Shape derivative method and application to optimal design problems

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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

$$\int_{\Omega} \chi(x) \, dx = q_\alpha.$$ 

Conductivity can be expressed as

$$A(\chi) := \chi \alpha I + (1 - \chi) \beta I,$$
State functions $u_i \in H^1_0(\Omega)$, $i = 1, 2, \ldots, m$ are given as a solution of the following boundary value problems:

\[
\begin{cases}
-\text{div}(A \nabla u_i) = f_i & \text{in } \Omega \\
u = 0 & \text{on } \partial \Omega,
\end{cases}
\tag{S}
\]

with $A = \chi \alpha I + (1 - \chi) \beta I$. Denote $u = (u_1, \ldots, u_m)$.

Energy functional:

\[
J(\chi) := \sum_{i=1}^{m} \mu_i \int_{\Omega} f_i(\mathbf{x}) u_i(\mathbf{x}) \, d\mathbf{x},
\]

where $\mu_i > 0$, $i = 1, 2, \ldots, m$. 
Statement of the problem

Optimal design problem:

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

If solution \( \chi \) exists for (P) we call it \textit{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:

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

with

\[\int_{\Omega} \theta \, d\mathbf{x} := q_\alpha.\]

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

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

$$\lambda_\theta^+ = \theta \alpha + (1 - \theta) \beta$$

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

Relaxed design:

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

Relaxed problem can be written as:

\[
\text{(A)} \quad \max_{(\theta, A) \in \mathcal{A}} J(\theta, A) = \max_{(\theta, A) \in \mathcal{A}} \sum_{i=1}^{m} \mu_i \int_\Omega f_i u_i \, dx
\]

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

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

and with it

\[
\text{(B)} \quad \max_{(\theta, A) \in \mathcal{B}} J(\theta, A) = \max_{(\theta, A) \in \mathcal{B}} \sum_{i=1}^{m} \mu_i \int_\Omega f_i u_i \, dx
\]
Rewrite $B$ as a max-min problem

Define $S := \{ \sigma = (\sigma_1, \sigma_2, \ldots, \sigma_m) \mid \sigma_i \in L^2(\Omega, \mathbb{R}^d), \quad -\text{div}(\sigma_i) = f_i \}$

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

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

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

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

$$= \max_{(\theta, B) \in C} \min_{\sigma \in S} \sum_{i=1}^{m} \mu_i \int_{\Omega} B \sigma_i \cdot \sigma_i$$
Observe that

\[ L(\sigma, (\theta, B)) = \sum_{i=1}^{m} \mu_i \int_{\Omega} B \sigma_i \cdot \sigma_i \]

\( \sigma \mapsto L(\sigma, (\theta, B)) \)

\( (\theta, B) \mapsto L(\sigma, (\theta, B)) \)

- quadratic (strictly convex)
- linear (concave)
- continuous in \( L^2(\Omega) \) (l.s.c.)
- continuous in \( L^{\infty*} \) (u.s.c.)
- \( \exists (\theta, B) \) \( \sigma \mapsto L(\sigma, (\theta, B)) \)
- \( \lim_{\|\sigma\| \to +\infty} L(\sigma, (\theta, B)) = +\infty \)
- set \( C \) is compact (in \( L^{\infty*} \)).
Min-max theory

Previous conclusions for the Lagrange functional $L$ implies:
- set of saddle points $S_0 \times C_0 \subset S \times C$ is not empty
- min and max are interchangeable
- $\sigma \mapsto L(\sigma, (\theta, B))$ is strictly convex $\Rightarrow S_0 = \{\sigma^*\}$.

