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CONNECTIONS BETWEEN TOPOLOGICAL SENSITIVITY ANALYSIS AND MATERIAL INTERPOLATION SCHEMES IN TOPOLOGY OPTIMIZATION

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Abstract. Material interpolation schemes, like SIMP, are very popular in topology optimization. They convert the difficult 0-1 problem into a nonlinear programming problem defined over a convex set by involving an interpolation (or penalization) function, usually constructed in rather empirical ways. This paper gives an insight into such methods with the help of the notion of topological sensitivity, and in particular provides some arguments for the choice of the penalization function. A simple algorithm based on these concepts is proposed and illustrated by numerical experiments.

1. Introduction

Let D be a bounded domain of $\mathbb{R}^d$, $d = 2$ or 3, with a Lipschitz boundary Γ made of two disjoint parts Γ_D and Γ_N, with Γ_D of nonzero measure and Γ_N of class $\mathcal{C}^1$. We focus on the following minimization problem, with the notation specified below:

$$\min_{(\gamma,u)\in\mathcal{E}\times\mathcal{V}} J(\gamma,u) \tag{1}$$

$$\text{subject to } \int_D \gamma\nabla u.\nabla\eta dx = \int_{\Gamma_N} \varphi\eta ds \qquad \forall\eta\in\mathcal{V}. \tag{2}$$

The symbol ∇ stands for the gradient operator, and the dot notation is used for the canonical scalar product of $\mathbb{R}^d$. For the two unknowns γ and u the feasible sets are respectively

$$\mathcal{E} := \{\gamma : D \to \{\gamma^-,\gamma^+\}, \gamma \text{ measurable}\},$$
$$\mathcal{V} := \{u \in H^1(D), u_{|\Gamma_D=0}\}.$$

The constants $\gamma^+ > \gamma^- > 0$, the distribution $\varphi \in H^{-1/2}(\Gamma_N)$, and the functional $J : \mathcal{E}\times\mathcal{V} \to \mathbb{R}$ are given data. For convenience we denote by $j(\gamma) := J(\gamma, u_\gamma)$ the reduced cost, or objective, with u_γ the solution of (2). Subsequently γ and u_γ will be referred to as the density (or conductivity) and the state, respectively. Note that, in many applications, the weak phase approximates an empty region, which means that $\gamma^- \ll \gamma^+$.

Due to the "bang-bang" nature of the targeted density γ, Problem (1)-(2) falls into the framework of topology optimization. A number of methods have been devised for its solution, which we briefly recall. A first class of methods, sometimes known as classical shape optimization [19, 27], relies on the control of the interface Γ_γ where γ jumps. The sensitivity analysis of the objective with respect to the position of Γ_γ leads to the notion of shape derivative. Algorithms based on the shape derivative produce in principle smooth variations of Γ_γ, in particular, the number of its connected components cannot change. This is a serious drawback in many applications. An important exception must nevertheless be mentioned. It concerns level set methods [4, 22, 23], where Γ_γ is represented as the zero level set of a smooth function ψ defined over D. A Hamilton-Jacobi equation is then often used to move the interface in the desired direction. Within this setting, connected

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components can cancel or merge, but can hardly be created, at least in two dimensions. In fact, these methods lack a nucleation mechanism. The topological sensitivity analysis aims precisely at evaluating the variation of the objective when γ is switched within a small region. This concept has been introduced in [15], mathematically justified in [16, 26], and then developed by several authors, see, e.g., [6, 7, 17, 20, 21]. Therefore, the topological sensitivity may be advantageously combined with level set methods [3, 8, 13]. A basically different class of methods consists in relaxing the constraint $\gamma(x) \in \{\gamma^-, \gamma^+\}$. This is usually achieved by invoking the homogenization theory [1, 10]. This latter approach benefits from nice theoretical properties, like differentiability and existence of global minimizers. However, eventually retrieving a feasible solution requires a rather heuristic penalization post-processing. Simplified methods, called material interpolation schemes or methods of fictitious materials [9, 11, 12, 25], are very popular in the engineering community. They are based on the two following principles. Firstly, the set of admissible values $\{\gamma^-, \gamma^+\}$ is simply extended to its convex hull $[\gamma^-, \gamma^+]$, thus the whole theory of homogenization is not needed. Secondly, the penalization is directly included in the optimization process by a modification of the state equation. Typically, in the SIMP model (Solid Isotropic Material with Penalization), the density γ in (2) is replaced by a power law $\theta(\gamma) = \gamma^p$ which, for some objective functions, tends to enforce extremal values. This formulation has proven particularly simple and efficient in many important cases. However, it has no proper theoretical justification, and the choice of the exponent p is mainly empirical.

The purpose of this paper is to give an insight into material interpolation schemes by interpreting the associated first order necessary optimality conditions in terms of topological sensitivity. We show that special penalization functions θ can be related to isotropic topological perturbations, which provides a clear meaning to the solutions obtained through this model. The power law penalization is retrieved in particular cases.

The paper is organized as follows. The notion of topological sensitivity is recalled in Section 2. The aforementioned relations between material interpolation schemes and topological sensitivity are exhibited in Section 3. The case of anisotropic perturbations is discussed in Section 4, complemented by Appendix A. The extension to the linear elasticity setting is addressed in Section 5. A gradient-like algorithm based on these concepts is described in Section 6. Numerical experiments are reported in Sections 7 and 8.

2. Topological sensitivity and optimality conditions

In the sequel we shall use the following standard notation. The dot product of two vectors $x, y \in \mathbb{R}^d$ is denoted, as in the introduction, by $x.y$, while the Euclidean norm of x is denoted by $|x|$. The open ball of center $\hat{x} \in \mathbb{R}^d$ and radius $\rho > 0$ is denoted by $B(\hat{x}, \rho) := \{x \in \mathbb{R}^d, |x - \hat{x}| < \rho\}$. If A is a subset of $\mathbb{R}^d$, $|A|$ stands for the d-dimensional Lebesgue measure of A. In addition, χ_A stands for the characteristic function of A, i.e., $\chi_A(x) = 1$ if $x \in A$, $\chi_A(x) = 0$ if $x \notin A$. The interior of A is denoted by $\operatorname{int} A$, i.e., $\operatorname{int} A := \{x \in A \text{ s.t. } \exists \rho > 0, B(x, \rho) \subset A\}$. For any $\gamma \in \mathcal{E}$ we define the sets

$$[\gamma = \gamma^+] := \{x \in D, \gamma(x) = \gamma^+\}, \qquad [\gamma = \gamma^-] := \{x \in D, \gamma(x) = \gamma^-\},$$

$$D_\gamma^+ := \operatorname{int}[\gamma = \gamma^+], \qquad D_\gamma^- := \operatorname{int}[\gamma = \gamma^-].$$

We also define the function $s_\gamma : D_\gamma^+ \cup D_\gamma^- \to \mathbb{R}$ by

$$s_\gamma(x) = \begin{cases} 1 & \text{if} \quad x \in D_\gamma^-, \\ -1 & \text{if} \quad x \in D_\gamma^+. \end{cases}$$

Below we define a notion of local optimality relative to a particular class of perturbations. More general perturbations are considered in Section 4.

