Irregularity of shape optimization problems and an improvement technique

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Abstract

Shape optimization problems of linear elastic bodies, flow fields, magnetic fields, etc. for equilibrium types can be generalized as optimization problems of domains in which elliptic boundary value problems are defined. This paper shows that ordinary domain optimization problems do not have sufficient regularity and proposes a technique to overcome this irregularity. It briefly describes the derivation of the shape gradient functions for a self-adjoint shape optimization problem, and shape identification problems of the Dirichlet type, Neumann type and subdomain gradient assigned type. Using these shape gradient functions, the irregularity of ordinary domain optimization problems is shown through a discussion of the ill-posedness that occurs when the gradient method in Hilbert space is applied directly. To overcome this irregularity, the idea of a smoothing gradient method in Hilbert space is proposed. It is conclusively shown that a numerical method based on this idea coincides with the traction method previously proposed by one of the authors and this conclusion is verified by numerical experiments.

1 Introduction

Essential issues in mechanical or structural design include the determination of layouts and shapes of components. To improve the performance of machines or structures, techniques for optimizing layouts and shapes are thus required. Various optimization techniques have been researched and implemented with an eye toward achieving greater efficiency and economy. One way of classifying these techniques is according to the procedure for dealing with the topology of structures or the layout of components:
Another way is to classify them according to the types of design variables:

A) vector (parametric)
B) distributed function (nonparametric)

These classifications can be combined to yield four categories. Zero-one programming problems of structural components fall under the category of a)-A) and have been investigated by many researchers. The topology optimization technique based on the homogenization method is a typical approach that has achieved great success in the category of a)-B). Another successful approach falling in the category of a)-B) is to solve the optimum topology related to continuum problems involving distributed grilles. Parametric optimization problems using CAD data are included in category b)-A) and have been solved with integrated CAE software in recent years using the mathematical programming techniques. Approaches that limit the degrees of freedom defining geometrical shapes to a finite number, such as by using the basis vectors or the spline functions, fall under the category of b)-A). However, no effective approaches have been found in the category b)-B).

The reason why approaches in category b)-B) have failed is related to the irregularity of shape optimization problems. Shape optimization problems in category b)-B) are stated as a domain optimization problem in which the objective functional depends on the geometrical shape of the domain through the solution of a boundary value problem defined on the domain. In this paper, for simplicity, we deal with the elliptic type of boundary value problem that arises in shape optimization problems of linear elastic bodies, flow fields, magnetic fields and the like.

This domain optimization problem is formulated by selecting a one parameter family of continuous mapping functions as the design variable that is defined in an initial domain and yields a variable domain as shown by Cea\textsuperscript{1} and Zolesio.\textsuperscript{2} The shape sensitivity function, also known as the shape gradient function, for an objective functional relative to domain variation can be derived using the Lagrange multiplier method, also known as the adjoint method,\textsuperscript{3} and the theory related with the material derivative in continuum mechanics.

Following the gradient method, we can consider a technique for deforming the shape of the domain by moving the boundary to the outside in proportion to the negative value of the shape gradient function. However, it is known that an iteration in which a shape is varied by moving the nodes of the finite element model in proportion to the value of the shape gradient function that is also evaluated using a finite element model in advance often results in an oscillating shape. Imam\textsuperscript{4} in 1982 pointed out this irregularity and proposed methods for limiting the degrees of freedom. Braibant and Fleury\textsuperscript{5} in 1984 presented numerical results that indicated an unrealistic shape was generated by moving the nodes in a finite element mesh. Based on that observation, they proposed the use of B-spline curves to control shapes. Kikuchi, Chung, Torigaki and Taylor\textsuperscript{6} in 1986 showed that the optimal shape strongly depends on the shape of finite elements near the
design boundary. As a remedy, they proposed the application of adaptive finite element methods.

The necessity of regularity concerning a boundary on which an elliptic boundary value problem is defined is known as Lipschitz continuity of the boundary. A numerical result showing that optimal shape can not be obtained without the constraint condition of Lipschitz continuity is found in a monograph published by Haslinger and Neittaanmaki\(^7\) in 1988. The necessity of this condition in the formulation of ordinary domain optimization problems in engineering, however, has not been discussed thoroughly.

The objective of this paper is to show that ordinary domain optimization problems do not have sufficient regularity and to propose a technique for overcoming this irregularity. This paper briefly describes the derivation of the shape gradient function. Based on theoretical results obtained with the direct gradient method in Hilbert space with support on the boundary, we use a theorem related to the regularity of elliptic boundary problems to show that ordinary domain optimization problems lack sufficient regularity. The basic idea of the gradient method in Hilbert space can be found in Cea’s 1981 work.\(^1\)

To overcome this irregularity, we introduce the idea of a smoothing gradient method in Hilbert space. With this method, the domain variation is determined by using a coercive bilinear form in Hilbert space of the first order with support in the domain. That the renewed domain has the same boundary smoothness as the original boundary can be confirmed using the regularity theorem.

Considering that the bilinear form defined for variational strain energy in an elastic continuum problem is an explicit form of the coercive bilinear form, we reach the conclusion that the traction method proposed by Azegami\(^8\) in 1994 is a concrete form of the smoothing gradient method. The traction method was proposed as a technique for determining the domain variation as a displacement of a pseudo-elastic body defined in the design domain by applying a pseudo-external force in proportion to the negative value of the shape gradient function under constraints on the displacement of the invariable boundaries or subdomain.\(^9\) To conduct a numerical analysis, we can use any technique applicable to linear elastic problems, such as the finite element method or boundary element method.

The smoothing gradient method will be compared with the direct gradient method in actual problems by numerical experiments using a finite element model.

