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Chapter 8

Topology Optimization Problems of Density Variation Type

From this chapter, we finally examine shape optimization problems in continua. Firstly, let us think about a problem seeking the appropriate arrangement of holes in a domain where the boundary value problem of a partial differential equation is defined. Such a problem is known as the [topology optimization problem](#). Here, the term topology refers to the study of geometrical properties and spatial relation of objects unaffected by the continuous change of their shape or size. In mathematics, two mathematical objects are said to belong to the same topology if they are images of two homotopic maps; that is, if one can be continuously deformed into the other. Therefore, letting n be a natural number, a set of n -connected domains are regarded as belonging to the same homotopy groups. Here, the term “topology optimization” in the topology optimization problem refers to the determination of the connectivity of the design domain that optimizes an object’s material distribution through insertion and arrangement of holes in its structure. However, as will be explained in detail later, the shape of the holes actually becomes the target. Therefore, the problems dealt with in this chapter also become included in shape optimization problems in a wider sense. In this book, it will be referred to as the topology optimization problem in the sense that topology is also in the scope of the design.

Until now, various problem formulations with respect to the topology optimization problem and solutions to these problems have been proposed. By setting up a fixed domain in which a design target is included, a way to choose the [characteristic function](#) (an L^∞ -class function which takes the value 0 in holes and 1 in a domain) of the domain as the design variable was considered. In such a problem, we determine a state determination problem as a boundary value problem multiplying the characteristic function with the coefficient of the partial differential equation, and define the cost function by the characteristic function

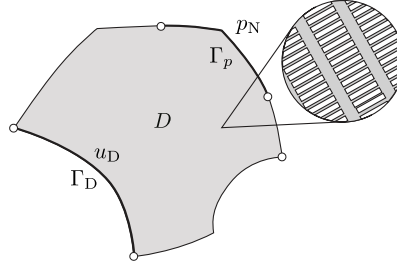


Fig. 8.1: Rank 2 material.

and the solutions of the boundary value problem. However, it was shown that such a problem does not always have a solution [31]. The basic reason for this is that a set of L^∞ -class functions does not induce enough regularity to keep the compactness of the admissible set of design variables [2]. Subsequently, the idea of applying a method (homogenization technique) for describing a continuum problem with a microstructure was shown [3, 19–22, 24, 25]. In particular, with respect to a $d \in \{2, 3\}$ -dimensional linear elastic body, the material constructed of microlayers of d types crossing over one another such as that in Fig. 8.1 are referred to as **rank d material**. Since the homogenized material constant of the rank d material could be analytically obtained, it was investigated in a lot of papers, see, for instance, [5, 7, 18, 32]. As a result, it was shown that in a uniform stress field, if each layer density in the direction of each principal stress is determined in proportion to the value of each principal stress, the mean compliance will be minimized as the volume is constrained [18]. However, no results could be obtained which recognize macro holes. Moreover, since rank d material has no rigidity with respect to shearing deformation, there was an issue with it not being applicable as a mechanical structure.

The generation of holes was confirmed when a continuum with a rectangular hole in a microcell Y similar to the one in Fig. 8.2 was assumed [6, 9, 26, 38]. This problem is constructed as a function optimization problem with the design variable as $(a_1, a_2, \theta)^\top : D \rightarrow \mathbb{R}^3$ in Fig. 8.2. The numerical solution of this problem was obtained by an iterative method satisfying the optimality criteria [38]. If such a numerical solution is obtained, we can define the density by the ratio of the magnitude of holes to the microcell and determine the shapes of holes from the isosurface of the density with an appropriate threshold.

After that, it was shown that even if a microstructure is not assumed, when function $\phi : D \rightarrow [0, 1]$ (in reality, in order to avoid the discontinuity of the solution of state determination problem occurring at $\phi \rightarrow 0$, $\phi : D \rightarrow [c, 1]$ is used with some small constant c) representing density is set to be the design variable, the same topology can be obtained as per the case of micro rectangular holes [28, 41]. In this case, a material characteristic (a coefficient of a partial differential equation) k was assumed to be given by

$$k(\phi) = k_0 \phi^\alpha,$$

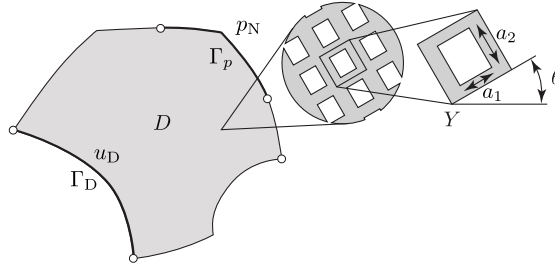


Fig. 8.2: A two-dimensional continuum with micro rectangular holes.

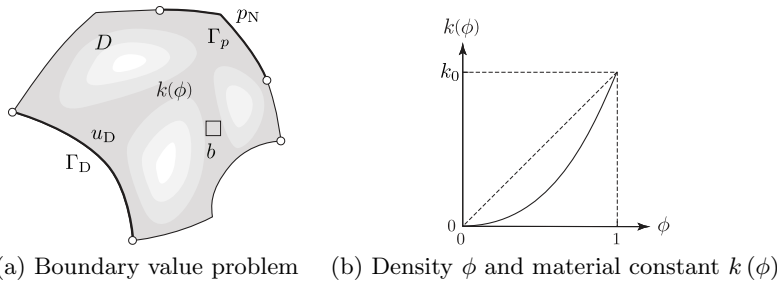


Fig. 8.3: SIMP model.

where k_0 is the existing material constant and $\alpha > 1$ is a constant. Figure 8.3 shows the image of a topology optimization problem in that case. Figure 8.3 (a) shows an example of a state determination problem (boundary value problem). Figure 8.3 (b) shows the relationship between density ϕ (function defined on D) and material characteristic $k(\phi)$ (function defined on D). If the density which is the design variable ϕ varies, the material characteristic $k(\phi)$ varies via the function in Fig. 8.3 (b) and causes the solution of the boundary value problem of Fig. 8.3 (a) to vary. A topology optimization problem defined in this way is referred to as **topology optimization problem of density type**. Moreover, this problem is also referred to as the **SIMP** (solid isotropic material with penalization) model [35]. The reason for this can be explained in the following way. With respect to mid-level density ($\phi = 0.5$), for materials with homogeneous material such as in Fig. 8.4 (a), the material characteristic k becomes 0.5^α . But if, as in Fig. 8.4 (b), it splits into $\phi = 0$ and $\phi = 1$, k becomes 0.5 . For $0.5^\alpha < 0.5$, it becomes a model which gives a penalty to materials split into $\phi = 0$ and $\phi = 1$ as having a greater material characteristic value compared with uniform materials.

With respect to the topology optimization problem of density type, the Fréchet derivatives of cost functions are calculated via the finite element method using an evaluation method such as one shown later. However, if a constant density is assumed for each finite element and moved in the negative direction of the Fréchet derivative, it has been pointed out that the density is seen to vibrate

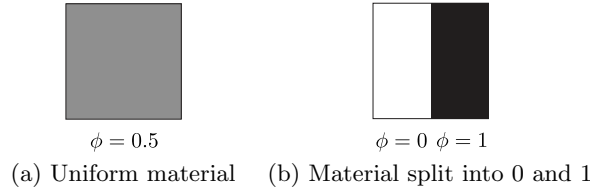


Fig. 8.4: Microstructures when density is 0.5.

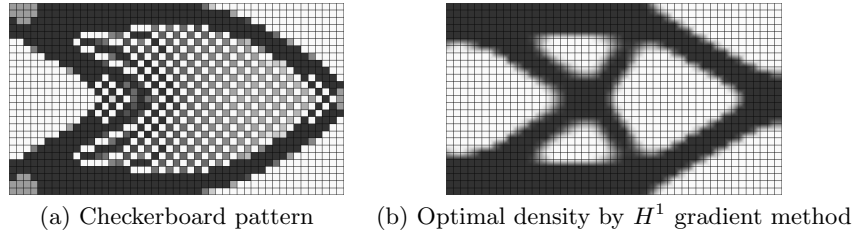


Fig. 8.5: Numerical example of density-type topology optimization problem for linear elastic body (provided by Quint Corporation).

in a checkerboard pattern [10]. Figure 8.5 (a) shows the results of numerical analysis with respect to a mean compliance minimization problem (Problem 8.9.3) of a two-dimensional linear elastic body. In a state determination problem, an external force pointing in the downward direction acts on the center of the right edge while the left edge is fixed. The black and white elements show that ϕ is close to 1 and 0, respectively. When this type of phenomenon occurs, it can be avoided by implementing post-processing such as filtering, etc. [17, 23, 37]. Moreover, methods to approximate the distribution of material parameters in a microstructure with continuous basis functions were shown [27]. However, it has been pointed out that a different issue called the island phenomenon, etc., may arise [34]. Moreover, to remove the intermediate density regions, methods using projection from intermediate density to zero one values were proposed [36, 40].

In contrast, in this chapter, we shall think about the numerical analysis of density-type topology optimization problem along the framework of abstract optimization design problem shown in Chap. 7. However, in this chapter, a function θ defined on D is newly chosen as the design variable rather than choosing directly the density to be the design variable, for reasons shown later. Hence, the density-type topology optimization problem in such a scenario will be referred to as the [topology optimization problem of \$\theta\$ -type](#). The framework of the logic used in this chapter is shown clearly in the paper [4]. Figure 8.5 (b) is the result obtained from the algorithm shown in Sect. 8.7. The fact that no numerical instability phenomenon such as the checkerboard pattern is generated can be seen.

This chapter is constructed in the following way. In Sect. 8.1, the admissible set of the design variable θ is defined in order to construct a topology

optimization problem in continuum. In Sect. 8.2, a θ -type Poisson problem is defined as a state determination problem assuming that a design variable is given. Using the design variable and the solution (state variables) of the state determination problem, the topology optimization problem of θ -type will be defined in Sect. 8.3. Here, a cost function of general form will be used. The existence of a solution to the topology optimization problem of θ -type is shown in Sect. 8.4. In Sect. 8.5, by referring to the Fréchet derivatives of cost functions with respect to variation of the design variable θ as θ -derivatives, the process for obtaining the θ -derivatives and second-order θ -derivatives of cost functions will be seen based on the methods for seeking Fréchet derivatives of cost functions shown in Section 7.5. As a result, depending on the setting of the state determination problem, it becomes apparent that the θ -derivatives of the cost functions do not have regularity such that it would be included in the admissible set of design variables. In Sect. 8.6, the abstract gradient method and abstract Newton method are specified with respect to the topology optimization problem of θ -type. It becomes apparent that the variation of θ which can be obtained from such methods have the regularity such that it could be included in the admissible set of design variable. In Sect. 8.7, the algorithm for solving the topology optimization problem of θ -type will be considered. However, the basic construction is the algorithm as shown in Section 3.7. Error estimations when numerical analyses are conducted via this algorithm are considered in Sect. 8.8. Here, the results of error estimation from the numerical analysis shown in Section 6.6 are used. Once the method for solving a Poisson-problem-related topology optimization problem of θ -type has been confirmed, we define a mean compliance minimization problem of a linear elastic body and an energy loss minimization problem of a Stokes flow field as topology optimization problems of θ -type and show the process for seeking the θ -derivatives of their cost functions in Sections 8.9 and 8.10. Moreover, a numerical example with respect to a simple problem is shown in each section.

8.1 Set of Design Variables

Firstly, let us define a set of design variables in order to construct a topology optimization problem of a continuum. In this chapter, as shown in Fig. 8.3 (a), D is taken to be a $d \in \{2, 3\}$ -dimensional Lipschitz domain. $\Gamma_D \subset \partial D$ is taken to be a Dirichlet boundary and $|\Gamma_D| \neq 0$. $\Gamma_N \subset \partial D \setminus \bar{\Gamma}_D$ is a Neumann boundary.

In research so far, the range of density ϕ is limited to $[0, 1]$. The set of functions with restricted range such as this cannot be a linear space. Hence in this book, $\theta : D \rightarrow \mathbb{R}$ is set to be the design variable and the density is assumed to be given by a sigmoid function $\phi \in C^\infty(\mathbb{R}; \mathbb{R})$ with respect to θ . Several functions are known to be [sigmoid functions](#). Here, either

$$\phi(\theta) = \frac{1}{\pi} \tan^{-1} \theta + \frac{1}{2} \quad (8.1.1)$$

or

$$\phi(\theta) = \frac{1}{2} \tanh \theta + \frac{1}{2} \quad (8.1.2)$$

is used. These graphs are shown in Fig. 8.6. At this point, there is a need to note that $\phi : \mathbb{R} \rightarrow \mathbb{R}$ is a function which returns $(0, 1)$ when θ is given, and is not a function defined in D . However, because θ is a function with the domain D , $\phi(\theta)$ becomes a function defined in D .

With respect to this type of design variable θ , let us use the framework of an abstract optimal design problem (Problem 7.3.1) to define the **linear space of design variables**. As seen in Section 7.1, if the use of the gradient method is considered, the linear space of design variables needs to be a real Hilbert space. Hence, the linear space of design variable θ is set to be

$$X = \{ \theta \in H^1(D; \mathbb{R}) \mid \theta = 0 \text{ in } \bar{\Omega}_C \}, \quad (8.1.3)$$

where $\bar{\Omega}_C \subset \bar{D}$ is a boundary or a domain on which a variation of θ is compressed according to the design demands. If a function $\theta_C : D \rightarrow \mathbb{R}$ is specified and it is assumed that $\theta = \theta_C$ is established on Ω_C , $\tilde{\theta} = \theta - \theta_C$ is assumed to be an element of X . In particular, if Ω_C is not required, $\theta \in X = H^1(D; \mathbb{R})$ is assumed.

Furthermore, in order to be able to determine a Lipschitz continuous boundary from the isosurfaces of θ and to be compact in X , we assume that the **admissible set of design variables** is, at least, given by

$$\mathcal{D} = \left\{ \theta \in X \cap H^2(D; \mathbb{R}) \cap C^{0,1}(D; \mathbb{R}) \mid \max \left\{ \|\theta\|_{H^2(D; \mathbb{R})}, \|\theta\|_{C^{0,1}(D; \mathbb{R})} \right\} \leq \beta \right\} \quad (8.1.4)$$

where β is a positive constant. The requirement that \mathcal{D} is a compact set in X is assured by $H^2(D; \mathbb{R}) \Subset H^1(D; \mathbb{R})$ obtained from the Rellich–Kondrachov compact embedding theorem (Theorem 4.4.15). Moreover, in the same manner as Chap. 1, we consider that the boundedness constraint with norm is a **side constraint** and assume that θ is an interior point of \mathcal{D} ($\theta \in \mathcal{D}^\circ$) and when the side constraint is activated, we include it in the inequality constraints.

8.2 State Determination Problem

The linear space X and the admissible set \mathcal{D} of design variables have been defined, hence let us next define the boundary value problem of a partial differential equation which is a state determination problem. Here, the Poisson problem is considered for simplicity.

A Poisson problem (Problem 5.1.1) is defined in Chap. 5. Here, the Poisson problem when θ is a design variable is called the θ -type Poisson problem and its definition is shown based on the framework of an abstract optimal design problem (Problem 7.3.1).

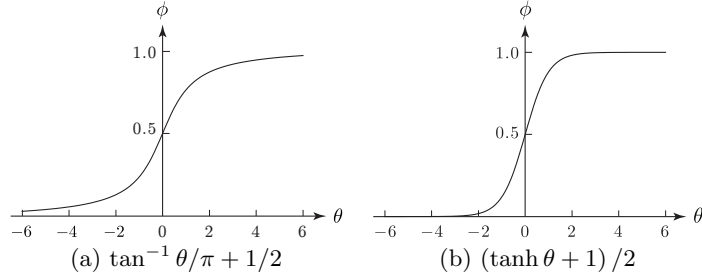


Fig. 8.6: Sigmoid functions for density $\phi(\theta)$ with respect to the design variable θ .

The [linear space of state variables](#) (real Hilbert space) containing the homogeneous solution (which is given by $\tilde{u} = u - u_D$ with a known function u_D provided for Dirichlet condition) of θ -type Poisson problem is set to be

$$U = \{u \in H^1(D; \mathbb{R}) \mid u = 0 \text{ on } \Gamma_D\}. \quad (8.2.1)$$

Furthermore, in order for the variation of θ obtained by the gradient method which will be shown later to be included in \mathcal{D} of Eq. (8.1.4), the [admissible set of state variables](#) \tilde{u} of the homogeneous form with respect to the state determination problem is set to be

$$\mathcal{S} = \{u \in U \cap W^{1,2q_R}(D; \mathbb{R}) \mid \partial_\nu u|_{\Gamma_D} \in L^2(\Gamma_D; \mathbb{R})\}, \quad (8.2.2)$$

where we let q_R be an integer satisfying $q_R > d$.

In order for the homogeneous solution \tilde{u} with respect to a state determination problem to be in \mathcal{S} , from the results seen in Section 5.3, the following assumptions are set with respect to the regularity of the known function.

Hypothesis 8.2.1 (Regularity of given functions) With respect to $q_R > d$, it is assumed that

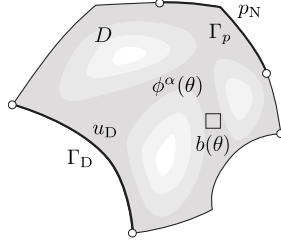
$$b \in C^1(X; L^{2q_R}(D; \mathbb{R})), \quad p_N \in W^{1,2q_R}(D; \mathbb{R}), \quad u_D \in H^2(D; \mathbb{R}),$$

where $C^1(\cdot; \cdot)$ denotes the set of Fréchet differentiables (Definition 4.5.4). \square

Moreover, the following assumption is established with respect to the regularity of the boundary.

Hypothesis 8.2.2 (Opening angle of corner point) Let D be a two-dimensional domain. In relation to the corner points on the boundary, and with respect to the Dirichlet boundary and Neumann boundary,

- (1) if the opening angle β is on the same type of boundary, $\beta < 2\pi$,
- (2) if it is on a mixed boundary, $\beta < \pi$.

Fig. 8.7: θ -type Poisson problem.

Meanwhile, if D is a three-dimensional domain, the corner line on the boundary is smooth and it is assumed that the aforementioned relationship holds on the corner points of the boundary at a plane perpendicular to the corner line. Furthermore, the crossing points of the corner lines or the apexes of the conical boundaries are assumed not to have such singularities as they go beyond the framework within this book. \square

If Hypotheses 8.2.1 and 8.2.2 hold, the fact that u is included in $W^{1,2q_R}(D; \mathbb{R})$ can be confirmed as below. If Hypothesis 8.2.1 holds with respect to given functions, as seen in Section 5.3.1, u is included in $W^{1,2q_R}$ class at all points except those around the corner. Furthermore, from Proposition 5.3.1, if

$$\omega > 1 - \frac{2}{2q_R} \quad (8.2.3)$$

holds, u becomes included in the $W^{1,2q_R}$ class. Here, in the neighborhood around corner points on the homogeneous boundary of Dirichlet or Neumann boundary type, $\omega = \pi/\beta$, hence the condition (1) in Hypothesis 8.2.2 can be obtained. Moreover, at the neighborhood of a corner point of the mixed boundary, from the fact that $\omega = \pi/(2\beta)$, the condition (2) of Hypothesis 8.2.2 is obtained.

Let us use the hypotheses above to define the **state determination problem**. For simplicity, we consider a Poisson problem such as in Fig. 8.7. Here, $\nu \cdot \nabla$ is also to be written as ∂_ν .

Problem 8.2.3 (θ -type Poisson problem) With respect to $\theta \in \mathcal{D}$, suppose that Hypotheses 8.2.1 and 8.2.2 are satisfied. Let $\alpha > 1$ be a constant and $\phi(\theta)$ a function given by Eq. (8.1.1) or Eq. (8.1.2). In this case, obtain $u : D \rightarrow \mathbb{R}$ which satisfies

$$\begin{aligned} -\nabla \cdot (\phi^\alpha(\theta) \nabla u) &= b(\theta) && \text{in } D, \\ \phi^\alpha(\theta) \partial_\nu u &= p_N && \text{on } \Gamma_N, \\ u &= u_D && \text{on } \Gamma_D. \end{aligned}$$

\square

The unique existence of a weak solution to Problem 8.2.3 is guaranteed by the Lax–Milgram theorem (Theorem 5.2.4) with respect to $\tilde{u} = u - u_D \in U$.

Subsequently, \tilde{u} will be used to mean $u - u_D$. Moreover, if Hypotheses 8.2.1 and 8.2.2 are satisfied, $u - u_D \in \mathcal{S}$ is guaranteed.

