Numerical approximation of classical optimal design on annuli

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The necessary and sufficient condition of optimality

Statement of the problem

Let $\Omega \subset \mathbb{R}^d$ be open and bounded set. It consists of two phases each with different isotropic conductivity: α, β $(0 < \alpha < \beta)$.
q_α is the prescribed volume of the first phase α $(0 < q_\alpha < |\Omega|)$.
$\chi \in L^\infty(\Omega, \{0,1\})$ a measurable characteristic function.

Conductivity can be expressed as

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

where

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

State functions $u_i \in \mathrm{H}_0^1(\Omega)$, $i = 1, 2, ..., m$ are solutions of the following boundary value problems:

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

Energy functional:

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

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

Optimal design problem:

$$(2) \qquad \begin{cases} I(\chi) = \sum_{i=1}^m \mu_i \int_\Omega f_i u_i \,\mathrm{d}\boldsymbol{x} \to \max \\ \text{s.t.} \quad \chi \in L^\infty(\Omega, \{0,1\}), \quad \int_\Omega \chi\,\mathrm{d}\boldsymbol{x} = q_\alpha, \\ \boldsymbol{u} \text{ solves (1) with } \mathbf{A} = \chi\alpha\mathbf{I} + (1-\chi)\beta\mathbf{I}. \end{cases}$$

If solution χ exists for (2) we call it *classical solution.*

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

Relaxed design: Effective conductivity

For characteristic functions relaxation consists of:

$$(3) \qquad \chi \in L^\infty(\Omega, \{0,1\}) \quad \rightsquigarrow \quad \theta \in L^\infty(\Omega, [0,1]),$$

with $\int_\Omega \theta\,\mathrm{d}\boldsymbol{x} := q_\alpha$.

Set of effective conductivities $\mathcal{K}(\theta)$:
$\mathbf{A} \in \mathcal{K}(\theta)$ iff there exists sequence of characteristic functions

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

Visual representation of a set $\mathcal{K}(\theta)$

$\mathcal{K}(\theta)$ is given in terms of eigenvalues

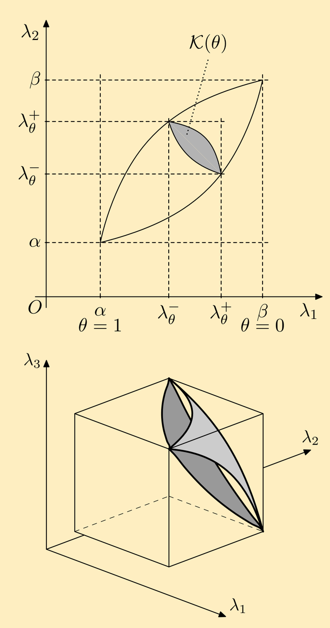
$$\lambda_\theta^- \le \lambda_j \le \lambda_\theta^+ \quad j = 1, \dots, d$$

$$\sum_{j=1}^d \frac{1}{\lambda_j - \alpha} \le \frac{1}{\lambda_\theta^- - \alpha} + \frac{d-1}{\lambda_\theta^+ - \alpha}$$

$$\sum_{j=1}^d \frac{1}{\beta - \lambda_j} \le \frac{1}{\beta - \lambda_\theta^-} + \frac{d-1}{\beta - \lambda_\theta^+},$$

where

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



Relaxed problem A:

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

Relaxed problem can be written as:

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

Generalized (convex) problem B

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

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

and with it

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

Using fluxes one can rewrite problem (B) as max-min problem and prove:

Theorem
Optimization problem (B) is equivalent to following optimization problem:

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

∎

The necessary and sufficient condition of optimality

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 $c \ge 0$ such that

$$(4) \qquad \begin{array}{l} \psi = \sum_{i=1}^m \mu_i |\boldsymbol{\sigma}_i^*|^2 > c \Rightarrow \theta^* = 1, \\ \psi = \sum_{i=1}^m \mu_i |\boldsymbol{\sigma}_i^*|^2 < c \Rightarrow \theta^* = 0. \end{array}$$