### 2 Elliptic boundary value problem

For simplicity, we consider an (strong) elliptic boundary value problem of the second order related to a real-valued scalar state function \(u\) defined in a bounded open domain \(\Omega \in \mathbb{R}^n\) (closed domain \(\bar{\Omega}\)), \(n = 2, 3\), with a boundary \(\partial \Omega = \Gamma\):

\[
-\nabla \cdot (\tilde{A}(\bar{x}) \nabla u(\bar{x})) + a(\bar{x})u(\bar{x}) = f(\bar{x}), \quad \forall \bar{x} \in \Omega \tag{1}
\]

\[
u(\bar{x}) = u_\Gamma(\bar{x}), \quad \forall \bar{x} \in \Gamma_0 \subseteq \Gamma \quad \text{(Dirichlet condition)} \tag{2}
\]

\[
\tilde{A}(\bar{x}) \nabla u(\bar{x}) \cdot \bar{n}(\bar{x}) = g(\bar{x}), \quad \forall \bar{x} \in \Gamma \setminus \Gamma_0 \quad \text{(Neumann condition)} \tag{3}
\]
where the real-valued symmetric $n \times n$ matrix function $\tilde{A}(\vec{x}) = \tilde{A}(\vec{x})^T$ and the real-valued scalar function $a(\vec{x})$ holds that
\[
\exists \alpha > 0 : a \geq \alpha, \quad \vec{z} \cdot \tilde{A} \vec{z} \geq \alpha |\vec{z}|^2, \quad \forall \vec{z} \in \mathbb{R}^n.
\]
(4)

In this paper, $\langle \cdot \rangle$ is used for $n$ dimensional vectors, $(\cdot)$ denotes the subtraction between sets, $(\cdot)^T$ denotes the transpose, $\nabla$ denotes the gradient vector and $\vec{n}$ denotes the outer normal vector well defined at almost all points of $\Gamma$. We term the problems with the complete Dirichlet and Neumann conditions on $\Gamma$ the Dirichlet and Neumann problems respectively. When considering the Neumann problem, the following relation is needed in addition:
\[
\int_{\Omega} (f - au) \, dx = \int_{\Gamma} g \, d\Gamma.
\]
(5)

3 Regularity of the solution

To prepare for the discussion, we review the theorem about the regularity of elliptic boundary value problems. This theorem can be found in the references\textsuperscript{10},\textsuperscript{11}

Definitions: Boundary $\Gamma$ is of class $C^{l+\alpha}$ if
\[
\exists \rho > 0 : S = \Gamma \cap B(\vec{x}, \rho) \text{ is a connected boundary, } \forall \vec{x} \in \Gamma,
B(\vec{x}, \rho) = \{z \in \mathbb{R}^n \mid |\vec{x} - \vec{z}| \leq \rho\}
\]
and, selecting a local Cartesian coordinate system $\{y_i\}_{i=1}^n$ with the origin at $\vec{x}$ and the $y_n$-axis in the outer normal direction to $\Omega$,
\[
\exists w \in C^{l+\alpha}(\bar{S}) \text{ where } y_n = w(y_1, y_2, \ldots, y_{n-1}) \text{ is the equation of } S.
\]
(7)

In particular, we term $C^{0,\alpha}$, $\alpha > 0$, a Lipschitz boundary. The symbol $C^{l+\alpha}(\Omega_{s})$ denotes the set of $l$-times differentiable functions defined in $\Omega_{s}$ of which the $l$th derivative is H"{o}lder continuous with exponent $\alpha > 0$.

Theorem: If $\Gamma \in C^{2+\alpha}$ class, $\tilde{A} \in (C^{1-\delta,\alpha}(\bar{\Omega}))^{n \times n}$, $a, f \in C^{0,\alpha}(\bar{\Omega})$, $g \in C^{1,\alpha}(\Gamma)$ and $u_{\Gamma} \in C^{2,\alpha}(\Gamma)$, then the solution $u \in C^{2,\alpha}(\bar{\Omega})$ is obtained where $\delta = 1$ for the Dirichlet problem and $\delta = 0$ for the Neumann problem.

4 Domain variation

Suppose that the domain $\Omega$ is variable in a given bounded domain $\Omega_{\text{limit}} \in \mathbb{R}^n$, $n = 2, 3$. One approach to describing the variation is to use the following one parameter family which is mapped from the initial closed domain $\bar{\Omega}$ to the varied closed domain $\bar{\Omega}_{s}$ as shown in Figure 1:
\[
\begin{align*}
\bar{T}_s(\bar{\Omega}) : \bar{X} \in \bar{\Omega} & \mapsto \bar{x} \in \bar{\Omega}_{s} \subset \bar{\Omega}_{\text{limit}}, \\
\bar{T}_s^{-1}(\bar{\Omega}_{s}) : \bar{x} \in \bar{\Omega}_{s} & \mapsto \bar{X} \in \bar{\Omega}, \ s \geq 0, \ \bar{T}_0(\bar{\Omega}) = \bar{\Omega}.
\end{align*}
\]
(8)
Keeping the topology of $\Omega$ and assuming a set $\Theta$ of restrictions on domain variation, the admissible set of the mapping function $\bar{T}_s(\Omega)$ is given by

$$D = \{ \bar{T}_s(\Omega) \in (C^{0,\alpha}(\bar{\Omega}))^n : \Theta : set \ of \ kinematic \ conditions \ of \ domain \ variation \}. \quad (9)$$

When a domain functional $J_{\Omega_s}$ and a boundary functional $J_{\Gamma_s}$ of a distributed function $\phi_s$ are considered, their derivatives $\dot{J}_{\Omega_s}$ and $\dot{J}_{\Gamma_s}$ with respect to $s$ are given by the formulae of the material derivative assuming $s$ as time:

$$J_{\Omega_s} = \int_{\Omega_s} \phi_s \, dx, \quad \dot{J}_{\Omega_s} = \int_{\Omega_s} \phi'_s \, dx + \int_{\Gamma_s} \phi_s \vec{n} \cdot \vec{V} \, d\Gamma, \quad (10)$$

$$J_{\Gamma_s} = \int_{\Gamma_s} \phi_s \, d\Gamma, \quad \dot{J}_{\Gamma_s} = \int_{\Gamma_s} \left\{ \phi'_s + (\nabla_n \phi_s + \phi_s \kappa) \vec{n} \cdot \vec{V} \right\} \, d\Gamma, \quad (11)$$

where $\nabla_n (\cdot) \equiv \nabla(\cdot) \cdot \vec{n}$ and $\kappa$ denotes the mean curvature. The shape derivative $\phi'_s$ of the distributed function $\phi_s$ indicates the derivatives under a spatially fixed condition. The derivative $\bar{V}(\Omega_s)$ of $\bar{T}_s(\Omega)$ with respect to $s$ defined on $\bar{\Omega}_s$ is given by

$$\bar{V}(\Omega_s) = \frac{\partial \bar{T}_s}{\partial s} (\bar{T}_s^{-1}(\bar{\Omega}_s)) \quad (12)$$

and called velocity function because of the analogy between $s$ and time.

