Shape derivative method for optimal design in conductivity problem

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Let $\Omega \subset \mathbb{R}^d$ be open and bounded set. Two phases each with different isotropic conductivity: $\alpha, \beta$ ($0 < \alpha < \beta$).

$q_\alpha$ is the prescribed volume of the first phase $\alpha$ ($0 < q_\alpha < |\Omega|$). $\chi \in L^\infty(\Omega)$ such that $\chi(1 - \chi) = 0$.

State function $u \in H^1_0(\Omega)$ is a solution of the following boundary value problem:

\begin{equation}
\begin{cases}
- \text{div}(A \nabla u) = f & \text{in } \Omega \\
 u = 0 & \text{on } \partial \Omega,
\end{cases}
\end{equation}

Energy functional:

\[ J(\chi) := \int_{\Omega} f(\boldsymbol{x})u(\boldsymbol{x}) \, d\boldsymbol{x}. \]

Conductivity can be expressed as

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

where

\[ \int_{\Omega} \chi(\boldsymbol{x}) \, d\boldsymbol{x} = q_\alpha. \]
Statement of the problem

Optimal design problem:

\[
\begin{align*}
J(\chi) &= \int_{\Omega} fu \, dx \rightarrow \max \\
\text{s.t.} & \quad \chi \in L^\infty(\Omega, \{0, 1\}), \quad \int_{\Omega} \chi \, dx = q\alpha, \\
& \quad u \text{ solves (1) with } A = \chi\alpha I + (1 - \chi)\beta I.
\end{align*}
\]

If solution $\chi$ exists for (P) we call it \textit{classical solution}.

\textbf{Important: } For general optimal design problems the classical solutions usually does not exist.

\textbf{Aim of this talk:}

- to present examples of classical solutions on annuli.
- solve problem numerically using shape derivative method.
Relaxed design

For characteristic functions relaxation consists of:

\[(2) \quad \chi \in L^\infty(\Omega, \{0, 1\}) \leadsto \theta \in L^\infty(\Omega, [0, 1]),\]

with

\[\int_\Omega \theta \, dx := q_\alpha.\]

Notion of H-convergence is introduced for conductivity $A$.

**Effective conductivities:**

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

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

\[
\left\{
\begin{array}{l}
\chi_n \xrightarrow{L^\infty} \theta \\
A^n = \chi_n \alpha I + (1 - \chi_n) \beta I \xrightarrow{H} A.
\end{array}
\right.
\]
Effective conductivities - set $\mathcal{K}(\theta)$

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

$$\lambda_\theta^- \leq \lambda_j \leq \lambda_\theta^+ \quad j = 1, \ldots, d$$

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

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

where

$$\begin{align*}
\lambda_\theta^+ &= \theta \alpha + (1 - \theta) \beta \\
\frac{1}{\lambda_\theta^-} &= \frac{\theta}{\alpha} + \frac{1 - \theta}{\beta}.
\end{align*}$$
Generalized (convex) problem

Relaxed design:

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

Relaxed problem can be written as:

\[ (A) \quad \max_{(\theta, \mathbf{A}) \in A} J(\theta, \mathbf{A}) = \max_{(\theta, \mathbf{A}) \in A} \int_\Omega f u \, d\mathbf{x} \]

Unfortunately, \( A \) is not a convex set. To achieve convexity, an enlarged set is introduced:

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

and with it

\[ (B) \quad \max_{(\theta, \mathbf{A}) \in B} J(\theta, \mathbf{A}) = \max_{(\theta, \mathbf{A}) \in B} \int_\Omega f u \, d\mathbf{x} \]
Rewrite $B$ as a max-min problem

Define $S := \{\sigma \in L^2(\Omega, \mathbb{R}^d), \ - \text{div}(\sigma) = f\}$

One can rewrite functional $J$ in terms of fluxes:

$$J(\theta, A) = \min_{\sigma \in S} \int_{\Omega} A^{-1} \sigma \cdot \sigma$$

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

$$\max_{(\theta, A) \in B} J(\theta, A) = \max_{(\theta, A) \in B} \min_{\sigma \in S} \int_{\Omega} A^{-1} \sigma \cdot \sigma$$

$$= \max_{(\theta, B) \in C} \min_{\sigma \in S} \int_{\Omega} B \sigma \cdot \sigma$$
Conclusions

Next step is to apply theory of saddle points. First, one can conclude that $\sigma^*$ is unique. Second, instead of solving convex problem $B$, one can solve the following optimization problem:

\[
\begin{aligned}
I(\theta) &= \int_{\Omega} f u \, dx \to \max \\
\text{s.t. } &\theta \in L^\infty(\Omega, [0, 1]), \int_{\Omega} \theta = q_\alpha, \text{ where } u \text{ satisfies} \\
&- \text{div}(\lambda^\theta \nabla u) = f, \quad u \in H^1_0(\Omega)
\end{aligned}
\]

Define $\psi := |\sigma^*|^2$.

