Optimal design on annulus: numerical approximation obtained by the shape gradient method

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Introduction

Let $\Omega \subset \mathbb{R}^d$ be open and bounded set.

Two phases each with different isotropic conductivity: α, β $(0 < \alpha < \beta)$.

 q_{α} is the prescribed volume of the first phase α ($0 < q_{\alpha} < |\Omega|$). $\chi \in L^{\infty}(\Omega)$ such that

$$\begin{cases} \chi = 1, & \text{phase } \alpha \\ \chi = 0, & \text{phase } \beta \end{cases}$$

Conductivity can be expressed as

$$\mathbf{A}(\chi) := \chi \alpha \, \mathbf{I} + (1 - \chi) \beta \, \mathbf{I},$$

where

$$\int_{\Omega} \chi(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} = q_{\alpha}.$$



Introduction

State functions $u_i \in H_0^1(\Omega)$, i = 1, 2, ..., m are given as a solution of the following boundary value problems:

(S)
$$\begin{cases} -\operatorname{div}(\mathbf{A}\nabla u_i) = f_i & \text{in } \Omega\\ u = 0 & \text{on } \partial\Omega, \end{cases} \quad i = 1, 2, ..., m,$$

with $\mathbf{A} = \chi \alpha \mathbf{I} + (1 - \chi) \beta \mathbf{I}$. Denote $\boldsymbol{u} = (u_1, ..., u_m)$. Energy functional:

$$J(\chi) := \sum_{i=1}^{m} \mu_i \int_{\Omega} f_i(\boldsymbol{x}) u_i(\boldsymbol{x}) \, \mathrm{d} \boldsymbol{x},$$

where $\mu_i > 0, \ i = 1, 2, ..., m$.

Statement of the problem

Optimal design problem:

(P)
$$\begin{cases} J(\chi) = \sum_{i=1}^{m} \mu_i \int_{\Omega} f_i u_i \, \mathrm{d}\boldsymbol{x} \to \max\\ \text{s.t.} \quad \chi \in L^{\infty}(\Omega, \{0, 1\}), \quad \int_{\Omega} \chi \, \mathrm{d}\boldsymbol{x} = q_{\alpha},\\ \boldsymbol{u} \text{ solves (S) with } \mathbf{A} = \chi \alpha \mathbf{I} + (1 - \chi) \beta \mathbf{I}. \end{cases}$$

If solution χ exists for (P) we call it *classical solution*.

Important: For general optimal design problems the classical solutions usually do not exist.

Assumptions:

- $\Omega \subset \mathbb{R}^d$ is ball or annulus,
- right hand sides f_i are radial functions.

With this assumptions one can construct classical solutions.

Relaxed design

For characteristic functions relaxation consists of:

(1)
$$\chi \in \mathcal{L}^{\infty}(\Omega, \{0, 1\}) \quad \rightsquigarrow \quad \theta \in \mathcal{L}^{\infty}(\Omega, [0, 1]),$$

with

$$\int_{\Omega} heta \, \mathrm{d} oldsymbol{x} := q_{lpha}.$$

Notion of H-convergence is introduced for conductivity **A**. **Effective conductivities:**

 $\mathcal{K}(\theta) \subset M_d(\mathbb{R})$ with local fraction $\theta \in [0, 1]$.

Precisely, $A \in \mathcal{K}(\theta)$ iff there exists sequence of characteristic functions

$$\begin{cases} \chi_n \xrightarrow{L^{\infty_*}} \theta \\ \mathbf{A}^n = \chi_n \alpha \mathbf{I} + (1 - \chi_n) \beta \mathbf{I} \xrightarrow{H} A. \end{cases}$$

Effective conductivities - set $\mathcal{K}(\theta)$

 $\mathcal{K}(\theta) \text{ is given in terms of eigenvalues}$ $\lambda_{\theta}^{-} \leq \lambda_{j} \leq \lambda_{\theta}^{+} \quad j = 1, \dots, d$ $\sum_{j=1}^{d} \frac{1}{\lambda_{j} - \alpha} \leq \frac{1}{\lambda_{\theta}^{-} - \alpha} + \frac{d - 1}{\lambda_{\theta}^{+} - \alpha}$ $\sum_{j=1}^{d} \frac{1}{\beta - \lambda_{j}} \leq \frac{1}{\beta - \lambda_{\theta}^{-}} + \frac{d - 1}{\beta - \lambda_{\theta}^{+}},$

where

$$\begin{aligned} \lambda_{\theta}^{+} &= \theta \alpha + (1 - \theta) \beta \\ \frac{1}{\lambda_{\theta}^{-}} &= \frac{\theta}{\alpha} + \frac{1 - \theta}{\beta}. \end{aligned}$$





