Methods based on shape derivative for the optimal design on annulus

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VIII Partial differential equations, optimal design and numerics
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Part I: Construction of classical solutions for optimal design problems
Introduction

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

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

where

Conductivity can be expressed as

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

$\beta$
$\Omega$
$\alpha$
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:

\[
\begin{align*}
\text{(S)} & \quad \begin{cases}
-\text{div}(A \nabla u_i) = f_i & \text{in } \Omega \\
u = 0 & \text{on } \partial \Omega,
\end{cases} \\
& \quad i = 1, 2, \ldots, m,
\end{align*}
\]

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 $\mu_i > 0, \ i = 1, 2, \ldots, m$. 
Optimal design problem:

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

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

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

\textbf{Important:} For general optimal design problems the classical solutions usually do not exist.
Results from general theory

\[
I(\theta) = \sum_{i=1}^{m} \mu_i \int_{\Omega} f_i u_i \, d\mathbf{x} \rightarrow \text{max}
\]

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

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

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 if \( \theta^*_R \) is classical it is also a solution of problem \( (P) \). Also, state functions \( u_i \) and fluxes \( \sigma_i = a \nabla u_i \) are radial functions and \( \sigma_i \) are unique.
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

\begin{align*}
\Psi > c & \Rightarrow \theta^* = 1, \\
\Psi < c & \Rightarrow \theta^* = 0.
\end{align*}

(1)
Single state optimal design problem

Single state equation:

\[
\begin{aligned}
(2) \quad & \begin{cases} 
- \text{div}(\lambda_\theta(x) \nabla u) = 1 & \text{in } \Omega \\
  u = 0 & \text{on } \partial \Omega
\end{cases} \\
& \text{where } \lambda_\theta(x) = \left( \frac{\theta(x)}{\alpha} + \frac{1 - \theta(x)}{\beta} \right)^{-1}.
\end{aligned}
\]

Optimization problem:

\[
\begin{aligned}
(3) \quad & \begin{cases} 
I(\theta) = \int_{\Omega} u \, dx \rightarrow \text{max} \\
  s.t. \quad & \theta \in L^\infty(\Omega, [0, 1]), \quad \int_{\Omega} \theta = q_\alpha, \text{ where } u \text{ satisfies (2)}
\end{cases}
\end{aligned}
\]
Single state optimal design problem

One can rewrite (2) 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 $\sigma$ 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 $\theta^*$ 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) $\theta^*(r) = \begin{cases} 
0, & r \in [r_1, r_-) \\
1, & r \in (r_-, r_2]
\end{cases}$
Simplification to a non-linear system

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

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

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.
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 \( q_\alpha \) is small design 2) is optimal.

\[ \text{alpha-beta} \quad (q_\alpha < \text{critical value}) \]

\[ \text{alpha-beta-alpha} \quad (q_\alpha > \text{critical value}) \]
Part II: Numerical methods based on shape derivative

description of methods, numerical solutions in 2D & 3D.
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.
Single state problem

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

\[
\begin{cases}
J(\chi) = \int_{\Omega} fu \, dx \rightarrow \max \\
\text{s.t.} \quad \chi \in L^\infty(\Omega, \{0, 1\}), \quad \int_{\Omega} \chi \, dx = q_\alpha,
\end{cases}
\]

\[u \text{ solves (S) with } A = \chi \alpha I + (1 - \chi) \beta I\]

shape derivative is given with:

\[
J'(\Omega, \psi) = \int_{\Omega} A(- \text{div}(\psi) + \nabla \psi + \nabla \psi^\top) \nabla u \cdot \nabla u \, dx
\]

\[+ \int_{\Omega} 2 \text{div}(f \psi) u \, dx\]

where \(u\) is solution of BVP (S) on domain \(\Omega\) with \(A = \chi \alpha I + (1 - \chi) \beta I\).
Gradient method based on shape derivative

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

Algorithm 1: iteration of the method

1. Input: interface is given implicitly (LSF) or explicitly as discretized set of points - triangulation mesh $\mathcal{T}_k$

2. Create function space $Vh_{\mathcal{T}_k}$ (P1,P2,...)

3. Determine ascent vector $\psi \in Vh$ from shape derivative (consists of solving several PDEs)

4. Output: update interface (depends highly on considered representation of interface)

- above implemented methods are fairly stable with minimal user intervention
- in 2D it quickly approximates the optimal shape and script is under 100 lines of code
Numerical results