5 Shape optimization problems

Let us formulate some basic shape optimization problems as elliptic boundary value problems paying no attention to the regularity of the shapes.
5.1 Self-adjoint problem

A natural formulation is to select the following linear form \( l(u) \) as an objective functional:

\[
\begin{aligned}
\text{Given } & \Omega, \Omega_{\text{limit}} \in \mathbb{R}^n, \ 0 < M \in \mathbb{R} \\
A & \in (L^\infty(\Omega_{\text{limit}}))^{n \times n}, \ a \in L^\infty(\Omega_{\text{limit}}), \\
f & \in H^{-1}(\Omega_{\text{limit}}), \ u_{\Gamma} \in H^1(\Omega_{\text{limit}}), \\
g & \in H^{-1}(\Omega_{\text{limit}}), \\
\text{find } & \Omega_s = \vec{T}_s(\Omega) \in D \\
\text{that minimize} & \ l(u), u - u_0 \in U \\
\text{subject to} & \ a(u - u_0, v) = l(v), \ \forall v \in U \\
& \ \text{meas}(\Omega_s) = \int_{\Omega_s} dx \leq M
\end{aligned}
\]

where the elliptic boundary problem is described by the variational form using the following bilinear form \( a(\cdot, \cdot) \) and the linear form \( l(\cdot) \),

\[
\begin{aligned}
a(u, v) & = \int_{\Omega_s} (\vec{\nabla} u \cdot \vec{A} \vec{\nabla} v + auv) \ dx \\
l(v) & = \int_{\Omega_s} fv \ dx + \int_{\vec{T}_s(\Gamma_\Omega \setminus \Gamma_\Omega)} gv \ d\Gamma.
\end{aligned}
\]

The set \( U \) of the admissible state function \( u - u_0 \) is given by

\[
U = \{ u(\Omega_s) \in H^1(\Omega_s) | u(\Gamma_0) = 0, \int_{\Omega_s} u \ dx = 0 \text{ for the Neumann problem} \}
\]

where \( u_0 \in H^1(\Omega_s) \) is a real-valued function satisfying the Dirichlet condition of Eq. (2). The symbols \( L^\infty(\Omega_{\text{limit}}), H^m(\Omega_{\text{limit}}) \) and \( H^{-m}(\Omega_{\text{limit}}) \) denote the space of bounded functions, the space of square integrable functions until \( m \)th derivatives, i.e. Hilbert (Sobolev) space of order \( m \), and the dual space of \( H^m(\Omega_{\text{limit}}) \) defined in the invariable domain \( \Omega_{\text{limit}} \) respectively. Although the coefficient functions of \( \vec{A}, a, f \) and \( g \) are assumed fixed in the domain during domain variation, for simplicity, we can assume that these are variable in accordance with certain rules, such as fixed in material or covariation with the material as shown in the reference.12

Applying the Lagrange multiplier method, the problem given by Eq. (13) can be rendered into a stationalization problem of the Lagrange functional

\[
L(u, v, A, \vec{T}_s) = l(u) - a(u - u_0, v) + l(v) + A(\text{meas}(\Omega_s) - M) \\
v \in U, \ 0 \leq A \in \mathbb{R}.
\]

where \( v \) and \( A \) are used for the Lagrange multipliers. The derivative \( \dot{L} \) with respect to \( s \) is derived using the formulae of Eqs. (10) and (11):

\[
\begin{aligned}
\dot{L} = & \ l(u') - a(u', v) - a(u - u_0, v') + l(v') \\
& + A(\text{meas}(\Omega_s) - M) + (G\vec{n}, \vec{V})_{(H^0(\vec{T}_s(\Gamma))))^n}
\end{aligned}
\]
where the linear form \((G\tilde{n}, \tilde{V})(H^0(\tilde{T}_s(\Gamma)))^n\) with respect to \(\tilde{V}\) is given by

\[
(G\tilde{n}, \tilde{V})(H^0(\tilde{T}_s(\Gamma)))^n = \int_{\tilde{T}_s(\Gamma)} G\tilde{n} \cdot \tilde{V} \, d\Gamma
\]

\[
G = -\tilde{\nabla}(u - u_0) \cdot A\tilde{\nabla}v - a(u - u_0)v + f(u + v)
+ \nabla_n g(u + v) + g\nabla_n(u + v) + g(u + v)\kappa + \Lambda.
\]

The coefficient vector function \(G\tilde{n}\) with respect to the velocity function \(\tilde{V}\) has the meaning of a sensitivity function relative to domain variation and is the so-called the shape gradient function. The scalar function \(G\) is called the shape gradient density function. In Eq. (20), the term \(\nabla_n g(u + v) + g\nabla_n(u + v) + g(u + v)\kappa\) is evaluated only on the Neumann condition boundary.

From Eq. (18), some of the Kuhn-Tucker conditions for \(u\), \(v\) and \(A\) are obtained by

\[
a(u - u_0, v') = l(v'), \quad \forall v' \in U
\]

\[
a(u', v) = l(u'), \quad \forall u' \in U
\]

\[
A(\text{meas}(\Omega_s) - M) = 0 \quad \text{and} \quad \text{meas}(\Omega_s) \leq M
\]

that indicate the variational form of the original elliptic boundary value problem for \(u\), the variational form for \(v\), which we call an adjoint equation and an adjoint state function for \(v\), and the governing equations for \(A\) respectively. Comparing Eqs. (21) and (22), we obtain the following self-adjoint relation in this problem.

\[
u - u_0 = v
\]

By factoring in this relation, Eq. (20) becomes

\[
G = -\tilde{\nabla}(u - u_0) \cdot A\tilde{\nabla}(u - u_0) - a(u - u_0)^2 + f(2u - u_0)
+ \{\nabla_n g(2u - u_0) + g\nabla_n(2u - u_0) + g(2u - u_0)\kappa}\} + \Lambda.
\]

