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Technical Note

Design of materials with prescribed elastic properties using D-functions

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1. Introduction

The inverse homogenization method has been used to design a lot of materials that meet some prescribed properties, such as Sigmund (1994, 2000), Liu *et al.* (2001), Guest and Prevost (2007). In this paper, D-functions are used as the distance between the equivalent and prescribed elastic tensors in the objective function. This generalized distance D-functions have a variety of forms which were first proposed by Bregman (1967). The 2 norm and cross entropy objective function are obtained as special cases. The convergence of the model can be assured by properties of D-functions. The numerical study is carried out to demonstrate that the proposed method can actually be used to design materials with prescribed elastic properties, including materials with negative poissons ratio and with bulk modulus on the upper HS bound.

2. D-functions (Distance Functions)

Definition (D-function) Let $S \subseteq R^n$ be a nonempty open convex set and $\overline{S}$ denote its closure. Let $F:\overline{S} \to R$ be a strictly convex function that is differentiable on S. The function $D_F:\overline{S} \times S \to R$ defined by

$$D_F(x,y) = F(x) - F(y) - <\nabla F(y), x - y> \tag{1}$$

is called D-function or Bregman distance.

By the strict convexity of F, the following relations are satisfied: $D_F(x,y) \geq 0$; $D_F(x,y) = 0$ iff $x = y$; $D_F(x,y)$ is a strictly convex function on $\overline{S}$. So we can interpret D-function as a generalized

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distance function. Furthermore, function F imposed on some additional requirements for the efficiency of the algorithms is called Bregman function (Censor and Zenios 1992). In this paper, two typical Bregman functions are chosen: $F_1(\mathbf{x}) = \mathbf{x}^2$, $F_2(\mathbf{x}) = \mathbf{x}\log(\mathbf{x})$. And their corresponding D-functions are 2 norm and cross entropy distances:

$$D_1(\mathbf{x}, \mathbf{x}_0) = \|\mathbf{x} - \mathbf{x}_0\|^2, \quad D_2(\mathbf{x}, \mathbf{x}_0) = \sum_{i=1}^{n}[x_i \log(x_i/x_{0(i)}) - x_i + x_{0(i)}] \tag{2}$$

where $\mathbf{x} = (x_1, \ldots, x_n)$, $\mathbf{x}_0 = (x_{0(1)}, \ldots, x_{0(n)})$.

3. Optimization model for material design

We are concerned with the material design problem in two-dimensional linear elasticity. For convenience, the abbreviation of the constitutive tensor are defined by

$$E_{1111} = E_1, E_{2222} = E_2, E_{1212} = E_3, E_{1122} = E_4, E_{1112} = E_5, E_{2212} = E_6 \quad (E_{ijkl} \to E_I) \tag{3}$$

The target materials are composed of two phases: solid and void. In this paper, we use D-functions to describe the distance between the equivalent elastic tensor $\mathbf{E}^H$ of the base cell and the prescribed elastic tensor $\mathbf{E}^*$. Then, the optimization model for material design in discretized form is

$$\begin{aligned} &\min \Phi = D_F(\mathbf{E}^H, \mathbf{E}^*) + \alpha \sum_{e=1}^{NE} x^e(1 - x^e) \\ &s.t. \quad [\mathbf{S}]\{\mathbf{D}\}_{ij} = \{\mathbf{R}\}_{ij} \\ &\quad E^H_{ijkl} = \frac{1}{Y}\sum_{e=1}^{NE} x^e(\{\mathbf{d}_0^e\}_{ij} - \{\mathbf{d}^e\}_{ij})^T[\mathbf{s}_0^e](\{\mathbf{d}_0^e\}_{kl} - \{\mathbf{d}^e\}_{kl}) \\ &\quad \sum_{e=1}^{NE} x^e \le \rho Y \\ &\quad 0 < x_{\min} \le x^e \le 1 \quad e = 1, \ldots, NE \end{aligned} \tag{4}$$

where $[\mathbf{S}]\{\mathbf{D}\}_{ij} = \{\mathbf{R}\}_{ij}$ is the finite element(FE) formulation of the test strain fields $\{\boldsymbol{\varepsilon}_0\}_{ij}$, $[\mathbf{s}^e] = x^e[\mathbf{s}_0^e]$ is the local stiffness matrices, Y is the base cell area, $\{\mathbf{d}_0^e\}_{ij}$ is the initial element displacement vector, $\{\mathbf{d}^e\}_{ij}$ is the element displacement vector of FE solution, α is the penalty factor, $x_{\min}$ is the lower bound on design variable to prevent the singularity of the stiffness matrix, ρ is the bound on the volume fraction, $x^e = 0$ and 1 denote void and solid phases in the element e respectively, 2 norm distance $D_1 = \sum_{I=1}^{6}(E_I^H - E_I^*)^2$ and cross entropy distance $D_2 = \sum_{I=1}^{6}[E_I^H \log(E_I^H/E_I^*) - E_I^H + E_I^*]$ are chosen as $D_F(\mathbf{E}^H, \mathbf{E}^*)$.