The graph shows the relationship between the radius $r_+$ and the parameter $\eta$. The blue line represents the optimal radius $r_+$, while the red squares represent the numerical radius $r_+$. The data points are plotted at $\eta = 0.3, 0.4, 0.5, 0.6, 0.7, 0.8$, with corresponding values of $r_+$. The graph visually demonstrates how $r_+$ increases with $\eta$. The values for $\eta$ range from 0.3 to 0.8, and the $r_+$ values are approximately 1.15, 1.2, 1.25, 1.3, 1.35, and 1.4, respectively.
Numerical results

$\begin{align*}
\eta & \quad r_- \quad \text{optimal} \\
0.3 & \quad 1.8 \\
0.4 & \quad 1.7 \\
0.5 & \quad 1.6 \\
0.6 & \quad 1.5 \\
0.7 & \quad 1.4 \\
0.8 & \quad 1.3
\end{align*}$
(a) 3D representation of material $\beta$ (yellow)  
(b) slice of volume representation at $z = 0$
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Part III: Second order shape derivative

Work in progress
We are interested in the second order expansions of $J$:

$$J((\text{Id} + \psi)\Omega) = J(\Omega) + J'(\Omega; \psi) + \frac{1}{2} J''(\Omega; \psi, \psi) + o(\|\psi\|^2_k)$$

**Important:** This is not a variations of first order shape derivative

$$J''(\Omega; \psi_1, \psi_2) \neq (J'(\Omega; \psi_1))'(\Omega; \psi_2) = \lim_{t \to 0} \frac{1}{t} (J'(\text{Id} + t\psi_2)\Omega; \psi_1) - J'(\Omega; \psi_1).$$

but the following identity holds

$$J''(\Omega; \psi_1, \psi_2) = (J'(\Omega; \psi_1))'(\Omega; \psi_2) - J'(\Omega; \nabla\psi_1\psi_2).$$
By standard method of using local derivative $u'(\psi)$:

\[
J''(\Omega; \psi_1, \psi_2) = \\
\alpha \int_{\Gamma} (\psi_1 \cdot n_\alpha)(\psi_2 \cdot n_\alpha) \left\{ \mathbf{H} \left[ 2 \left| \frac{\partial u_\alpha}{\partial n_\alpha} \right|^2 - |\nabla u_\alpha|^2 \right] + \frac{\partial}{\partial n_\alpha} \left[ 2 \left| \frac{\partial u_\alpha}{\partial n_\alpha} \right|^2 - |\nabla u_\alpha|^2 \right] \right\} \, dS \\
- \beta \int_{\Gamma} (\psi_1 \cdot n_\alpha)(\psi_2 \cdot n_\alpha) \left\{ \mathbf{H} \left[ 2 \left| \frac{\partial u_\beta}{\partial n_\alpha} \right|^2 - |\nabla u_\beta|^2 \right] + \frac{\partial}{\partial n_\alpha} \left[ 2 \left| \frac{\partial u_\beta}{\partial n_\alpha} \right|^2 - |\nabla u_\beta|^2 \right] \right\} \, dS \\
- \frac{2(\beta + \alpha)\alpha}{\beta - \alpha} \int_{\Omega_\alpha} \nabla u'_\alpha(\psi_1) \cdot \nabla u'_\alpha(\psi_2) \, dx + \frac{2(\beta + \alpha)\beta}{\beta - \alpha} \int_{\Omega_\beta} \nabla u'_\beta(\psi_1) \cdot \nabla u'_\beta(\psi_2) \, dx \\
+ \frac{2\alpha\beta}{\beta - \alpha} \int_{\Gamma} u'_\beta(\psi_1) \frac{\partial u'_\alpha(\psi_2)}{\partial n_\alpha} + u'_\alpha(\psi_2) \frac{\partial u'_\beta(\psi_1)}{\partial n_\alpha} + u'_\alpha(\psi_1) \frac{\partial u'_\beta(\psi_2)}{\partial n_\alpha} + u'_\beta(\psi_2) \frac{\partial u'_\alpha(\psi_1)}{\partial n_\alpha} \, dS \\
+ \alpha \int_{\Gamma} Z(\psi_1, \psi_2) \left[ 2 \left| \frac{\partial u_\alpha}{\partial n_\alpha} \right|^2 - |\nabla u_\alpha|^2 \right] \, dS - \beta \int_{\Gamma} Z(\psi_1, \psi_2) \left[ 2 \left| \frac{\partial u_\beta}{\partial n_\alpha} \right|^2 - |\nabla u_\beta|^2 \right] \, dS
\]
where