Definition 2.1. We say that $\gamma \in \mathcal{E}$ is a local minimizer of j if, for every family $(x_1, ..., x_N) \in (D_\gamma^+ \cup D_\gamma^-)^N$, $N \in \mathbb{N} \setminus \{0\}$, there exists $\bar{\rho} > 0$ such that, for all $(\rho_1, ..., \rho_N) \in \mathbb{R}_+^N$,

$$\max_{i=1,...,N} \rho_i < \bar{\rho} \Longrightarrow j\left(\gamma + (\gamma^+ - \gamma^-) \sum_{i=1}^{N} s_\gamma(x_i) \chi_{B(x_i,\rho_i)}\right) \geq j(\gamma).$$

In other words, the domain $[\gamma = \gamma^+]$ is said to be locally optimal if $j(\gamma)$ cannot be decreased by the creation of an arbitrary set of small spherical inclusions. The concept of topological derivative gives a quantitative information on the variation of $j(\gamma)$ with respect to such perturbations.

Definition 2.2. We say that the functional j admits a topological derivative $g(\hat{x})$ at the point $\hat{x} \in D_\gamma^+ \cup D_\gamma^-$ if the following asymptotic expansion holds when $\rho \to 0$:

$$j(\gamma + s_\gamma(\hat{x})(\gamma^+ - \gamma^-)\chi_{B(\hat{x},\rho)}) - j(\gamma) = s_\gamma(\hat{x})(\gamma^+ - \gamma^-)|B(\hat{x},\rho)|g_\gamma(\hat{x}) + o(|B(\hat{x},\rho)|), \tag{3}$$

with $\lim_{\rho\to 0} \frac{o(|B(\hat{x},\rho)|)}{|B(\hat{x},\rho)|} = 0$.

As a straightforward consequence of Definitions 2.2 and 2.1 we derive the following result.

Lemma 2.3. *Suppose that γ is a local minimizer of j and j admits a topological derivative $g_\gamma(x)$ at all point $x \in D_\gamma^+ \cup D_\gamma^-$. Then*

$$\begin{array}{ll} g_\gamma(x) \geq 0 & \forall x \in D_\gamma^-, \\ g_\gamma(x) \leq 0 & \forall x \in D_\gamma^+. \end{array} \tag{4}$$

Proof. We choose a single perturbation centered at a point $\hat{x}$, for instance $\hat{x} \in D_\gamma^-$. By Definition 2.2 we have

$$j(\gamma + (\gamma^+ - \gamma^-)\chi_{B(\hat{x},\rho)}) - j(\gamma) = (\gamma^+ - \gamma^-)|B(\hat{x},\rho)|g_\gamma(\hat{x}) + o(|B(\hat{x},\rho)|).$$

In view of Definition 2.1 this quantity is nonnegative as soon as ρ is sufficiently small. Dividing by $|B(\hat{x},\rho)|$ and passing to the limit as $\rho \to 0$ entails $g_\gamma(\hat{x}) \geq 0$. Likewise $g_\gamma(\hat{x}) \leq 0$ when $\hat{x} \in D_\gamma^+$. □

To fix ideas, we assume henceforth that the objective functional is of the form

$$J(\gamma, u) = \int_{\Gamma_N} \psi u ds + \ell \int_D \gamma dx, \tag{5}$$

with $\psi \in H^{-1/2}(\Gamma_N)$. The scalar constant ℓ can be seen as a Lagrange multiplier associated with a volume constraint. The following result is proven in [6].

Proposition 2.4. *When J is defined by (5), the reduced cost j admits a topological derivative $g_\gamma(x)$ at each point $x \in D_\gamma^\pm$ given by*

$$g_\gamma(x) = k^\pm \gamma(x) \nabla u_\gamma(x).\nabla v_\gamma(x) + \ell,$$

where the adjoint state $v_\gamma \in \mathcal{V}$ solves

$$\int_D \gamma \nabla v_\gamma.\nabla \eta dx = -\int_{\Gamma_N} \psi \eta ds \qquad \forall \eta \in \mathcal{V}, \tag{6}$$

and the expression of $k^\pm$ is reported in Table 1.

d	2	3
k^-	$\frac{2}{\gamma^+ + \gamma^-}$	$\frac{3}{\gamma^+ + 2\gamma^-}$
k^+	$\frac{2}{\gamma^+ + \gamma^-}$	$\frac{3}{2\gamma^+ + \gamma^-}$

TABLE 1. Expressions of $k^{\pm}$ for the conductivity problem.

3. Connection with material interpolation schemes

We now consider the auxiliary problem

$$\min_{(\gamma,u)\in\tilde{\mathcal{E}}\times\mathcal{V}} J(\gamma,u) \tag{7}$$

$$\text{subject to } \int_D \theta(\gamma)\nabla u.\nabla\eta dx = \int_{\Gamma_N} \varphi\eta ds \qquad \forall\eta\in\mathcal{V}. \tag{8}$$

Compared with (1)-(2), γ is sought in the convex set

$$\tilde{\mathcal{E}} := \{\gamma : D \to [\gamma^-,\gamma^+], \gamma \text{ measurable}\},$$

and the state equation is modified by the introduction of a smooth (at least $\mathcal{C}^1$) function $\theta : (\gamma^{--},\gamma^{++}) \to (\gamma^{--},\gamma^{++})$, with $0 < \gamma^{--} < \gamma^- < \gamma^+ < \gamma^{++}$. We assume further that θ is increasing and satisfies

$$\theta(\gamma^-) = \gamma^-, \qquad \theta(\gamma^+) = \gamma^+.$$

For this problem we denote by $j_\theta(\gamma) := J(\gamma, u_{\theta,\gamma})$ the reduced cost, with $u_{\theta,\gamma}$ the solution of (8).

We will afterwards use standard notions of differential calculus in Banach spaces. The reader who is not familiar with this field may refer, e.g., to [14, 18]. More specifically, the following proposition is a direct application of the adjoint method for the calculus of derivatives (see, e.g., [2, 18]).