For later use, the Lagrange function with respect to Problem 8.2.3 is defined as

$$\begin{aligned} \mathcal{L}_S(\theta, u, v) &= \int_D (-\phi^\alpha(\theta) \nabla u \cdot \nabla v + b(\theta) v) \, dx \\ &\quad + \int_{\Gamma_N} p_N v \, d\gamma + \int_{\Gamma_D} \{(u - u_D) \phi^\alpha(\theta) \partial_\nu v + v \phi^\alpha(\theta) \partial_\nu u\} \, d\gamma, \end{aligned} \quad (8.2.4)$$

where u is not necessarily the solution of Problem 8.2.3, and $v \in \mathcal{S}$ was introduced as a Lagrange multiplier. That $v \in U$ is a Lagrange multiplier with respect to Problem 8.2.3 can be confirmed by recalling that in the process to obtain the weak form of the Poisson problem (Problem 5.1.1) in Chap. 5, $v \in U$ was introduced as a Lagrange multiplier. In Eq. (8.2.4), the third term on the right-hand side is a term which was removed in Chap. 5 using $u - u_D, v \in U$ when seeking the weak form of the Poisson problem. In reality, by removing this term, u and v could be viewed as H^1 -class functions (in order for $\partial_\nu v$ to have meaning on Γ_D , v needs to be a H^2 -class function). Here, however, that term will be left. The reason for this is because when a cost function f_i includes the boundary integral on Γ_D , it becomes apparent that the boundary condition of the adjoint problem with respect to f_i is seen from the boundary integral on Γ_D in the Lagrange function of f_i by using this term. Matching the definition by Eq. (7.2.3) of a Lagrange function with respect to the abstract variational problem in Chap. 7, using $\tilde{u} = u - u_D$, we write

$$\mathcal{L}_S(\theta, u, v) = -a(\theta)(u, v) + l(\theta)(v) = -a(\theta)(\tilde{u}, v) + \hat{l}(\theta)(v), \quad (8.2.5)$$

where

$$a(\theta)(u, v) = \int_D \phi^\alpha(\theta) \nabla u \cdot \nabla v \, dx, \quad (8.2.6)$$

$$l(\theta)(v) = \int_D b(\theta) v \, dx + \int_{\Gamma_N} p_N v \, d\gamma, \quad (8.2.7)$$

$$\hat{l}(\theta)(v) = l(\theta)(v) + a(\theta)(u_D, v). \quad (8.2.8)$$

When u is the solution to Problem 8.2.3,

$$\mathcal{L}_S(\theta, u, v) = 0,$$

holds for all $v \in U$. This equation is equivalent to the weak form of Problem 8.2.3.

8.3 Topology Optimization Problem of θ -Type

The design variable θ and solution u of the state determination problem (state variable) were already defined. Hence, let us use these to define the topology

optimization problem of θ -type. Here, we will consider a general cost function. Let u be the solution of a state determination problem (Problem 8.2.3) with respect to $\theta \in \mathcal{D}$ and set the cost function for each $i \in \{0, 1, \dots, m\}$ as

$$\begin{aligned} f_i(\theta, u) = & \int_D \zeta_i(\theta, u, \nabla u) \, dx + \int_{\Gamma_N} \eta_{Ni}(u) \, d\gamma \\ & - \int_{\Gamma_D} \eta_{Di}(\phi^\alpha(\theta) \partial_\nu u) \, d\gamma - c_i, \end{aligned} \quad (8.3.1)$$

where c_i is a constant and is determined so that some $(\theta, \tilde{u}) \in \mathcal{D} \times \mathcal{S}$ exists that satisfies $f_i \leq 0$ for all $i \in \{1, \dots, m\}$ (Slater constraint qualification is satisfied). Moreover, ζ_i , η_{Ni} and η_{Di} are assumed to be given by the following. These hypotheses will be used in an adjoint problem (Problem 8.5.1) to satisfy appropriate regularity requirements. To obtain the second-order θ derivatives of cost functions, additional hypotheses are needed but we will not specify them further. Nevertheless, we will only assume that sufficient conditions are satisfied by the state and adjoint state variables for us to be able to carry out a second-order differentiation of the cost functions with respect to θ .

Hypothesis 8.3.1 (Regularity of cost functions) For cost functions f_i ($i \in \{0, 1, \dots, m\}$) of Eq. (8.3.1), assume that $\zeta_i \in C^1(\mathbb{R} \times \mathbb{R} \times \mathbb{R}^d; \mathbb{R})$, $\eta_{Ni} \in C^1(\mathbb{R}; \mathbb{R})$ and $\eta_{Di} \in C^1(\mathbb{R}; \mathbb{R})$, and with respect to $(\theta, u, \nabla u, \partial_\nu u) \in \mathcal{D} \times \mathcal{S} \times \mathcal{G} \times \mathcal{G}_{\Gamma_D}$ ($\mathcal{G} = \{\nabla u \mid u \in \mathcal{S}\}$, $\mathcal{G}_{\Gamma_D} = \{\partial_\nu u|_{\Gamma_D} \mid u \in \mathcal{S}\}$),

$$\begin{aligned} \zeta_i(\theta, u, \nabla u) & \in L^1(D; \mathbb{R}), \quad \zeta_{i\theta}(\theta, u, \nabla u) \in L^{qR}(D; \mathbb{R}), \\ \zeta_{iu}(\theta, u, \nabla u) & \in L^{2qR}(D; \mathbb{R}), \quad \zeta_{i(\nabla u)^\top}(\theta, u, \nabla u) \in W^{1, 2qR}(D; \mathbb{R}^d), \\ \eta_{Ni}(u) & \in L^1(\Gamma_N; \mathbb{R}), \quad \eta'_{Ni}(u) \in L^2(\Gamma_N; \mathbb{R}), \\ \eta_{Di}(\phi^\alpha(\theta) \partial_\nu u) & \in L^1(\Gamma_D; \mathbb{R}), \quad \eta'_{Di}(\phi^\alpha(\theta) \partial_\nu u) \in W^{1, 2qR}(\Gamma_D; \mathbb{R}). \end{aligned}$$

□

As a supplementary explanation, if we are worried that $\partial_\nu u$ in the third term on the right-hand side of Eq. (8.3.1) cannot be defined from the assumption of $u - u_D \in \mathcal{S}$, it is remarked that this term will disappear due to the Dirichlet condition of adjoint problem (Problem 8.5.1) with respect to f_i shown later.

Using cost functions f_0, f_1, \dots, f_m of Eq. (8.3.1) and the framework of an abstract optimal design problem (Problem 7.3.1), the [topology optimization problem of \$\theta\$ -type](#) is defined as follows.

Problem 8.3.2 (Topology optimization problem of θ -type) Let \mathcal{D} and \mathcal{S} be given by Eq. (8.1.4) and Eq. (8.2.2), respectively. Suppose $f_0, \dots, f_m : X \times U \rightarrow \mathbb{R}$ are given by Eq. (8.3.1). In this case, obtain θ which satisfies

$$\min_{(\theta, u - u_D) \in \mathcal{D} \times \mathcal{S}} \{f_0(\theta, u) \mid f_1(\theta, u) \leq 0, \dots, f_m(\theta, u) \leq 0, \text{ Problem 8.2.3}\}.$$

□

Based on the definition of a Lagrange function in Eq. (7.3.2) with respect to the abstract optimal design problem in Chap. 7, the Lagrange function with respect to Problem 8.3.2 is set to be

$$\begin{aligned} \mathcal{L}(\theta, u, v_0, v_1, \dots, v_m, \lambda_1, \dots, \lambda_m) \\ = \mathcal{L}_0(\theta, u, v_0) + \sum_{i \in \{1, \dots, m\}} \lambda_i \mathcal{L}_i(\theta, u, v_i), \end{aligned} \quad (8.3.2)$$

where $\boldsymbol{\lambda} = \{\lambda_1, \dots, \lambda_m\}^\top \in \mathbb{R}^m$ are Lagrange multipliers with respect to $f_1 \leq 0, \dots, f_m \leq 0$. Moreover,

$$\begin{aligned} \mathcal{L}_i(\theta, u, v_i) &= f_i(\theta, u) + \mathcal{L}_S(\theta, u, v_i) \\ &= \int_D (\zeta_i(\theta, u, \nabla u) - \phi^\alpha(\theta) \nabla u \cdot \nabla v_i + b(\theta) v_i) dx \\ &\quad + \int_{\Gamma_N} (\eta_{Ni}(u) + p_N v_i) d\gamma \\ &\quad + \int_{\Gamma_D} \left\{ (u - u_D) \phi^\alpha(\theta) \partial_\nu v_i \right. \\ &\quad \left. + (v_i \phi^\alpha(\theta) \partial_\nu u - \eta_{Di}(\phi^\alpha(\theta) \partial_\nu u)) \right\} d\gamma - c_i \end{aligned} \quad (8.3.3)$$

is a Lagrange function with respect to f_i . Here, \mathcal{L}_S is the Lagrange function with respect to Problem 8.2.3 defined in Eq. (8.2.4). Moreover, v_i is a Lagrange multiplier with respect to a state determination problem prepared for f_i and assumes $v_i - \eta'_{Di} \in U$. Furthermore, when thinking about the solution of the topology optimization problem of θ -type, the admissible set of $\tilde{v}_i = v_i - \eta'_{Di}$ (admissible set of adjoint variables) needs to be a subset of \mathcal{S} .

8.4 Existence of an Optimum Solution

The existence of an optimum solution of Problem 8.3.2 can be assured by Theorem 7.4.4 in Chap. 7. To use it, we need to show the compactness of

$$\mathcal{F} = \{(\theta, \tilde{u}(\theta)) \in \mathcal{D} \times \mathcal{S} \mid \text{Problem 8.2.3}\} \quad (8.4.1)$$

and the (lower semi) continuity of f_0 . Here, we use $\tilde{u} = u - u_D \in U$.

The compactness of \mathcal{F} is presented in the following lemma.

Lemma 8.4.1 (Compactness of \mathcal{F}) Suppose that Hypothesis 8.2.1 and Hypothesis 8.2.2 are satisfied. With respect to an arbitrary Cauchy sequence $\theta_n \rightarrow \theta$ in X which is uniformly convergent in \mathcal{D} and the solutions $\tilde{u}_n = \tilde{u}(\theta_n) \in U$ ($n \rightarrow \infty$) of Problem 8.2.3, the convergence

$$\tilde{u}_n \rightarrow \tilde{u} \quad \text{strongly in } U$$

holds, and $\tilde{u} = \tilde{u}(\theta) \in U$ solves Problem 8.2.3. \square

Proof Concerning the solution \tilde{u}_n of Problem 8.2.3 for θ_n , the inequality

$$\alpha_n \|\tilde{u}_n\|_U^2 \leq a(\theta_n)(\tilde{u}_n, \tilde{u}_n) = \hat{l}(\theta_n)(\tilde{u}_n) \leq \left\| \hat{l}(\theta_n) \right\|_{U'} \|\tilde{u}_n\|_U$$

holds, where $a(\theta_n)$ and $\hat{l}(\theta_n)$ are defined in Eq. (8.2.5), and α_n is a positive constant used in the definition of coerciveness for $a(\theta_n)$ (see (1) in the answer to Exercise 5.2.5). When $\theta_n \rightarrow \theta$ (uniform convergence in \mathcal{D}), α_n can be replaced by a positive constant α not depending with n . The norm $\left\| \hat{l}(\theta_n) \right\|_{U'} = \|l(\theta_n) + a(\theta_n)(u_D, \cdot)\|_{U'}$ ($l(\theta_n)$ is defined in Eq. (8.2.5)) being bounded can be shown using (3) in the answer to Exercise 5.2.5 via the convergence $\phi^\alpha(\theta_n) \rightarrow \phi^\alpha(\theta)$ for $\theta_n \rightarrow \theta$ (uniform convergence in \mathcal{D}), where $\hat{l}(v)$ and Ω in Exercise 5.2.5 are replaced by $\hat{l}(\theta_n)(v)$ and D , respectively. Hence, there exists a subsequence such that $\tilde{u}_n \rightarrow \tilde{u}$ weakly in U .

Next, we will show that \tilde{u} solves Problem 8.2.3 for θ . From the definition of Problem 8.2.3, we have

$$\lim_{n \rightarrow \infty} a(\theta_n)(\tilde{u}_n, v) = \lim_{n \rightarrow \infty} \hat{l}(\theta_n)(v), \quad (8.4.2)$$

with respect to an arbitrary $v \in U$. The right-hand side of Eq. (8.4.2) becomes

$$\lim_{n \rightarrow \infty} \hat{l}(\theta_n)(v) = \hat{l}(\theta)(v). \quad (8.4.3)$$

Indeed, from Hypothesis 8.2.1, the inequality

$$\begin{aligned} \left| \hat{l}(\theta_n)(v) - \hat{l}(\theta)(v) \right| &= \left| \int_D (b(\theta_n) - b(\theta))v \, dx \right| \\ &\leq \|b(\theta_n) - b(\theta)\|_{L^2(D; \mathbb{R})} \|v\|_{L^2(D; \mathbb{R})} \rightarrow 0 \quad (n \rightarrow \infty) \end{aligned}$$

holds. The left-hand side of Eq. (8.4.2) becomes

$$\lim_{n \rightarrow \infty} a(\theta_n)(\tilde{u}_n, v) = a(\theta)(\tilde{u}, v). \quad (8.4.4)$$

This is due to the fact that, since $\tilde{u}_n \rightarrow \tilde{u}$ weakly in U , we then have

$$\begin{aligned} &|a(\theta_n)(\tilde{u}_n, v) - a(\theta)(\tilde{u}, v)| \\ &= \left| \int_D (\phi^\alpha(\theta_n) - \phi^\alpha(\theta)) \nabla \tilde{u}_n \cdot \nabla v \, dx \right| + \left| \int_D \phi^\alpha(\theta) \nabla(\tilde{u}_n - \tilde{u}) \cdot \nabla v \, dx \right| \\ &\leq \|\phi^\alpha(\theta_n) - \phi^\alpha(\theta)\|_{C^{0,1}(D; \mathbb{R})} \|\tilde{u}_n\|_{H^1(D; \mathbb{R})} \|v\|_{H^1(D; \mathbb{R})} + |a(\theta)(\tilde{u}_n - \tilde{u}, v)| \\ &\rightarrow 0 \quad (n \rightarrow \infty). \end{aligned}$$

Substituting Eq. (8.4.3) and Eq. (8.4.4) into Eq. (8.4.2), the weak form of Problem 8.2.3 is obtained. It means that $\tilde{u} = \tilde{u}(\theta) \in U$ solves Problem 8.2.3.

Since the weak convergence of $\{u_n\}_{n \in \mathbb{N}}$ to u was shown, the strong convergence can be confirmed by showing

$$\|u_n\|_U \rightarrow \|u\|_U \quad (n \rightarrow \infty). \quad (8.4.5)$$

Indeed, when we use $a(\theta)$ in Eq. (8.2.6) as a norm in U and define

$$\|v\| = a(\theta)(v, v),$$

we have

$$\begin{aligned}
\|u_n\| &= a(\theta)(u_n, u_n) = a(\theta - \theta_n)(u_n, u_n) + a(\theta_n)(u_n, u_n) \\
&= \int_D (\phi^\alpha(\theta) - \phi^\alpha(\theta_n)) \nabla u_n \cdot \nabla u_n \, dx + l(\theta_n)(u_n) \\
&\rightarrow l(\theta)(u) = \|u\| \quad (n \rightarrow \infty).
\end{aligned} \tag{8.4.6}$$

From the above relation, it follows that $u_n \rightarrow u$ strongly in U , as desired. \square

We consider that the condition of $\tilde{u}(\theta)$ included in \mathcal{S} is guaranteed in the setting of Problem 8.2.3 (Hypotheses 8.2.1 and 8.2.2).

The continuity of f_0 means that f_0 is continuous on

$$S = \{(\theta, \tilde{u}(\theta)) \in \mathcal{F} \mid f_1(\theta, u(\theta)) \leq 0, \dots, f_m(\theta, u(\theta)) \leq 0\}. \tag{8.4.7}$$

Then, we will confirm the continuity of f_0 by showing the continuity of f_i ($i \in \{0, 1, \dots, m\}$) by the following lemma and assuming that S is not empty.

Lemma 8.4.2 (Continuity of f_0) Let f_i be defined as in Eq. (8.3.1) under Hypothesis 8.3.1. Also, let $u_n \rightarrow u$ strongly in U which is determined by Lemma 8.4.1 with respect to an arbitrary Cauchy sequence $\theta_n \rightarrow \theta$ in X , which is uniformly convergent in \mathcal{D} , satisfy $\|\partial_\nu u_n - \partial_\nu u\|_{L^2(\Gamma_D; \mathbb{R})} \rightarrow 0$ ($n \rightarrow \infty$) on Γ_D . Then, f_i is continuous with respect to $\theta \in \mathcal{D}$. \square

Proof The proof will be completed when

$$\begin{aligned}
|f_i(\theta_n, u_n) - f_i(\theta, u)| &\leq \left| \int_D (\zeta_i(\theta_n, u_n, \nabla u_n) - \zeta_i(\theta, u, \nabla u)) \, dx \right| \\
&\quad + \left| \int_{\Gamma_N} (\eta_{Ni}(u_n) - \eta_{Ni}(u)) \, d\gamma \right| \\
&\quad + \left| \int_{\Gamma_D} (\eta_{Di}(\phi^\alpha(\theta_n)) \partial_\nu u_n - \eta_{Di}(\phi^\alpha(\theta)) \partial_\nu u) \, d\gamma \right| \\
&= e_D + e_{\Gamma_N} + e_{\Gamma_D} \rightarrow 0 \quad (n \rightarrow \infty)
\end{aligned} \tag{8.4.8}$$

is shown with respect to $\theta_n \rightarrow \theta$ ($\theta_n, \theta \in \mathcal{D}$). From $\tilde{u}_n \rightarrow \tilde{u}$ weakly in U , the convergence $e_D \rightarrow 0$ ($n \rightarrow \infty$) is obtained. Indeed, writing $\tilde{\zeta}_i(t) = \zeta_i(t\theta_n + (1-t)\theta, tu_n + (1-t)u, t\nabla u_n + (1-t)\nabla u)$ ($t \in [0, 1]$) and considering $\zeta_i \in C^1(\mathbb{R} \times \mathbb{R} \times \mathbb{R}^d; \mathbb{R})$ in Hypothesis 8.3.1, we get

$$\begin{aligned}
e_D &\leq \sup_{t \in [0, 1]} \left| \int_D \tilde{\zeta}_{i\theta}(t) [\theta_n - \theta] \, dx \right| + \sup_{t \in [0, 1]} \left| \int_D \tilde{\zeta}_{iu}(t) [u_n - u] \, dx \right| \\
&\quad + \sup_{t \in [0, 1]} \left| \int_D \tilde{\zeta}_{i\nabla u}(t) [\nabla u_n - \nabla u] \, dx \right| \\
&\leq \sup_{t \in [0, 1]} \left\| \tilde{\zeta}_{i\theta}(t) \right\|_{L^{q_R}(D; \mathbb{R})} \|\theta_n - \theta\|_X + \sup_{t \in [0, 1]} \left\| \tilde{\zeta}_{iu}(t) \right\|_{L^{2q_R}(D; \mathbb{R})} \|u_n - u\|_U \\
&\quad + \sup_{t \in [0, 1]} \left\| \tilde{\zeta}_{i\nabla u}(t) \right\|_{W^{1, 2q_R}(D; \mathbb{R}^d)} \|\nabla u_n - \nabla u\|_{L^2(D; \mathbb{R}^d)},
\end{aligned}$$

In the same way, we can obtain $e_{\Gamma_N} \rightarrow 0$. Meanwhile, the convergence $e_{\Gamma_D} \rightarrow 0$ ($n \rightarrow \infty$) can be shown in the following way. Writing $\tilde{\eta}_{D_i}(t) = \eta_{D_i}(\phi^\alpha(t\theta_n + (1-t)\theta)(t\partial_\nu u_n + (1-t)\partial_\nu u))$ ($t \in [0, 1]$) and considering $\eta_{D_i} \in C^1(\mathbb{R}; \mathbb{R})$ in Hypothesis 8.3.1, we see that the sequence of inequalities

$$\begin{aligned} e_{\Gamma_D} &\leq \sup_{t \in [0, 1]} \left| \int_{\Gamma_D} \tilde{\eta}'_{D_i}(t) [\phi^\alpha(\theta_n) \partial_\nu u_n - \phi^\alpha(\theta) \partial_\nu u] dx \right| \\ &= \sup_{t \in [0, 1]} \left| \int_{\Gamma_D} \tilde{\eta}'_{D_i}(t) [(\phi^\alpha(\theta_n) - \phi^\alpha(\theta)) \partial_\nu u_n + \phi^\alpha(\theta) (\partial_\nu u_n - \partial_\nu u)] dx \right| \\ &\leq \|\gamma_{\Gamma_D}\|^3 \sup_{t \in [0, 1]} \|\tilde{\eta}'_{D_i}(t)\|_{W^{1, 2q_R}(D; \mathbb{R})} \\ &\quad \times \left(\|\theta_n - \theta\|_X \|\partial_\nu u_n\|_{L^2(\Gamma_D; \mathbb{R})} + \|\theta\|_X \|\partial_\nu u_n - \partial_\nu u\|_{L^2(\Gamma_D; \mathbb{R})} \right) \end{aligned}$$

holds. Here, boundedness of the trace operator $\|\gamma_{\Gamma_D}\|$ (Eq. (5.2.4)) was used. In conclusion, we obtain Eq. (8.4.8). \square

From Lemma 8.4.1, the compactness of \mathcal{F} was confirmed. The continuity of f_0 was shown by Lemma 8.4.2 and by the assumption that S is not empty. Then, under these conditions, it can be assured that there exists an optimum solution to Problem 8.3.2 by Theorem 7.4.4 (existence of an optimum solution).

Regarding the solution of Problem 8.3.2, we state the following remark.