In addition, when we assume that the nonzero Neumann condition boundary \(\Gamma_1 = \{\tilde{x} \in \Gamma \setminus \Gamma_0 \mid g(\tilde{x}) \neq 0\}\) and nonzero gradient Neumann condition boundary \(\Gamma_2 = \{\tilde{x} \in \Gamma \setminus \Gamma_0 \mid \nabla_n g(\tilde{x}) \neq 0\}\) are invariable, i.e., \(\tilde{T}_s(\Gamma_1 \cup \Gamma_2) = \Gamma_1 \cup \Gamma_2\), the term \(\{\nabla_n g(2u - u_0) + g\nabla_n(2u - u_0) + g(2u - u_0)\kappa}\}\) does not need to be evaluated because \(\tilde{V}(\tilde{T}_s(\Gamma_1 \cup \Gamma_2)) = 0\).

Under the condition satisfying Eqs. (21), (23) and (24), the derivative of the Lagrange functional agrees with that of the objective functional and the linear form \((G\tilde{n}, \tilde{V})(H^0(\tilde{T}_s(\Gamma)))^n\) with respect to \(\tilde{V}\):

\[
\hat{L}_{u,v,A} = \hat{l}(u)_{u,v,A} = (G\tilde{n}, \tilde{V})(H^0(\tilde{T}_s(\Gamma)))^n
\]

5.2 Dirichlet identification problem

A shape determination problem where the state function \(u\) is specified with \(w\) on a subboundary \(\Gamma_D \subset \Gamma\) given at the initial shape can be regarded
as a shape identification problem of the Dirichlet type. This problem is formulated using a squared error integral

\[ E_{\Gamma_D}(u - w, u - w) = \int_{\tilde{T}_s(\Gamma_D)} (u - w)^2 \, d\Gamma \]  

as an objective functional by

\[
\begin{align*}
\text{Given } & \Omega, \Omega_{\text{limit}}, M, A, a, f, u_{\Gamma}, g \\
\text{in Eq(13) and } & w \in H^1(\Omega_{\text{limit}}), \\
\text{find } & \Omega_s = \tilde{T}_s(\Omega) \in D \\
\text{minimize } & E_{\Gamma_D}(u - w, u - w), \ u - u_0 \in U \\
\text{subject to } & a(u - u_0, v) = l(v), \ \forall v \in U \\
\text{meas}(\Omega_s) & \leq M.
\end{align*}
\]

The shape gradient density function given in the form of Eq. (19) for this problem is obtained in the manner of the previous subsection as

\[
G = 2(u - w)\nabla_n (u - w) + (u - w)^2\kappa - \nabla (u - u_0) \cdot A \nabla v - a(u - u_0)v + f + \nabla_n g + g \nabla_n v + g\kappa + A
\]

where \( u \) is the solution of the original elliptic boundary value problem and \( v \) is determined by the adjoint equation:

\[
a(u', v) = 2E_{\Gamma_D}(u - w, u'), \ \forall u' \in U.
\]

In Eq. (29), the term \( 2(u - w)\nabla_n (u - w) + (u - w)^2\kappa \) is evaluated only on the state function specified boundary \( \Gamma_D \). When we assume that the boundary \( \Gamma_D \) is invariable, i.e., \( \tilde{T}_s(\Gamma_D) = \Gamma_D \), evaluation of the terms \( 2(u - w)\nabla_n (u - w) + (u - w)^2\kappa \) is not needed because \( \nabla (\tilde{T}_s(\Gamma_D)) = \emptyset \).

### 5.3 Neumann identification problem

We can also consider a shape identification problem of the Neumann type where the gradient of the state function \( \nabla_n u \) is specified with \( w \) on a subboundary \( \Gamma_D \subset \Gamma \) given at the initial shape. Using the objective functional given by

\[ E_{\Gamma_D}(\nabla_n u - w, \nabla_n u - w) = \int_{\tilde{T}_s(\Gamma_D)} (\nabla_n u - w)^2 \, d\Gamma, \]

this problem is formulated by

\[
\begin{align*}
\text{Given } & \Omega, \Omega_{\text{limit}}, M, A, a, f, u_{\Gamma}, g \\
\text{in Eq(13) and } & w \in H^1(\Omega_{\text{limit}}), \\
\text{find } & \Omega_s = \tilde{T}_s(\Omega) \in D \\
\text{minimize } & E_{\Gamma_D}(\nabla_n u - w, \nabla_n u - w), \ u - u_0 \in U \\
\text{subject to } & a(u - u_0, v) = l(v), \ \forall v \in U \\
\text{meas}(\Omega_s) & \leq M.
\end{align*}
\]
The shape gradient density function is obtained as
\[
G = 2(u - w)\nabla_n(\nabla_n u - w) + (\nabla_n u - w)\nabla(\nabla_n u - u_0) \cdot A\nabla v - a(u - u_0)v + f v + \nabla_n gv + g\nabla_n v + gv + A \nabla v
\]
(33)
where the adjoint state function \( v \) is determined by
\[
a(u', v) = 2E_{\Gamma}(\nabla_n u - w, \nabla_n u'), \forall u' \in U.
\]
(34)