Proposition 3.1. *The reduced cost j_θ is Fréchet differentiable on $L^\infty(D,(\gamma^{--},\gamma^{++}))$ with the derivative in the direction $\delta\in L^\infty(D)$ given by*

$$Dj_\theta(\gamma)\delta = \int_D g_{\theta,\gamma}\delta dx, \tag{9}$$

with

$$g_{\theta,\gamma} := \theta'(\gamma)\nabla u_{\theta,\gamma}.\nabla v_{\theta,\gamma} + \ell,$$

and the adjoint state $v_{\theta,\gamma}\in\mathcal{V}$ solution of

$$\int_D \theta(\gamma)\nabla v_{\theta,\gamma}.\nabla\eta dx = -\int_{\Gamma_N}\psi\eta ds \qquad \forall\eta\in\mathcal{V}. \tag{10}$$

Proof. First, it stems from the implicit function theorem that the mapping $S : \gamma\in L^\infty(D,(\gamma^{--},\gamma^{++})) \mapsto u_{\theta,\gamma}\in\mathcal{V}$ is Fréchet differentiable. We write for simplicity $\dot{u}_{\theta,\gamma} := DS(u_{\theta,\gamma})\delta$ the derivative in the direction $\delta\in L^\infty(D)$. Then j_θ is differentiable by composition, and the chain rule yields

$$Dj_\theta(\gamma)\delta = \int_{\Gamma_N}\psi\dot{u}_{\theta,\gamma}ds + \ell\int_D\delta dx.$$

On using the adjoint equation (10) to rewrite the first integral we obtain

$$Dj_\theta(\gamma)\delta = -\int_D\theta(\gamma)\nabla v_{\theta,\gamma}.\nabla\dot{u}_{\theta,\gamma}dx + \ell\int_D\delta dx. \tag{11}$$

Now differentiating (8) yields

$$\int_D [\theta'(\gamma)\delta\nabla u_{\theta,\gamma}.\nabla\eta + \theta(\gamma)\nabla\dot{u}_{\theta,\gamma}.\nabla\eta]dx = 0 \qquad \forall\eta\in\mathcal{V}. \tag{12}$$

Combining (11) and (12) provides (9). □

For the optimality of j_θ we use the standard definition recalled below. For simplicity we denote by $\|.\|$ the L^∞ norm on D, i.e., $\|\gamma\| = \inf\{c, |\gamma| \le c \text{ a.e. in } D\}$.

Definition 3.2. We say that $\gamma\in\tilde{\mathcal{E}}$ is a local minimizer of j_θ if there exists $\alpha>0$ such that

$$\forall\tilde{\gamma}\in\tilde{\mathcal{E}}, \qquad \|\gamma-\tilde{\gamma}\|\le\alpha \Rightarrow j_\theta(\gamma)\le j_\theta(\tilde{\gamma}).$$

From Proposition 3.1 we derive the following necessary optimality conditions.

Corollary 3.3. *Suppose that γ is a local minimizer of j_θ. Then*

$$\begin{array}{lll} g_{\theta,\gamma}\ge 0 & a.e.\ on & [\gamma=\gamma^-],\\ g_{\theta,\gamma}= 0 & a.e.\ on & [\gamma^-<\gamma<\gamma^+],\\ g_{\theta,\gamma}\le 0 & a.e.\ on & [\gamma=\gamma^+]. \end{array} \tag{13}$$

Proof. By virtue of the convexity of $\tilde{\mathcal{E}}$ we have the optimality condition (see, e.g., [18])

$$Dj_\theta(\gamma)(\tilde{\gamma}-\gamma)\ge 0 \qquad \forall\tilde{\gamma}\in\tilde{\mathcal{E}}.$$

Consider an arbitrary pair $(\lambda,\delta)\in(\gamma^-,\gamma^+)\times L^\infty(D)$ with $\delta\ge 0$ a.e., and set

$$\tilde{\gamma} = \gamma + \chi_{[\gamma\le\lambda]}t\delta.$$

For $t>0$ sufficiently small we have $\tilde{\gamma}\in\tilde{\mathcal{E}}$, hence

$$Dj_\theta(\gamma)(\tilde{\gamma}-\gamma) = t\int_{[\gamma\le\lambda]} g_{\theta,\gamma}\delta dx \ge 0.$$

It follows that

$$\int_{[\gamma\le\lambda]} g_{\theta,\gamma}\delta dx\ge 0 \qquad \forall\delta\in L^\infty(D),\delta\ge 0,$$

and subsequently that

$$g_{\theta,\gamma}\ge 0 \text{ a.e. on } [\gamma\le\lambda].$$

Similarly we find that

$$g_{\theta,\gamma}\le 0 \text{ a.e. on } [\gamma\ge\lambda].$$

Using that $\lambda\in(\gamma^-,\gamma^+)$ is arbitrary completes the proof. □

From comparison of Lemma 2.3 and Corollary 3.3, it appears that, apart from the convexification of the feasible set, the two optimality systems essentially differ by the expression of the sensitivities. Then a natural question arises: is there a function θ such that those two sensitivities coincide? This question is addressed by the following theorem.

Theorem 3.4. *There exists a unique polynomial function $\gamma\mapsto\theta(\gamma)$ of degree not larger than 3 such that $\theta(\gamma(x))=\gamma(x)$ and $g_{\theta,\gamma}(x)=g_\gamma(x)$ for all $\gamma\in\mathcal{E}$ and all $x\in D_\gamma^-\cup D_\gamma^+$. This function is given by*

$$\begin{array}{ll} \theta(\gamma) = \dfrac{\gamma^2+\gamma^+\gamma^-}{\gamma^++\gamma^-} & \text{if } d=2,\\ \theta(\gamma) = \dfrac{-\gamma^3+3(\gamma^++\gamma^-)\gamma^2+2\gamma^+\gamma^-(\gamma^++\gamma^-)}{(2\gamma^++\gamma^-)(\gamma^++2\gamma^-)} & \text{if } d=3. \end{array} \tag{14}$$

If θ is chosen as above, $\gamma\in\mathcal{E}$ and $|D\setminus D_\gamma^-\setminus D_\gamma^+|=0$, then $j_\theta(\gamma)=j(\gamma)$ and the conditions (4) and (13) are equivalent.