Remark 8.4.3 (Existence of an optimum solution) The compactness of \mathcal{F} defined in Eq. (8.4.1) is based on the compactness of θ 's admissible set \mathcal{D} defined in Eq. (8.1.4). In Eq. (8.1.4), the condition $\max \left\{ \|\theta\|_{H^2(D; \mathbb{R})}, \|\theta\|_{C^{0, 1}(D; \mathbb{R})} \right\} \leq \beta$ with a positive constant β is added. This condition corresponds to the condition called a [side constraint](#) in Chap. 1. Such a side constraint is usually neglected, but it should be considered as a non-equality constraint when the condition becomes active. \square

Moreover, regarding the selection of the linear space X and the admissible set \mathcal{D} for the design variable, the following remark is left for reference.

Remark 8.4.4 (Selection of X and \mathcal{D}) The existence of a solution to Problem 8.3.2 was confirmed by Theorem 7.4.4 in Chap. 7. In the assumption of the theorem, it is necessary to assume that \mathcal{D} is a compact subset in X . In this chapter, this relation was satisfied by taking X as a function space of class H^1 and \mathcal{D} as a set of functions of $(H^2 \cap C^{0, 1})$ -class based on the Rellich–Kondrachov compact embedding theorem (Theorem 4.4.15). However, there are other selections. For instance, it is possible to select X as a function space of C^0 class and \mathcal{D} as a set of functions of $C^{0, 1}$ class. In this case, the [Ascoli–Arzelà theorem](#) (Theorem A.10.1) is used to show that \mathcal{D} is a compact subset in X [15, proof in Theorem 2.1, p. 16]. When those are selected, the assumptions and lemmas are changed to show the existence of a solution. In this book, since a gradient method in a Hilbert space is considered, X and \mathcal{D} were selected as noted above. \square

8.5 Derivatives of Cost Functions

From this point onward, we will consider a solution to Problem 8.3.2 given that the conditions for its existence are satisfied. The Fréchet derivative of cost function f_i with respect to the variation of design variable θ will be referred to as a θ -derivative. Let us seek the θ -derivative of f_i by the Lagrange multiplier method such as that looked at in Section 7.5.2. Furthermore, let us seek the second-order θ -derivative of f_i using a method such as that seen in Section 7.5.3.

8.5.1 θ -Derivatives of Cost Functions

Let us focus on the Lagrange function \mathcal{L}_i of f_i defined in Eq. (8.3.3). The Fréchet derivative of \mathcal{L}_i with respect to an arbitrary variation $(\vartheta, \hat{u}, \hat{v}_i) \in X \times U \times U$ of (θ, u, v_i) becomes

$$\begin{aligned} \mathcal{L}'_i(\theta, u, v_i)[\vartheta, \hat{u}, \hat{v}_i] &= \mathcal{L}_{i\theta}(\theta, u, v_i)[\vartheta] + \mathcal{L}_{iu}(\theta, u, v_i)[\hat{u}] + \mathcal{L}_{iv_i}(\theta, u, v_i)[\hat{v}_i]. \end{aligned} \quad (8.5.1)$$

The third term on the right-hand side of Eq. (8.5.1) becomes

$$\mathcal{L}_{iv_i}(\theta, u, v_i)[\hat{v}_i] = \mathcal{L}_{Sv_i}(\theta, u, v_i)[\hat{v}_i] = \mathcal{L}_S(\theta, u, \hat{v}_i). \quad (8.5.2)$$

Equation (8.5.2) is the Lagrange function of the state determination problem (Problem 8.2.3). Here, if u is the weak solution of the state determination problem, the third term on the right-hand side of Eq. (8.5.1) is zero.

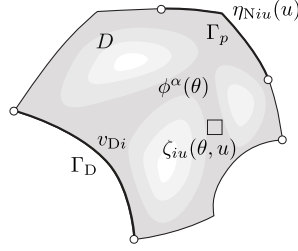
Moreover, the second term on the right-hand side of Eq. (8.5.1) becomes

$$\begin{aligned} \mathcal{L}_{iu}(\theta, u, v_i)[\hat{u}] &= \int_D \left(-\phi^\alpha(\theta) \nabla v_i \cdot \nabla \hat{u} + \zeta_{iu} \hat{u} + \zeta_{i(\nabla u)^\top} \cdot \nabla \hat{u} \right) dx \\ &\quad + \int_{\Gamma_N} \eta'_{Ni} \hat{u} \, d\gamma + \int_{\Gamma_D} \{ \hat{u} \phi^\alpha(\theta) \partial_\nu v + (v_i - \eta'_{Di}) \phi^\alpha(\theta) \partial_\nu \hat{u} \} \, d\gamma, \end{aligned} \quad (8.5.3)$$

where $\zeta_{iu}(\theta, u, \nabla u)[\hat{u}]$, $\zeta_{i(\nabla u)^\top}(\theta, u, \nabla u)[\nabla \hat{u}]$, $\eta'_{Ni}(u)[\hat{u}]$ and $\eta'_{Di}(u)[\phi^\alpha(\theta) \partial_\nu \hat{u}]$ were written as $\zeta_{iu} \hat{u}$, $\zeta_{i(\nabla u)^\top} \cdot \nabla \hat{u}$, $\eta'_{Ni} \hat{u}$ and $\eta'_{Di} \phi^\alpha(\theta) \partial_\nu \hat{u}$, respectively. Here, if v_i is determined so that Eq. (8.5.3) becomes zero, the second term on the right-hand side of Eq. (8.5.1) becomes zero. This relationship is the weak form of the adjoint problem with respect to f_i shown next. Here, when v_i is the weak solution of Problem 8.5.1, the second term of the right-hand side of Eq. (8.5.1) vanishes. The boundary condition of Problem 8.5.1 is as shown in Fig. 8.8.

Problem 8.5.1 (Adjoint problem with respect to f_i) For $\theta \in \mathcal{D}^\circ$, supposing the solution u is given to Problem 8.2.3, obtain $v_i : D \rightarrow \mathbb{R}$ which satisfies

$$-\nabla \cdot (\phi^\alpha(\theta) \nabla v_i) = \zeta_{iu}(\theta, u, \nabla u) - \nabla \cdot \left(\zeta_{i(\nabla u)^\top}(\theta, u, \nabla u) \right) \quad \text{in } D,$$


 Fig. 8.8: Adjoint problem with respect to f_i .

$$\begin{aligned}\phi^\alpha(\theta) \partial_\nu v_i &= \eta'_{Ni}(u) + \zeta_{i(\nabla u)^\top} \cdot \boldsymbol{\nu} \quad \text{on } \Gamma_N, \\ v_i &= \eta'_{Di} \quad \text{on } \Gamma_D.\end{aligned}$$

□

Similarly to the solution u of the state determination problem, when Hypotheses 8.3.1 and 8.2.2 are satisfied, the solution $\tilde{v}_i = v_i - \eta'_{Di}$ of Problem 8.5.1 is guaranteed to be included in S .

Furthermore, the first term on the right-hand side of Eq. (8.5.1) becomes

$$\begin{aligned}\mathcal{L}_{i\theta}(\theta, u, v_i)[\vartheta] &= \int_D (\zeta_{i\theta} + b'v_i - \alpha\phi^{\alpha-1}\phi' \nabla u \cdot \nabla v_i) \vartheta \, dx \\ &\quad + \int_{\Gamma_D} \alpha\phi^{\alpha-1}\phi' \{(u - u_D) \partial_\nu v_i + (v_i - \eta'_{Di}) \partial_\nu u\} \, d\gamma.\end{aligned}\quad (8.5.4)$$

In the above equation, u and v_i are assumed to be the weak solutions of Problems 8.2.3 and 8.5.1, respectively. If we denote $f_i(\theta, u)$ here by $\tilde{f}_i(\theta)$, we can write

$$\tilde{f}'_i(\theta)[\vartheta] = \mathcal{L}_{i\theta}(\theta, u, v_i)[\vartheta] = \langle g_i, \vartheta \rangle, \quad (8.5.5)$$

where

$$g_i = \zeta_{i\theta} + b'v_i - \alpha\phi^{\alpha-1}\phi' \nabla u \cdot \nabla v_i. \quad (8.5.6)$$

When Eq. (8.1.1) is used in $\phi(\theta)$, we get

$$\phi'(\theta) = \frac{1}{\pi} \frac{1}{1 + \theta^2}. \quad (8.5.7)$$

Moreover, when Eq. (8.1.2) is used,

$$\phi'(\theta) = \frac{1}{2} \operatorname{sech}^2 \theta = \frac{1}{2} \frac{1}{\cosh^2 \theta} = \frac{1}{(e^\theta + e^{-\theta})^2}. \quad (8.5.8)$$

From the above, the following results can be obtained with respect to θ -derivative g_i of f_i .

Theorem 8.5.2 (θ -derivative of f_i) For $\theta \in \mathcal{D}^\circ$, suppose u and v_i are the weak solutions of Problems 8.2.3 and 8.5.1 and these are said to be in \mathcal{S} of Eq. (8.2.2) (Hypotheses 8.2.1, 8.2.2 and 8.3.1 are satisfied). In this case, the θ -derivative of f_i becomes Eq. (8.5.5). Hence, g_i of Eq. (8.5.6) is in X' . Furthermore, $g_i \in L^{q_R}(D; \mathbb{R})$. \square

Proof The fact that the θ -derivative of f_i becomes the g_i of Eq. (8.5.5) is as seen above. The following results can be obtained in respect of the regularity of g_i . If Hölder's inequality (Theorem A.9.1) and Poincaré's inequality (Corollary A.9.4) are used in Eq. (8.5.5),

$$\begin{aligned} & |\langle g_i, \vartheta \rangle|_{L^1(D; \mathbb{R})} \\ & \leq \left(\|\zeta_i \theta\|_{L^{q_R}(D; \mathbb{R})} + \|b'\|_{L^{2q_R}(D; \mathbb{R})} \|v_i\|_{L^{2q_R}(D; \mathbb{R})} \right. \\ & \quad \left. + \|\alpha \phi^{\alpha-1} \phi'\|_{C^\infty(\mathbb{R}; \mathbb{R})} \|\nabla u\|_{L^{2q_R}(D; \mathbb{R}^d)} \|\nabla v_i\|_{L^{2q_R}(D; \mathbb{R}^d)} \right) \|\vartheta\|_{L^2(D; \mathbb{R})} \\ & \leq \left(\|\zeta_i \theta\|_{L^{q_R}(D; \mathbb{R})} + \|b'\|_{L^{2q_R}(D; \mathbb{R})} \|v_i\|_{L^{2q_R}(D; \mathbb{R})} \right. \\ & \quad \left. + \|\alpha \phi^{\alpha-1} \phi'\|_{C^\infty(\mathbb{R}; \mathbb{R})} \|u\|_{W^{1, 2q_R}(D; \mathbb{R})} \|v_i\|_{W^{1, 2q_R}(D; \mathbb{R})} \right) \|\vartheta\|_X \end{aligned}$$

is obtained. The term (\cdot) on the right-hand side of the equation above is completely bounded due to the hypotheses. Hence, g_i is included in X' . Moreover, from the fact that each term within (\cdot) is in $L^{q_R}(D; \mathbb{R})$, $g_i \in L^{q_R}(D; \mathbb{R})$ can be obtained. \square

From Theorem 8.5.2, the following can be said about the regularity of the topology optimization problem of θ -type.

Remark 8.5.3 (Irregularity of topology optimization problem of θ -type)

If in Theorem 8.5.2, Hypotheses 8.2.1, 8.2.2 and 8.3.1 are made more strict and a problem is constructed such that u and v_i are included in $W^{2, \infty}(D; \mathbb{R})$, g_i would be included in $C^{0,1}(D; \mathbb{R})$. In this case, the design variable $\theta + \epsilon \vartheta$ (ϵ is a positive constant) updated via the gradient method such that $-g_i$ is replaced by ϑ would be included in the admissible set of design variables \mathcal{D} . However, in such a case, it is necessary that the corner points permitted by Hypothesis 8.2.2 are removed, there is no boundary between the Dirichlet and Neumann boundaries, such as a Robin problem, or the neighborhoods of such points are included in $\bar{\Omega}_C$ in order to fix θ .

If these conditions are not satisfied, g_i is not included in $C^{0,1}(D; \mathbb{R})$. Hence, in a gradient method such that $-g_i$ is replaced by ϑ , $\theta + \epsilon \vartheta$ is not included in the admissible set \mathcal{D} of design variables. This result is thought to be one of the reasons for numerical instability phenomena in which a checkerboard pattern appears such as that in Fig. 8.5. \square

8.5.2 Second-Order θ -Derivative of Cost Functions

Furthermore, let us seek the second-order derivative (Hessian) of the cost function with respect to the variation of the design variable. In Section 7.5.3, the way to seek a second-order Fréchet derivative with respect to an abstract

optimal design problem has already been shown. Hence, let us follow that method in order to seek the second-order θ -derivative of f_i with respect to f_i given in Eq. (8.3.1).

The following assumption is established in order to obtain the second-order θ -derivative of f_i .

Hypothesis 8.5.4 (Second-order θ -derivative of \tilde{f}_i) With respect to the state determination problem (Problem 8.2.3) and the cost function f_i defined in Eq. (8.3.1), assume respectively that:

- (1) b is not a function of θ ,
- (2) ζ_i is not a function of u (it is a function of θ and ∇u).

□

Hypothesis 8.5.4 will be used in Eq. (8.5.16) to obtain Eq. (8.5.17). However, in the method shown in Sect. 8.5.3, this hypothesis will not be required.

The Lagrange function \mathcal{L}_i of f_i is defined by Eq. (8.3.3). Viewing (θ, u) as a design variable and putting its admissible set and admissible set of directions as

$$S = \{(\theta, u) \in \mathcal{D} \times \mathcal{S} \mid \mathcal{L}_S(\theta, u, v) = 0 \text{ for all } v \in U\},$$

$$T_S(\theta, u) = \{(\vartheta, \hat{v}) \in X \times U \mid \mathcal{L}_{S\theta u}(\theta, u, v)[\vartheta, \hat{v}] = 0 \text{ for all } v \in U\},$$

the second-order Fréchet partial derivative of \mathcal{L}_i with respect to arbitrary variations $(\vartheta_1, \hat{v}_1), (\vartheta_2, \hat{v}_2) \in T_S(\theta, u)$ of $(\theta, u) \in S$, similarly to Eq. (7.5.21), becomes

$$\begin{aligned} & \mathcal{L}_{i(\theta, u)(\theta, u)}(\theta, u, v_i)[(\vartheta_1, \hat{v}_1), (\vartheta_2, \hat{v}_2)] \\ &= \mathcal{L}_{i\theta\theta}(\theta, u, v_i)[\vartheta_1, \vartheta_2] + \mathcal{L}_{i\theta u}(\theta, u, v_i)[\vartheta_1, \hat{v}_2] \\ & \quad + \mathcal{L}_{i\theta u}(\theta, u, v_i)[\vartheta_2, \hat{v}_1] + \mathcal{L}_{iuu}(\theta, u, v_i)[\hat{v}_1, \hat{v}_2]. \end{aligned} \quad (8.5.9)$$

Each term on the right-hand side of Eq. (8.5.9) becomes

$$\mathcal{L}_{i\theta\theta}(\theta, u, v_i)[\vartheta_1, \vartheta_2] = \int_D \{ \zeta_{i\theta\theta} - (\phi^\alpha(\theta))'' \nabla u \cdot \nabla v_i \} \vartheta_1 \vartheta_2 \, dx, \quad (8.5.10)$$

$$\begin{aligned} & \mathcal{L}_{i\theta u}(\theta, u, v_i)[\vartheta_1, \hat{v}_2] \\ &= \int_D \left\{ \zeta_{i\theta(\nabla u)^\top} \cdot \nabla \hat{v}_2 - (\phi^\alpha(\theta))' \nabla \hat{v}_2 \cdot \nabla v_i \right\} \vartheta_1 \, dx, \end{aligned} \quad (8.5.11)$$

$$\begin{aligned} & \mathcal{L}_{i\theta u}(\theta, u, v_i)[\vartheta_2, \hat{v}_1] \\ &= \int_D \left\{ \zeta_{i\theta(\nabla u)^\top} \cdot \nabla \hat{v}_1 - (\phi^\alpha(\theta))' \nabla \hat{v}_1 \cdot \nabla v_i \right\} \vartheta_2 \, dx, \end{aligned} \quad (8.5.12)$$

$$\mathcal{L}_{iuu}(\theta, u, v_i)[\hat{v}_1, \hat{v}_2] = 0. \quad (8.5.13)$$

Here, the fact that $u - u_D, v_i - \eta'_{D_i}, \hat{v}_1$ and \hat{v}_2 become zero on Γ_D was used. Moreover,

$$(\phi^\alpha(\theta))' = \alpha \phi^{\alpha-1}(\theta) \phi'(\theta), \quad (8.5.14)$$

$$(\phi^\alpha(\theta))'' = \alpha(\alpha-1)\phi^{\alpha-2}(\theta)\phi'^2(\theta) + \alpha\phi^{\alpha-1}(\theta)\phi''(\theta). \quad (8.5.15)$$

On the other hand, with respect to arbitrary variations $(\vartheta_j, \hat{v}_j) \in T_S(\theta, u)$ for $j \in \{1, 2\}$, the Fréchet partial derivative of \mathcal{L}_S becomes

$$\begin{aligned} & \mathcal{L}_{S\theta u}(\theta, u, v)[\vartheta_j, \hat{v}_j] \\ &= \int_D \{ -(\phi^\alpha(\theta))' \vartheta \nabla u - \phi^\alpha(\theta) \nabla \hat{v}_j \} \cdot \nabla v \, dx \\ &= 0 \end{aligned} \quad (8.5.16)$$

with respect to an arbitrary $v \in U$. Here, Hypothesis 8.5.4 and the fact that v and \hat{v}_j are both zero on Γ_D were used. From Eq. (8.5.16), we can obtain

$$\nabla \hat{v}_j = -\frac{(\phi^\alpha(\theta))'}{\phi^\alpha(\theta)} \vartheta_j \nabla u \quad \text{in } D. \quad (8.5.17)$$

This relation becomes possible the following argument.

Substituting \hat{v}_j of Eq. (8.5.17) into \hat{v}_j in Eq. (8.5.9), and considering Dirichlet boundary conditions in the state determination problem and the adjoint problems with respect to f_1, \dots, f_m , as well as $\hat{v}_j = 0$ on Γ_D , we have

$$\begin{aligned} & \mathcal{L}_{i\theta u}(\theta, u, v_i)[\vartheta_1, \hat{v}_2] = \mathcal{L}_{i\theta}(\theta, u, v_i)[\hat{v}_1, \vartheta_2] \\ &= \int_D \frac{(\phi^\alpha(\theta))'}{\phi^\alpha(\theta)} \left\{ (\phi^\alpha(\theta))' \nabla v_i - \zeta_{i\theta(\nabla u)^\top} \right\} \cdot \nabla u \vartheta_1 \vartheta_2 \, dx. \end{aligned} \quad (8.5.18)$$

Summarizing the results above, from Eq. (8.5.10), Eq. (8.5.13) and Eq. (8.5.18), the second-order θ -derivative of \tilde{f}_i becomes

$$\begin{aligned} & h_i(\theta, u, v_i)[\vartheta_1, \vartheta_2] \\ &= \int_D \left[\left\{ 2 \frac{(\phi^\alpha(\theta))^2}{\phi^\alpha(\theta)} - (\phi^\alpha(\theta))'' \right\} \nabla u \cdot \nabla v_i \right. \\ & \quad \left. + \zeta_{i\theta\theta} - 2 \frac{(\phi^\alpha(\theta))'}{\phi^\alpha(\theta)} \zeta_{i\theta(\nabla u)^\top} \cdot \nabla u \right] \vartheta_1 \vartheta_2 \, dx \\ &= \int_D \left(\beta(\alpha, \theta) \nabla u \cdot \nabla v_i + \zeta_{i\theta\theta} - 2\alpha \frac{\phi'(\theta)}{\phi(\theta)} \zeta_{i\theta(\nabla u)^\top} \cdot \nabla u \right) \vartheta_1 \vartheta_2 \, dx, \end{aligned} \quad (8.5.19)$$

where

$$\beta(\alpha, \theta) = \alpha(\alpha+1)\phi^{\alpha-2}(\theta)\phi'^2(\theta) - \alpha\phi^{\alpha-1}(\theta)\phi''(\theta). \quad (8.5.20)$$

When $\phi(\theta)$ is given by Eq. (8.1.1) or Eq. (8.1.2), they respectively become

$$\beta(\alpha, \theta) = \alpha(\alpha+1) \left(\frac{1}{\pi} \tan^{-1} \theta + \frac{1}{2} \right)^{\alpha-2} \left\{ \frac{1}{\pi(1+\theta^2)} \right\}^2$$

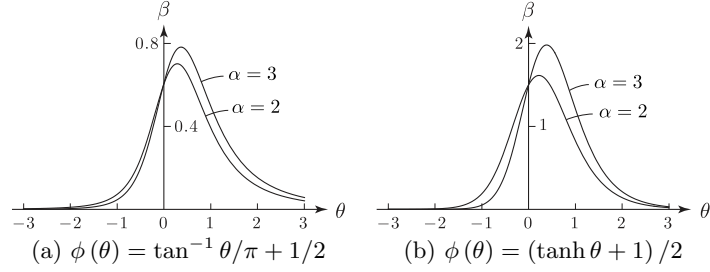


Fig. 8.9: Coefficient function $\beta(\alpha, \theta)$ in the second-order θ -derivative of the cost function.

$$-\alpha \left(\frac{1}{\pi} \tan^{-1} \theta + \frac{1}{2} \right)^{\alpha-1} \left\{ -\frac{2\theta}{\pi(1+\theta^2)^2} \right\} \quad (8.5.21)$$

or

$$\begin{aligned} \beta(\alpha, \theta) &= \alpha(\alpha+1) \left(\frac{1}{2} \tanh \theta + \frac{1}{2} \right)^{\alpha-2} \left(\frac{\operatorname{sech}^2 \theta}{2} \right)^2 \\ &\quad - \alpha \left(\frac{1}{2} \tanh \theta + \frac{1}{2} \right)^{\alpha-1} (-\operatorname{sech}^2 \theta \tanh \theta). \end{aligned} \quad (8.5.22)$$

Figure 8.9 shows the graph of $\beta(\alpha, \theta)$. From these graphs, the fact that $\beta(\alpha, \theta) > 0$ holds can be confirmed. Furthermore, if the remainder term in (\cdot) on the right-hand side of Eq. (8.5.19) is positive and bounded, $h_i(\theta, u, v_i)[\cdot, \cdot]$ becomes a coercive and bounded bilinear form on X .