5.4 Subdomain gradient identification problem
Another shape identification problem is considered where the gradient of the state function \( \nabla u \) is specified with \( \vec{w} \) in subdomain \( \Omega_D \subset \Omega \). Using the objective functional given by
\[
E_{\Omega_D}(\nabla u - \vec{w}, \nabla u - \vec{w}) = \int_{\tilde{T}_s(\partial\Omega_D)} (\tilde{\nabla} u - \tilde{w}) \cdot (\tilde{\nabla} u - \tilde{w}) \, dx,
\]
(35)
this problem is formulated by
\[
\begin{align*}
\text{Given } & \Omega, \Omega_{\text{limit}}, M, A, a, f, g, u, u_0, \Gamma, \\
\text{in Eq}(13) \text{ and } & \vec{w} \in (H^1(\Omega_{\text{limit}}))^n, \\
\text{find } & \Omega_s = \tilde{T}_s(\Omega) \subset D \text{ that } \\
\text{minimize } & E_{\Omega_D}(\nabla u - \vec{w}, \nabla u - \vec{w}), \ u - u_0 \in U \\
\text{subject to } & a(u - u_0, v) = l(v), \forall v \in U \\
& \text{meas}(\Omega_s) \leq M.
\end{align*}
\]
(36)
The linear form \((G\vec{n}, \vec{V})_{(H^1(\tilde{T}_s(\partial\Omega_D \cup \Gamma)))^n}\) corresponding to Eq. (19) is given as
\[
(G\vec{n}, \vec{V})_{(H^1(\tilde{T}_s(\partial\Omega_D \cup \Gamma)))^n} = \int_{\tilde{T}_s(\partial\Omega_D)} G_{\vec{n}} \cdot \vec{V} \, d\Gamma + \int_{\tilde{T}_s(\Gamma)} G_{\vec{n}} \cdot \vec{V} \, d\Gamma
\]
(37)
\[
\begin{align*}
G_{\vec{n}} &= (\tilde{\nabla} u - \tilde{w}) \cdot (\tilde{\nabla} u - \tilde{w}) \\
G_{\vec{\Gamma}} &= -\tilde{\nabla}(u - u_0) \cdot A\tilde{\nabla} v - a(u - u_0)v + f v \\
& + \nabla_n gv + g\nabla_n v + gv + A
\end{align*}
\]
(38)
where \( \partial\Omega_D \) denotes the boundary of \( \Omega_D \) and \( v \) is determined by
\[
a(u', v) = 2E_{\Omega_D}(\tilde{\nabla} u - \tilde{w}, \tilde{\nabla} u'), \forall u' \in U
\]
(40)

6 Gradient methods
A conventional approach to solving optimization problems where the sensitivity or gradient can be evaluated is to apply the gradient method. However, in the shape optimization problems formulated in the previous section, the shape gradient functions were derived as functions distributed on the boundary. Accordingly, we have to use the gradient method defined in a function space. In this section, we review the gradient method in Hilbert space, apply this method directly to the shape optimization problems and propose the concept of a smoothing gradient method that will play a significant role later.
6.1 Gradient method in Hilbert space

In general optimization problems, the first variation of the objective function (functional) is obtained as the scalar product of the gradient and the variation of the design variable. Therefore, a general theory of the gradient method is given in the space where a scalar product is defined, i.e., Hilbert space.

Let us consider a minimization problem of an objective functional $I(\vec{z}(s))$ which is given with a design variable of a one parameter family of functions $\vec{z}(s) \in Z \subset (H^m(\Omega))^n$, integer $m \geq 0$. The derivative of $I(\vec{z}(s))$ with respect to $s$ (the first variation of $I(\vec{z}(s))$) is obtained as the following scalar product.

$$\dot{I} = (\vec{I}_z, \dot{\vec{z}})_{(H^m(\Omega))^n}$$

where $(\cdot , \cdot)_{(H^m(\Omega))^n}$ represents the scalar product in $(H^m(\Omega))^n$. The gradient method is a general technique for determining the variation of design function $\dot{\vec{z}}$ as follows.

$$\text{Find } \dot{\vec{z}} \in Z \text{ such that } b(\dot{\vec{z}}, \vec{y})_{(H^m(\Omega))^n} = -(\vec{I}_z, \vec{y})_{(H^m(\Omega))^n}, \forall \vec{y} \in Z \quad (42)$$

where $b(\cdot , \cdot)_{(H^m(\Omega))^n}$ is a coercive (elliptic) bilinear form in $(H^m(\Omega))^n$:

$$\exists \alpha > 0 : b(\vec{y}, \vec{y})_{(H^m(\Omega))^n} \geq \alpha \| \vec{y} \|^2_{(H^m(\Omega))^n}, \forall \vec{y} \in (H^m(\Omega))^n$$

and $\| \cdot \|_{(H^m(\Omega))^n}$ denotes the norm in $(H^m(\Omega))^n$. A concrete example of $b(\cdot , \cdot)_{(H^m(\Omega))^n}$ is the scalar product $(\cdot , \cdot)_{(H^m(\Omega))^n}$ on $(H^m(\Omega))^n$. That the variation of design function $\dot{\vec{z}}(s)$ reduces the objective functional $I$ can be confirmed by

$$\dot{I} = -b(\dot{\vec{z}}, \dot{\vec{z}})_{(H^m(\Omega))^n} \leq -\alpha \| \dot{\vec{z}} \|^2_{(H^m(\Omega))^n} \leq 0. \quad (44)$$

6.2 Direct gradient method

Let $(G\vec{n}, \vec{V})_{(H^0(\partial\Omega, \Gamma_D))^n}$ defined by Eq. (19) be a scalar product in the Hilbert space $(H^0(\partial\Omega, \Gamma_D))^n$ and $(G\vec{n}, \vec{V})_{(H^0(\partial\Omega_D + \Gamma))^n}$ defined by Eq. (37) be a scalar product in the Hilbert space $(H^0(\partial\Omega_D + \Gamma))^n$ when we consider the subdomain gradient identification problem. Then, the gradient method in $(H^0(\partial\Omega, \Gamma_D))^n$ can be obtained as follows.

$$\text{Find } \vec{V} \in D \text{ such that } b(\vec{V}, \vec{y})_{(H^0(\partial\Omega, \Gamma_D))^n} = -(G\vec{n}, \vec{y})_{(H^0(\partial\Omega_D + \Gamma))^n}, \forall \vec{y} \in D \quad (45)$$

where the coercive bilinear form $b(\cdot , \cdot)_{(H^0(\partial\Omega, \Gamma_D))^n}$ is chosen arbitrarily in $(H^0(\partial\Omega, \Gamma_D))^n$. We call this solution the direct gradient method for the reason that there is no restriction on the derivation process, and will discuss the regularity of the shape optimization problems from the standpoint of whether the solution obtained by this method maintains the Lipschitz boundary or not.
6.3 Smoothing gradient method

As a possibility, let us consider a gradient method in \((H^1(\Omega_s))^n\). Selecting \(b(\cdot, \cdot)_{(H^1(\Omega_s))^n}\) for a coercive bilinear form in \((H^1(\Omega_s))^n\), the gradient method is written as follows.

\[
\text{Find } \vec{V} \in D \text{ such that } \quad b(\vec{V}, \vec{y})_{(H^1(\Omega_s))^n} = -(G\vec{n}, \vec{y})_{(H^0(\Gamma_1))^n}, \forall \vec{y} \in D \tag{46}
\]

Based on the trace theorem that if \(\vec{y}(\Omega_s) \in (H^1(\Omega_s))^n\) then \(\vec{y}(\vec{T}_s(\Gamma)) \in (H^{1/2}(\vec{T}_s(\Gamma)))^n \subset (H^0(\vec{T}_s(\Gamma)))^n\), we can confirm that the solution obtained by this method is smoother than that obtained by the direct gradient method. From this relation, we call this solution the smoothing gradient method.