Proof. In order to fulfill the assertions of the theorem we need to construct a smooth function θ such that

$$\theta(\gamma^-) = \gamma^-, \qquad \theta(\gamma^+) = \gamma^+, \qquad \theta'(\gamma^-) = k^-\gamma^-, \qquad \theta'(\gamma^+) = k^+\gamma^+. \tag{15}$$

For a polynomial interpolation of the form

$$\theta(\gamma) = a_3\gamma^3 + a_2\gamma^2 + a_1\gamma + a_0,$$

the conditions (15) are equivalent to

$$\left\{\begin{array}{l} a_3(\gamma^-)^3 + a_2(\gamma^-)^2 + a_1\gamma^- + a_0 = \gamma^-, \\ a_3(\gamma^+)^3 + a_2(\gamma^+)^2 + a_1\gamma^+ + a_0 = \gamma^+, \\ 3a_3(\gamma^-)^2 + 2a_2\gamma^- + a_1 = k^-\gamma^-, \\ 3a_3(\gamma^+)^2 + 2a_2\gamma^+ + a_1 = k^+\gamma^+. \end{array}\right. \tag{16}$$

By Gauss elimination, we find that the above system admits a unique solution given by

$$\begin{aligned} a_3 &= \frac{k^+\gamma^+ + k^-\gamma^- - 2}{(\gamma^+ - \gamma^-)^2}, \\ a_2 &= \frac{(1-k^+\gamma^+)(\gamma^+ + 2\gamma^-) + (1-k^-\gamma^-)(2\gamma^+ + \gamma^-)}{(\gamma^+ - \gamma^-)^2}, \\ a_1 &= 1 - \frac{(1-k^+\gamma^+)\gamma^-(2\gamma^+ + \gamma^-) + (1-k^-\gamma^-)\gamma^+(\gamma^+ + 2\gamma^-)}{(\gamma^+ - \gamma^-)^2}, \\ a_0 &= \frac{\gamma^+\gamma^-}{(\gamma^+ - \gamma^-)^2}\left[(1-k^+\gamma^+)\gamma^- + (1-k^-\gamma^-)\gamma^+\right]. \end{aligned}$$

Now using the expressions of k^+ and k^- from Table 1 results in (14). □

Remark 3.5. For $\gamma^+ = 1$ and $\gamma^- \to 0$ we have

$$\begin{array}{ll} \theta(\gamma) \sim \gamma^2 & \text{if } d = 2, \\ \theta(\gamma) \sim -\dfrac{1}{2}\gamma^3 + \dfrac{3}{2}\gamma^2 & \text{if } d = 3. \end{array} \tag{17}$$

These functions are plotted in Figure 1.

Remark 3.6. By virtue of the relations

$$\begin{aligned} |D \setminus D_\gamma^- \setminus D_\gamma^+| &= |[\gamma = \gamma^+] \setminus \mathrm{int}[\gamma = \gamma^+]| + |[\gamma = \gamma^-] \setminus \mathrm{int}[\gamma = \gamma^-]| \\ &\leq |\partial[\gamma = \gamma^+]| + |\partial[\gamma = \gamma^-]|, \end{aligned}$$

the condition $|D \setminus D_\gamma^- \setminus D_\gamma^+| = 0$ will be fulfilled as soon as the sets $\partial[\gamma = \gamma^+]$ and $\partial[\gamma = \gamma^-]$ have zero d-dimensional Lebesgue measure. This will hold true whenever those sets have some smoothness, for instance, when they are Lipschitz.

Remark 3.7. Of course, Theorem 3.4 does not imply that Problems (1)-(2) and (7)-(8) are equivalent since there is no guarantee that the solutions (global or local) to (7)-(8) belong to $\mathcal{E}$. We mention in this respect the paper [24], where it is proven that, for $\theta(\gamma) = \gamma^p$, in the self-adjoint case and for a discrete version, solutions to (7)-(8) are necessarily in $\mathcal{E}$ for p sufficiently high.

4. On optimality with respect to elliptic perturbations

This section deals with the extension of the previous concepts of topological sensitivity analysis and related optimality conditions to non spherical inclusions. This means that, in the asymptotic expansion (3), $B(\hat{x}, \rho)$ is replaced by

$$\omega(\hat{x}, \rho) := \hat{x} + \rho\omega,$$

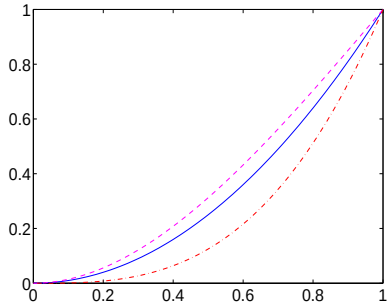

FIGURE 1. Function θ for $\gamma^+ = 1$ and $\gamma^- \to 0$, from top to bottom: conductivity 3D, conductivity 2D, linear elasticity 2D.

where ω is an arbitrary reference domain. When it exists, the associated topological derivative is denoted by $g_{\gamma,\omega}$. The following result is proven in [6].

Proposition 4.1. *When J is defined by (5), the reduced cost j admits a topological derivative $g_{\gamma,\omega}(x)$ at each point $x \in D_\gamma^\pm$ given by*

$$g_{\gamma,\omega}(x) = P_{\omega,r}\nabla u_\gamma(x).\nabla v_\gamma(x) + \ell, \tag{18}$$

where the adjoint state $v_\gamma \in \mathcal{V}$ solves

$$\int_D \gamma \nabla v_\gamma.\nabla \eta dx = -\int_{\Gamma_N} \psi \eta ds \qquad \forall \eta \in \mathcal{V}. \tag{19}$$

The polarization matrix $P_{\omega,r}$ is always symmetric and depends only on ω and the density contrast r, i.e., $r = \gamma^+/\gamma^-$ if $x \in D_\gamma^-$, $r = \gamma^-/\gamma^+$ if $x \in D_\gamma^+$. If ω is the ellipse with semi major and minor axes of length 1 and e, respectively, directed along the main axes of the coordinate system, then the polarization matrix admits the expression

$$P_{\omega,r} = Q_{r,e} := \begin{pmatrix} \dfrac{1+e}{1+re} & 0 \\ 0 & \dfrac{1+e}{e+r} \end{pmatrix}.$$

Detailed properties of polarization matrices can be found in [5]. In particular, if $\omega' = R\omega$ where R belongs to the set $\mathcal{U}$ of unitary transformations of $\mathbb{R}^2$, then the associated polarization matrix becomes

$$P_{\omega',r} = RP_{\omega,r}R^T.$$

The following theorem states topological optimality conditions with respect to the class of all elliptic inclusions. The proof, which is fairly technical, is deferred to Appendix A.