8.5.3 Second Order θ -Derivative of Cost Function Using Lagrange Multiplier Method

When the Lagrange multiplier method is used to obtain the second-order θ -derivative of a cost function, we use the same idea as proposed in Section 7.5.4. Fixing ϑ_1 , we define the Lagrange function with respect to $\tilde{f}'_i(\theta)[\vartheta_1] = \langle g_i, \vartheta_1 \rangle$ in Eq. (8.5.5) by

$$\mathcal{L}_{I_i}(\theta, u, v_i, w_i, z_i) = \langle g_i, \vartheta_1 \rangle + \mathcal{L}_S(\theta, u, w_i) + \mathcal{L}_{A_i}(\theta, v_i, z_i), \quad (8.5.23)$$

where \mathcal{L}_S is given by Eq. (8.2.4), and

$$\begin{aligned} &\mathcal{L}_{A_i}(\theta, v_i, z_i) \\ &= \int_D \left(-\phi^\alpha(\theta) \nabla v_i \cdot \nabla z_i + \zeta_{iu} z_i + \zeta_{i(\nabla u)^\top} \cdot \nabla z_i \right) dx \\ &\quad + \int_{\Gamma_N} \eta'_{N_i} z_i \, d\gamma + \int_{\Gamma_D} \{ z_i \phi^\alpha(\theta) \partial_\nu v + (v_i - \eta'_{D_i}) \phi^\alpha(\theta) \partial_\nu z_i \} \, d\gamma \end{aligned} \quad (8.5.24)$$

is the Lagrange function with respect to the adjoint problem (Problem 8.5.1) with respect to f_i . $w_i \in U$ and $z_i \in U$ are the adjoint variables provided for u and v_i in g_i .

With respect to arbitrary variations $(\vartheta_2, \hat{u}, \hat{v}_i, \hat{w}_i, \hat{z}_i) \in X \times U^4$ of $(\theta, u, v_i, w_i, z_i)$, the Fréchet derivative of \mathcal{L}_i is written as

$$\begin{aligned} & \mathcal{L}'_i(\theta, u, v_i, w_i, z_i) [\vartheta_2, \hat{u}, \hat{v}_i, \hat{w}_i, \hat{z}_i] \\ &= \mathcal{L}_{i\theta}(\theta, u, v_i, w_i, z_i) [\vartheta_2] + \mathcal{L}_{iu}(\theta, u, v_i, w_i, z_i) [\hat{u}] \\ & \quad + \mathcal{L}_{iv_i}(\theta, u, v_i, w_i, z_i) [\hat{v}_i] + \mathcal{L}_{iw_i}(\theta, u, v_i, w_i, z_i) [\hat{w}_i] \\ & \quad + \mathcal{L}_{iz_i}(\theta, u, v_i, w_i, z_i) [\hat{z}_i]. \end{aligned} \quad (8.5.25)$$

The fourth term on the right-hand side of Eq. (8.5.25) vanishes if u is the solution of the state determination problem. If v_i can be determined as the solution of the adjoint problem, the fifth term of Eq. (8.5.25) also vanishes.

The second term on the right-hand side of Eq. (8.5.25) is

$$\begin{aligned} & \mathcal{L}_{iu}(\theta, u, v_i, w_i, z_i) [\hat{u}] \\ &= \int_D \left[\left\{ \left(\zeta_{i\theta u} + \zeta_{iuu} z_i + \zeta_{i(\nabla u)^\top u} \cdot \nabla z_i \right) \hat{u} - \alpha \phi^{\alpha-1} \phi' \nabla v_i \cdot \nabla \hat{u} \right\} \vartheta_1 \right. \\ & \quad \left. - \phi^\alpha \nabla w_i \cdot \nabla \hat{u} \right] dx. \end{aligned} \quad (8.5.26)$$

Here, the condition that Eq. (8.5.26) is zero for arbitrary $\hat{u} \in U$ is equivalent to setting w_i to be the solution of the following adjoint problem.

Problem 8.5.5 (Adjoint problem of w_i with respect to $\langle g_i, \vartheta_1 \rangle$) Under the assumption of Problem 8.3.2, letting $\vartheta_1 \in X$ be given, find $w_i = w_i(\vartheta_1) \in U$ satisfying

$$\begin{aligned} -\nabla \cdot (\phi^\alpha \nabla w_i) &= \left(\nabla \cdot (\alpha \phi^{\alpha-1} \phi' \nabla v_i) + \zeta_{i\theta u} + \zeta_{iuu} z_i + \zeta_{i(\nabla u)^\top u} \cdot \nabla z_i \right) \vartheta_1 \\ & \quad \text{in } D, \\ \phi^\alpha \partial_\nu w_i &= \alpha \phi^{\alpha-1} \phi' \partial_\nu v_i \vartheta_1 \quad \text{on } \Gamma_N, \\ w_i &= 0 \quad \text{on } \Gamma_D. \end{aligned}$$

□

The third term on the right-hand side of Eq. (8.5.25) is

$$\begin{aligned} & \mathcal{L}_{iv_i}(\theta, u, v_i, w_i, z_i) [\hat{v}_i] \\ &= \int_D \left\{ (b' \hat{v}_i - \alpha \phi^{\alpha-1} \phi' \nabla u \cdot \nabla \hat{v}_i) \vartheta_1 - \phi^\alpha \nabla z_i \cdot \nabla \hat{v}_i \right\} dx. \end{aligned} \quad (8.5.27)$$

Here, the condition that Eq. (8.5.27) is zero for arbitrary $\hat{v}_i \in U$ is equivalent to setting z_i to be the solution of the following adjoint problem.

Problem 8.5.6 (Adjoint problem of z_i with respect to $\langle g_i, \vartheta_1 \rangle$) Under the assumption of Problem 8.3.2, letting $\vartheta_1 \in X$ be given, find $z_i = z_i(\vartheta_1) \in U$ satisfying

$$\begin{aligned} -\nabla \cdot (\phi^\alpha \nabla z_i) &= (\nabla \cdot (\alpha \phi^{\alpha-1} \phi' \nabla u) + b') \vartheta_1 \quad \text{in } D, \\ \phi^\alpha \partial_\nu z_i &= \alpha \phi^{\alpha-1} \phi' \partial_\nu u \vartheta_1 \quad \text{on } \Gamma_N, \\ z_i &= 0 \quad \text{on } \Gamma_D. \end{aligned}$$

□

Finally, the first term on the right-hand side of Eq. (8.5.25) becomes

$$\begin{aligned} &\mathcal{L}_{i\theta}(\theta, u, v_i, w_i, z_i)[\vartheta_2] \\ &= \int_D \left[\{ \zeta_{i\theta\theta} u + b'' v_i - (\alpha(\alpha-1)\phi^{\alpha-2}\phi'^2 + \alpha\phi^{\alpha-1}\phi'') \nabla u \cdot \nabla v_i \} \vartheta_1 \right. \\ &\quad \left. - \alpha\phi^{\alpha-1}\phi' (\nabla u \cdot \nabla w_i + \nabla v_i \cdot \nabla z_i) + b'(w_i + z_i) \right] \vartheta_2 \, dx. \end{aligned}$$

Here, u , v_i , $w_i(\vartheta_1)$ and $z_i(\vartheta_1)$ are assumed to be the weak solutions of Problems 8.2.3, 8.5.1, 8.5.5 and 8.5.6, respectively. If we denote $f_i(\theta, u)$ here by $\tilde{f}_i(\theta)$, we have the relation:

$$\begin{aligned} \mathcal{L}_{i\theta}(\theta, u, v_i, w_i(\vartheta_1), z_i(\vartheta_1))[\vartheta_2] &= \tilde{f}_i''(\theta)[\vartheta_1, \vartheta_2] \\ &= \langle g_{Hi}(\theta, \vartheta_1), \vartheta_2 \rangle, \end{aligned} \tag{8.5.28}$$

where the Hesse gradient g_{Hi} of f_i is given by

$$\begin{aligned} &g_{Hi}(\theta, \vartheta_1) \\ &= \{ -(\alpha(\alpha-1)\phi^{\alpha-2}\phi'^2 + \alpha\phi^{\alpha-1}\phi'') \nabla u \cdot \nabla v_i + \zeta_{i\theta\theta} u + b'' v_i \} \vartheta_1 \\ &\quad - \alpha\phi^{\alpha-1}\phi' (\nabla u \cdot \nabla w_i(\vartheta_1) + \nabla v_i \cdot \nabla z_i(\vartheta_1)) \\ &\quad + b'(w_i(\vartheta_1) + z_i(\vartheta_1)). \end{aligned} \tag{8.5.29}$$

We obtained two different expressions for the second-order derivative $\tilde{f}_i''(\theta)[\vartheta_1, \vartheta_2]$. Under the assumption of Hypothesis 8.5.4, they accord when using the same ϑ_1 and ϑ_2 . This relation will be confirmed in Sections 8.9 and 8.10.

8.6 Descent Directions of Cost Functions

In Remark 8.5.3, it was shown that the topology optimization problem of θ -type becomes irregular unless a special assumption of regularity is set. Here, let us consider the gradient method and Newton method on the linear space X of design variables with the functionality of regularizing θ -derivative of a cost function. Here, with respect to the $i \in \{0, \dots, m\}$ th cost function f_i , assume that the gradient $g_i \in X'$ of Eq. (8.5.6) and Hessian $h_i \in \mathcal{L}^2(X \times X; \mathbb{R})$ of Eq. (8.5.19) are given and think about the method to obtain a descent direction of f_i using the gradient method and Newton method on the linear space X of design variables.

8.6.1 H^1 Gradient Method

The method for obtaining the aforementioned descent direction vector using the solution $\vartheta_{g_i} \in X$ to the next problem will be referred to as the H^1 gradient method of θ -type.

Problem 8.6.1 (H^1 gradient method of θ -type) Let X and \mathcal{D} be Eq. (8.1.3) and Eq. (8.1.4), respectively. Let $a_X : X \times X \rightarrow \mathbb{R}$ be a bounded and coercive bilinear form on X . In other words, it is supposed that some positive constants α_X and β_X exist and that

$$a_X(\vartheta, \vartheta) \geq \alpha_X \|\vartheta\|_X^2, \quad |a_X(\vartheta, \psi)| \leq \beta_X \|\vartheta\|_X \|\psi\|_X \quad (8.6.1)$$

holds with respect to arbitrary $\vartheta \in X$ and $\psi \in X$. For each $f_i \in C^1(\mathcal{D}; \mathbb{R})$, let $g_i(\theta_k) \in X'$ be its corresponding θ -derivative at $\theta_k \in \mathcal{D}^\circ$ which is not a local minimum point. In this case, obtain $\vartheta_{g_i} \in X$ which satisfies

$$a_X(\vartheta_{g_i}, \psi) = -\langle g_i(\theta_k), \psi \rangle \quad (8.6.2)$$

with respect to an arbitrary $\psi \in X$. \square

There is an arbitrary property for choosing $a_X : X \times X \rightarrow \mathbb{R}$ which was assumed in Problem 8.6.1. Several specific examples will be shown below.

Method Using the Inner Product of H^1 Space

An inner product in a real Hilbert space is coercive. Hence, let us use the inner product as

$$a_X(\vartheta, \psi) = \int_D (\nabla \vartheta \cdot \nabla \psi + c_D \vartheta \psi) \, dx, \quad (8.6.3)$$

Here, it is assumed that c_D is a uniformly bounded element of $L^\infty(D; \mathbb{R})$ which is positive almost everywhere. In this case a_X is a coercive bilinear form on X (see solution to Exercise 5.2.7 (1)). Moreover, the following can be said for the way to choose c_D . If c_D takes a large value, the second term in the integral of the right-hand side of Eq. (8.6.3) is dominant compared to the first term and suppresses the smoothing functionality. Hence, it becomes a result closer to when $-g_i$ is chosen to be the direct search vector. Here, the size of the search vector (step size) is considered to be adjusted by the size of the positive constant c_a used in the algorithm in Section 7.7.1 (same as Section 3.7).

The strong form of H^1 gradient method when using Eq. (8.6.3) is as below.

Problem 8.6.2 (H^1 gradient method using H^1 inner product) Let $\theta \in \mathcal{D}^\circ$, and $g_i \in X'$ of Eq. (8.5.6) be given. Find $\vartheta_{g_i} : D \rightarrow \mathbb{R}$ which satisfies

$$\begin{aligned} -\Delta \vartheta_{g_i} + c_D \vartheta_{g_i} &= -g_i \quad \text{in } D, \\ \partial_\nu \vartheta_{g_i} &= 0 \quad \text{on } \partial D. \end{aligned}$$

\square

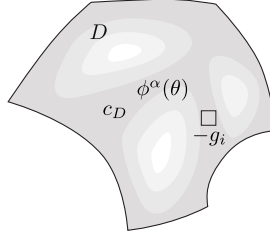


Fig. 8.10: H^1 gradient method using inner product in H^1 space.

Figure 8.10 shows the image of Problem 8.6.2. This problem is a boundary value problem of an elliptic partial differential equation when Ω in the extended Poisson problem of Problem 5.1.3 has changed to D , and $c_{\partial D} = 0$ is set. Hence, numerical solutions can be obtained via numerical analysis methods such as the finite element method.

Method Using Boundary Conditions

Moreover, even if the Dirichlet condition or Robin condition with respect to θ are used, the bilinear form $a_X : X \times X \rightarrow \mathbb{R}$ can be made coercive.

Firstly, let us think about using the Dirichlet boundary condition. On Eq. (8.1.3) where the linear space X of the design variable is defined, $\Omega_C \subset \bar{D}$ was defined to be a boundary or domain in which θ is fixed under the design demand. Here, the measure of the boundary or domain for $\bar{\Omega}_C$ is assumed to have a positive value. In this case,

$$a_X(\vartheta, \psi) = \int_{D \setminus \bar{\Omega}_C} \nabla \vartheta \cdot \nabla \psi \, dx \quad (8.6.4)$$

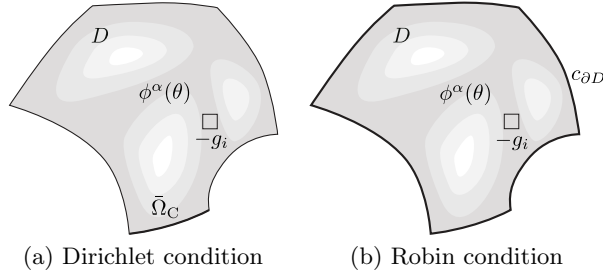
is a bounded and coercive bilinear form on X as seen in the solution for Exercise 5.2.5. The strong form equation of H^1 gradient method in this case is as follows.

Problem 8.6.3 (H^1 gradient method using Dirichlet condition) Let $g_i \in X'$ of Eq. (8.5.6) be given with respect to $\theta \in \mathcal{D}^\circ$. Obtain $\vartheta_{g_i} : D \setminus \bar{\Omega}_C \rightarrow \mathbb{R}$ which satisfies

$$\begin{aligned} -\Delta \vartheta_{g_i} &= -g_i && \text{in } D \setminus \bar{\Omega}_C, \\ \partial_\nu \vartheta_{g_i} &= 0 && \text{on } \partial D \setminus \bar{\Omega}_C, \\ \vartheta_{g_i} &= 0 && \text{in } \bar{\Omega}_C. \end{aligned}$$

□

Problem 8.6.3 is a problem replacing Ω and Γ_D in the Poisson problem of Problem 5.1.1 with $D \setminus \bar{\Omega}_C$ and $\partial \Omega_C$, respectively. Figure 8.11 (a) shows its image. The numerical solution of this problem can also be obtained via numerical analysis method such as the finite element method.

Fig. 8.11: H^1 gradient method using boundary conditions.

Furthermore, if the Robin condition is used, even if $\bar{\Omega}_C = \emptyset$ is assumed in Eq. (8.1.3), the coerciveness of $a_X(\vartheta, \psi)$ can be obtained. Some positive-valued and uniformly bounded function $c_{\partial D} \in L^\infty(\partial D; \mathbb{R})$ is chosen and

$$a_X(\vartheta, \psi) = \int_D \nabla \vartheta \cdot \nabla \psi \, dx + \int_{\partial D} c_{\partial D} \vartheta \psi \, d\gamma. \quad (8.6.5)$$

The fact that this a_X becomes a coercive bilinear form in X is shown in the solution of Exercise 5.2.7 (2). In this case, the strong form is as follows.

Problem 8.6.4 (H^1 gradient method using the Robin condition) Let $g_i \in X'$ of Eq. (8.5.6) be given at $\theta \in \mathcal{D}^\circ$. Obtain $\vartheta_{g_i} : D \rightarrow \mathbb{R}$ which satisfies

$$\begin{aligned} -\Delta \vartheta_{g_i} &= -g_i && \text{in } D, \\ \partial_\nu \vartheta_{g_i} + c_{\partial D} \vartheta_{g_i} &= 0 && \text{on } \partial D. \end{aligned}$$

□

Figure 8.11 (b) shows an image of Problem 8.6.4. The Robin condition for this problem is a condition typically used for a heat transfer boundary when a Poisson problem is viewed as a stationary heat transfer problem. The external temperature at the boundary is set to zero and the heat transfer coefficient is set to be $c_{\partial D}$. Here, the numerical solutions of this problem can be obtained via a numerical analysis method, such as the finite element method.

Regularity of H^1 Gradient Method

The following results can be obtained with respect to the weak solutions of the H^1 gradient method (Problems 8.6.2 to 8.6.4) with respect to the topology optimization problem of θ -type. Here, in this section, vicinities of the singular points as follows are denoted as B : when D is a two-dimensional domain, concave corner points on ∂D and corner points on $\partial\Gamma_D$ in mixed boundary conditions for which the opening angle is greater than $\pi/2$, and when D is a three-dimensional domain, concave edges on ∂D and edges on $\partial\Gamma_D$ in mixed boundary conditions for which the opening angle is greater than $\pi/2$. Moreover, $f_i(\theta, u)$ when u is the solution to Problem 8.2.3 is written as $\tilde{f}_i(\theta)$.

Theorem 8.6.5 (H^1 gradient method of θ -type) With respect to $g_i \in L^{q_R}(D; \mathbb{R})$ in Theorem 8.5.2, the weak solutions ϑ_{g_i} of Problems 8.6.2 to 8.6.4 exist uniquely, and ϑ_{g_i} is in the $H^2(D; \mathbb{R}) \cap C^{0,1}$ class on $D \setminus \bar{B}$. Moreover, ϑ_{g_i} is a descent direction for this function. \square

Proof From the fact that g_i is in $L^{q_R}(D; \mathbb{R}) \subset X'$, the Lax–Milgram theorem says that the weak solutions ϑ_{g_i} of Problems 8.6.2 to 8.6.4 uniquely exist. Moreover, the following results can be obtained regarding the regularity of the solution ϑ_{g_i} . From the fact that ϑ_{g_i} satisfies an elliptic partial differential equation, the differentiability increases by two orders compared to g_i ; it becomes $W^{2, q_R} \subset H^2(D; \mathbb{R})$ class on $D \setminus \bar{B}$. If Sobolev's embedding theorem (Theorem 4.3.14) is applied to this, when $q_R > d$,

$$2 - \frac{d}{q_R} = 1 + \sigma > 1$$

holds, where $\sigma \in (0, 1)$. Therefore, in Theorem 4.3.14 (3), when $p = q_R$, $q = \infty$, $k = 1$ and $j = 1$,

$$W^{2, q_R}(D \setminus \bar{B}, \mathbb{R}) \subset C^{0,1}(D \setminus \bar{B}, \mathbb{R})$$

holds on $D \setminus \bar{B}$. Then, ϑ_{g_i} becomes $H^2(D; \mathbb{R}) \cap C^{0,1}$ class on $D \setminus \bar{B}$. Furthermore, with respect to the weak solutions ϑ_{g_i} of Problems 8.6.2 to 8.6.4 and for some positive constant $\bar{\epsilon}$, the estimate

$$\begin{aligned} \tilde{f}_i(\theta + \bar{\epsilon}\vartheta_{g_i}) - \tilde{f}_i(\theta) &= \bar{\epsilon} \langle \mathbf{g}_i, \vartheta_{g_i} \rangle + o(|\bar{\epsilon}|) = -\bar{\epsilon} a_X(\vartheta_{g_i}, \vartheta_{g_i}) + o(|\bar{\epsilon}|) \\ &\leq -\bar{\epsilon} \alpha_X \|\vartheta_{g_i}\|_X^2 + o(|\bar{\epsilon}|) \end{aligned}$$

holds. Here, if $\bar{\epsilon}$ is taken to be sufficiently small, $\tilde{f}_i(\theta)$ decreases. \square

If the direction of variation of the design variable is determined using the H^1 gradient method, a solution is found in the admissible set \mathcal{D} of design variables excepting the neighborhood of singular points from Theorem 8.6.5. From this, it is thought that the H^1 gradient method is a regular gradient method.