7 Ill-posedness of direct gradient method

This section discusses the regularity of the shape optimization problems in reference to the smoothness of the boundary renewed by the direct gradient method.

To avoid a complicated explanation, the discussion excludes the boundary except the boundary of the subboundary assigned the Dirichlet condition and the boundary of the specified subboundary or subdomain, where sufficient smoothness, which is assumed in the subsections, can not be assumed respectively.

7.1 Self-adjoint problem

Let us consider the assumption used in the regularity theorem in Section 3, i.e., \(\Gamma \in C^{2,\alpha}\) class, \(A \in (C^{1-\delta,\alpha}(\bar{\Omega}))^{n \times n}, \delta = 0\) for the Dirichlet problem and \(\delta = 1\) for the Neumann problem, \(a, f \in C^{0,\alpha}(\bar{\Omega}), g \in C^{1,\alpha}(\Gamma)\) and \(u_\Gamma \in C^{2,\alpha}(\Gamma)\) at the initial shape, i.e., \(s = 0\). Then, the solution is obtained as \(u \in C^{2,\alpha}(\bar{\Omega})\) by the theorem. In addition, the boundary of the nonzero Neumann condition \(\Gamma_1 = \{ \vec{x} \in \Gamma \setminus \Gamma_0 | g(\vec{x}) \neq 0 \}\) belongs to the \(C^{3,\alpha}\) class so that \(\kappa \in C^{3,\alpha}(\Gamma_1)\). Then, the shape gradient density function \(G\) given by Eq. (20) belongs to \(C^{1,\alpha}(\Gamma)\). Applying the direct gradient method of Eq. (45), the velocity function is obtained as \(\vec{V} \in C^{1,\alpha}(\Gamma)\). This result means that the renewed boundary obtained with this velocity function, i.e., \(\vec{T}_s(\Delta_s) = \vec{V}(\Gamma)\Delta_s\) for infinitesimal \(\Delta_s > 0\), belongs to the \(C^{2,\alpha}\) class that reduces the differentiability by one order from the original \(C^{2,\alpha}\) class on \(\Gamma \setminus \Gamma_1\) and two orders from the original \(C^{3,\alpha}\) class on \(\Gamma_1\). Therefore, we can conclude that the iteration of the boundary variation with the velocity function \(\vec{V}\) obtained by the direct gradient method deteriorates the smoothness of the boundary progressively.

In general cases, we can surmise that the relative relation of decreasing the smoothness step by step of the iteration still remains. Considering that the direct gradient method was derived without any restriction, this conclusion shows the irregularity of the shape optimization problem of self-adjoint type.
7.2 Identification problems

The shape gradient density function for the Dirichlet identification problem was obtained as Eq. (29). Let us assume the same strict smoothness of the given functions and the boundary at the initial shape, i.e., \( s = 0 \), that was used in the previous subsection. Then, the solution is obtained as \( u \in C^{2,\alpha}(\bar{\Omega}) \), by the theorem. In addition, let \( v \in C^{2,\alpha}(\bar{\Omega}_{\text{init}}) \). Then, the solution of the adjoint state function obtained by Eq. (30) is given at least as \( v \in C^{2,\alpha}(\bar{\Omega}) \), because \( v \) is the solution of an elliptic boundary value problem where \( 2(u - w) \in C^{2,\alpha}(\Gamma_D) \subset C^{1,\alpha}(\Gamma_D) \) is assumed instead of \( g \in C^{1,\alpha}(\Gamma_1) \) in the original elliptic boundary value problem. Moreover, let \( \Gamma_D \) belong to the \( C^{3,\alpha} \) class so that \( \kappa \in C^{1,\alpha}(\Gamma_D) \). Then, the shape gradient density function \( G \) given by Eq. (29) belongs to \( C^{1,\alpha}(\Gamma) \). Using this result, we reach the same conclusion about irregularity as in the previous subsection.

The same conclusion can be derived for the identification problems of the Neumann type and the subdomain gradient type.

8 Well-posedness of smoothing gradient method

Let us consider the case of applying the smoothing gradient method to the shape optimization problems.

8.1 Self-adjoint problem

Based on the result in Subsection 7.1, we obtained \( G \in C^{1,\alpha}(\Gamma) \) by assuming \( \Gamma \in C^{2,\alpha} \) class, \( \Gamma_1 \in C^{3,\alpha} \) class and sufficient smoothness of the given functions. When we apply the smoothing gradient method, the solution of the velocity function \( \tilde{V} \) falls into \( C^{2,\alpha}(\bar{\Omega}) \) by the theorem that is obtained by expanding the regularity theorem in Section 3 for the elliptic boundary value problem of a scalar function to that for the elliptic boundary value problem of a \( n \) dimensional vector function. Therefore, \( \tilde{V} \in C^{2,\alpha}(\bar{\Omega}) \) means that the renewed domain, i.e., \( \Omega_{\Delta s} = \tilde{V}(\bar{\Omega}) \Delta s \) for infinitesimal \( \Delta s > 0 \), has the boundary of the \( C^{2,\alpha} \) class that agrees with the original smoothness of the \( C^{2,\alpha} \) class on \( \Gamma \setminus \Gamma_1 \). Although the smoothness on the boundary \( \Gamma_1 \) has been reduced, if we assume the condition \( \kappa(\tilde{T}_s(I_1)) = \kappa(\Gamma_1) \) in \( D \), such as \( \kappa(\tilde{T}_s(I_1)) = 0 \) or \( \tilde{V}(\bar{T}_s(I_1)) \cdot \tilde{n}(\bar{T}_s(I_1)) = 0 \), we can escape this difficulty.