\[ Z(\psi_1, \psi_2) = \nabla n_\alpha^T (\psi_1)_{\Gamma} \cdot (\psi_2)_{\Gamma} - \nabla_{\Gamma} (\psi_1 \cdot n_\alpha) \cdot (\psi_2)_{\Gamma} - \nabla_{\Gamma} (\psi_2 \cdot n_\alpha) \cdot (\psi_1)_{\Gamma} \]

and \( u \) is a solution of (S). Local derivative \( u'(\psi) \in H^1(\Omega_\alpha \cup \Omega_\beta) \) is a solution of the following transmission problem with discontinuous jumps on the interface:

\[
\begin{aligned}
\Delta u'(\psi) &= 0 \quad \text{in } \Omega_\alpha \cup \Omega_\beta, \\
\left\{ \begin{array}{l}
    u'_\alpha(\psi) - u'_\beta(\psi) = \frac{\alpha - \beta}{\beta} (\nabla u_\alpha \cdot n_\alpha)(\psi \cdot n_\alpha) \\
    \alpha \nabla u'_\alpha(\psi) \cdot n_\alpha - \beta \nabla u'_\beta(\psi) \cdot n_\alpha = (\alpha - \beta) \text{div}_{\Gamma} (\nabla_{\Gamma} u(\psi \cdot n_\alpha)) \\
    u'(\psi) = 0
\end{array} \right. \quad \text{on } \Gamma, \\
& \quad \text{on } \partial \Omega.
\end{aligned}
\]
Volume representation:

\[ J''(\Omega; \psi_1, \psi_2) = \int_{\Omega} a \left[ - \text{div} \psi_1 \text{div} \psi_2 \mathbf{I} + \nabla \psi_1 : \nabla \psi_2^T \mathbf{I} - \nabla \psi_1 \nabla \psi_2^T - \nabla \psi_2 \nabla \psi_1^T \right] \nabla u \cdot \nabla u \, dx \]

\[ + \int_{\Omega} a \left[ - \nabla \psi_1 \nabla \psi_2 - \nabla \psi_2 \nabla \psi_1 - \nabla \psi_1^T \nabla \psi_2^T - \nabla \psi_2^T \nabla \psi_1^T \right] \nabla u \cdot \nabla u \, dx \]

\[ + \int_{\Omega} a \left[ \text{div} \psi_1 (\nabla \psi_2 + \nabla \psi_2^T) + \text{div} \psi_2 (\nabla \psi_1 + \nabla \psi_1^T) \right] \nabla u \cdot \nabla u \, dx \]

\[ + 2 \int_{\Omega} [f \text{div} \psi_1 \text{div} \psi_2 + \psi_1 \cdot \nabla f \text{div} \psi_2 + \psi_2 \cdot \nabla f \text{div} \psi_1 + Hf \psi_2 \cdot \psi_1] u \, dx \]

\[ - 2 \int_{\Omega} \nabla \psi_1 : \nabla \psi_2^T f u \, dx + \frac{1}{2} \int_{\Omega} a \nabla v(\psi_1) \cdot \nabla v(\psi_2) \, dx \]

where \( u \) is a solution of (S) and \( v(\psi) \in H^1_0(\Omega) \) satisfies following equality for any \( \varphi \in H^1_0(\Omega) \):

\[ \int_{\Omega} a \nabla v(\psi) \cdot \nabla \varphi \, dx = 2 \int_{\Omega} \text{div}(f\psi) \varphi \, dx + 2 \int_{\Omega} a \left[ - \text{div}(\psi) \mathbf{I} + \nabla \psi + \nabla \psi^T \right] \nabla u \cdot \nabla \varphi \, dx. \]


Henrot, A., Pierre M. *Shape Variation and Optimization* (2018)
