Properties of Cost Functionals in Free Material Design

Cristian Barbarosie¹, Sérgio Lopes¹,²

¹CMAF, Av. Professor Gama Pinto, 2, 1649-003, Lisboa, Portugal. E-mail: {barbaros,slopes}@ptmat.fc.ul.pt
²ISEL, Rua Conselheiro Emídio Navarro, 1, 1959-007, Lisboa, Portugal. E-mail: slopes@deea.isel.pt

Abstract
We study several properties of integral functionals arising in free material optimization as cost functions. The framework could be that of linearly elastic solids, but for simplicity of presentation purposes we consider scalar equations that model other physical phenomena such as heat or electrical conductivity (thus making the dependence of the cost functions less complicated – a matrix variable instead of an elastic tensor variable.)

Keywords: Free material design, lower semicontinuity, homogenization.

1. Introduction
The identification of adequate cost functions is essential to any optimization problem and the purpose of the talk is to establish a class of such admissible functions, covering both practical and theoretical aspects. Natural properties deriving from mechanical considerations (such as isotropy and monotonicity) are imposed.

The study focuses on two main properties: subadditivity and lower semicontinuity. Subadditivity is a requirement emerging from the practical observation that by superimposing two materials (which corresponds to the sum of the material coefficients) one should obtain a material whose cost is not greater to the sum of the costs of the two base materials. However the mathematical characterization of this property is a difficult problem. The lower semicontinuity of the cost function (together with the compactness of the design space) ensures the well-posedness of the optimization problem. This latter aspect raises the question of what notion of convergence should be considered in the design space, a problem often mistreated in the literature, usually by means of introducing a topology that, despite being mathematically sound, does not reflect well the physical reality. It is known for several years that the H-convergence (under which we develop our analysis) models correctly the mechanical behaviour of fine mixtures of materials.

The lower semicontinuity of the cost functional is related (but not equivalent) to the convexity of the integrand. A particular functional emerging from the homogenization theory, equal to the minimum amount of material needed to build a certain composite, is given special attention and its relevancy is discussed regarding subadditivity and lower semicontinuity. The majority of the results here presented can be found in [1].

2. Setting of the Problem
Let \( \Omega \) be a bounded domain in \( \mathbb{R}^n \); let \( \alpha \) and \( \beta \) be two real constants such that \( 0 < \alpha < \beta \). Denote by \( M^{\alpha,\beta}_n \) the set of symmetric \( n \times n \) matrices \( A \) such that \( \alpha I \leq A \leq \beta I \) (that is, \( A - \alpha I \) and \( \beta I - A \) are positive semidefinite matrices) and let \( M^{\alpha,\beta}_n(\Omega) \) be the set of matrix functions \( A : \Omega \to M^{\alpha,\beta}_n \) whose components are measurable functions (and therefore belong to \( L^\infty(\Omega) \)). The goal is to study functionals defined over \( M^{\alpha,\beta}_n(\Omega) \) of the form

\[
\Phi(A) = \int_\Omega \phi(A(x)) \, dx,
\]

with \( \phi : M^{\alpha,\beta}_n \to [0, +\infty[ \) being some scalar function, that typically arise in free material optimization settings (see Section 5) by means of an optimization problem

\[
\min_{A \in A} J(A),
\]

where, for a fixed, given \( c > 0 \),

\[
A = \{ A \in M^{\alpha,\beta}_n(\Omega) : \Phi(A) = c \}.
\]

One should distinguish between the objective functional \( J \) (the one to be minimized) which measures the performance of the structure according to some criteria, and the cost functional \( \Phi \) (giving the constraint)
which measures the price of the structure (the fabrication cost). The functional $\mathcal{J}$ depends on $A$ through the solution $u_A$ of some elliptic problem in $\Omega$; the matrix $A$ represents the material coefficients for the state equation

$$-\text{div}(A\nabla u_A) = f.$$  

Note that boundary conditions should be added to Eq. (4); we do not need to specify these boundary conditions due to the local character of the $H$-convergence and also because our study focuses on the properties of the cost functional $\Phi$ which does not depend on the elliptic problem.

### 3. Basic Properties

Along our study, we shall assume that the function $\phi$ is smooth enough. Continuity is a natural requirement, but more smoothness will be assumed when necessary. Note that, although the function $\phi$ should be defined on the set $M^+_s$, one may find it easier to consider $\phi$ defined on the whole set $M^+_s$ of symmetric positive definite matrices in order to obtain statements and properties independent of the parameters $\alpha$ and $\beta$.