Theorem 4.2. *Set $U = \nabla u_\gamma$, $V = \nabla v_\gamma$, $M = (U \otimes V + V \otimes U)/2$, and denote by Λ^+ and Λ^- the largest and smallest eigenvalues of M, respectively, i.e.,*

$$\Lambda^+ = \frac{U.V + |U||V|}{2}, \qquad \Lambda^- = \frac{U.V - |U||V|}{2}. \tag{20}$$

Define

$$g_\gamma^\star = \begin{cases} \dfrac{\gamma^-}{\gamma^+}\Lambda^+ + \Lambda^- + \ell \quad in \quad D_\gamma^-, & (a) \\ \dfrac{\gamma^+}{\gamma^-}\Lambda^+ + \Lambda^- + \ell \quad in \quad D_\gamma^+. & (b) \end{cases} \tag{21}$$

A necessary optimality condition for $\gamma \in \mathcal{E}$ to be a local minimizer of j with respect to arbitrary elliptic inclusions is

$$\begin{array}{ll} g_\gamma^\star(x) \geq 0 & \forall x \in D_\gamma^-, \quad (a) \\ g_\gamma^\star(x) \leq 0 & \forall x \in D_\gamma^+. \quad (b) \end{array} \tag{22}$$

Let us now give some practical implications of Theorem 4.2.

(1) In the self-adjoint case $v_\gamma = -u_\gamma$ (i.e., $\psi = \varphi$) we derive

$$g_\gamma^\star = -|\nabla u_\gamma|^2 + \ell \text{ in } D_\gamma^- \cup D_\gamma^+.$$

Then solving the optimality conditions (22) amounts to finding a solution $(\gamma, u) \in \mathcal{E} \times \mathcal{V}$ of (7)-(8) with the interpolation function $\theta(\gamma) = \gamma$ (see Proposition 3.1 and Corollary 3.3). It is well known (see, e.g., [2]) that this problem admits solutions in $\tilde{\mathcal{E}} \times \mathcal{V}$, but the corresponding γ is usually not of bang-bang type. This suggests that (22) has few chances to admit a solution in $\mathcal{E}$.

(2) Consider now a non self-adjoint case and a point $x \in D_\gamma^+$ where $\nabla u_\gamma(x) \neq -\nabla v_\gamma(x)$. Hence $\Lambda^+(x) > 0$, and (22)(b) reads

$$\frac{\gamma^+}{\gamma^-}\Lambda^+(x) + \Lambda^-(x) + \ell \leq 0.$$

When $\gamma^- \ll \gamma^+$, the above condition is hardly fulfilled, which again suggests the absence of local minimizer relative to elliptic inclusions.

We therefore conclude that imposing optimality with respect to the class of all elliptic inclusions is generally too strong to allow for the existence of solutions in $\mathcal{E}$. This implies that interpolation methods attempting to solve these conditions are likely to generate regions of intermediate density, which are usually undesirable due to their unclear mechanical interpretation [2, 11]. Accordingly, we subsequently limit ourselves to spherical inclusions.

5. Generalization to linear elasticity

We consider now a linear elasticity problem in two space dimensions. The domain D is defined as before. The state is the displacement field

$$u \in \mathcal{V} := \{u \in (H^1(D))^2, u_{|\Gamma_D = 0}\},$$

and the equilibrium equation reads

$$\int_D \gamma \sigma(u) : \nabla^s \eta = \int_{\Gamma_N} \varphi.\eta ds \qquad \forall \eta \in \mathcal{V}.$$

Here $\sigma(u)$ is the stress normalized to a unitary Young modulus, $\nabla^s \eta := (\nabla \eta + \nabla^T \eta)/2$ is the symmetric gradient (strain), and $\varphi \in (H^{-1/2}(\Gamma_N))^2$ is a prescribed load. The stress is computed by the Hooke law

$$\sigma(u) = \lambda \mathrm{tr} \nabla^s u + 2\mu \nabla^s u,$$

where (λ, μ) are the Lamé coefficients. The following result is taken from [6].

Proposition 5.1. *When J is defined by (5), the reduced cost j admits a topological derivative $g(x)$ at each point $x \in D_\gamma^\pm$ given by*

$$g_\gamma(x) = \frac{\kappa + 1}{2(\kappa r^\pm + 1)} \left[2\sigma(u_\gamma)(x) : \nabla^s v_\gamma(x) + \frac{(r^\pm - 1)(\kappa - 2)}{\kappa + 2r^\pm - 1} tr\sigma(u_\gamma)(x) tr\nabla^s v_\gamma(x) \right] + \ell,$$

where

$$\kappa = \frac{\lambda + 3\mu}{\lambda + \mu}, \qquad r^+ = \frac{\gamma^-}{\gamma^+}, \qquad r^- = \frac{\gamma^+}{\gamma^-},$$

and the adjoint state $v_\gamma \in \mathcal{V}$ *solves*

$$\int_D \gamma\sigma(v_\gamma) : \nabla^s \eta dx = -\int_{\Gamma_N} \psi.\eta ds \qquad \forall \eta \in \mathcal{V}. \tag{23}$$

Henceforth we place ourselves in the plane stress case. Then the Lamé coefficients are related to the Poisson ratio ν by

$$\lambda = \frac{\nu}{1-\nu^2}, \qquad \mu = \frac{1}{2(1+\nu)},$$

which entails

$$\kappa = \frac{3-\nu}{1+\nu}.$$

Obviously, Lemma 2.3, Proposition 3.1 and Corollary 3.3 straightforwardly extend to the linear elasticity case for the gradient

$$g_{\theta,\gamma} = \theta'(\gamma)\sigma(u_{\theta,\gamma}) : \nabla^s v_{\theta,\gamma} + \ell.$$

In order to be able to match $g_{\theta,\gamma}$ and g_γ with the help of a scalar-valued interpolation function, we restrict ourselves to the Poisson ratio $\nu = 1/3$, which is a rather standard value. In this case we have $\kappa = 2$, and the topological derivative admits the simpler expression

$$g_\gamma(x) = k^\pm \gamma(x)\sigma(u_\gamma)(x) : \nabla^s v_\gamma(x) + \ell \qquad \forall x \in D_\gamma^\pm,$$

with

$$k^- = \frac{3}{2\gamma^+ + \gamma^-}, \qquad k^+ = \frac{3}{\gamma^+ + 2\gamma^-}.$$

By arguing as in Theorem 3.4, we obtain the following result.