This means that there exists unique $\sigma^*$ such that this holds

$$
\max_{(\theta, A) \in B} J(\theta, A) = \max_{(\theta, B) \in C} \min_{\sigma \in S} L(\sigma, (\theta, B))
$$

$$
= \max_{(\theta, B) \in C} L(\sigma^*, (\theta, B))
$$

$$
= \max_{(\theta, B) \in C} \sum_{i=1}^{m} \mu_i \int_{\Omega} B \sigma^*_i \cdot \sigma^*_i
$$
Conclusions

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

\[
\begin{align*}
I(\theta) &= \sum_{i=1}^{m} \mu_i \int_{\Omega} f_i u_i \, d\mathbf{x} \to \text{max} \\
\text{s.t.} \quad \theta &\in L^\infty(\Omega, [0, 1]), \quad \int_{\Omega} \theta = q_\alpha, \text{ where } u_i \text{ satisfies} \\
-\text{div}(\lambda_\theta^{-} \nabla u_i) &= f_i, \quad u_i \in H_0^1(\Omega), \quad i = 1, 2, \ldots, m
\end{align*}
\]

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 \( \theta^*_R \) of (I).

In particular, it can be shown that

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

Define

\[ \Psi := \sum_{i=1}^{m} \mu_i |\sigma_i^*|^2. \]

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

\[(2) \quad \Psi > c \quad \Rightarrow \quad \theta^* = 1, \]

\[ \Psi < c \quad \Rightarrow \quad \theta^* = 0. \]
Single state optimal design problem

Single state equation:

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

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

Optimization problem:

\[
I(\theta) = \int_{\Omega} u \, d\mathbf{x} \rightarrow \max
\]

\[
\text{s.t. } \theta \in L^\infty(\Omega, [0, 1]), \quad \int_{\Omega} \theta = q_{\alpha}, \text{ where } u \text{ satisfies (3)}
\]
Single state optimal design problem

One can rewrite \((3)\) in polar coordinates:

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

Observe that \(\sigma\) satisfies

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

\(\sigma(r) : \langle 0, \infty \rangle \rightarrow \mathbb{R}\) is a strictly decreasing function.
The necessary and sufficient condition of optimality for $\theta^*$ states

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

There are only three possible candidates for optimal design:

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

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 $\gamma, c, r_+, r_-$) is created:

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

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

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

If $q_\alpha$ is small design 2) is optimal.

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**alpha-beta**  \hspace{2cm} (q_\alpha < \text{critical value})

**alpha-beta-alpha**  \hspace{2cm} (q_\alpha > \text{critical value})
Shape derivative

Perturbation of the set $\Omega$ is given with

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

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

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.
For single state optimal design problem (with transmission condition):

\[
J(\chi) = \int_{\Omega} f u \, d\mathbf{x} \rightarrow \max \\
\text{s.t. } \chi \in L^\infty(\Omega, \{0, 1\}), \quad \int_{\Omega} \chi \, d\mathbf{x} = q_\alpha, \\
u \text{ solves } (S) \text{ with } A = \chi \alpha \mathbf{I} + (1 - \chi) \beta \mathbf{I}
\]

(5)

shape derivative is given with:

\[
J'(\Omega, \psi) = \int_{\Omega} A(-\text{div}(\psi) + \nabla \psi + \nabla \psi^T) \nabla u_0 \cdot \nabla u_0 \, d\mathbf{x} \\
+ \int_{\Omega} 2(\text{div}(\psi)f + \nabla f \cdot \psi)u_0 \, d\mathbf{x}
\]

where \(u_0\) is solution of BVP (S) on domain \(\Omega\) with

\[A = \chi \alpha \mathbf{I} + (1 - \chi) \beta \mathbf{I}.\]
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 $\psi \in Vh$ 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 $\mathcal{T}_{k+1} = (Id + t_0\psi)\mathcal{T}_k$

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.
Numerical results

The graph shows the relationship between the angle $\eta$ and the radius $r_+$.

- The blue line with circles represents the optimal radius $r_+$.
- The red line with squares represents the numerical radius $r_+$.

The data points are marked at specific values of $\eta$ and correspond to the numerical results.
Numerical results

![Graph showing two lines: one for $r_-$ optimal and another for $r_-$ numerical. The x-axis represents $\eta$ ranging from 0.3 to 0.8, and the y-axis represents the radius $r_-$ ranging from 1.8 to 1.6. The lines show a linear relationship between $\eta$ and $r_-$.](image-url)
References