We make the usual assumption in free material design of invariance under rotations of the cost function. This is a difficult condition to characterize in the elasticity framework; but since we restrict ourselves to scalar problems, we can accommodate it by simply imposing the condition

$$\forall A \in M^+_s \quad \forall Q \in \mathbb{R}^{n \times n} : QQ^t = I \quad \phi(Q^tAQ) = \phi(A).$$  

Equivalently, $\phi$ should depend solely on the invariants or on the eigenvalues (taken, for instance, in decreasing order) of its argument.

Another natural hypothesis is that “stronger structures should be more expensive”, that is, if $A, B \in M^+_{s,\beta}(\Omega)$ are two coefficient matrices such that $A(x) \leq B(x)$, a.e. $x \in \Omega$, then $A$ should be cheaper than $B$: $\Phi(A) \leq \Phi(B)$. This is equivalent to the monotonicity of $\phi$:

$$\forall A, B \in M^+_{s,\beta} \quad A \leq B \implies \phi(A) \leq \phi(B).$$

Note that this assumption is quite natural when one is looking for rigid structures (for instance, when minimizing the compliance, or some norm of the stress). It is far less obvious for cases like mechanism design. Being aware of that, we shall nevertheless impose this property on $\phi$ in the sequel.

By subadditivity we mean

$$\forall A, B \in M^+_{s,\beta} \quad \phi(A + B) \leq \phi(A) + \phi(B).$$  

There are reasons (of mechanical nature) for taking this property into consideration. Roughly speaking, it states that the cost of a material built by superimposing two base materials should not be higher than their combined prices. Note that the opposite operation is also legitimate: if one has a certain material $A$ at a certain cost $\phi(A)$, it is natural to require that the cost of the material $A/2$ (obtained by slicing the material $A$ in two halves) be less than or equal to $\phi(A)/2$. These two operations imply that the integrand $\phi$ should be positively homogeneous, that is,

$$\forall A \in M^+_{s,\beta}, \forall s > 0, \phi(sA) = s\phi(A).$$

The mathematical implications of properties (7) and (8) on the structure of the integrand $\phi$ are not yet clear.

### 4. Semicontinuity of $\Phi$

It is well known that, for the optimization problem (2) to be well-posed, one usually requires the lower semicontinuity of both the objective and the cost functionals. Now the question of the topology arises: one should check the lower semicontinuity of $\phi$ with respect to some topology on $M^+_{s,\beta}(\Omega)$ such that $M^+_{s,\beta}(\Omega)$ be compact. A natural choice is the weak* topology of $M^+_{s,\beta}(\Omega)$, as a subset of $L^\infty(\Omega; \mathbb{R}^{n \times n})$.

This is also convenient, since lower semicontinuous integral functionals for this topology are known to be those with a convex integrand (see [2]).

However, a closer look at the mechanical problem reveals that the weak* topology of $M^+_{s,\beta}(\Omega)$ is not an appropriate model: when the material coefficients oscillate at a small scale (the case of microstructures), the limit behaviour of the material is correctly described not by the weak* limit of the coefficient matrices, but by their $H$-limit. The notion of $H$-convergence is associated with a metrizable topology, the $H$-topology, for which $M^+_{s,\beta}(\Omega)$ is still a compact set.
Unfortunately, there is no simple characterization of lower semicontinuity with respect to the $H$-topology. Nevertheless, the following assertion stands: suppose $\phi$ is a continuous nondecreasing function, in the sense of Eq. (6); if the functional $\Phi$ defined by Eq. (1) is lower semicontinuous with respect to the weak* topology of $\mathcal{M}_{s}^{\alpha,\beta}(\Omega)$, then $\Phi$ is also lower semicontinuous with respect to the $H$-topology of $\mathcal{M}_{s}^{\alpha,\beta}(\Omega)$.

This result, together with the earlier observation about semicontinuous integral functionals for the weak* topology of $\mathcal{M}_{s}^{\alpha,\beta}(\Omega)$, implies that, under the monotonicity assumption Eq. (6), convexity of integrands is a sufficient condition of lower semicontinuity (with respect to the $H$-topology of $\mathcal{M}_{s}^{\alpha,\beta}(\Omega)$) for all integral functionals defined by Eq. (1).

In the particular case where $\phi$ depends only on the trace of its argument, that is $\phi(A) = \varphi(\text{tr} A)$ for all $A \in \mathcal{M}_{s}^{\alpha,\beta}$, it is possible to show that, under the monotonicity assumption, fulfilled by considering a nondecreasing real function $\varphi$, the convexity of $\varphi$ (equivalent to the one of $\phi$) is not only sufficient but necessary as well – for lower semicontinuity of the integral functional (1) with respect to the $H$-topology of $\mathcal{M}_{s}^{\alpha,\beta}(\Omega)$.