8.6.2 H^1 Newton Method

Furthermore, if it is possible to calculate the second-order derivative (Hessian) $h_i \in \mathcal{L}^2(X \times X; \mathbb{R})$ of the cost function f_i , the Newton method on $X = H^1(D; \mathbb{R})$ can be considered. Such a method is referred to as the H^1 Newton method of θ -type.

Problem 8.6.6 (H^1 Newton method of θ -type) Let X and \mathcal{D} be Eq. (8.1.3) and Eq. (8.1.4), respectively. For $f_i \in C^2(\mathcal{D}; \mathbb{R})$, its θ -derivative and second-order θ -derivative at $\theta_k \in \mathcal{D}^\circ$, which is not a local minimum point, are taken respectively to be $g_i(\theta_k) \in X'$ and $h_i(\theta_k) \in \mathcal{L}^2(X \times X; \mathbb{R})$. Moreover, let $a_X : X \times X \rightarrow \mathbb{R}$ be a coercive and bounded bilinear form on X . Here, obtain $\vartheta_{g_i} \in X$ which satisfies

$$h_i(\theta_k)[\vartheta_{g_i}, \psi] + a_X(\vartheta_{g_i}, \psi) = -\langle g_i(\theta_k), \psi \rangle \quad (8.6.6)$$

with respect to an arbitrary $\psi \in X$. \square

In Problem 8.6.6, if the left-hand side of Eq. (8.6.6) is made to be just h_i , it cannot be expected to fix the irregularity of $g_i(\theta_k)$ pointed out in Remark 8.5.3. In reality, h_i calculated with Eq. (8.5.19) does not include the term of $\nabla\vartheta_1 \cdot \nabla\vartheta_2$. Hence, in Problem 8.6.6, a bilinear form a_X was added in order to ensure coerciveness and boundedness of the left-hand side of Eq. (8.6.6) on X and the regularity of ϑ_{g_i} . For example, if Eq. (8.6.3) using an inner product on X is to be used as a basis, let:

$$a_X(\vartheta, \psi) = \int_D (c_{D1} \nabla\vartheta \cdot \nabla\psi + c_{D0} \vartheta\psi) \, dx. \quad (8.6.7)$$

Here, c_{D0} and c_{D1} are positive constants for achieving the coerciveness and regularity respectively. These have the same meaning as that explained after Eq. (8.6.3).

Furthermore, in the case of the Newton method when the second-order θ -derivative of $f_i(\theta)$ is given by the Hesse gradient, Problem 8.6.6 is replaced with the following problem.

Problem 8.6.7 (Newton method of θ -type using Hesse gradient) Let X and \mathcal{D} be Eq. (8.1.3) and Eq. (8.1.4), respectively. For $f_i \in C^2(\mathcal{D}; \mathbb{R})$, the gradient of the θ -derivative of f_i , search vector, which is obtained in the previous step by the H^1 gradient method or H^1 Newton method of θ -type using the Hesse gradient, and Hesse gradient of f_i at a non-local minimum point $\theta_k \in \mathcal{D}^\circ$ are denoted as $g_i(\theta_k) \in X'$, $\vartheta_{g_i} \in X$ and $g_{Hi}(\theta_k, \vartheta_{g_i}) \in X'$, respectively. $a_X : X \times X \rightarrow \mathbb{R}$ is a coercive and bounded bilinear form on X . Here, obtain a $\vartheta_{g_i} \in X$ which satisfies

$$a_X(\vartheta_{g_i}, \psi) = -\langle (g_i(\theta_k) + g_{Hi}(\theta_k, \vartheta_{g_i})), \psi \rangle \quad (8.6.8)$$

with respect to an arbitrary $\psi \in X$. □

8.7 Solution of Topology Optimization Problem of θ -Type

The abstract optimal design problem (Problem 7.3.1) and topology optimization problem of θ -type (Problem 8.3.2) can be dealt with as in Table 8.1. Therefore by appropriate replacements, the gradient method and Newton method with respect to constrained problems shown in Section 7.7.1 (Section 3.7) and Section 7.7.2 (Section 3.8) can be applied.

8.7.1 Gradient Method for Constrained Problems

The gradient method with respect to a constrained problem can have a simple algorithm such as Algorithm 3.7.2 shown in Section 3.7.1, which can be used by applying changes such as those below:

- (1) Replace the design variable \mathbf{x} and its variation \mathbf{y} as θ and ϑ , respectively.

Table 8.1: Correspondence between abstract optimal design problem (Problem 7.3.1) and topology optimization problem of θ -type (Problem 8.3.2).

	Abstract problem	Topology optimization problem
Design variable	$\phi \in X$	$\theta \in X = H^1(D; \mathbb{R})$
State variable	$u \in U$	$u \in U = H^1(D; \mathbb{R})$
Fréchet derivative of f_i	$g_i \in X'$	$g_i \in X' = H^{1'}(D; \mathbb{R})$
Solution of gradient method	$\varphi_{g_i} \in X$	$\vartheta_{g_i} \in X = H^1(D; \mathbb{R})$

- (2) Equation (3.7.10) providing the gradient method is replaced by conditions that establish

$$c_a a_X(\vartheta_{g_i}, \psi) = -\langle g_i, \psi \rangle \quad (8.7.1)$$

with respect to an arbitrary $\psi \in X$, where $a_X(\vartheta_{g_i}, \psi)$ is a bilinear form on X used as the weak form of Problems 8.6.2 to 8.6.4.

- (3) Replace Eq. (3.7.11) seeking the search vector with

$$\vartheta_g = \vartheta_{g_0} + \sum_{i \in I_A} \lambda_i \vartheta_{g_i}, \quad (8.7.2)$$

where $I_A = \{i \in \{1, \dots, m\} \mid \tilde{f}_i(\theta) \geq 0\}$.

- (4) Replace Eq. (3.7.12) seeking the Lagrange multipliers with

$$(\langle g_i, \vartheta_{g_j} \rangle)_{(i,j) \in I_A^2} (\lambda_j)_{j \in I_A} = -(f_i + \langle g_i, \vartheta_{g_0} \rangle)_{i \in I_A}. \quad (8.7.3)$$

Equation (8.7.3) is solved possibly several times, removing each time the constraints where the associated Lagrange multiplier is negative ([active set method](#)).

Furthermore, if a complicated algorithm such as Algorithm 3.7.6 is to be used, the following changes should be added to (1) to (4) above:

- (5) The Armijo criterion Eq. (3.7.26) is replaced, with respect to $\xi \in (0, 1)$, with

$$\mathcal{L}(\theta + \vartheta_g, \lambda_{k+1}) - \mathcal{L}(\theta, \lambda) \leq \xi \left\langle g_0 + \sum_{i \in I_A} \lambda_i g_i, \vartheta_g \right\rangle. \quad (8.7.4)$$

- (6) Replace the Wolfe criterion Eq. (3.7.27), with respect to μ ($0 < \xi < \mu < 1$), with

$$\mu \left\langle g_0 + \sum_{i \in I_A} \lambda_i g_i, \vartheta_g \right\rangle$$

$$\leq \left\langle g_0(\theta + \vartheta_g) + \sum_{i \in I_A} \lambda_{i, k+1} g_i(\theta + \vartheta_g), \vartheta_g \right\rangle. \quad (8.7.5)$$

(7) Replace Eq. (3.7.21) for updating λ_{k+1} based on the Newton–Raphson method by

$$\begin{aligned} \delta \lambda &= (\delta \lambda_j)_{j \in I_A} \\ &= - \left(\langle g_i(\lambda_{k+1} l), \vartheta_{gj}(\lambda_{k+1} l) \rangle_{(i,j) \in I_A^2} \right)^{-1} (f_i(\lambda_{k+1} l))_{i \in I_A}. \end{aligned} \quad (8.7.6)$$

Let us look at the points to be aware of when solving a topology optimization problem of θ -type such as the one above.

In the topology optimization problem of θ -type (Problem 8.3.2), the solution of the state determination problem with respect to a design variable $\theta \in X$ or cost function becomes a non-convex non-linear mapping. This is because the coefficient $\phi^\alpha(\theta)$ of a partial differential equation used in a SIMP model is a composite function of a sigmoid function and a power function. Hence, depending on the definitions of cost functions and boundary conditions, there may be cases when several local minimum points exist. In that case, the initial distribution of θ needs to be changed and the convergence results need to be compared.

Moreover, the initial distribution of θ must be in the admissible set \mathcal{D} of design variables defined in Eq. (8.1.4). In other words, it needs to be a continuous function. If the initial distribution of θ is given by the characteristic function (an L^∞ class function) corresponding to the location of some holes, caution needs to be taken that the discontinuities of θ at the boundaries of the holes are not removed, even when the methods above are used.

Furthermore, in topology optimization problems of θ -type shown in this chapter, a sigmoid function is used to change θ to ϕ . Therefore, as ϕ nears 0 and 1, there is a disadvantage that the gradient of ϕ with respect to θ becomes small and convergence is slowed. This issue will hopefully be improved using the Newton method shown in the next section.

8.7.2 Newton Method for Constrained Problems

If the second-order θ -derivatives are computable in addition to the θ -derivatives of the cost functions, the gradient method with respect to a constrained problem can be changed to a Newton method with respect to a constrained problem. In this case, $h_i(\theta_k)[\vartheta_{gi}, \psi]$ of Eq. (8.6.6) is replaced by

$$h_{\mathcal{L}}(\theta_k)[\vartheta_{gi}, \psi] = h_0(\theta_k)[\vartheta_{gi}, \psi] + \sum_{i \in I_A(\theta_k)} \lambda_{ik} h_i(\theta_k)[\vartheta_{gi}, \psi]. \quad (8.7.7)$$

In other words, let Eq. (8.6.6) be

$$c_h h_{\mathcal{L}}(\theta_k)[\vartheta_{gi}, \psi] + a_X(\vartheta_{gi}, \psi) = - \langle g_i(\theta_k), \psi \rangle, \quad (8.7.8)$$

where a_X is defined by Eq. (8.6.7), and c_h , c_{D0} and c_{D1} are positive constants to control the step size. Under this situation, a simple algorithm such as Algorithm 3.8.4 shown in Section 3.8.1 can be utilized after the following replacements:

- (1) Replace the design variable \mathbf{x} and its variation \mathbf{y} with θ and ϑ respectively.
- (2) Replace Eq. (3.7.10) with the solution of Eq. (8.7.8).
- (3) Replace Eq. (3.7.11) with Eq. (8.7.2).
- (4) Replace Eq. (3.7.12) with Eq. (8.7.3).

When the second-order θ -derivative of $f_i(\theta)$ is obtained as a [Hesse gradient](#), Eq. (8.7.7) and Eq. (8.7.8) are replaced with

$$g_{\mathcal{H}\mathcal{L}}(\theta_k, \bar{\vartheta}_g) = g_{\mathcal{H}0}(\theta_k, \bar{\vartheta}_g) + \sum_{i \in I_A(\theta_k)} \lambda_{ik} g_{\mathcal{H}i}(\theta_k, \bar{\vartheta}_g), \quad (8.7.9)$$

$$a_X(\vartheta_{gi}, \psi) = -\langle (g_i(\theta_k) + c_h g_{\mathcal{H}\mathcal{L}}(\theta_k, \bar{\vartheta}_g)), \psi \rangle, \quad (8.7.10)$$

respectively. Using the definitions, the following is added:

- (5) Replace Eq. (3.8.11) with Eq. (8.7.10).

Furthermore, when considering the complicated algorithm shown in Section 3.8.2, all sorts of innovations in response to the additional functionalities and characteristics of problems become necessary.

8.8 Error Estimation

If an algorithm such as the one shown in Sect. 8.7 is to be used to solve the topology optimization problem of θ -type (Problem 8.3.2), the search vector ϑ_g can be obtained via Eq. (8.7.2). In this regard, there is a need to obtain the solutions to the boundary value problems of three elliptic partial differential equations. In other words, the solution u to the state determination problem (Problem 8.2.3), the solutions $v_0, v_{i_1}, \dots, v_{i_{|I_A|}}$ of the adjoint problems (Problem 8.5.1) with respect to $f_0, f_{i_1}, \dots, f_{i_{|I_A|}}$ and the solutions $\vartheta_0, \vartheta_{i_1}, \dots, \vartheta_{i_{|I_A|}}$ from the H^1 gradient method of θ -type (Problem 8.6.1). Furthermore, there is a need to seek the Lagrange multipliers $\lambda_{i_1}, \dots, \lambda_{i_{|I_A|}}$ with Eq. (8.7.3). Here, the numerical solutions with respect to the three boundary value problems are assumed to be obtained by the finite element method, so let us use the results of error estimation with respect to the numerical solutions from the finite element method looked at in Section 6.6 in order to conduct the error estimation of the search vector ϑ_g [29, 30].

Furthermore, if instead of the H^1 gradient method, the H^1 Newton method is to be used, evaluations of the second-order derivatives of cost functions are required. However, these will be omitted for now.

In this section, D is assumed to be a polygon in two dimensions; a polyhedron in three dimensions and a **regular finite element division** $\mathcal{T} = \{D_i\}_{i \in \mathcal{E}}$ with respect to D is considered. Moreover, we define the maximum diameter h of finite elements as $h(\mathcal{T})$ of Eq. (6.6.2) and consider a sequence $\{\mathcal{T}_h\}_{h \rightarrow 0}$ of finite element divisions. Hereinafter, notation such as that below will be used:

- (1) Let the exact solutions of a state determination problem (Problem 8.2.3) and adjoint problems (Problem 8.5.1) with respect to $f_0, f_{i_1}, \dots, f_{i_{|I_A|}}$ be u and $v_0, v_{i_1}, \dots, v_{i_{|I_A|}}$, respectively. Moreover, their numerical solutions from the finite element method can be written, with respect to $i \in I_A \cup \{0\}$, as

$$u_h = u + \delta u_h, \quad (8.8.1)$$

$$v_{ih} = v_i + \delta v_{ih}. \quad (8.8.2)$$

- (2) Let the numerical solutions of θ -derivatives of cost functions $f_0, f_{i_1}, \dots, f_{i_{|I_A|}}$ be

$$g_{ih} = g_i + \delta g_{ih}, \quad (8.8.3)$$

where g_i and g_{ih} are functions of $u, v_0, v_{i_1}, \dots, v_{i_{|I_A|}}$ and $u_h, v_{0h}, v_{i_1h}, \dots, v_{i_{|I_A|h}}$, respectively.

- (3) Let the exact solutions from the H^1 gradient method (for example, Problem 8.6.2) calculated using the exact solutions $g_0, g_{i_1}, \dots, g_{i_{|I_A|}}$ of θ -derivatives be $\vartheta_{g_0}, \vartheta_{g_{i_1}}, \dots, \vartheta_{g_{i_{|I_A|}}}$. Moreover, the exact solutions from the H^1 gradient method calculated using the numerical solutions $g_{0h}, g_{i_1h}, \dots, g_{i_{|I_A|h}}$ are written, with respect to $i \in I_A \cup \{0\}$, as

$$\hat{\vartheta}_{g_i} = \vartheta_{g_i} + \delta \hat{\vartheta}_{g_i}. \quad (8.8.4)$$

- (4) Let the numerical solutions from the H^1 gradient method calculated using the numerical solutions $g_{0h}, g_{i_1h}, \dots, g_{i_{|I_A|h}}$, with respect to $i \in I_A \cup \{0\}$, be

$$\vartheta_{g_{ih}} = \hat{\vartheta}_{g_i} + \delta \hat{\vartheta}_{g_{ih}} = \vartheta_{g_i} + \delta \vartheta_{g_{ih}}. \quad (8.8.5)$$

- (5) The coefficient matrix $(\langle g_i, \vartheta_{gj} \rangle)_{(i,j) \in I_A^2}$ of Eq. (8.7.3) constructed using $g_0, g_{i_1}, \dots, g_{i_{|I_A|}}$ and $\vartheta_{g_0}, \vartheta_{g_{i_1}}, \dots, \vartheta_{g_{i_{|I_A|}}}$ as \mathbf{A} . Moreover, the coefficient matrix $(\langle g_{ih}, \vartheta_{gjh} \rangle)_{(i,j) \in I_A^2}$ of Eq. (8.7.3) constructed from $g_{0h}, g_{i_1h}, \dots, g_{i_{|I_A|h}}$ and $\vartheta_{g_{0h}}, \vartheta_{g_{i_1h}}, \dots, \vartheta_{g_{i_{|I_A|h}}}$ is denoted as $\mathbf{A}_h = \mathbf{A} + \delta \mathbf{A}_h$. Here, we assume that $f_i = 0$ and denote $-(\langle g_i, \vartheta_{g_0} \rangle)_{i \in I_A}$ as \mathbf{b} . Moreover, $-(\langle g_{ih}, \vartheta_{g_{0h}} \rangle)_{i \in I_A}$ is denoted as $\mathbf{b}_h = \mathbf{b} + \delta \mathbf{b}_h$. Furthermore, the exact solution of the Lagrange multiplier is written as $\boldsymbol{\lambda} = \mathbf{A}^{-1} \mathbf{b}$. Furthermore, its numerical solution is written as

$$\boldsymbol{\lambda}_h = (\lambda_{ih})_{i \in I_A} = \mathbf{A}_h^{-1} \mathbf{b}_h = \boldsymbol{\lambda} + \delta \boldsymbol{\lambda}_h. \quad (8.8.6)$$

- (6) Equation (8.7.2) constructed by $\lambda_{i_1 h}, \dots, \lambda_{i_{|I_A|} h}$ and numerical solutions $\vartheta_{g_0 h}, \vartheta_{g_{i_1 h}}, \dots, \vartheta_{g_{i_{|I_A|} h}}$ is written as

$$\vartheta_{gh} = \vartheta_{g_0 h} + \sum_{i \in I_A} \lambda_{ih} \vartheta_{gih} = \vartheta_g + \delta \vartheta_{gh}. \quad (8.8.7)$$

In the definition above, $\delta \vartheta_{gh}$ defined in Eq. (8.8.7) represents the error of the search vector. In this section, the aim is to evaluate the order of its norm $\|\delta \vartheta_{gh}\|_X$ with respect to h . Here, the following hypothesis is established.

Hypothesis 8.8.1 (Error estimation of ϑ_g) In a state determination problem and adjoint problems with respect to $f_0, f_{i_1}, \dots, f_{i_{|I_A|}}$, let $\alpha > 1$. Moreover, the following is assumed with respect to $q_R > d$ and $k, j \in \{1, 2, \dots\}$:

- (1) The homogeneous form for the exact solutions u of a state determination problem and $v_0, v_{i_1}, \dots, v_{i_{|I_A|}}$ of adjoint problems with respect to $f_0, f_{i_1}, \dots, f_{i_{|I_A|}}$ are elements of

$$\mathcal{S}_k = U \cap W^{k+1, 2q_R}(D; \mathbb{R}). \quad (8.8.8)$$

In order for this condition to be established, Hypotheses 8.2.1, 8.2.2 and 8.3.1 need to be amended.

- (2) The integrand of the cost function f_i is, with respect to $i \in I_A \cup \{0\}$,

$$\zeta_i \vartheta_u \in L^{2q_R}(D; \mathbb{R}).$$

- (3) There exist positive constants c_1, c_2, c_3 which do not depend on h and for $i \in I_A \cup \{0\}$,

$$\|\delta u_h\|_{W^{j, 2q_R}(D; \mathbb{R})} \leq c_1 h^{k+1-j} |u|_{W^{k+1, 2q_R}(D; \mathbb{R})}, \quad (8.8.9)$$

$$\|\delta v_{ih}\|_{W^{j, 2q_R}(D; \mathbb{R})} \leq c_2 h^{k+1-j} |v_i|_{W^{k+1, 2q_R}(D; \mathbb{R})}, \quad (8.8.10)$$

$$\|\delta \hat{\vartheta}_{gih}\|_{W^{j, 2q_R}(D; \mathbb{R})} \leq c_3 h^{k+1-j} \left| \hat{\vartheta}_{gi} \right|_{W^{k+1, 2q_R}(D; \mathbb{R})}, \quad (8.8.11)$$

is satisfied, where $|\cdot|$ expresses a semi-norm (see Eq. (4.3.12)).

- (4) With respect to the coefficient matrix \mathbf{A}_h in Eq. (8.8.6), a positive constant c_4 exists and

$$\|\mathbf{A}_h^{-1}\|_{\mathbb{R}^{|I_A| \times |I_A|}} \leq c_4$$

is satisfied, where $\|\cdot\|_{\mathbb{R}^{|I_A| \times |I_A|}}$ represents the norm of a matrix (see Eq. (4.4.3)).

□

In (1) of Hypothesis 8.8.1, since $k \in \{1, 2, \dots\}$, it is a stronger condition than \mathcal{S} defined in Eq. (8.2.2). The reason for this is because in (3) of Hypothesis 8.8.1, u and $v_0, v_{i_1}, \dots, v_{i_{|r_A|}}$ on the right-hand side of Eq. (8.8.9) and Eq. (8.8.10) need to be in the $W^{k+1, 2q_R}$ class. Hypothesis 8.8.1 (3) is based on Corollary 6.6.4. Hypothesis 8.8.1 (4) is a condition which is established when $g_{i_1}, \dots, g_{i_{|r_A|}}$ are linearly independent.