Theorem 5.2. *Set*

$$\theta(\gamma) = \frac{2\gamma^3 + 3\gamma^+\gamma^-\gamma + 2\gamma^+\gamma^-(\gamma^+ + \gamma^-)}{(\gamma^+ + 2\gamma^-)(2\gamma^+ + \gamma^-)}, \tag{24}$$

and suppose that $\gamma \in \mathcal{E}$ *and* $|D \setminus D_\gamma^- \setminus D_\gamma^+| = 0$. *Then* $j_\theta(\gamma) = j(\gamma)$, $g_{\theta,\gamma} = g_\gamma$, *and the conditions* (4) *and* (13) *are equivalent.*

Remark 5.3. For $\gamma^+ = 1$ and $\gamma^- \to 0$ we have

$$\theta(\gamma) \sim \gamma^3. \tag{25}$$

Interestingly, this cubic power law penalization is the most frequently used within the SIMP model.

6. Optimization algorithm

In view of the preceding findings, we replace the solution of (1)-(2) by that of the interpolated problem (7)-(8), that is

$$\min_{\gamma \in \tilde{\mathcal{E}}} j_\theta(\gamma).$$

The function θ is chosen according to Theorems 3.4 (in conductivity) or 5.2 (in elasticity). Two classes of methods are of common usage in topology optimization with material interpolation schemes, for which we refer to [12]. On one hand the so-called optimality criteria methods are efficient in some cases but they are quite heuristic. On the other hand convex approximations methods, like the Method of Moving Asymptotes (MMA), consist in iteratively solving simpler subproblems constructed so as to account for approximations of the objective and possible constraints, with the property of being separable in the elements. Here we simply use a projected gradient algorithm.

Algorithm 1. (1) *Initialization: choose* $\beta > 0$, $\alpha \in (0,1)$, $\gamma_0 \in \tilde{\mathcal{E}}$.

(2) *Loop while* $\|\gamma_{n+1}-\gamma_n\|/\|\gamma_n\| \leq \beta$*:*

$$\gamma_{n+1} = \max(\gamma^-, \min(\gamma^+, \gamma_n - t_n \nabla j_\theta(\gamma_n))),$$

where $t_n = t_n^0 \alpha^m$ *and* m *is the smallest integer such that*

$$j_\theta(\gamma_{n+1}) < j_\theta(\gamma_n).$$

In the computations we have always used $\alpha = 0.5$, $\gamma_0 \equiv (\gamma^- + \gamma^+)/2$, and $t_n^0 = \|\gamma_n\|/\|\nabla j_\theta(\gamma_n)\|$. In this latter expression, as well as in the stopping criterion, the L^2 norm on D has been chosen.

For the discretization of the state equation we use finite elements with piecewise linear shape functions on a triangular mesh. We denote by $\mathcal{V}_h$ the finite element space and by $\{e_1, ..., e_N\}$ the finite element basis. The density γ is also represented on this basis, as

$$\gamma = \sum_{i=1}^{N} \gamma_i e_i,$$

and the vector $(\gamma_1, ..., \gamma_N)$ is the design variable. The equivalent density within each element is computed by applying a linear interpolation operator $S \in \mathcal{L}(\mathcal{V}_h, \mathcal{T}_h)$, where $\mathcal{T}_h$ is the set of functions defined on D which are constant per element. Then the discrete state $u_{\theta,\gamma} \in \mathcal{V}_h$ is computed by

$$\int_D \theta(S\gamma) \nabla u_{\theta,\gamma}.\nabla \eta dx = \int_{\Gamma_N} \varphi \eta ds \qquad \forall \eta \in \mathcal{V}_h,$$

and the discrete cost is defined by

$$j_\theta(\gamma) = \int_{\Gamma_N} \psi u_{\theta,\gamma} ds + \ell \int_D S\gamma dx.$$

Arguing as in Proposition 3.1, we find that the derivative of the discrete cost is

$$Dj_\theta(\gamma)\delta = \int_D [\theta'(S\gamma) \nabla u_{\theta,\gamma}.\nabla v_{\theta,\gamma} S\delta + \ell S\delta] dx,$$

with the discrete adjoint state $v_{\theta,\gamma}$ solution of

$$\int_D \theta(S\gamma) \nabla v_{\theta,\gamma}.\nabla \eta dx = -\int_{\Gamma_N} \psi \eta ds \qquad \forall \eta \in \mathcal{V}_h.$$

Denoting by $S^\star$ the adjoint operator of S with respect to the inner product of $L^2(D)$ we obtain the gradient

$$\nabla j_\theta(\gamma) = S^\star \left(\theta'(S\gamma) \nabla u_{\theta,\gamma}.\nabla v_{\theta,\gamma} + \ell\right).$$

Remark 6.1. Piecewise linear finite elements are seldom used in topology optimization because they are known to produce instabilities in the form of checkerboard patterns [2, 12]. However in all the numerical tests performed this phenomenon has not been encountered. Probably this is due to the fact that the design variable is here defined at the nodes, whereas it is usually attached to the elements. Hence, thanks to the possibility to use low order triangular finite elements, the present algorithm proves to be of remarkably simple implementation and appropriate for arbitrary domains.

In the following two sections we show some applications of this algorithm to conductivity and linear elasticity academic problems. The main feature which stands out from those experiments is that, at convergence, the intermediate densities are almost confined to the elements located at the interface between the two extremal materials. Therefore, this region can be made arbitrarily small by mesh refinement.

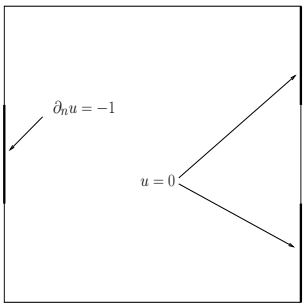

FIGURE 2. Conductor: computational domain and boundary conditions.

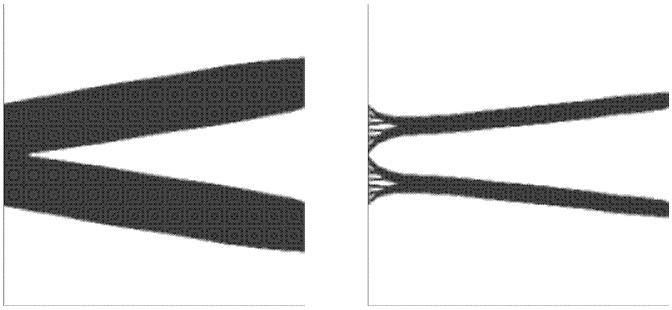

FIGURE 3. Conductor: optimal density for $\ell = 1$ (left), and $\ell = 10$ (right).