Therefore, in the case of strict smoothness, we can conclude that the smoothing gradient method has well-posedness with respect to the self-adjoint shape optimization problem under the constraint on \( \Gamma_1 \).

In general cases, we can surmise that the boundary smoothness is maintained in the iteration by the smoothing gradient method. This relation will be verified through a numerical experiment in Section 10.

8.2 Identification problems

For the identification problem of the Dirichlet type, using the result in Subsection 7.2, we can obtain the same conclusion as in the previous subsection that the renewed domain has the same smoothness by assuming the condition \( \kappa(\tilde{T}_s(I_1 \cup \Gamma_D)) = \kappa(I_1 \cup \Gamma_D) \) in \( D \).
For the Neumann identification problem, we need to add a strict condition of \( \vec{V}(\vec{T}_s(\Gamma_D)) \cdot \vec{n}(\vec{T}_s(\Gamma_D)) = 0 \) to the conclusion for the Dirichlet identification problem because the term \( 2(u - w)\nabla_n(\nabla_n u - w) \) in Eq. (33) falls into \( C^{0,\alpha}(\Gamma_D) \). The same conclusion can be obtained for the subdomain gradient identification problem as for the self adjoint problem.

9 Traction method

The smoothing gradient method was proposed using the arbitrary coercive bilinear form \( b(\cdot, \cdot)_{(H^1(\Omega_s))^n} \) as shown in Eq. (46). To execute this method, we have to give the coercive bilinear form in \( (H^1(\Omega_s))^n \) concretely.

One of the most familiar coercive bilinear forms in \( (H^1(\Omega_s))^n \) is that for the variational strain energy \( a(\cdot, \cdot)_{(H^1(\Omega_s))^n} \) in an elastic continuum problem under rigid motion constraint defined by

\[
a(\vec{u}, \vec{v})_{(H^1(\Omega_s))^n} = \int_{\Omega_s} C_{ijkl} u^{k,l} v^{i,j} \, dx \tag{48}
\]

where \( C_{ijkl} \in L^\infty(\Omega_s) \), \( i, j, k, l = \{1, 2, \ldots, n\} \), denotes the Hooke stiffness tensor. In the tensor notation, the summation convention and the gradient notation \( (\cdot)_i = \partial(\cdot)/\partial x_i \) are used. The smoothing gradient method using \( a(\cdot, \cdot)_{(H^1(\Omega_s))^n} \) is expressed as follows.

\[
\text{Find } \vec{V} \in D \text{ such that } \\
a(\vec{V}, \vec{y})_{(H^1(\Omega_s))^n} = -(G\vec{n}, \vec{y})_{(H^0(\Gamma_t))^n}, \forall \vec{y} \in D \tag{49}
\]
When a rigid motion is allowed in $D$, Eq. (49) is applied under rigid motion constraint after incremental rigid motions of $\Delta s \vec{V}$ determined by $\vec{V} \cdot \vec{y} = -\left( \int_{\Gamma} G \vec{n} \, d\Gamma \right) \cdot \vec{y}, \forall \vec{y} \in D$, until $\int_{\Gamma} G \vec{n} \, d\Gamma = 0$ holds. This expression agrees with the traction method proposed by one of authors and described earlier (refer to Figure 2).

To determine the Lagrange multiplier $\Lambda$ for the domain measure constraint, we can also apply the traction method. Since $\Lambda$ contributes to the pseudo force $-G\vec{n}$ as a uniform boundary force, the relation between the variation of the uniform boundary force $\Delta \Lambda \vec{n}$, the variation of the velocity $\Delta \vec{V}$ and the variation of the measure of the domain $\Delta \text{meas}(\Omega_s)$ is obtained by an elastic deformation analysis based on the following equation loaded with the uniform boundary force $\Delta \Lambda \vec{n}$ as shown in Figure 3.

$$\text{Find } \Delta \vec{V} \in D \text{ such that } \begin{cases} a(\Delta \vec{V}, \vec{y})_{H^1(\Omega_s)^n} = - (\Delta \Lambda \vec{n}, \vec{y})_{H^0(\Gamma)} \forall \vec{y} \in D \end{cases}$$

$$\Delta \text{meas}(\Omega_s) = \int_{\Gamma} \vec{n} \cdot \Delta \vec{V} \, d\Gamma$$

Using the relation between $\Delta \Lambda$ and $\Delta \text{meas}(\Omega_s)$, we can determine $\Lambda$ that satisfies Eq. (23).

The procedure of the traction method can be summarized as follows.

1) Solve the original elliptic boundary value problem and the adjoint equation, if necessary, depending on problems involved.

2) Calculate the shape gradient function on the design boundary, where some arbitrary value is substituted for $\Lambda \geq 0$, such as the average of $G - \Lambda$ at the first step and the value determined in the previous step.

3) Solve $\vec{V}$ by Eq. (49), deform the domain with $\Delta s \vec{V}$ using some $\Delta s > 0$ and evaluate the domain measure.

4) Solve $\Delta \vec{V}$ with $\Delta \Lambda \vec{n}$ by Eq. (50) and calculate Eq. (51). Using the results, modify $\Delta s \vec{V}$ by varying $\Lambda \geq 0$ so that Eq. (23) is satisfied

5) Update the domain with the modified $\Delta s \vec{V}$ and return to 1).

6) Terminate the procedure based on the results of the state function analysis.