∎

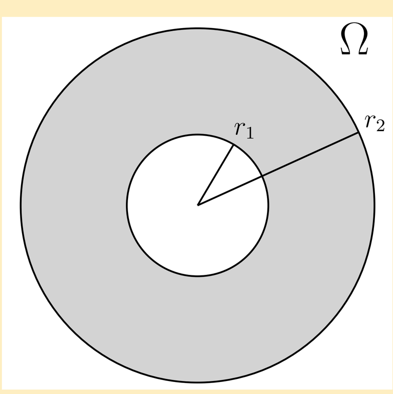
Analytical example on annulus for single state problem

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

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



$\Omega = \overline{K}(0, r_2) \backslash K(0, r_1)$

Single state equation:

$$(5) \qquad \begin{cases} -\mathrm{div}(\lambda_\theta^-(x)\nabla u) = 1 & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega \end{cases}$$

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

Optimization problem:
For $\theta \in \mathcal{T} :=$
$\{\theta \in L^\infty(\Omega, [0,1]) : \int_\Omega \theta\,\mathrm{d}x = q_\alpha\}$

$$I(\theta) = \int_\Omega u\,\mathrm{d}x \to \max$$

One can rewrite (5) in polar coordinates :

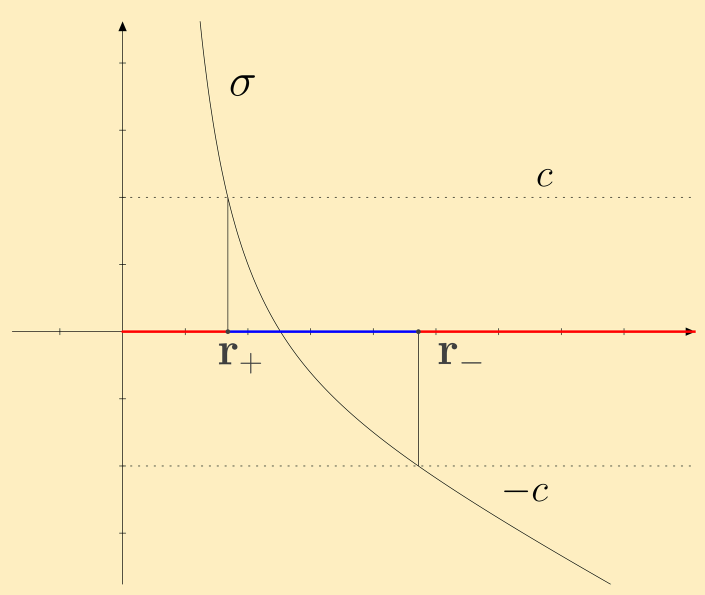
$$-\frac{1}{r^{d-1}}(r^{d-1}\underbrace{\lambda_\theta^- u'(r)}_{\sigma})' = 1 \text{ in } \langle r_1, r_2\rangle, \quad u(r_1) = u(r_2) = 0.$$

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

$$|\sigma^*| > c \Rightarrow \theta^* = 1,$$
$$|\sigma^*| < c \Rightarrow \theta^* = 0.$$



There are only three possible candidates for optimal design:

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

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

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

Direct calculations

Necessary and sufficient condition of optimality can also be expressed as a non-linear system (unknowns $\gamma, c, r_+ r_-$):