Here, Theorem 8.8.5 shown later can be obtained. In order to show this result, the following three lemmas are used.

Lemma 8.8.2 (Error estimation of g_i) When the assumptions (1) and (2) in Hypothesis 8.8.1 as well as Eq. (8.8.9) and Eq. (8.8.10) are satisfied, with respect to δg_{ih} of Eq. (8.8.3), there exists a positive constant c_5 which does not depend on h and the estimate

$$\langle \delta g_{ih}, \vartheta \rangle \leq c_5 h^k \|\vartheta\|_X$$

is established with respect to an arbitrary $\vartheta \in X$. \square

Proof δg_{ih} is yielded by the numerical error of δu_h and δv_{ih} . Hence, from Eq. (8.5.5),

$$|\langle \delta g_i, \vartheta \rangle| \leq |\mathcal{L}_{i\theta u}(\theta, u, v_i)[\vartheta, \delta u_h] + \mathcal{L}_{i\theta v_i}(\theta, u, v_i)[\vartheta, \delta v_{ih}]| \quad (8.8.12)$$

is established. If with respect to the right-hand side of Eq. (8.8.12), Hölder's inequality (Theorem A.9.1) and Poincaré's inequality (Corollary A.9.4) are used,

$$\begin{aligned} & |\mathcal{L}_{i\theta u}(\theta, u, v_i)[\vartheta, \delta u_h] + \mathcal{L}_{i\theta v_i}(\theta, u, v_i)[\vartheta, \delta v_{ih}]| \\ & \leq \left\{ \|\zeta_{i\theta u}\|_{L^{2q_R}(D; \mathbb{R})} \|\delta u_h\|_{L^{2q_R}(D; \mathbb{R})} + \|b'\|_{L^{2q_R}(D; \mathbb{R})} \|\delta v_{ih}\|_{L^{2q_R}(D; \mathbb{R})} \right. \\ & \quad + \|\alpha \phi^{\alpha-1} \phi'\|_{L^\infty(D; \mathbb{R})} \|\nabla \delta u_h\|_{L^{2q_R}(D; \mathbb{R}^d)} \|\nabla v_i\|_{L^{2q_R}(D; \mathbb{R}^d)} \\ & \quad \left. + \|\alpha \phi^{\alpha-1} \phi'\|_{L^\infty(D; \mathbb{R})} \|\nabla u_h\|_{L^{2q_R}(D; \mathbb{R}^d)} \|\nabla \delta v_{ih}\|_{L^{2q_R}(D; \mathbb{R}^d)} \right\} \|\vartheta\|_X \\ & \leq \left\{ \|\zeta_{i\theta u}\|_{L^{2q_R}(D; \mathbb{R})} \|\delta u_h\|_{W^{1, 2q_R}(D; \mathbb{R})} + \|b'\|_{L^{2q_R}(D; \mathbb{R})} \|\delta v_{ih}\|_{W^{1, 2q_R}(D; \mathbb{R})} \right. \\ & \quad + \|\alpha \phi^{\alpha-1} \phi'\|_{L^\infty(D; \mathbb{R})} \|\delta u_h\|_{W^{1, 2q_R}(D; \mathbb{R})} \|v_i\|_{W^{1, 2q_R}(D; \mathbb{R})} \\ & \quad \left. + \|\alpha \phi^{\alpha-1} \phi'\|_{L^\infty(D; \mathbb{R})} \|u_h\|_{W^{1, 2q_R}(D; \mathbb{R})} \|\delta v_{ih}\|_{W^{1, 2q_R}(D; \mathbb{R})} \right\} \|\vartheta\|_X \end{aligned}$$

is established. Here, Eq. (8.8.9) and Eq. (8.8.10) in which $j = 1$ as well as Hypothesis 8.8.1 (1) leads to the result of the lemma. \square

Lemma 8.8.3 (Error estimation of ϑ_{g_i}) When Hypothesis 8.8.1 (1), (2) and (3) are satisfied, with respect to $\delta \vartheta_{g_i}$ of Eq. (8.8.5), the positive constant c_6 which does not depend on h exists and the inequality

$$\|\delta \vartheta_{g_{ih}}\|_X \leq c_6 h^k$$

is established. \square

Proof The following is established from Eq. (8.8.4) and Eq. (8.8.5):

$$\|\delta\vartheta_{gih}\|_X \leq \left\| \delta\hat{\vartheta}_{gi} \right\|_X + \left\| \delta\hat{\vartheta}_{gih} \right\|_X. \quad (8.8.13)$$

Here $\left\| \delta\hat{\vartheta}_{gi} \right\|_X$ represents the error of the exact solution of the H^1 gradient method (for example, Problem 8.6.2) by δg_{ih} in Lemma 8.8.2 and $\left\| \delta\hat{\vartheta}_{gih} \right\|_X$ represents the error with respect to the numerical solution of H^1 gradient method. $\left\| \delta\hat{\vartheta}_{gi} \right\|_X$ of Eq. (8.8.13) satisfies

$$\alpha_X \left(\delta\hat{\vartheta}_{gi}, \vartheta \right) = - \langle \delta g_{ih}, \vartheta \rangle$$

with respect to an arbitrary $\vartheta \in X$. Here, if $\vartheta = \delta\hat{\vartheta}_{gi}$, the bound

$$\alpha_X \left\| \delta\hat{\vartheta}_{gi} \right\|_X^2 \leq \left| \langle \delta g_{ih}, \delta\hat{\vartheta}_{gi} \rangle \right| \quad (8.8.14)$$

is established, where α_X is a positive constant used in Eq. (8.6.1). If Lemma 8.8.2 is used with respect to δg_{ih} of Eq. (8.8.14), the estimate

$$\left\| \delta\hat{\vartheta}_{gi} \right\|_X \leq \frac{c_5}{\alpha_X} h^k \quad (8.8.15)$$

can be obtained. On the other hand, $\left\| \delta\hat{\vartheta}_{gih} \right\|_X$ satisfies the inequality

$$\left\| \delta\hat{\vartheta}_{gih} \right\|_X \leq \left\| \delta\hat{\vartheta}_{gih} \right\|_{W^{1,2q_R}(D;\mathbb{R})} \leq c_3 h^k \left\| \hat{\vartheta}_{gi} \right\|_{W^{k+1,2q_R}(D;\mathbb{R})} \quad (8.8.16)$$

from Eq. (8.8.11) in which $j = 1$. In Eq. (8.8.16), $\left\| \hat{\vartheta}_{gi} \right\|_{W^{k+1,2q_R}(D;\mathbb{R})}$ is bounded. This is because if Hypothesis 8.8.1 (1) is used in the proof of Theorem 8.6.5, $\hat{\vartheta}_{gi} \in W^{k+1,\infty}(D;\mathbb{R})$ can be obtained. Hence, if Eq. (8.8.15) and Eq. (8.8.16) are substituted into Eq. (8.8.13), the result for the lemma can be obtained. \square

Lemma 8.8.4 (Error estimation of λ_h) When Hypothesis 8.8.1 is satisfied, there exists a positive constant c_7 which is not dependent on h , and the estimate

$$\|\delta\lambda_h\|_{\mathbb{R}^{|I_A|}} \leq c_7 h^k$$

holds with respect to λ_h of Eq. (8.8.6). \square

Proof With respect to λ_h of Eq. (8.8.6), the equation

$$\begin{aligned} \delta\lambda_h &= \mathbf{A}_h^{-1} (-\delta\mathbf{A}_h \lambda + \delta\mathbf{b}_h) \\ &= \mathbf{A}_h^{-1} \left\{ - \left((\langle \delta g_{ih}, \vartheta_{gj} \rangle)_{(i,j) \in I_A^2} + (\langle g_i, \delta\vartheta_{gjh} \rangle)_{(i,j) \in I_A^2} \right) \lambda \right. \\ &\quad \left. + (\langle \delta g_{ih}, \vartheta_{g0} \rangle)_{i \in I_A} + (\langle g_i, \delta\vartheta_{g0h} \rangle)_{i \in I_A} \right\} \end{aligned} \quad (8.8.17)$$

is established. If in Eq. (8.8.17), Hypothesis 8.8.1 (4) is used, the estimate

$$\|\delta\lambda_h\|_{\mathbb{R}^{|I_A|}}$$

$$\leq c_4 \left(1 + |I_A| \max_{i \in I_A} |\lambda_i| \right) \max_{(i,j) \in I_A \times (I_A \cup \{0\})} (|\langle \delta g_{ih}, \vartheta_{gj} \rangle| + |\langle g_i, \delta \vartheta_{gjh} \rangle|) \quad (8.8.18)$$

holds. Since $|I_A|$ is bounded, with respect to $|\langle \delta g_{ih}, \vartheta_{gj} \rangle|$ of Eq. (8.8.18), the bound

$$|\langle \delta g_{ih}, \vartheta_{gj} \rangle| \leq c_5 h^k \|\vartheta_{gj}\|_X \quad (8.8.19)$$

is obtained from Lemma 8.8.2. Moreover, with respect to $|\langle g_i, \delta \vartheta_{gjh} \rangle|$,

$$|\langle g_i, \delta \vartheta_{gjh} \rangle| \leq c_6 h^k \|g_i\|_X \quad (8.8.20)$$

can be obtained from Lemma 8.8.3. In Eq. (8.8.20), $\|g_i\|_X$ is bounded. This is because if Hypothesis 8.8.1 (1) is used in the proof of Theorem 8.5.2, $g_i \in W^{k, q_{\mathbb{R}}}(D; \mathbb{R})$ can be obtained. Hence, if Eq. (8.8.18) and Eq. (8.8.19) are substituted into Eq. (8.8.17), the result of the lemma can be obtained. \square

The following results can be obtained based on these lemmas.

Theorem 8.8.5 (Error estimation of ϑ_g) When Hypothesis 8.8.1 is satisfied, there exists a positive constant c not dependent on h , and

$$\|\delta \vartheta_{gh}\|_X \leq ch^k$$

is satisfied with respect to $\delta \vartheta_{gh}$ of Eq. (8.8.7). \square

Proof The following is established based on Eq. (8.8.7):

$$\delta \vartheta_{gh} = \delta \vartheta_{g0h} + \sum_{i \in I_A} (\delta \lambda_{ih} \vartheta_{gi} + \lambda_i \delta \vartheta_{gih}). \quad (8.8.21)$$

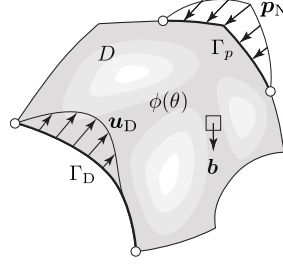
From Eq. (8.8.21),

$$\begin{aligned} \|\delta \vartheta_{gh}\|_X &\leq \left(1 + |I_A| \max_{i \in I_A} |\lambda_i| \right) \max_{i \in I_A \cup \{0\}} \|\delta \vartheta_{gih}\|_X \\ &\quad + \|\delta \lambda_h\|_{\mathbb{R}|I_A|} |I_A| \max_{i \in I_A} \|\vartheta_{gi}\|_X \end{aligned} \quad (8.8.22)$$

can be obtained. If Eq. (8.8.22) is substituted with the results of Lemmas 8.8.3 and 8.8.4, the result of the theorem can be obtained. \square

From Theorem 8.8.5, the following can be said with respect to error estimation of finite element solutions with respect to the topology optimization problem of θ -type.

Remark 8.8.6 (Error estimation of finite element solution ϑ_{gh}) When the numerical solutions of the three boundary value problems (the state determination problem, the adjoint problems and the H^1 gradient method) are obtained by the finite element method with $k = 1$ order basis functions, from Theorem 8.8.5, the error $\|\delta \vartheta_{gh}\|_X$ of search vector ϑ_{gh} reduces to the first order of h with respect to a sequence $\{\mathcal{T}_h\}_{h \rightarrow 0}$ of finite element divisions. \square

Fig. 8.12: θ -type linear elastic body.

8.9 Topology Optimization Problem of Linear Elastic Body

Let us change the state determination problem of θ -type topology optimization problem to a linear elastic problem. Here, a mean compliance minimization problem of a linear elastic body is defined, and let us look at the θ -derivative and second-order θ -derivative. If θ -derivatives and second-order θ -derivatives of the cost functions can be obtained, such a problem can be solved in a similar way to the Poisson problem.

Let D , Γ_D and Γ_N be the domain, Dirichlet boundary and Neumann boundary of a linear elastic problem, similar to the θ -type Poisson problem (Problem 8.2.3). For X and \mathcal{D} , Eq. (8.1.3) and Eq. (8.1.4) respectively will be used.

8.9.1 State Determination Problem

Let us define a linear elastic problem as a state determination problem. Let the linear space U and admissible set \mathcal{S} of state variables be

$$U = \{ \mathbf{u} \in H^1(D; \mathbb{R}^d) \mid \mathbf{u} = \mathbf{0}_{\mathbb{R}^d} \text{ on } \Gamma_D \}, \quad (8.9.1)$$

$$\mathcal{S} = U \cap W^{1,2q_R}(D; \mathbb{R}^d). \quad (8.9.2)$$

Moreover, Hypothesis 8.2.1 is changed in the following way.

Hypothesis 8.9.1 (Regularity of known functions) With respect to $q_R > d$, assume

$$\begin{aligned} \mathbf{b} &\in C^1(X; L^{2q_R}(D; \mathbb{R}^d)), \quad \mathbf{p}_N \in L^{2q_R}(\Gamma_N; \mathbb{R}^d), \\ \mathbf{u}_D &\in H^2(D; \mathbb{R}^d), \quad \mathbf{C} \in L^\infty(D; \mathbb{R}^{d \times d \times d \times d}). \end{aligned}$$

□

On top of this, a problem such as the following is defined with respect to a θ -type linear elastic body such as the one in Fig. 8.12.

Problem 8.9.2 (θ -type linear elastic problem) Let us suppose that Hypotheses 8.9.1 and 8.2.2 hold. Moreover, let $\alpha > 1$ be a constant and $\phi(\theta)$ is given by Eq. (8.1.1) or Eq. (8.1.2) with respect to $\theta \in \mathcal{D}$. In this case, obtain $\mathbf{u} : D \rightarrow \mathbb{R}^d$ satisfying

$$-\nabla^\top (\phi^\alpha(\theta) \mathbf{S}(\mathbf{u})) = \mathbf{b}^\top(\theta) \quad \text{in } D, \quad (8.9.3)$$

$$\phi^\alpha(\theta) \mathbf{S}(\mathbf{u}) \boldsymbol{\nu} = \mathbf{p}_N \quad \text{on } \Gamma_N, \quad (8.9.4)$$

$$\mathbf{u} = \mathbf{u}_D \quad \text{on } \Gamma_D. \quad (8.9.5)$$

□

For later use, define the Lagrange function with respect to Problem 8.9.2 as

$$\begin{aligned} \mathcal{L}_S(\theta, \mathbf{u}, \mathbf{v}) &= \int_D (-\phi^\alpha(\theta) \mathbf{S}(\mathbf{u}) \cdot \mathbf{E}(\mathbf{v}) + \mathbf{b}(\theta) \cdot \mathbf{v}) \, dx + \int_{\Gamma_N} \mathbf{p}_N \cdot \mathbf{v} \, d\gamma \\ &\quad + \int_{\Gamma_D} \{(\mathbf{u} - \mathbf{u}_D) \cdot (\phi^\alpha(\theta) \mathbf{S}(\mathbf{v}) \boldsymbol{\nu}) + \mathbf{v} \cdot (\phi^\alpha(\theta) \mathbf{S}(\mathbf{u}) \boldsymbol{\nu})\} \, d\gamma, \end{aligned}$$

where \mathbf{u} is not necessarily the solution of Problem 8.9.2. $\mathbf{v} \in U$ is a Lagrange multiplier. If \mathbf{u} is the solution of Problem 8.9.2,

$$\mathcal{L}_S(\theta, \mathbf{u}, \mathbf{v}) = 0$$

holds with respect to an arbitrary $\mathbf{v} \in U$.

8.9.2 Mean Compliance Minimization Problem

Let us define a topology optimization problem of θ -type with respect to a linear elastic problem. Define the cost function as follows. With respect to the solution \mathbf{u} of Problem 8.9.2,

$$f_0(\theta, \mathbf{u}) = \int_D \mathbf{b}(\theta) \cdot \mathbf{u} \, dx + \int_{\Gamma_N} \mathbf{p}_N \cdot \mathbf{u} \, d\gamma - \int_{\Gamma_D} \mathbf{u}_D \cdot (\phi^\alpha(\theta) \mathbf{S}(\mathbf{u}) \boldsymbol{\nu}) \, d\gamma \quad (8.9.6)$$

is referred to as the **mean compliance**. Moreover, the functional

$$f_1(\theta) = \int_D \phi(\theta) \, dx - c_1 \quad (8.9.7)$$

is referred to as the constraint function with respect to the domain measure of the linear elastic body. Here, c_1 is taken to be a positive constant, such that $f_1(\theta) \leq 0$ holds with respect to some $\theta \in \mathcal{D}$. The reason that the functional f_0 in Eq. (8.9.6) is called mean compliance is as follows. The first and second terms on the right-hand side of Eq. (8.9.6) are the work conducted by the volume force \mathbf{b} and traction \mathbf{p}_N , respectively. Since \mathbf{b} and \mathbf{p}_N are fixed, work conducted here being small means that \mathbf{u} is small. It can be referred to as external work if there are only these two terms. However, the third term on the right-hand side of

Eq. (8.9.6) is the negative value of the work done by \mathbf{u}_D . It is because the larger work done by \mathbf{u}_D means that the resistance force with respect to deformation is stronger. Based on these, f_0 will be called mean compliance in the sense that it is the mean value for ease of deformation (compliance).

Using these definitions, the mean compliance minimization problem is defined as follows.

Problem 8.9.3 (Mean compliance minimization problem) Let \mathcal{D} and \mathcal{S} be Eq. (8.1.4) and Eq. (8.9.2), respectively. Let f_0 and f_1 be Eq. (8.9.6) and Eq. (8.9.7), respectively. In this case, obtain θ which satisfies

$$\min_{(\theta, \mathbf{u}-\mathbf{u}_D) \in \mathcal{D} \times \mathcal{S}} \{f_0(\theta, \mathbf{u}) \mid f_1(\theta) \leq 0, \text{ Problem 8.9.2}\}.$$

□

8.9.3 θ -Derivatives of Cost Functions

Let us obtain the θ -derivative of $f_0(\theta, \mathbf{u})$ using the adjoint variable method. Let the Lagrange function of f_0 be

$$\begin{aligned} \mathcal{L}_0(\theta, \mathbf{u}, \mathbf{v}_0) &= f_0(\theta, \mathbf{u}) + \mathcal{L}_S(\theta, \mathbf{u}, \mathbf{v}_0) \\ &= \int_D \{-\phi^\alpha(\theta) \mathbf{S}(\mathbf{u}) \cdot \mathbf{E}(\mathbf{v}_0) + \mathbf{b}(\theta) \cdot (\mathbf{u} + \mathbf{v}_0)\} dx \\ &\quad + \int_{\Gamma_N} \mathbf{p}_N \cdot (\mathbf{u} + \mathbf{v}_0) d\gamma \\ &\quad + \int_{\Gamma_D} \{(\mathbf{u} - \mathbf{u}_D) \cdot (\phi^\alpha(\theta) \mathbf{S}(\mathbf{v}_0) \boldsymbol{\nu}) \\ &\quad \quad + (\mathbf{v}_0 - \mathbf{u}_D) \cdot (\phi^\alpha(\theta) \mathbf{S}(\mathbf{u}) \boldsymbol{\nu})\} d\gamma. \end{aligned} \quad (8.9.8)$$

The Fréchet derivative of \mathcal{L}_0 with respect to arbitrary variation $(\vartheta, \hat{\mathbf{u}}, \hat{\mathbf{v}}_0) \in X \times U \times U$ of $(\theta, \mathbf{u}, \mathbf{v}_0)$ can be written as

$$\begin{aligned} \mathcal{L}'_0(\theta, \mathbf{u}, \mathbf{v}_0)[\vartheta, \hat{\mathbf{u}}, \hat{\mathbf{v}}_0] &= \mathcal{L}_{0\theta}(\theta, \mathbf{u}, \mathbf{v}_0)[\vartheta] + \mathcal{L}_{0\mathbf{u}}(\theta, \mathbf{u}, \mathbf{v}_0)[\hat{\mathbf{u}}] + \mathcal{L}_{0\mathbf{v}_0}(\theta, \mathbf{u}, \mathbf{v}_0)[\hat{\mathbf{v}}_0]. \end{aligned} \quad (8.9.9)$$

Each term is considered below.

The third term on the right-hand side of Eq. (8.9.9) becomes

$$\mathcal{L}_{0\mathbf{v}_0}(\theta, \mathbf{u}, \mathbf{v}_0)[\hat{\mathbf{v}}_0] = \mathcal{L}_{S\mathbf{v}_0}(\theta, \mathbf{u}, \mathbf{v}_0)[\hat{\mathbf{v}}_0] = \mathcal{L}_S(\theta, \mathbf{u}, \hat{\mathbf{v}}_0). \quad (8.9.10)$$

Equation (8.9.10) is a Lagrange function of the state determination problem (Problem 8.9.2). Hence, if \mathbf{u} is the weak solution of the state determination problem, the third term of the right-hand side of Eq. (8.9.9) is zero.