7. Numerical examples in conductivity

We use the parameters $\gamma^+ = 1$, $\gamma^- = 10^{-5}$ and $\beta = 10^{-2}$. In the example under consideration the domain D is a square of size 1.5, with the boundary conditions indicated on Figure 2. In the objective functional we take $\psi = \varphi$, hence the problem is self-adjoint, i.e., $v_{\theta,\gamma} = -u_{\theta,\gamma}$. We use a mesh containing $N = 29041$ nodes. Figures 3 shows the results of two computations, corresponding to the Lagrange multipliers $\ell = 1$ and $\ell = 10$. The implementation is done in Matlab.

8. Numerical examples in elasticity

For structural optimization problems, in order to reduce the risk to fall in local minima and save computer time, we use a sequence of iteratively refined meshes, like in [8]. The optimization is first performed on a coarse mesh. After convergence, the mesh is refined, the density γ is projected onto the new mesh, and the optimization is continued. This procedure is repeated up to the final desired mesh. We present three examples.

8.1. **Cantilever.** Here and in the subsequent section 8.2 we use $\gamma^+ = 1$, $\gamma^- = 10^{-5}$ and $\beta = 10^{-3}$. Again we place ourselves in the self-adjoint case ($\psi = \varphi$), which corresponds to the standard compliance minimization problem. The domain D is a rectangle of size 2×1 (see Figure 4, left). The Lagrange multiplier is chosen as $\ell = 100$. The successive meshes consist of 431, 1661, 6521 and 25841 nodes. The obtained distribution of material is depicted on Figure 4, right.

8.2. **Mast.** The domain D is shown on Figure 5, left, where the vertical and horizontal branches are rectangles of sizes 2×4 and 4×2, respectively. The Lagrange multiplier is chosen as $\ell = 50$.

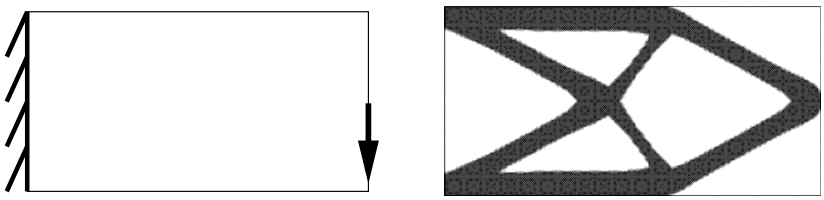

FIGURE 4. Cantilever: boundary conditions (left) and optimal density (right)

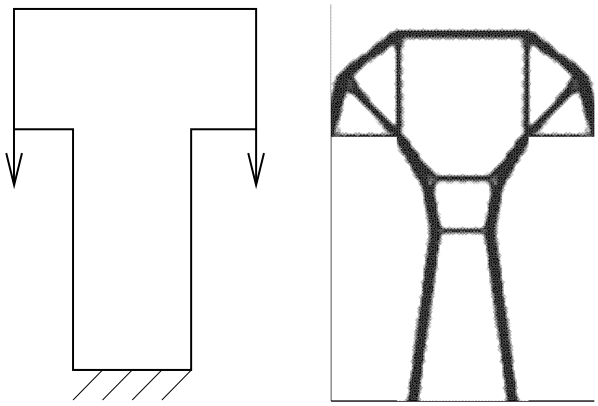

FIGURE 5. Mast: boundary conditions (left) and optimal density (right)

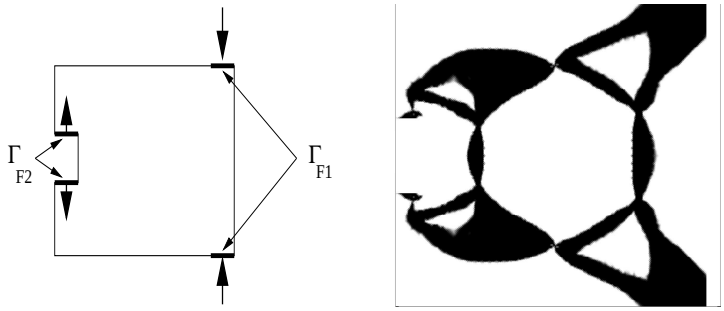

FIGURE 6. Gripping mechanism: boundary conditions (left) and optimal density (right)

The successive meshes consist of 851, 3301 and 13001 nodes. The obtained solution is depicted on Figure 5, right.

8.3. **Gripping mechanism.** We consider a simplified model of gripping mechanism. The loaded part of the boundary is split into $\Gamma_F = \Gamma_{F1} \cup \Gamma_{F2}$, see Figure 6, left. The functions φ and ψ are defined as

$$\varphi = \varphi_1 \chi_{\Gamma_{F1}} + \varphi_2 \chi_{\Gamma_{F2}}, \qquad \psi = \psi_1 \chi_{\Gamma_{F1}} + \psi_2 \chi_{\Gamma_{F2}},$$

with $\varphi_1 = 1$, $\varphi_2 = 10$, $\psi_1 = 1$, $\psi_2 = 0$. The Lagrange multiplier is chosen as $\ell = 0.3$. We use the parameters $\gamma^+ = 1$, $\gamma^- = 10^{-2}$, $\beta = 10^{-2}$, and successive meshes containing 3467, 13693 and 54425 nodes. The obtained solution is depicted on Figure 6, right.

Appendix A. Mathematical complements

The goal of this appendix is to prove Theorem 4.2. We begin by two preliminary lemmas.

Lemma A.1. *Let $\mathcal{S}$ be the set of polarization matrices generated by arbitrary ellipses, i.e,*

$$\mathcal{S} = \{RQ_{r,e}R^T, R \in \mathcal{U}, 0 < e \leq 1\}.$$

Then $\mathcal{S}$ is the set of all 2×2 symmetric positive definite matrices P verifying

$$\textit{trace}\ (P^{-1}) = 1 + r, \qquad \textit{trace}\ (P) < 1 + \frac{1}{r}. \tag{26}$$

Proof. If $P \in \mathcal{S}$, one easily checks (26). Suppose that P satisfies (26) and denote by λ_1, λ_2 the eigenvalues of P, which satisfy

$$\frac{1}{\lambda_1} + \frac{1}{\lambda_2} = 1 + r, \qquad \lambda_1 + \lambda_2 < 1 + \frac{1}{r}. \tag{27}$$