Lemma

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

\[
\psi > c \Rightarrow \theta^* = 1, \\
\psi < c \Rightarrow \theta^* = 0.
\]
Spherical symmetry

For spherically symmetric problem such that:

- $\Omega = R(\Omega)$ for any rotation $R$
- $f$ is radial function

it can be proved that there exists radial solution $\theta^*_R$ of (I).

In particular, it can be shown that

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

Design problems with spherical symmetry were studied for ball:

- **Single state equations**

- **Multiple state equations**
Single state optimal design problem

\[ \Omega = K(0, r_2) \setminus K(0, r_1) \]

Single state equation:

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

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

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

\[
I(\theta) = \int_\Omega u \, dx \rightarrow \max
\]

One can rewrite (4) in polar coordinates:

\[- \frac{1}{r^{d-1}} \left( r^{d-1} \lambda_\theta^{-1} u' \right)' = 1 \text{ in } (r_1, r_2), \quad u(r_1) = u(r_2) = 0.\]
The necessary and sufficient condition of optimality for $\theta^*$ states

$$|\sigma^*| > c \implies \theta^* = 1,$$

$$|\sigma^*| < c \implies \theta^* = 0.$$ 

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) $\theta^*(r) = \begin{cases} 
0, & r \in [r_1, r_-] \\
1, & r \in [r_-, r_2] 
\end{cases}$
Necessary and sufficient condition of optimality can also be expressed as a non-linear system (unknowns $\gamma, c, r_+ r_-)$:

\[
\begin{aligned}
S_d \int_{r_1}^{r_2} \theta(\rho) \rho^{d-1} \, d\rho &= q_\alpha \\
\sigma(r_+) &= c, \quad \sigma(r_-) = -c, \quad \text{where } c > 0
\end{aligned}
\]

where

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

With this you can easily calculate the shape of domain.
Analytical solution:
\[ f = 1, \text{ domain } \Omega \text{ is annulus and amount } q_\alpha \text{ is not scarce one can prove that shape design } \alpha - \beta - \alpha \text{ is optimal solution.} \]

Remark:
- Problem can be generalized to multi-state problem where functional is given with \( J(\chi) = \sum_{i=1}^{m} \mu_i \int_{\Omega} f_i u_i. \)
- Existence of such solutions is important for any numerical method like shape derivative method.
Shape derivative

Perturbation of the set $\Omega$ is given with

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

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

This allows us to define shape derivative:

If $t$ is small (i.e. $\|t\psi\|_{W^{k,\infty}} \ll 1$) mapping $\text{Id} + t\psi$ is homeomorphism.

### Definition (Shape derivative)

Let $J = J(\Omega)$ be a shape functional. $J$ is said to be shape differentiable at $\Omega$ in direction $\psi$ 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 optimal design problem:

\[
\begin{cases}
  J(\chi) = \int_\Omega fu \, dx \to \max \\
  \text{s.t. } \chi \in L^\infty(\Omega, \{0, 1\}), \quad \int_\Omega \chi \, dx = q_\alpha, \\
  u \text{ solves (1) with } A = \chi \alpha I + (1 - \chi) \beta I.
\end{cases}
\]

shape derivative is given with:

\[
J'(\Omega, \psi) = \int_\Omega A(- \text{div}(\psi) + \nabla \psi + \nabla \psi^\tau) \nabla u_0 \cdot \nabla u_0 \, dx \\
+ \int_\Omega 2(\text{div}(\psi) f + \nabla f \cdot \psi) u_0 \, dx
\]

where $u_0$ is solution of BVP (1) on domain $\Omega$ with $A$. 
Choice of vector field $\psi$:
Vector field $\psi \in H_0^1(\Omega)$ can be constructed from variational formulation:

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

With this approach regularity of $\psi$ is higher than usual ($L^2$) which is particularly good regardless the method.
Observe that thus created $\psi$ is ascent direction for our problem because

$$J(\Omega_t) = J(\Omega) + tJ'(\Omega, \psi) + o(t)$$

and

$$J'(\Omega, \psi) = \|\psi\|_{H^1}^2 > 0 \text{ (by construction)}$$
Lagrangian method using shape derivative

It is important to note:

- outer boundaries stays the same
- only boundary between phases is changing.

This is implemented using `movemesh` from freefem++. Remeshing is necessary with this approach.

⇒ one step $\phi_t$
Numerical results - simple connected set
Numerical results