Generalized (convex) problem

Relaxed design:

$$\mathcal{A} = \left\{ (\theta, \mathbf{A}) \in L^{\infty}(\Omega, [0, 1] \times \operatorname{Sym}_d) \middle| \begin{array}{c} \int_{\Omega} \theta \, \mathrm{d}\boldsymbol{x} = q_{\alpha}, \\ \mathbf{A}(\boldsymbol{x}) \in \mathcal{K}(\theta(\boldsymbol{x})), \text{ a.e. } \boldsymbol{x} \end{array} \right\}$$

Relaxed problem can be written as:

(A)
$$\max_{(\theta, \mathbf{A}) \in \mathcal{A}} J(\theta, \mathbf{A}) = \max_{(\theta, \mathbf{A}) \in \mathcal{A}} \sum_{i=1}^{m} \mu_i \int_{\Omega} f_i u_i \, \mathrm{d}\boldsymbol{x}$$

Unfortunately, \mathcal{A} is not a convex set. To achieve convexity, an enlarged set is introduced:

$$\mathcal{B} = \left\{ (\theta, \mathbf{A}) \in L^{\infty}(\Omega, [0, 1] \times \operatorname{Sym}_d) \middle| \begin{array}{c} \int_{\Omega} \theta \, \mathrm{d}\boldsymbol{x} = q_{\alpha}, \\ \lambda^{-}_{\theta(\boldsymbol{x})} \mathbf{I} \leq \mathbf{A}(\boldsymbol{x}) \leq \lambda^{+}_{\theta(\boldsymbol{x})} \mathbf{I}, \text{ a.e. } \boldsymbol{x} \end{array} \right\}$$

and with it

(B)
$$\max_{(\theta, \mathbf{A}) \in \mathcal{B}} J(\theta, \mathbf{A}) = \max_{(\theta, \mathbf{A}) \in \mathcal{B}} \sum_{i=1}^{m} \mu_i \int_{\Omega} f_i u_i \, \mathrm{d} \boldsymbol{x}$$

Rewrite B as a max-min problem

Define
$$\mathcal{S} := \left\{ \boldsymbol{\sigma} = (\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2, ..., \boldsymbol{\sigma}_m) \mid \boldsymbol{\sigma}_i \in \mathrm{L}^2(\Omega, \mathbb{R}^d), -\mathrm{div}(\boldsymbol{\sigma}_i) = f_i \right\}$$

One can rewrite functional J in terms of fluxes:

$$J(\theta, \mathbf{A}) = \min_{\boldsymbol{\sigma} \in \mathcal{S}} \sum_{i=1}^{m} \mu_i \int_{\Omega} \mathbf{A}^{-1} \, \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_i$$

With notation $C = \{(\theta, \mathbf{A}) | (\theta, \mathbf{A}^{-1}) \in \mathcal{B}\}$

$$\max_{(\theta, \mathbf{A}) \in \mathcal{B}} J(\theta, \mathbf{A}) = \max_{(\theta, \mathbf{A}) \in \mathcal{B}} \min_{\boldsymbol{\sigma} \in \mathcal{S}} \sum_{i=1}^{m} \mu_i \int_{\Omega} \mathbf{A}^{-1} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_i$$
$$= \max_{(\theta, \mathbf{B}) \in \mathcal{C}} \min_{\boldsymbol{\sigma} \in \mathcal{S}} \sum_{i=1}^{m} \mu_i \int_{\Omega} \mathbf{B} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_i$$

Observe that

$$L(\boldsymbol{\sigma}, (\theta, \mathbf{B})) = \sum_{i=1}^{m} \mu_i \int_{\Omega} \mathbf{B} \, \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_i$$

 $\pmb{\sigma}\mapsto L(\pmb{\sigma},(\theta,\mathbf{B}))$

- quadratic (strictly convex)
- continuous in $L^2(\Omega)$ (l.s.c.)
- $(\exists (\theta, \mathbf{B})) \quad \boldsymbol{\sigma} \mapsto L(\boldsymbol{\sigma}, (\theta, \mathbf{B}))$ $\lim_{\|\boldsymbol{\sigma}\| \to +\infty} L(\boldsymbol{\sigma}, (\theta, \mathbf{B}))) = +\infty$

 $(\theta,\mathbf{B})\mapsto L(\pmb{\sigma},(\theta,\mathbf{B}))$

- linear (concave)
- continuous in L^{∞} * (u.s.c.)
- set C is compact (in $L^{\infty}*$).