10 Numerical verification

Sections 7 and 8 described the ill-posedness of the direct gradient method and the well-posedness of the smoothing gradient method under a condition of strict smoothness of the given distributed functions and the boundary. This section will show that these conclusions can be expanded to shape optimization problems with less smoothness through numerical analysis using the finite element method. A static linear elastic problem will be considered here as an elliptic boundary value problem.
10.1 Self-adjoint problem

A self-adjoint shape optimization problem involving a static linear elastic continuum represents a minimization problem of external work in which the objective is to maximize stiffness. In that sense, it can be called a mean compliance minimization problem. Assuming no body force and a boundary restriction on domain variation of a nonzero Neumann condition boundary, this problem is stated as follows:

Given \( \Omega, \Omega_{\text{limit}}, M, \) in Eq(13) and
\[
C_{ijkl} \in L^\infty(\Omega_{\text{limit}}), \ i, j, k, l = \{1, 2, \ldots, n\},
\]
\[
\vec{g} \in (H^{-1}(\Omega_{\text{limit}}))^n,
\]
find \( \Omega_s = \hat{T}(\Omega) \in D \) that
\[
\text{minimize } l(\vec{u}), \vec{u} \in U
\]
subject to
\[
a(\vec{u}, \vec{v})(H^1(\Omega_s))^n = l(\vec{v}), \forall \vec{v} \in U
\]
\[
\text{meas}(\Omega_s) \leq M
\]
(52)

where \( a(\cdot, \cdot)(H^1(\Omega_s))^n \) is defined by Eq. (48) and \( l(\cdot) \) is defined by
\[
l(\vec{v}) = \int_{\hat{T}(\Gamma \setminus \Gamma_0)} \vec{g} \cdot \vec{v} d\Gamma,
\]
(53)

\( U \) is the set of the admissible displacements satisfying \( \vec{u}(\Gamma_0) = 0 \). The shape gradient density function is derived as
\[
G = -C_{ijkl}u_{k,l}u_{i,j} + \Lambda
\]
(54)

where \( \Lambda \) is the Lagrange multiplier of the domain measure constraint.

The boundary condition for the original elastic problem and the results obtained by the direct gradient method and the smoothing gradient method are shown in Figure 4. Plane stress was assumed. Admissible domain variation was assumed only in the perpendicular direction on the slope. The direct gradient method was executed by giving the compulsory displacement in the perpendicular direction in proportion to the shape gradient density function at the nodes of the finite elements on the slope. For the smoothing gradient method, the traction method was applied where the traction force in proportion to the shape gradient density function was loaded in the perpendicular direction at the nodes of the finite elements on the slope. The general purpose FEM program I-DEAS 6.1 and its four-node elements were used in this investigation. The result indicate that a smooth boundary was obtained by the smoothing gradient method, although oscillation occurred with the direct gradient method.

10.2 Dirichlet identification problem

Assuming no body force and boundary restrictions on domain variation of a nonzero Neumann condition boundary and the displacement prescribed boundary, i.e., \( \{\hat{T}(\Gamma_1 \cup \Gamma_D) \cdot \vec{n}(\hat{T}(\Gamma_1 \cup \Gamma_D)) = 0\} \in \Theta \) in Eq. (9), the Dirichlet identification problem of the static linear elastic problem is stated as
Given $\Omega$, $\Omega_{\text{limit}}$, $M$, in Eq(13) and

\[
C_{ijkl} \in L^\infty(\Omega_{\text{limit}}), \ i, j, k, l = \{1, 2, \ldots, n\},
\]
\[
g \in (H^{-1}(\Omega_{\text{limit}}))^n, \ \bar{w} \in (H^1(\Omega_{\text{limit}}))^n,
\]
\[
\text{find } \Omega_s = \mathcal{T}_s(\Omega) \in D \text{ that}
\]
\[
\text{minimize } E_{\Gamma_D}(\bar{u} - \bar{w}, \bar{u} - \bar{w}), \ \bar{u} \in U
\]
\[
\text{subject to } a(\bar{u}, \bar{v})(H^1(\Omega_s))^n = l(\bar{v}), \ \forall \bar{v} \in U
\]
\[
\text{meas}(\Omega_s) \leq M
\]

where

\[
E_{\Gamma_D}(\bar{u} - \bar{w}, \bar{u} - \bar{w}) = \int_{\mathcal{T}_s(\Gamma_D)} (\bar{u} - \bar{w}) \cdot (\bar{u} - \bar{w}) \, d\Gamma.
\]
The shape gradient density function is derived as

\[ G = -C_{ijkl}u_{k,l}v_{i,j} + A \] (57)

where the adjoint state function \( \vec{v} \) is determined by

\[ a(\vec{u}', \vec{v})_{(H^1(\Omega_S))^n} = 2E_{\Gamma_D}(\vec{u} - \vec{w}, \vec{u}'), \quad \forall \vec{u}' \in U. \] (58)

As an example of this problem, we considered a shape optimization problem of a connecting rod having less displacement around a hole so as to avoid seizure. The boundary condition for the original elastic problem and the results obtained by the direct gradient method and the smoothing gradient method are shown in Figure 5. Plane stress was assumed. The outer shape where no load was applied was defined as the design boundary. The displacement prescribed boundary \( \Gamma_D \) was given with the right half of the hole defined as a free. The target displacement was \( \vec{w} = \vec{0} \). The direct gradient method was executed by giving the compulsory displacement at the nodes of the finite elements on the design boundary obtained by taking average of the normal vectors obtained from adjoining elements in proportion to the shape gradient density function. For the smoothing gradient method, the traction method was applied where the traction force in proportion to the shape gradient density function was loaded in the normal direction at the nodes of the finite elements on the design boundary by calculating the nodal force using the shape function. The general purpose FEM program ANSYS 5.1 and its three-node elements were used in the calculations.

The results also indicate that a smooth boundary was obtained by the smoothing gradient method compared with the oscillating boundary seen for the direct gradient method.

11 Conclusion

A self-adjoint shape optimization problem and shape identification problems of the Dirichlet type, Neumann type and subdomain gradient assigned type were formulated using a one parameter family of functions for mapping from the initial domain to the varied domain. Their shape gradient functions were derived using the formulae of the material derivatives. Based on the notion of the gradient method in Hilbert space, we introduced the concepts of a direct gradient method and a smoothing gradient method with these shape gradient functions. The irregularity of shape optimization problems was discussed by showing the ill-posedness when the direct gradient method was applied. On the other hand, the regularity of the smoothing gradient method was discussed by showing the well-posedness when this method is applied. It was shown conclusively that a numerical method based on the smoothing gradient method coincides with the traction method previously proposed by one of the authors. The results of numerical experiments substantiated these theoretical conclusions.
References