Moreover, the second term on the right-hand side of Eq. (8.9.9) becomes

$$\mathcal{L}_{0\mathbf{u}}(\theta, \mathbf{u}, \mathbf{v}_0)[\hat{\mathbf{u}}]$$

$$\begin{aligned}
&= \int_D (-\phi^\alpha(\theta) \mathbf{S}(\hat{\mathbf{u}}) \cdot \mathbf{E}(\mathbf{v}_0) + \mathbf{b}(\theta) \cdot \hat{\mathbf{u}}) \, dx + \int_{\Gamma_N} \mathbf{p}_N \cdot \hat{\mathbf{u}} \, d\gamma \\
&\quad + \int_{\Gamma_D} \{ \hat{\mathbf{u}} \cdot (\phi^\alpha(\theta) \mathbf{S}(\mathbf{v}_0) \boldsymbol{\nu}) + (\mathbf{v}_0 - \mathbf{u}_D) \cdot (\phi^\alpha(\theta) \mathbf{S}(\hat{\mathbf{u}}) \boldsymbol{\nu}) \} \, d\gamma \\
&= \mathcal{L}_S(\theta, \mathbf{v}_0, \hat{\mathbf{u}}).
\end{aligned} \tag{8.9.11}$$

Here, if \mathbf{v}_0 is chosen so that Eq. (8.9.11) becomes zero, the second term on the right-hand side of Eq. (8.9.9) vanishes. This relationship shows that the [self-adjoint relationship](#)

$$\mathbf{u} = \mathbf{v}_0 \tag{8.9.12}$$

holds.

Furthermore, the first-term on the right-hand side of Eq. (8.9.9) becomes

$$\mathcal{L}_{0\theta}(\theta, \mathbf{u}, \mathbf{v}_0)[\vartheta] = \int_D \{ \mathbf{b}' \cdot (\mathbf{u} + \mathbf{v}_0) - \alpha \phi^{\alpha-1} \phi' \mathbf{S}(\mathbf{u}) \cdot \mathbf{E}(\mathbf{v}_0) \} \vartheta \, dx. \tag{8.9.13}$$

Hence, \mathbf{u} is taken to be a weak solution of Problem 8.9.2 and the self-adjoint relationship (Eq. (8.9.12)) is assumed to hold. If $f_0(\theta, \mathbf{u})$ in this case is denoted as $\tilde{f}_0(\theta)$, we can write

$$\tilde{f}'_0(\theta)[\vartheta] = \mathcal{L}_{0\theta}(\theta, \mathbf{u}, \mathbf{v}_0)[\vartheta] = \langle g_0, \vartheta \rangle, \tag{8.9.14}$$

where

$$g_0 = 2\mathbf{b}' \cdot \mathbf{u} - \alpha \phi^{\alpha-1} \phi' \mathbf{S}(\mathbf{u}) \cdot \mathbf{E}(\mathbf{u}). \tag{8.9.15}$$

On the other hand, with respect to $f_1(\theta)$,

$$f'_1(\theta)[\vartheta] = \int_D \phi' \vartheta \, dx = \langle g_1, \vartheta \rangle \tag{8.9.16}$$

is established with respect to an arbitrary $\vartheta \in X$.

Based on the above results, the function space which contains g_0 of Eq. (8.9.15) becomes the same result as Theorem 8.5.2. Hence, by applying H^1 gradient method, the fact that the search vector ϑ_g is in class $C^{0,1}$ is guaranteed.

8.9.4 Second-Order θ -Derivatives of Cost Functions

Furthermore, the second-order θ -derivatives of mean compliance f_0 and the constraint cost function f_1 with respect to the domain measure of linear elastic body can also be obtained. Here, we will follow the procedure shown in Sect. 8.5.2.

Firstly, let us think about the second-order θ -derivative of f_0 . To correspond to Hypothesis 8.5.4 (1), here \mathbf{b} is assumed not to be a function of θ . The relationship corresponding to Hypothesis 8.5.4 (2) is satisfied here.

The Lagrange function \mathcal{L}_0 of f_0 is defined by Eq. (8.9.8). Viewing (θ, \mathbf{u}) as a design variable, its admissible set and admissible set of directions are set as

$$\begin{aligned} S &= \{(\theta, \mathbf{u}) \in \mathcal{D} \times \mathcal{S} \mid \mathcal{L}_S(\theta, \mathbf{u}, \mathbf{v}) = 0 \text{ for all } \mathbf{v} \in U\}, \\ T_S(\theta, \mathbf{u}) &= \{(\vartheta, \hat{\mathbf{v}}) \in X \times U \mid \mathcal{L}_{S\theta\mathbf{u}}(\theta, \mathbf{u}, \mathbf{v})[\vartheta, \hat{\mathbf{v}}] = 0 \text{ for all } \mathbf{v} \in U\}. \end{aligned}$$

The second-order Fréchet partial derivative of \mathcal{L}_0 of Eq. (8.9.8) with respect to arbitrary variations $(\vartheta_1, \hat{\mathbf{v}}_1), (\vartheta_2, \hat{\mathbf{v}}_2) \in T_S(\theta, \mathbf{u})$ of design variable $(\theta, \mathbf{u}) \in S$ becomes

$$\begin{aligned} &\mathcal{L}_{0(\theta, \mathbf{u})(\theta, \mathbf{u})}(\theta, \mathbf{u}, \mathbf{v}_0)[(\vartheta_1, \hat{\mathbf{v}}_1), (\vartheta_2, \hat{\mathbf{v}}_2)] \\ &= \mathcal{L}_{0\theta\theta}(\theta, \mathbf{u}, \mathbf{v}_0)[\vartheta_1, \vartheta_2] + \mathcal{L}_{0\theta\mathbf{u}}(\theta, \mathbf{u}, \mathbf{v}_0)[\vartheta_1, \hat{\mathbf{v}}_2] \\ &\quad + \mathcal{L}_{0\theta\mathbf{u}}(\theta, \mathbf{u}, \mathbf{v}_0)[\vartheta_2, \hat{\mathbf{v}}_1] + \mathcal{L}_{0\mathbf{u}\mathbf{u}}(\theta, \mathbf{u}, \mathbf{v}_0)[\hat{\mathbf{v}}_1, \hat{\mathbf{v}}_2]. \end{aligned} \quad (8.9.17)$$

Each term on the right-hand side of Eq. (8.9.17) becomes

$$\mathcal{L}_{0\theta\theta}(\theta, \mathbf{u}, \mathbf{v}_0)[\vartheta_1, \vartheta_2] = \int_D -(\phi^\alpha(\theta))'' \mathbf{S}(\mathbf{u}) \cdot \mathbf{E}(\mathbf{v}_0) \vartheta_1 \vartheta_2 \, dx, \quad (8.9.18)$$

$$\mathcal{L}_{0\theta\mathbf{u}}(\theta, \mathbf{u}, \mathbf{v}_0)[\vartheta_1, \hat{\mathbf{v}}_2] = \int_D -(\phi^\alpha(\theta))' \mathbf{S}(\hat{\mathbf{v}}_2) \cdot \mathbf{E}(\mathbf{v}_0) \vartheta_1 \, dx, \quad (8.9.19)$$

$$\mathcal{L}_{0\theta\mathbf{u}}(\theta, \mathbf{u}, \mathbf{v}_0)[\vartheta_2, \hat{\mathbf{v}}_1] = \int_D -(\phi^\alpha(\theta))' \mathbf{S}(\hat{\mathbf{v}}_1) \cdot \mathbf{E}(\mathbf{v}_0) \vartheta_2 \, dx, \quad (8.9.20)$$

$$\mathcal{L}_{0\mathbf{u}\mathbf{u}}(\theta, \mathbf{u}, \mathbf{v}_0)[\hat{\mathbf{v}}_1, \hat{\mathbf{v}}_2] = 0. \quad (8.9.21)$$

Here, $\mathbf{u} - \mathbf{u}_D$, $\mathbf{v}_0 - \mathbf{u}_D$, $\hat{\mathbf{v}}_1$ and $\hat{\mathbf{v}}_2$ use the fact that $\mathbf{0}_{\mathbb{R}^d}$ on Γ_D . Moreover, $(\phi^\alpha(\theta))'$ and $(\phi^\alpha(\theta))''$ are Eq. (8.5.14) and Eq. (8.5.15), respectively. Here, with respect to an arbitrary variation $(\vartheta_j, \hat{\mathbf{v}}_j) \in T_S(\theta, \mathbf{u})$ for $j \in \{1, 2\}$, the Fréchet partial derivative of Lagrange function \mathcal{L}_S of the state determination problem becomes

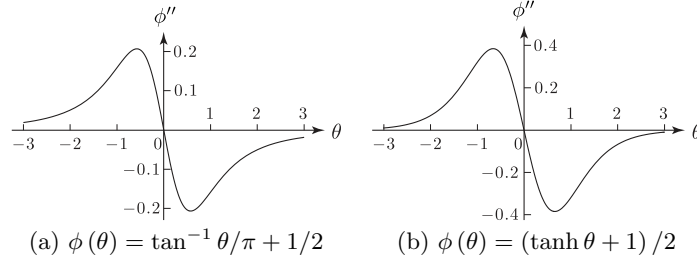
$$\begin{aligned} &\mathcal{L}_{S\theta\mathbf{u}}(\theta, \mathbf{u}, \mathbf{v})[\vartheta_j, \hat{\mathbf{v}}_j] \\ &= \int_D \{ -(\phi^\alpha(\theta))' \vartheta_j \mathbf{S}(\mathbf{v}) - \phi^\alpha(\theta) \mathbf{S}(\hat{\mathbf{v}}_j) \} \cdot \mathbf{E}(\mathbf{v}) \, dx \\ &= 0 \end{aligned} \quad (8.9.22)$$

with respect to an arbitrary $\mathbf{v} \in U$. Here, the fact that \mathbf{v} and $\hat{\mathbf{v}}_j$ are $\mathbf{0}_{\mathbb{R}^d}$ on Γ_D is used. From Eq. (8.9.22), the equation

$$\mathbf{S}(\hat{\mathbf{v}}_j) = -\frac{(\phi^\alpha(\theta))'}{\phi^\alpha(\theta)} \vartheta_j \mathbf{S}(\mathbf{u}) \quad \text{in } D \quad (8.9.23)$$

can be obtained. Hence, substituting $\hat{\mathbf{v}}_j$ of Eq. (8.9.23) into $\hat{\mathbf{v}}_1$ in Eq. (8.9.20) and $\hat{\mathbf{v}}_2$ in Eq. (8.9.19), and considering Dirichlet boundary conditions in the state determination problem and the adjoint problems with respect to f_1, \dots, f_m as well as $\hat{\mathbf{v}}_j = \mathbf{0}_{\mathbb{R}^d}$ on Γ_D , the equations

$$\mathcal{L}_{0\theta\mathbf{u}}(\theta, \mathbf{u}, \mathbf{v}_0)[\vartheta_1, \hat{\mathbf{v}}_2] = \mathcal{L}_{0\theta\mathbf{u}}(\theta, \mathbf{u}, \mathbf{v}_0)[\vartheta_2, \hat{\mathbf{v}}_1]$$

Fig. 8.13: Coefficient functions $\phi''(\theta)$ in h_1 .

$$= \int_D \frac{(\phi^\alpha(\theta))'^2}{\phi^\alpha(\theta)} \mathbf{S}(\mathbf{u}) \cdot \mathbf{E}(\mathbf{v}_0) \vartheta_1 \vartheta_2 \, dx \quad (8.9.24)$$

is obtained.

Summarizing the results above, by substituting Eq. (8.9.24) and Eq. (8.9.18) into Eq. (8.9.17), the second-order θ -derivative of mean compliance f_0 becomes

$$\begin{aligned} h_0(\theta, \mathbf{u}, \mathbf{v}_0)[\vartheta_1, \vartheta_2] &= \int_D \left\{ 2 \frac{(\phi^\alpha(\theta))'^2}{\phi^\alpha(\theta)} - (\phi^\alpha(\theta))'' \right\} \mathbf{S}(\mathbf{u}) \cdot \mathbf{E}(\mathbf{v}_0) \vartheta_1 \vartheta_2 \, dx \\ &= \int_D \beta(\alpha, \theta) \mathbf{S}(\mathbf{u}) \cdot \mathbf{E}(\mathbf{v}_0) \vartheta_1 \vartheta_2 \, dx, \end{aligned} \quad (8.9.25)$$

where $\beta(\alpha, \theta)$ is given by Eq. (8.5.20). Furthermore, if a self-adjoint relationship is used, $\mathbf{S}(\mathbf{u}) \cdot \mathbf{E}(\mathbf{v}_0) > 0$ and $h_0(\theta, \mathbf{u}, \mathbf{v}_0)[\cdot, \cdot]$ becomes a coercive and bounded bilinear form on X .

On the other hand, the second-order θ -derivative of $f_1(\theta)$ becomes

$$h_1(\theta)[\vartheta_1, \vartheta_2] = f_1''(\theta)[\vartheta_1, \vartheta_2] = \int_D \phi''(\theta) \vartheta_1 \vartheta_2 \, dx \quad (8.9.26)$$

with respect to an arbitrary $\vartheta_1, \vartheta_2 \in X$. Here, when $\phi(\theta)$ of Eq. (8.1.1) is used, we get

$$\phi''(\theta) = -\frac{1}{\pi} \frac{2\theta}{(1 + \theta^2)^2}. \quad (8.9.27)$$

Moreover, when $\phi(\theta)$ is given by Eq. (8.1.2), the equation

$$\phi''(\theta) = -\operatorname{sech}^2 \theta \tanh \theta \quad (8.9.28)$$

holds. Figure 8.13 shows the graphs of $\phi''(\theta)$.

In this way, in the mean compliance minimization problem, the second-order θ -derivative of the object cost function f_0 is coercive but the second-order θ -derivative of the constraint function f_1 is not. Hence, if using the Newton method (Problem 8.6.6), an additional term for capturing coerciveness becomes necessary.

8.9.5 Second-Order θ -Derivative of Cost Function Using Lagrange Multiplier Method

When the Lagrange multiplier method is used to obtain the second-order θ -derivative of the mean compliance f_0 , it becomes as follows. Fixing ϑ_1 , we define the Lagrange function for $\tilde{f}'_0(\theta)[\vartheta_1] = \langle g_0, \vartheta_1 \rangle$ in Eq. (8.9.14) by

$$\mathcal{L}_{10}(\theta, \mathbf{u}, \mathbf{w}_0) = \langle g_0, \vartheta_1 \rangle + \mathcal{L}_S(\theta, \mathbf{u}, \mathbf{w}_0), \quad (8.9.29)$$

where \mathcal{L}_S is the Lagrange function of Problem 8.9.2, and $\mathbf{w}_0 \in U$ is the adjoint variable provided for \mathbf{u} in \mathbf{g}_0 .

With respect to arbitrary variations $(\vartheta_2, \hat{\mathbf{u}}, \hat{\mathbf{w}}_0) \in X \times U^2$ of $(\theta, \mathbf{u}, \mathbf{w}_0)$, the Fréchet derivative of \mathcal{L}_{10} is written as

$$\begin{aligned} & \mathcal{L}'_{10}(\theta, \mathbf{u}, \mathbf{w}_0)[\vartheta_2, \hat{\mathbf{u}}, \hat{\mathbf{w}}_0] \\ &= \mathcal{L}_{10\theta}(\theta, \mathbf{u}, \mathbf{w}_0)[\vartheta_2] + \mathcal{L}_{10\mathbf{u}}(\theta, \mathbf{u}, \mathbf{w}_0)[\hat{\mathbf{u}}] \\ & \quad + \mathcal{L}_{10\mathbf{w}_0}(\theta, \mathbf{u}, \mathbf{w}_0)[\hat{\mathbf{w}}_0]. \end{aligned} \quad (8.9.30)$$

The third term on the right-hand side of Eq. (8.9.30) vanishes if \mathbf{u} is the solution of the state determination problem.

The second term on the right-hand side of Eq. (8.9.30) is

$$\begin{aligned} & \mathcal{L}_{10\mathbf{u}}(\theta, \mathbf{u}, \mathbf{w}_0)[\hat{\mathbf{u}}] \\ &= \int_D \{ (2\mathbf{b}' \cdot \hat{\mathbf{u}} - 2\alpha\phi^{\alpha-1}\phi' \mathbf{S}(\mathbf{u}) \cdot \mathbf{E}(\hat{\mathbf{u}})) \vartheta_1 - \phi^\alpha \mathbf{S}(\mathbf{w}_0) \cdot \mathbf{E}(\hat{\mathbf{u}}) \} dx. \end{aligned} \quad (8.9.31)$$

Here, the condition that Eq. (8.9.31) is zero for arbitrary $\hat{\mathbf{u}} \in U$ is equivalent to setting \mathbf{w}_0 to be the solution of the following adjoint problem.

Problem 8.9.4 (Adjoint problem of \mathbf{w}_0 with respect to $\langle g_0, \vartheta_1 \rangle$) Under the assumption of Problem 8.9.2, let $\vartheta_1 \in X$ be given. Find $\mathbf{w}_0 = \mathbf{w}_0(\vartheta_1) \in U$ satisfying

$$\begin{aligned} -\nabla^\top(\phi^\alpha \mathbf{S}(\mathbf{w}_0)) &= 2 \left(\nabla^\top(\alpha\phi^{\alpha-1}\phi' \mathbf{S}(\mathbf{u})) + \mathbf{b}'^\top \right) \vartheta_1 \quad \text{in } D, \\ \phi^\alpha \mathbf{S}(\mathbf{w}_0) \boldsymbol{\nu} &= 2\alpha\phi^{\alpha-1}\phi' \mathbf{S}(\mathbf{u}) \boldsymbol{\nu} \vartheta_1 \quad \text{on } \Gamma_N, \\ \mathbf{w}_0 &= \mathbf{0}_{\mathbb{R}^d} \quad \text{on } \Gamma_D. \end{aligned}$$

□

Finally, the first term on the right-hand side of Eq. (8.9.30) becomes

$$\begin{aligned} & \mathcal{L}_{10\theta}(\theta, \mathbf{u}, \mathbf{w}_0)[\vartheta_2] \\ &= \int_D \left[\{ 2\mathbf{b}'' \cdot \mathbf{u} - (\alpha(\alpha-1)\phi^{\alpha-2}\phi'^2 + \alpha\phi^{\alpha-1}\phi'') \mathbf{S}(\mathbf{u}) \cdot \mathbf{E}(\mathbf{u}) \} \vartheta_1 \right. \\ & \quad \left. - \alpha\phi^{\alpha-1}\phi' \mathbf{S}(\mathbf{u}) \cdot \mathbf{E}(\mathbf{w}_0) + \mathbf{b}' \cdot \mathbf{w}_0 \right] \vartheta_2 dx. \end{aligned}$$

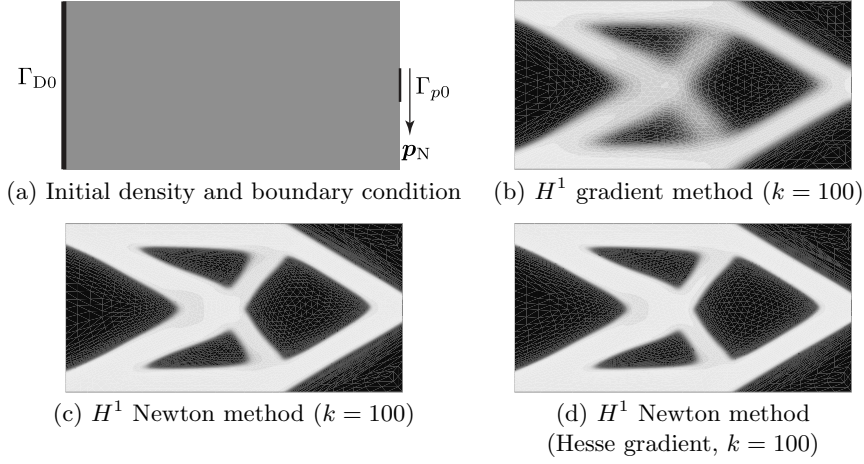


Fig. 8.14: Numerical example of mean compliance minimization: density

Here, \mathbf{u} and $\mathbf{w}_0(\vartheta_1)$ are assumed to be the weak solutions of Problems 8.9.2 and 8.9.4, respectively. If we denote $f_i(\theta, \mathbf{u})$ by $\tilde{f}_i(\theta)$, we have the relation:

$$\begin{aligned} \mathcal{L}_{10\theta}(\theta, \mathbf{u}, \mathbf{v}_0, \mathbf{w}_0(\vartheta_1), \mathbf{z}_0(\vartheta_1))[\vartheta_2] &= \tilde{f}'_0(\theta)[\vartheta_1, \vartheta_2] \\ &= \langle g_{H0}(\theta, \vartheta_1), \vartheta_2 \rangle, \end{aligned} \quad (8.9.32)$$

where the **Hesse gradient** g_{H0} of the mean compliance is given by

$$\begin{aligned} g_{H0}(\theta, \vartheta_1) &= \left\{ -(\alpha(\alpha-1)\phi^{\alpha-2}\phi'^2 + \alpha\phi^{\alpha-1}\phi'') \mathbf{S}(\mathbf{u}) \cdot \mathbf{E}(\mathbf{u}) + 2\mathbf{b}'' \cdot \mathbf{u} \right\} \vartheta_1 \\ &\quad - \alpha\phi^{\alpha-1}\phi' \mathbf{S}(\mathbf{u}) \cdot \mathbf{E}(\mathbf{w}_0(\vartheta_1)) + \mathbf{b}' \cdot \mathbf{w}_0(\vartheta_1). \end{aligned} \quad (8.9.33)$$

If \mathbf{b} is not a function of θ , with respect to the solution \mathbf{w}_0 of Problem 8.9.4,

$$\mathbf{E}(\mathbf{w}_0(\vartheta_1)) = -2 \frac{\alpha\phi'}{\phi} \mathbf{E}(\mathbf{v}_0) \vartheta_1 \quad (8.9.34)$$

holds. Substituting Eq. (8.9.34) into Eq. (8.9.33), it can be confirmed that Eq. (8.9.32) accords with Eq. (8.9.25).