Min-max theory

Previous conclusions for the Lagrange functional L implies:

- set of saddle points $\mathcal{S}_0 \times \mathcal{C}_0 \subset \mathcal{S} \times \mathcal{C}$ is not empty
- min and max are interchangeable
- $\boldsymbol{\sigma} \mapsto L(\boldsymbol{\sigma}, (\theta, \mathbf{B}))$ is strictly convex $\Rightarrow \mathcal{S}_0 = \{\boldsymbol{\sigma}^*\}.$

This means that there exists **unique** σ^* such that this holds

$$\max_{(\theta, \mathbf{A}) \in \mathcal{B}} J(\theta, \mathbf{A}) = \max_{(\theta, \mathbf{B}) \in \mathcal{C}} \min_{\boldsymbol{\sigma} \in \mathcal{S}} L(\boldsymbol{\sigma}, (\theta, \mathbf{B}))$$
$$= \max_{(\theta, \mathbf{B}) \in \mathcal{C}} L(\boldsymbol{\sigma}^*, (\theta, \mathbf{B}))$$
$$= \max_{(\theta, \mathbf{B}) \in \mathcal{C}} \sum_{i=1}^m \mu_i \int_{\Omega} \mathbf{B} \boldsymbol{\sigma}_i^* \cdot \boldsymbol{\sigma}_i^*$$

Conclusions

Instead of solving convex problem B, one can solve the following optimization problem:

(I)
$$\begin{cases} I(\theta) = \sum_{i=1}^{m} \mu_i \int_{\Omega} f_i u_i \, \mathrm{d} \boldsymbol{x} \to \max \\ s.t. \quad \theta \in L^{\infty}(\Omega, [0, 1]), \quad \int_{\Omega} \theta = q_{\alpha}, \text{ where } u_i \text{ satisfies} \\ -\operatorname{div}(\lambda_{\theta}^{-} \nabla u_i) = f_i, \quad u_i \in \mathrm{H}^1_0(\Omega), \ i = 1, 2, ..., m \end{cases}$$

For spherically symmetric problem such that:

- $\Omega = R(\Omega)$ for any rotation R
- f_i are radial functions

it can be proved that there exists radial solution θ_R^* of (I).

In particular, it can be shown that

$$\max_{(\theta, \mathbf{A}) \in \mathcal{A}} J(\theta, \mathbf{A}) = I(\theta_R^*).$$

Conclusions

Define

$$\Psi := \sum_{i=1}^m \mu_i |\boldsymbol{\sigma}_i^*|^2.$$

Lemma

The necessary and sufficient condition of optimality for solution θ^* of optimal design problem (I) simplifies to the existence of a Lagrange multiplier $c \geq 0$ such that

(2)
$$\begin{aligned} \Psi > c &\Rightarrow \theta^* = 1, \\ \Psi < c &\Rightarrow \theta^* = 0. \end{aligned}$$

Single state optimal design problem



Single state equation:

(3)
$$\begin{cases} -\operatorname{div}(\lambda_{\theta}^{-}(x)\nabla u) = 1 & \text{in } \Omega\\ u = 0 & \text{on } \partial\Omega \end{cases}$$

where
$$\lambda_{\theta}^{-}(x) = \left(\frac{\theta(x)}{\alpha} + \frac{1-\theta(x)}{\beta}\right)^{-1}$$
.

Optimization problem:

(4)
$$\begin{cases} I(\theta) = \int_{\Omega} u \, \mathrm{d}\boldsymbol{x} \to \max\\ s.t. \quad \theta \in \mathrm{L}^{\infty}(\Omega, [0, 1]), \quad \int_{\Omega} \theta = q_{\alpha}, \text{ where } u \text{ satisfies (3)} \end{cases}$$

One can rewrite (3) in polar coordinates :

$$-\frac{1}{r^{d-1}}(r^{d-1}\underbrace{\lambda_{\theta}^{-}u'(r)}_{\sigma})' = 1 \text{ in } \langle r_1, r_2 \rangle, \quad u(r_1) = u(r_2) = 0.$$

Observe that σ satisfies

$$\sigma = -\frac{r}{d} + \frac{\gamma}{r^{d-1}}, \quad \gamma > 0$$

 $\sigma(r): \langle 0, \infty \rangle \to \mathbb{R}$ is a strictly decreasing function.



The necessary and sufficient condition of optimality for θ^* states

$$\begin{aligned} |\sigma^*| > c &\Rightarrow \quad \theta^* = 1 \,, \\ |\sigma^*| < c &\Rightarrow \quad \theta^* = 0 \,. \end{aligned}$$

There are only three possible candidates for optimal design:

1)
$$\theta^*(r) = \begin{cases} 1, & r \in [r_1, r_+) \\ 0, & r \in [r_+, r_-) \\ 1, & r \in [r_-, r_2] \end{cases}$$

2) $\theta^*(r) = \begin{cases} 1, & r \in [r_1, r_+) \\ 0, & r \in [r_+, r_2) \end{cases}$
3) $\theta^*(r) = \begin{cases} 0, & r \in [r_1, r_-) \\ 1, & r \in [r_-, r_2) \end{cases}$

