2\left(\frac{\nu_{yx}}{E_y} - \frac{\nu^*_{yx}}{E^*_y}\right)^2 + \frac{1}{4}\left(\frac{1}{\mu} - \frac{1}{\mu^*}\right)^2 \tag{3}$$

But since the rank 4 tensor implementing the strain to stress mapping is not unique, this is not the only possible Frobenius norm. Furthermore, we could have flattened in a different way when formulating (2). For example, we could instead use the matrix mapping flattened stress to engineering strain (this matrix is no longer symmetric in general, and its entries are no longer in direct correspondence with the compliance tensor entries):

$$S' = \begin{pmatrix} \frac{1}{E_x} & -\frac{\nu_{yx}}{E_y} & 0 \\ -\frac{\nu_{yx}}{E_y} & \frac{1}{E_y} & 0 \\ 0 & 0 & \frac{1}{\mu} \end{pmatrix},$$

which would give the objective

$$J_{S'}(E_x, E_y, \nu_{yx}, \mu) = \left(\frac{1}{E_x} - \frac{1}{E_x^*}\right)^2 + \left(\frac{1}{E_y} - \frac{1}{E_y^*}\right)^2 + 2\left(\frac{\nu_{yx}}{E_y} - \frac{\nu_{yx}^*}{E_y^*}\right)^2 + \left(\frac{1}{\mu} - \frac{1}{\mu^*}\right)^2. \tag{4}$$

Carefully choosing one from the many possible "Frobenius norms" may not be worthwhile; the following objectives propose different weightings from those in (2) anyway.

2.3 Relative displacements objective function

We can weight the terms in another way that makes the quantities dimensionless and neatly separates the Young's modulus and Poisson ratio parameters. This is desirable in circumstances where the relative error of the displacements matters as opposed to the absolute error. For example, if one cares about fitting accurately small (nonzero!) Poisson ratios, a relative error measurement will prevent the Young's moduli terms of (2) from dominating.

Dividing each term in (2) by the corresponding target displacement quantity, we arrive at:

$$J_{rel} = \left(\frac{E_x^*}{E_x} - 1\right)^2 + \left(\frac{E_y^*}{E_y} - 1\right)^2 + 2\left(\frac{\nu_{yx}}{\nu_{yx}^*} - 1\right)^2 + \left(\frac{\mu^*}{\mu} - 1\right)^2$$

Now the objective is also independent of the "total force" of each scenario, which before was arbitrarily set to 1N. Of course, if absolute displacement under equal-force loading scenarios is what we care about (or if $\nu_{xy}^* = 0$), we're better off using the plain J_S.

3 Global displacement-aware objectives

We now attempt to formulate an objective that uses more information from the material optimization stage than just the target tensors. The full solution from the material optimization stage offers two extra pieces of information:

(a) The load on the cell under the "optimal" material field we're trying to fit.

(b) The sensitivity of the over-all objective, (1), to each parameter.

Using (a), we no longer need to consider the same arbitrary five 1N load scenarios that J_S does—we can focus on the particular load we expect the cell to bear. However, exactly fitting the strain under this load might not be the most important goal; some strain components are likely unimportant to the global displacement objective. Section 3.1 elaborates on this option.

Using (b), we have two options: we could use the sensitivity information to weight each term of J_S, or we could discard J_S entirely and use chain rule to directly optimize J_u (treating the material optimization stage + pattern lookup as giving an initial guess for pattern/shape optimization of J_u). Sections 3.2 and 3.3 elaborate on these two options.

3.1 Strain-fitting objective

Using the constant cell strain and stress from the material optimization stage, ϵ^* and σ, we can minimize:

$$J_{\text{strain}} = \|\epsilon - \epsilon^*\|_F^2 = \|S\sigma - S^*\sigma\|_F^2$$

Notice how this is essentially identical to the local step of the local-global material optimization algorithm. In fact, we could run a few iterations of the local-global material optimization algorithm, then project the material tensors into pattern parameter space with the look-up table (using J_{strain}) and run more local-global iterations in pattern parameter space (using the shape derivative of J_{strain} and taking ϵ^* from a Dirichlet solve). This merging of pattern and material optimization is similar in spirit to the approach in Section 3.3.

3.2 Sensitivity-weighted objective

Unfortunately, using the above objective doesn't solve one problem we've seen in practice. Some parameter (say, Poisson ratio), may be unimportant in achieving a particular target deformation. All objectives discussed so far consider all parameters (or in the case of J_{strain}, all strain components) as equally important. If the objective favors closely fitting an unimportant parameter at the expense of a more important parameter, the pattern optimizer likely will choose a suboptimal elasticity tensor with respect to the global displacement objective, J_u; we need some way of weighting the terms in J_S so that we choose good point on its Pareto curve.

One possible way to do this is to consider the analytic derivative of J_u with respect to $\frac{1}{Ex}$, $\frac{\nu_{yx}}{Ey}$, ... computed via the adjoint method. The magnitude of each derivative evaluated at C^* gives a sense of how important it is to fit the corresponding terms of J_S and could be used as a weight. Of course, if the C^* found by material optimization happens to be perfectly optimal (unlikely), these derivatives would all be zero, and one could instead evaluate at a nearby, perturbed point in material parameter space.

3.3 Global-displacement objective (i.e. massive chain rule)

Of course, it's possible to use more than just the magnitude of the derivatives of J_u; since we can compute derivatives of J_u with respect to $\frac{1}{Ex}$, $\frac{\nu_{yx}}{Ey}$, ..., and we can compute shape derivatives of these quantities, we can compute the full shape derivative of J_u and thus the derivative of J_u with respect to each pattern parameter.

This means that we would use the same energy for pattern optimization as material optimization, and the two stages (material optimization then pattern parameter optimization) could be interpreted as two levels of a multi-resolution optimization (an optimization at the macroscopic-scale followed by a projection to and an optimization at the microscopic scale).