Convoluity of $\varphi$ can be proven to be also necessary when $\phi$ depends solely on the determinant of its argument, that is $\phi(A) = \varphi(\det A)$ for all $A \in \mathcal{M}_{s}^{\alpha,\beta}$. It is easy to prove (see [4]) that convexity of determinants is a polyconvex function, thus being quasiconvex and also rank-1 convex, * all these types of convexity are excluded as sufficient conditions. In order for $\Phi$ to be lower semicontinuous with respect to the $H$-topology of $\mathcal{M}_{s}^{\alpha,\beta}(\Omega)$, $\phi$ has to be either convex or something strictly between convex and polyconvex (in fact, in the next section, we shall see that convexity of $\phi$ is necessary).

5. Examples
In this section we exhibit some lower semicontinuous cost functionals, with respect to the $H$-topology.

The first example is the most popular choice in free material optimization: $\phi(A) = \text{tr} A$. Lower semicontinuity of the corresponding cost functional follows directly from previous considerations.

The second example is the spectral radius: since only positive definite matrices are dealt with, we can express it in the form $\phi(A) = \max_{\|\xi\|=1} A \xi \cdot \xi$. Being the pointwise supremum of a family of convex functions, it is a convex function. The monotonicity, although not completely obvious, is a simple exercise. Lower semicontinuity of the corresponding cost functional again follows directly from previous discussion. The isotropy is straightforward: as an orthogonal matrix $Q$ yields an isometry, one has

$$\phi(Q^T AQ) = \max_{\|\xi\|=1} (Q^T AQ) \xi \cdot \xi = \max_{\|\xi\|=1} A(Q \xi) \cdot (Q \xi) = \max_{\|\eta\|=1} A \eta \cdot \eta = \phi(A).$$

The third example is the most significant one concerning the characterization of the integrand. We can perform optimization in the set of all possible mixtures between materials $\alpha I$ and $\beta I$. More precisely, an explicit description is available in the literature for the set $G_\theta$ of materials (coefficient matrices) attainable as mixtures between $\alpha I$ and $\beta I$ in proportions $1 - \theta$ and $\theta$, respectively ($\theta \in [0, 1]$) – the famous G-closure problem (see [3]). We then define the set $G = \bigcup_{0 \leq \theta \leq 1} G_\theta \subset \mathcal{M}_{s}^{\alpha,\beta}(\Omega)$. For each matrix $A \in G$, one can compute explicitly the lowest value $\theta$ such that $A \in G_\theta$; this represents the cheapest mixture between $\alpha I$ and $\beta I$ producing the material tensor $A$:

$$\phi(A) = \inf \{\theta \in [0, 1] : A \in G_\theta\}.$$

We obtain a cost functional $\Phi$ defined not on the entire $\mathcal{M}_{s}^{\alpha,\beta}(\Omega)$, but only on those matrix functions taking values in $G$. It is easy to prove the compactness of this set endowed with the $H$-topology.

As a direct result of the characterization of $G_\theta$, we obtain an explicit expression for $\phi$ in terms of eigenvalues of $A$. It follows immediately that $\phi$ is isotropic, continuous and nondecreasing (this latter aspect easily follows from a well known result in matrix analysis concerning eigenvalues). It can be seen that the corresponding cost functional is lower semicontinuous with respect to the $H$-topology; however, the integrand $\phi$ is not convex – we establish this through a characterization of isotropic convex functions of a matrix variable (see [4]); in fact, it is convex in some directions and concave in others.

Thus, Eq. (10) provides an example of a functional $\Phi$ which is lower semi-continuous with respect to the $H$-topology but is not lower semi-continuous with respect to the weak* topology of $\mathcal{M}_{s}^{\alpha,\beta}(\Omega)$. The

*These are all weaker notions of convexity.
complete characterization of the lower semicontinuity of integral functionals defined by Eq. (1) and satisfying Eq. (5) and Eq. (6) remains an open question. About the subadditivity property (7), and the related property of positive homogeneity (8), they only make mechanical sense if we consider mixtures between a given material $\beta I$ and void. This corresponds to letting the parameter $\alpha$ to go to zero. In this case, the analytical formula of the integrand $\phi$ defined by Eq. (10) becomes simpler:

$$\phi(A) = 1 - \frac{n-1}{\sum_{i=1}^{n} \frac{\beta}{\lambda_i} - 1},$$

where $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of $A$. It is interesting to note that this function is not subadditive; this can be checked by searching directly for matrices violating Eq. (7). This violation of the subadditivity property is quite puzzling. It implies that, for some material matrices $A \in \mathcal{G}$, the cheapest way to build the material $A$ is not by mixing directly $\beta I$ with void, but rather by building first two other mixtures $A_1$ and $A_2$ and then superimposing these two materials in order to obtain $A = A_1 + A_2$.

Also, the function $\phi$ defined by Eq. (11) is not positively homogeneous; along radial directions, it is strictly concave, thus violating Eq. (8).

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**References**