We deduce from (27) that

$$\lambda_1 > \frac{1}{1+r},$$
$$\lambda_1 + \lambda_2 - \left(1 + \frac{1}{r}\right) = \left(1 + \frac{1}{r}\right) \frac{(1 - r\lambda_1)(1 - \lambda_1)}{(1+r)\lambda_1 - 1} < 0,$$

which entails

$$(1 - \lambda_1)(r\lambda_1 - 1) > 0.$$

Hence $\hat{e} := (1 - \lambda_1)/(r\lambda_1 - 1) > 0$. If $\hat{e} \leq 1$, we set $e = \hat{e}$, so that $\lambda_1 = (1 + e)/(1 + re)$ and, using (27), $\lambda_2 = (1 + e)/(e + r)$. If $\hat{e} > 1$, we set $e = 1/\hat{e}$, so that $\lambda_1 = (1 + e)/(e + r)$ and, using (27), $\lambda_2 = (1 + e)/(1 + re)$. In both cases P has the same eigenvalues as $Q_{r,e}$, thus there exists $R \in \mathcal{U}$ such that $P = RQ_{r,e}R^T$. □

Lemma A.2. *The closure of $\mathcal{S}$ is the set of all symmetric positive definite matrices P verifying*

$$\textit{trace}\ (P^{-1}) = 1 + r, \qquad \textit{trace}\ (P) \leq 1 + \frac{1}{r}. \tag{28}$$

Proof. Clearly, (28) is fulfilled by all P belonging to the closure of $\mathcal{S}$, denoted by $\mathrm{cl}(\mathcal{S})$. In addition, every eigenvalue λ of a matrix $P \in \mathcal{S}$ satisfies $\lambda \geq 1/(1 + r)$. Hence each $P \in \mathrm{cl}(\mathcal{S})$ is symmetric positive definite. Suppose now that P is a symmetric positive definite matrix verifying

$$\mathrm{trace}\ (P^{-1}) = 1 + r, \qquad \mathrm{trace}\ (P) = 1 + \frac{1}{r}. \tag{29}$$

Using (29) we obtain that the eigenvalues of P are 1 and $1/r$. Therefore there exists $R \in \mathcal{U}$ such that

$$P = R \begin{pmatrix} 1 & 0 \\ 0 & 1/r \end{pmatrix} R^T.$$

Let (α_n) be a sequence of positive numbers such that

$$\alpha_n > \frac{1}{1+r} \qquad \forall n \in \mathbb{N}, \qquad \lim_{n\to\infty} \alpha_n \to 1,$$

and define

$$\beta_n = \frac{\alpha_n}{\alpha_n(1+r) - 1} > 0,$$
$$P_n = R \begin{pmatrix} \alpha_n & 0 \\ 0 & \beta_n \end{pmatrix} R^T.$$

By construction, we have for all n

$$\frac{1}{\alpha_n} + \frac{1}{\beta_n} = 1 + r,$$

$$a_n := \alpha_n + \beta_n - \left(1 + \frac{1}{r}\right) = \left(1 + \frac{1}{r}\right) \frac{(1-\alpha_n)(1-r\alpha_n)}{\alpha_n(1+r)-1}.$$

We choose (α_n) such that

$$\begin{aligned} \alpha_n &< 1 \quad \text{if} \quad r > 1, \\ \alpha_n &> 1 \quad \text{if} \quad r < 1. \end{aligned}$$

In each case, for n large enough, $a_n < 0$, hence $P_n \in \mathcal{S}$. As $\lim_{n\to\infty} P_n = P$, we conclude that $P \in \mathrm{cl}(\mathcal{S})$. □

We are now in position to prove Theorem 4.2. First, we easily check that, in the nontrivial case where $U, V \neq 0$, Λ^+ and Λ^- given by (20) are eigenvalues of M associated with the eigenvectors $U/|U| + V/|V|$ and $U/|U| - V/|V|$, respectively. Suppose that $\gamma \in \mathcal{E}$ is a local minimizer of j with respect to every elliptic inclusion, and choose $x \in D_\gamma^-$. According to Lemma 2.3, we have $g_{\gamma,\omega}(x) \geq 0$ for any ellipse ω. Then the condition (22)(a) will be fulfilled if we set

$$g_\gamma^\star(x) = \inf\{g_{\gamma,\omega}(x), \omega \text{ ellipse}\}.$$

We now check that the above infimum satisfies (21)(a). For each ellipse ω, we write (18) in the form

$$g_{\gamma,\omega}(x) = P_{\omega,r} : M(x) + \ell.$$

With the notation of Lemma A.1, we have

$$g_\gamma^\star(x) = \inf\{P : M + \ell, P \in \mathcal{S}\}.$$

As $\mathcal{S}$ is bounded, we also have

$$g_\gamma^\star(x) = \min\{P : M + \ell, P \in \mathrm{cl}(\mathcal{S})\}.$$

Let us consider an arbitrary $P \in \mathrm{cl}(\mathcal{S})$, which we write in the form

$$P = R\hat{P}R^T, \qquad \hat{P} = \begin{pmatrix} \lambda^+ & 0 \\ 0 & \lambda^- \end{pmatrix}, \qquad R \in \mathcal{U}, \qquad \lambda^+ \geq \lambda^- > 0.$$

Likewise, there exists $S \in \mathcal{U}$ such that

$$M = S\hat{M}S^T, \qquad \hat{M} = \begin{pmatrix} \Lambda^+ & 0 \\ 0 & \Lambda^- \end{pmatrix}.$$

Set $T = S^T R$. As $T \in \mathcal{U}$, there exists $\phi \in \mathbb{R}$ such that

$$T = \begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix} \text{ or } T = \begin{pmatrix} \cos\phi & \sin\phi \\ \sin\phi & -\cos\phi \end{pmatrix}.$$

We arrive in both cases at

$$P : M = (T\hat{P}T^T) : \hat{M} = (\lambda^+ - \lambda^-)(\Lambda^+ - \Lambda^-)\cos^2\phi + \Lambda^+\lambda^- + \Lambda^-\lambda^+. \tag{30}$$

Arguing as in Lemma A.1 with the characterization of $\mathrm{cl}(\mathcal{S})$ given by Lemma A.2, we obtain that

$$(1 - \lambda^\pm)(r\lambda^\pm - 1) \geq 0.$$

Since $x \in D_\gamma^-$, we have $r = \gamma^+/\gamma^- > 1$, hence the above inequality implies that $1/r \leq \lambda^- \leq \lambda^+ \leq 1$. Using that $\Lambda^- \leq 0 \leq \Lambda^+$ we derive

$$P : M \geq \frac{\Lambda^+}{r} + \Lambda^-.$$

In addition, this bound is attained for $\cos\phi = 0$, $\lambda^+ = 1$, $\lambda^- = 1/r$, which provides (21)(a). The case where $x \in D_\gamma^+$ can be treated in a similar way, with inf replaced by sup and $r = \gamma^-/\gamma^+ < 1$.

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