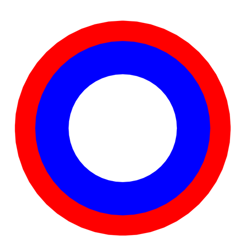
$$(6) \qquad \begin{cases} S_d \int_{r_1}^{r_2} \theta(\rho)\rho^{d-1}\,\mathrm{d}\rho = q_\alpha \\ u(r_2) = 0 \iff \gamma \int_{r_1}^{r_2} \left(\frac{1}{a(\rho)\rho^{d-1}}\right) \mathrm{d}\rho = \int_{r_1}^{r_2} \frac{\rho}{a(\rho)}\,\mathrm{d}\rho \\ \sigma(r_+) = c, \quad \sigma(r_-) = -c, \qquad \text{where } c > 0 \end{cases}$$

where

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

Results for $d = 2, 3$

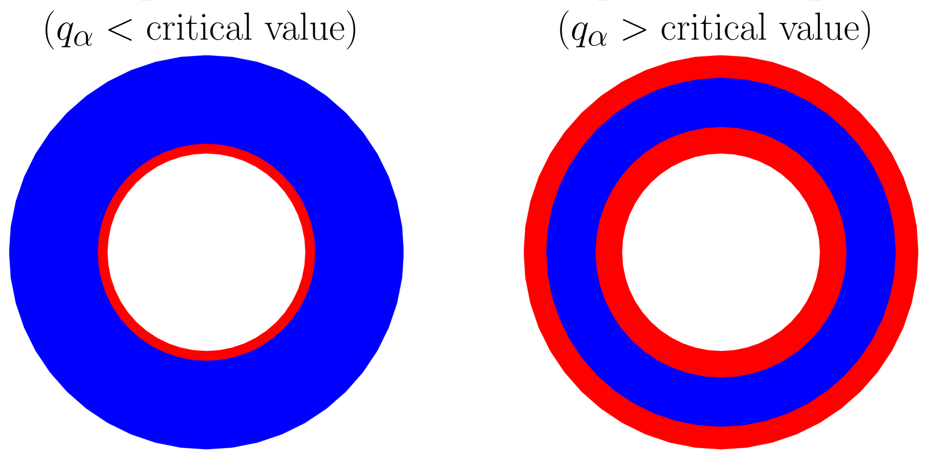
3) case beta-alpha



Non-linear system (6) does not admit a solution (proved for $d = 2$ and $d = 3$).

Therefore, cases: 1) and 2) should be considered as only possible solutions. One can easily prove if q_α is very small, case alpha-beta is always solution (for arbitrary chosen parameters α, β, r_1, r_2).

Furthermore, one can numerically obtain critical value for which optimal design changes from case alpha-beta to alpha-beta-alpha.



Remark:
- Problem can be easily generalized to multi-state problem for example $m = 2$;

$$f_1(r) = 1, \quad f_2(r) = \frac{b}{r(b-r)^2}, \qquad \text{where } b > r_2$$

- Existence of such solutions is important for any numerical method like shape derivative method.

Gradient method using shape derivative

Perturbation of the set Ω is given with

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

where $\psi \in W^{k,\infty}(\mathbb{R}^d, \mathbb{R}^d)$
If t is small (i.e. $\|t\psi\|_{W^{k,\infty}} \ll 1$) mapping $\mathrm{Id} + t\psi$ is homeomorphism. This allows us to define shape derivative:

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**.

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For our optimal design problem : shape derivative is given with:

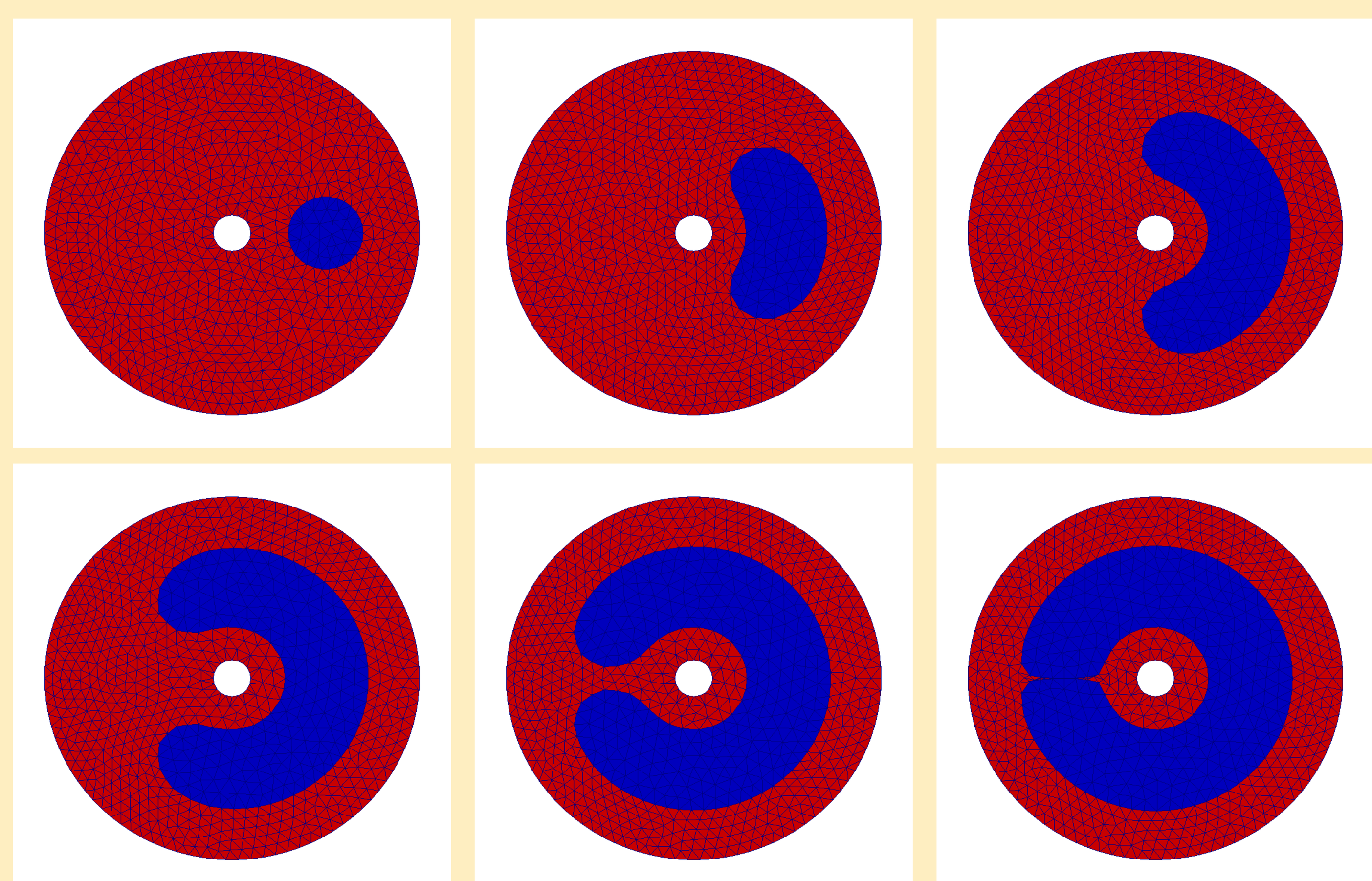
$$J'(\Omega, \psi) = \int_\Omega \mathbf{A}(-\mathrm{div}(\psi) + \nabla\psi + \nabla\psi^\tau)\nabla u_0 \cdot \nabla u_0 \,\mathrm{d}\boldsymbol{x} + \int_\Omega 2(\mathrm{div}(\psi)f + \nabla f \cdot \psi)u_0 \,\mathrm{d}\boldsymbol{x}$$

where u_0 is solution of BVP (1) on domain Ω with $\mathbf{A}$.
Vector field $\psi \in H_0^1(\Omega)$ is constructed from:

$$\int_\Omega \nabla\psi : \nabla\varphi + \int_\Omega \psi \cdot \varphi = J'(\Omega, \varphi), \quad \forall\varphi \in H_0^1(\Omega)$$

The shape is evolved by gradually moving the boundary between phases.

Numerical results:



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