Simplification to a non-linear system

From condition of optimality a non-linear system (with unknowns γ, c, r_+, r_-) is created:

(NS) $\begin{cases} S_d \int_{r_1}^{r_2} \theta(\rho) \rho^{d-1} d\rho = q_\alpha \\ u(r_2) = 0 \iff \gamma \int_{r_1}^{r_2} \left(\frac{1}{a(\rho)\rho^{d-1}}\right) d\rho = \int_{r_1}^{r_2} \frac{\rho}{a(\rho)} d\rho \\ \sigma(r_+) = c, \quad \sigma(r_-) = -c, \quad \text{where } c > 0 \end{cases}$

where

$$\sigma(r) = \frac{\gamma}{r^{d-1}} - \frac{r}{d}, \quad \& \quad a(r) = \left(\frac{\theta(r)}{\alpha} + \frac{1 - \theta(r)}{\beta}\right)^{-1}$$

Important: For solving (NS) optimal design is assumed.

(Optimal design for annulus d = 2, 3, f = 1)

With previous assumptions problem (I) admits optimal solution with two possible designs:

1)
$$\theta^{*}(r) = \begin{cases} 1, & r \in [r_{1}, r_{+}) \\ 0, & r \in [r_{+}, r_{-}) \\ 1, & r \in [r_{-}, r_{2}] \end{cases}$$
2)
$$\theta^{*}(r) = \begin{cases} 1, & r \in [r_{1}, r_{+}) \\ 0, & r \in [r_{+}, r_{2}) \end{cases}$$

If q_{α} is small design 2) is optimal.

alpha-beta-alpha

alpha-beta



alpha-beta-alpha $(q_{\alpha} > \text{critical value})$



Shape derivative

Perturbation of the set Ω is given with

 $\Omega_t = (\mathrm{Id} + t\psi)\Omega$

where $\psi \in W^{k,\infty}(\mathbb{R}^d, \mathbb{R}^d)$.



Definition (Shape derivative)

Let $J = J(\Omega)$ be a shape functional. J is said to be shape differentiable at Ω in direction ψ if

$$J'(\Omega,\psi) := \lim_{t \searrow 0} \frac{J(\Omega_t) - J(\Omega)}{t}$$

exists and the mapping $\psi \mapsto J'(\Omega, \psi)$ is linear and continuous. $J'(\Omega, \psi)$ is called the **shape derivative**.

Single state problem (general f)

For single state optimal design problem:

(5)
$$\begin{cases} J(\chi) = \int_{\Omega} f u \, \mathrm{d}\boldsymbol{x} \to \max\\ \text{s.t.} \quad \chi \in L^{\infty}(\Omega, \{0, 1\}), \quad \int_{\Omega} \chi \, \mathrm{d}\boldsymbol{x} = q_{\alpha},\\ u \text{ solves (S) with } \mathbf{A} = \chi \alpha \mathbf{I} + (1 - \chi) \beta \mathbf{I} \end{cases}$$

shape derivative is given with:

$$J'(\Omega, \psi) = \int_{\Omega} \mathbf{A}(-\operatorname{div}(\psi) + \nabla \psi + \nabla \psi^{\tau}) \nabla u_0 \cdot \nabla u_0 \, \mathrm{d}\boldsymbol{x} + \int_{\Omega} 2(\operatorname{div}(\psi)f + \nabla f \cdot \psi) u_0 \, \mathrm{d}\boldsymbol{x}$$

where u_0 is solution of BVP (S) on domain Ω with $\mathbf{A} = \chi \alpha \mathbf{I} + (1 - \chi) \beta \mathbf{I}$.

Gradient method, Lagrange approach

Heuristics: do several iterations of the method, check results and adapt parameters.

Algorithm 1: iteration of the method

- 1 Input : mesh \mathcal{T}_k boundary is discretized (it is desirable to make a new triangulation)
- 2 Create function space Vh na \mathcal{T}_k (P1,P2,...)
- **3** Determine ascent vector $\psi \in \mathsf{Vh}$ from shape derivative
- 4 Calculate size of the step $t_0 > 0$ \mathcal{T}_k (in order to avoid creating elements with negative volume)
- **5** Update mesh $\mathcal{T}_{k+1} = (\mathrm{Id} + t_0 \psi) \mathcal{T}_k$

The main drawback of implementation is the need for frequent triangulation of the domain.

Regardless, the above-implemented method is fairly stable and quickly approximates the optimal shape with minimal user intervention.























































































































































































































































































































































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iteration













0.87

















iteration



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iteration



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0.87





























0.87









iteration



0.78 0 10 20 30 40 50 60 70 80 90






































































































































































Numerical results



Numerical results



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