The gradient information of Φ required for the mathematical programming is obtained as

$$\frac{\partial \Phi_1}{\partial x^e} = \sum_{I=1}^{6} 2(E_I^H - E_I^*)\frac{\partial E_I^H}{\partial x^e} + \alpha(1 - 2x^e), \quad \frac{\partial \Phi_2}{\partial x^e} = \sum_{I=1}^{6} \log\left(\frac{E_I^H}{E_I^*}\right)\frac{\partial E_I^H}{\partial x^e} + \alpha(1 - 2x^e) \tag{5}$$

where $\dfrac{\partial E_I^H}{\partial x^e} = \dfrac{1}{Y}\sum_{e=1}^{NE}(\{\mathbf{d}_0^e\}_{ij} - \{\mathbf{d}^e\}_{ij})^T[\mathbf{s}_0^e](\{\mathbf{d}_0^e\}_{kl} - \{\mathbf{d}^e\}_{kl})$ is deduced from the homogenization formulations.

4. Examples

We will discuss two examples of material design: material with bulk modulus on the upper HS bound and negative poisson's ratio material. The base material has Poisson's ratio 0.3 and Young's modulus 0.91. The optimization problems are solved by the method of moving asymptotes (MMA) (Svanberg 1987).

4.1 Material with bulk modulus on the upper HS bound

The upper bound on bulk modulus of the two-phase composites is given by Hashin and Shtrikman (1963). If the volume fraction ρ and the possion's ratio of the target material is 0.3 and 0.75, respectively, the target constitutive tensor $\mathbf{E}^*$ is [0.0969 0.0969 0.0121 0.0727 0 0]. The unit cell is discretized by 21×12 equal-sized square four-node isoparametric finite elements. Because of the features of the homogenization method, the unit cell with hole is used as the initial distribution. And the initial distribution in the two optimization models of this example is the same. The iteration will terminate when $\sum_{I=1}^{6}\left|E_I^H - E_I^*\right| < 0.01$.

4.2 Negative poisson's ratio material

In this example, the volume fraction ρ is 0.4, the possion's ratio of the target material is –0.6 and the target constitutive tensor $\mathbf{E}^*$ is [0.04 0.04 0.032 –0.024 0 0]. The unit cell is discretized by 30×30 equal-sized square four-node isoparametric finite elements. Using the vertical symmetry, only a half of the finite elements need to be considered and the last two components in the target constitutive tensor needn't be added to the objective function. The same unit cell with hole is used as the initial distribution in the two models. The iteration will terminate when $\sum_{I=1}^{4}\left|E_I^H - E_I^*\right| < 0.005$.

From the comparison in Table 1 and Table 2, we can see that the cross entropy model is more efficient than the 2 norm model in the situation of this paper. This is because the cross entropy distance function is more convex than the 2 norm distance function around the target constitutive tensor. Generally, if the objective D-function is more convex around the target tensor, its' corresponding optimization model is more efficient. Since the convex features of diverse D-

Table 1 Results of two different optimization models for material with bulk modulus on the upper HS bound

Optimization model	Iteration number	The equivalent elastic tensor of the base cell
2 norm distance	1056	$\mathbf{E}^H$ = [0.0971 0.0968 0.0149 0.0663 0 0]
cross entropy distance	178	$\mathbf{E}^H$ = [0.0965 0.0967 0.0141 0.0653 0 0]

(a) (b) (c) (d)

Fig. 1 Microstructure with bulk modulus on the upper HS bound (a) one base cell by 2 norm optimization model, (b) 4×4 repeating unit cells of a, (c) one base cell by cross entropy optimization model, (d) 4×4 repeating unit cells of c

Table 2 Results of two different optimization models for negative poisson's ratio material

Optimization model	Iteration number	The equivalent elastic tensor of the base cell
2 norm distance	768	$\mathbf{E}^H$ = [0.0401 0.0402 0.0308 −0.0206 0 0]
cross entropy distance	367	$\mathbf{E}^H$ = [0.0410 0.0409 0.0310 −0.0220 0 0]

(a) (b) (c) (d)

Fig. 2 Microstructure with negative poisson's ratio (a) the upper half base cell by 2 norm optimization model, (b) 4×4 repeating unit cells of a, (c) the upper half base cell by cross entropy optimization model, (d) 4×4 repeating unit cells of c

functions around a certain value are different, we can choose the more convex one to make the model more efficient.

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