8.9.6 Numerical Example

The results of mean compliance minimization for a two-dimensional linear elastic body with a boundary condition referred to as the coat-hanging problem is shown in Figs. 8.14 to 8.16. The initial density ($\theta = 0$) and the boundary condition for the linear elastic problem are shown in Fig. 8.14 (a). A domain in which the density is constrained ($\bar{\Omega}_{C0}$ in Eq. (8.1.3)) was not set. The program is written using the programming language FreeFEM (<https://freefem.org/>) [16] using the finite element method. In the finite element analyses of the linear

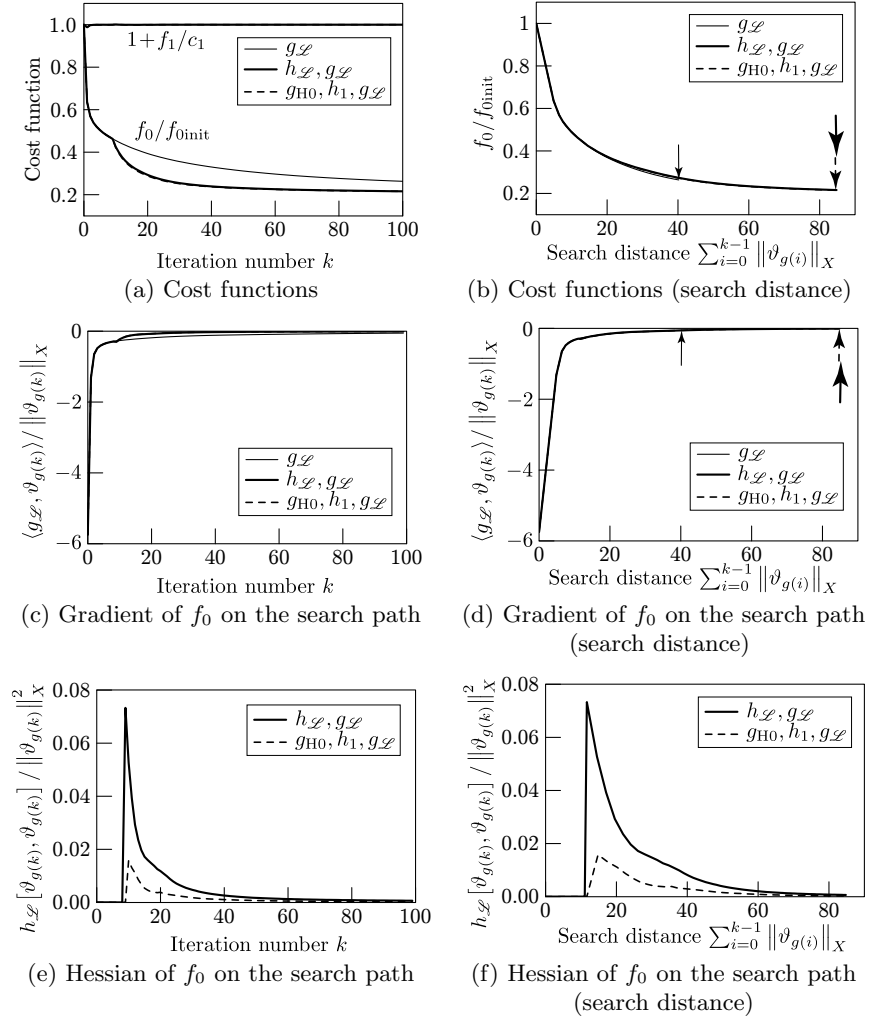


Fig. 8.15: Numerical example of mean compliance minimization: cost functions and gradients and Hessians of f_0 on the search path ($g_{\mathcal{L}}$: H^1 gradient method, $h_{\mathcal{L}}, g_{\mathcal{L}}$: H^1 Newton method, $g_{H0}, h_1, g_{\mathcal{L}}$: H^1 Newton method using the Hesse gradient).

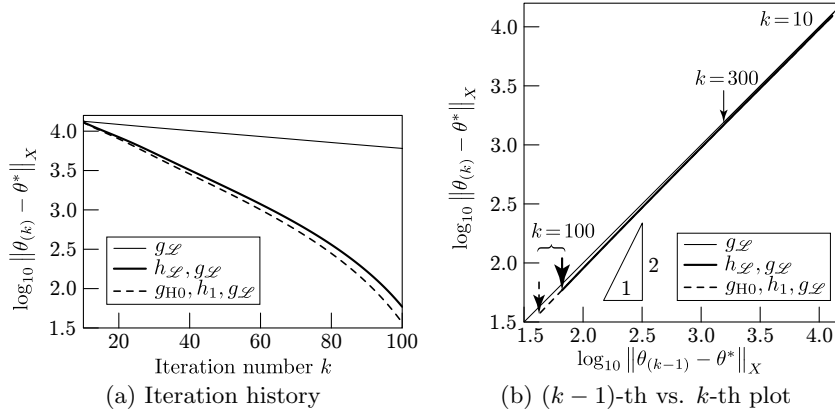


Fig. 8.16: Numerical example of mean compliance minimization problem: distance $\|\theta_k - \theta^*\|_X$ from an approximate minimum point θ^* ($g_{\mathcal{L}}$: the gradient method, $h_{\mathcal{L}}, g_{\mathcal{L}}$: the Newton method, $g_{H0}, h_1, g_{\mathcal{L}}$: the Newton method using the Hesse gradient).

elastic problem and the H^1 gradient method or the H^1 Newton method, the second-order triangular elements were used. In the case using the H^1 Newton method, the routine of the H^1 Newton method was started from $k_N = 10$. The results were changed with c_a in Eq. (8.7.1), c_D in Eq. (8.6.3), c_{D1} and c_{D0} in Eq. (8.6.7), c_h in Eq. (8.7.8) and the parameter (`errelas`) to control the error level in the adaptive mesh. For details, we refer the readers to the programs themselves.¹

Figure 8.14 (b) to (d) show the densities obtained by the three methods (H^1 gradient method using $g_{\mathcal{L}} = g_0 + \lambda_1 g_1$, H^1 Newton method using $h_{\mathcal{L}} = h_0 + \lambda_1 h_1$ and $g_{\mathcal{L}}$, and H^1 Newton method using $g_{H0}, h_1, g_{\mathcal{L}}$). Figure 8.15 (a) shows the cost functions $f_0/f_{0\text{init}}$ and $1 + f_1/c_1$ normalized with f_0 at the initial density denoted by $f_{0\text{init}}$ and c_1 set with the domain integral of the initial density (volume), respectively, with respect to the iteration number k . Figure 8.15 (b) shows those values with respect to the distance $\sum_{i=0}^{k-1} \|\vartheta_{g(i)}\|_X$ on the search path in X . The graphs of f_0 's gradient (the gradient of the Lagrange function $\mathcal{L} = \mathcal{L}_0 + \lambda_1 f_1$) calculated as $\langle g_{\mathcal{L}}, \vartheta_{g(k)} \rangle / \|\vartheta_{g(k)}\|_X$ are shown in Fig. 8.15 (c) and (d) with respect to the iteration number and the search distance, respectively. Moreover, Fig. 8.15 (e) and (f) show the graphs of f_0 's second-order derivative $h_{\mathcal{L}}[\vartheta_{g(k)}, \vartheta_{g(k)}] / \|\vartheta_{g(k)}\|_X^2$ (in the case of the Newton method using the Hesse gradient, $(\langle g_{H0}, \vartheta_{g(k)} \rangle + \lambda_1 h_1[\vartheta_{g(k)}, \vartheta_{g(k)}]) / \|\vartheta_{g(k)}\|_X^2$) with respect to the iteration number and the search distance, respectively. In these notations, the norm of the i -th search vector is defined by

$$\|\vartheta_{g(i)}\|_X = \left(\int_D (\nabla \vartheta_{g(i)} \cdot \nabla \vartheta_{g(i)} + \vartheta_{g(i)}^2) dx \right)^{1/2}. \quad (8.9.35)$$

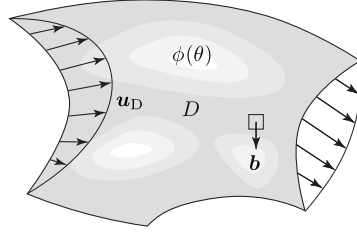
¹See Electronic supplementary material.

The computational times until $k = 100$ by PC were 6.897, 17.073 and 32.394 sec by the H^1 gradient method, the H^1 Newton method and the H^1 Newton method using the Hesse gradient, respectively.

We explain the numerical results and give some considerations as follows. The graphs in Fig. 8.15 (a) clearly show that the convergence speed with respect to the iteration number k is faster when using the H^1 Newton method than when applying the H^1 gradient method. However, when the H^1 Newton method started, c_{D1} and c_{D0} in Eq. (8.6.7) were replaced with smaller values so as to avoid any numerical instability during iterations. As a result, it can be considered that the convergence speed was increased by enlarging the step size. In reality, the following phenomenon was observed. When we set c_h to zero (H^1 gradient method), the computation fails at $k = k_N$. However, when we put a larger value for c_{D0} in Eq. (8.6.7), we have a convergence similar to the H^1 Newton method. Moreover, based on the fact that the three graphs plotted in Fig. 8.15 (b) coincide, we conclude that the search paths due from each methods are actually the same. Based on these observations, we infer that the H^1 Newton method is superior to the first-order method, in the sense that we can take larger values for the step size.

Based from the results shown in Fig. 8.15 (d) and (f), we also draw some particular observations around the minimum point as follows. Firstly, since the Hessian of f_0 on the search path has a positive value, we deduce that the point of convergence is a local minimum. Secondly, we noticed that both the first derivative and the Hessian eventually diminish to zero. This key finding is observed because we assumed a sigmoid function for the density of the design valuable θ , and obtained a small variation of the density around the minimum point where the density converges to 0 or 1 that causes a small variation of the cost functions.

In addition, Fig. 8.16 (a) shows the graphs of the distance $\|\theta_{(k)} - \theta^*\|_X$ from an approximate minimum point θ^* obtained by the three methods with respect to the iteration number k . The approximate minimum point θ^* was given by the numerical solution of θ when the iteration time is taken larger than the given value in the H^1 Newton method. From this figure, it can be confirmed that the convergence orders for the results by the H^1 Newton methods are more than the first order. However, Fig. 8.16 (b), plotting the k -th distance $\|\theta_k - \theta^*\|_X$ with respect to the $(k - 1)$ -th distance (the gradient of the graph shows the order of convergence as explained by using Eq. (3.8.13)), shows that the convergence order of the H^1 Newton method is less than the second order, while more than the first order. This result is possibly due to the fact that the bilinear form a_X in X was added to the original Hessian in order to ensure coerciveness and boundedness of the left-hand side of Eq. (8.6.6). By this addition, the H^1 Newton method has a different structure from the original Newton method. It is still unclear, however, whether a solution with second-order convergence exists for the problem analyzed in this section.

Fig. 8.17: Stokes flow field of θ -type.

8.10 Topology Optimization Problem of Stokes Flow Field

The fact that the topology optimization problem can be constructed even with respect to a flow field is shown in the literature [1, 8, 11–14, 33]. Here, the mean flow resistance minimization problem of the one-dimensional branched Stokes flow field mentioned in Section 1.3 is extended to a $d \in \{2, 3\}$ -dimensional topology optimization problem of θ -type. Here, θ -derivatives of cost functions and second-order θ -derivatives are shown up as far as can be sought. In this section, D is assumed to be a Stokes flow field and X and \mathcal{D} are taken to be defined in Eq. (8.1.3) and Eq. (8.1.4), respectively.

8.10.1 State Determination Problem

Let us define a Stokes problem as a state determination problem. A Stokes problem (Problem 5.5.1) was defined in Section 5.5 but here a Stokes flow field of θ -type such as the one in Fig. 8.17 is considered. In this regard, some definitions will be added. With respect to U and \mathcal{S} , Eq. (8.9.1) and Eq. (8.9.2) will be used respectively, but $\Gamma_D = \partial D$. Furthermore, with respect to $q_R > d$, put

$$P = \left\{ q \in L^2(D; \mathbb{R}) \mid \int_D q \, dx = 0 \right\}, \quad (8.10.1)$$

$$\mathcal{Q} = P \cap L^{2q_R}(D; \mathbb{R}). \quad (8.10.2)$$

In a topology optimization problem of a flow field, a flow field passing through porous media (penetration flow) is used. In an penetration flow, between the flow speed \mathbf{u} and pressure p , the [Darcy law](#) given by

$$\mathbf{u} = -\frac{k}{\mu} \nabla p$$

is assumed to hold. Here, k and μ are positive constants known as penetration and viscosity coefficients. In a topology optimization problem of a flow field, replace the constant μ/k representing the difficulty of penetration with

$$\psi(\phi) = \psi_1 \left\{ 1 - \frac{\phi(1+\alpha)}{\phi+\alpha} \right\} = \psi_1 \frac{\alpha(1-\phi)}{\alpha+\phi} \quad (8.10.3)$$

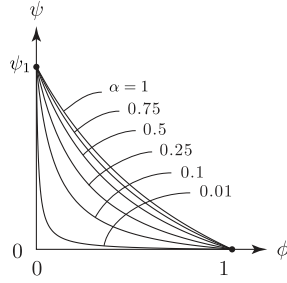


Fig. 8.18: Coefficient ψ expressing the flow resistance with respect to fluid content ϕ .

and ∇p in the Stokes equation with $\psi(\phi(\theta)) \mathbf{u} + \nabla p$. Here, ϕ represents the fluid content equivalent to the density of fluid and its range is assumed to be limited to $[0, 1]$. Hence, similarly to the density in the previous sections, ϕ is assumed to be given by the sigmoid function with respect to the design variable $\theta \in X$. Moreover, ψ_1 is a positive constant which gives the maximum value of the resistance to flow, α is a constant controlling the non-linearity and is chosen from $(0, 1]$. In the paper [1], it is changed from 0.01 to 1 along with calculation progression. Figure 8.18 shows the function $\psi(\phi)$.

Here, the following assumption is set.

Hypothesis 8.10.1 (Regularities of known functions) With respect to $q_R > d$,

$$\mathbf{b} \in L^{2q_R}(D; \mathbb{R}^d), \quad \mathbf{u}_D \in \{ \mathbf{u} \in W^{1,2q_R}(D; \mathbb{R}^d) \mid \nabla \cdot \mathbf{u} = 0 \text{ in } D \}$$

is assumed. □

Using these assumptions, a Stokes problem of θ -type is defined in the following way.

Problem 8.10.2 (θ -type Stokes problem) Let \mathbf{b} and \mathbf{u}_D satisfy Hypothesis 8.10.1, and Hypothesis 8.2.2 holds with respect to the opening angles of boundary corner points. Moreover, $\psi(\phi)$ is taken to be Eq. (8.10.3). Furthermore, $\phi(\theta)$ is assumed to be given by Eq. (8.1.1) or Eq. (8.1.2). Here, obtain $(\mathbf{u}, p) : D \rightarrow \mathbb{R}^{d+1}$ which satisfies

$$-\nabla^\top (\mu \nabla \mathbf{u}^\top) + \psi(\phi(\theta)) \mathbf{u}^\top + \nabla^\top p = \mathbf{b}^\top \quad \text{in } D, \quad (8.10.4)$$

$$\nabla \cdot \mathbf{u} = 0 \quad \text{in } D, \quad (8.10.5)$$

$$\mathbf{u} = \mathbf{u}_D \quad \text{on } \partial D, \quad (8.10.6)$$

$$\int_D p \, dx = 0. \quad (8.10.7)$$

□

For later use, the Lagrange function with respect to Problem 8.10.2 is defined as

$$\begin{aligned} \mathcal{L}_S(\theta, \mathbf{u}, p, \mathbf{v}, q) &= \int_D \{-\mu(\nabla \mathbf{u}^\top) \cdot (\nabla \mathbf{v}^\top) - \psi(\phi(\theta)) \mathbf{u} \cdot \mathbf{v} \\ &\quad + p \nabla \cdot \mathbf{v} + \mathbf{b} \cdot \mathbf{v} + q \nabla \cdot \mathbf{u}\} dx \\ &\quad + \int_{\partial D} \{(\mathbf{u} - \mathbf{u}_D) \cdot (\mu \partial_\nu \mathbf{v} - q \boldsymbol{\nu}) + \mathbf{v} \cdot (\mu \partial_\nu \mathbf{u} - p \boldsymbol{\nu})\} d\gamma, \end{aligned} \quad (8.10.8)$$

where (\mathbf{u}, p) is not necessarily the solution of Problem 8.10.2, and $(\mathbf{v}, q) \in U \times P$ is a Lagrange multiplier.

When (\mathbf{u}, p) is a solution to Problem 8.10.2, the equation

$$\mathcal{L}_S(\theta, \mathbf{u}, p, \mathbf{v}, q) = 0$$

is established with respect to an arbitrary $(\mathbf{v}, q) \in U \times P$.

8.10.2 Mean Flow Resistant Minimization Problem

Let us define a topology optimization problem of θ -type with respect to a Stokes flow field. Define the cost functions as follows. Firstly, let us define a cost function representing the resistance to flow as

$$f_0(\theta, \mathbf{u}, p) = - \int_D \mathbf{b} \cdot \mathbf{u} dx + \int_{\partial D} \mathbf{u}_D \cdot (\mu \partial_\nu \mathbf{u} - p \boldsymbol{\nu}) d\gamma. \quad (8.10.9)$$

The first term on the right-hand side of Eq. (8.10.9) represents the negative value of the rate of work due to the volume force. This value was given a negative sign because the greater it is, the greater the flow speed is. On the other hand, the second term on the right-hand side of Eq. (8.10.9) is equivalent to the energy per unit time lost through the viscosity inside Stokes flow field represented by the boundary integral. From the fact that these express the property of flow resistance, f_0 will be referred to as the **mean flow resistance**. With respect to this,

$$f_1(\theta) = \int_D \phi(\theta) dx - c_1 \quad (8.10.10)$$

is the cost function for constraint with respect to the domain measure of the flow field. Here, c_1 is a positive constant such that $f_1(\theta) \leq 0$ holds with respect to some $\theta \in \mathcal{D}$. Using these, the minimization problem of mean flow resistance is defined as follows.

Problem 8.10.3 (Mean flow resistance minimization problem) Let \mathcal{D} , \mathcal{S} and \mathcal{Q} be Eq. (8.1.4), Eq. (8.9.2) and Eq. (8.10.2), respectively. Let (\mathbf{u}, p) be

the solution of Problem 8.10.2 with respect to $\theta \in \mathcal{D}$ and f_0 and f_1 are given by Eq. (8.10.9) and Eq. (8.10.10). In this case, obtain θ which satisfies

$$\min_{(\theta, \mathbf{u}-\mathbf{u}_D, p) \in \mathcal{D} \times \mathcal{S} \times \mathcal{Q}} \{f_0(\theta, \mathbf{u}, p) \mid f_1(\theta) \leq 0, \text{ Problem 8.10.2}\}.$$

□

8.10.3 θ -Derivatives of Cost Functions

Let us obtain the θ -derivative of $f_0(\theta, \mathbf{u}, p)$ via the adjoint variable method. Let the Lagrange function of f_0 be

$$\begin{aligned} \mathcal{L}_0(\theta, \mathbf{u}, p, \mathbf{v}_0, q_0) &= f_0(\theta, \mathbf{u}, p) - \mathcal{L}_S(\theta, \mathbf{u}, p, \mathbf{v}_0, q_0) \\ &= \int_D \left\{ \mu (\nabla \mathbf{u}^\top) \cdot (\nabla \mathbf{v}_0^\top) + \psi(\phi(\theta)) \mathbf{u} \cdot \mathbf{v}_0 - p \nabla \cdot \mathbf{v}_0 \right. \\ &\quad \left. - \mathbf{b} \cdot (\mathbf{v}_0 + \mathbf{u}) - q_0 \nabla \cdot \mathbf{u} \right\} dx \\ &\quad - \int_{\partial D} \{(\mathbf{u} - \mathbf{u}_D) \cdot (\mu \partial_\nu \mathbf{v}_0 - q_0 \boldsymbol{\nu}) + (\mathbf{v}_0 - \mathbf{u}_D) \cdot (\mu \partial_\nu \mathbf{u} - p \boldsymbol{\nu})\} d\gamma. \end{aligned} \quad (8.10.11)$$

Comparing with Eq. (8.9.8) defining the Lagrange function with respect to mean compliance of linear elastic body, here a negative sign was put on \mathcal{L}_S . This change is so that a self-adjoint relationship can be obtained later. Although in the mean compliance minimization problem of a linear elastic body, the minimization of the displacement was the aim, in a Stokes flow field mean flow resistance minimization problem, the maximization of flow is aimed for. Hence, this type of difference arose. The Fréchet derivative of \mathcal{L}_0 with respect to an arbitrary variation $(\vartheta, \hat{\mathbf{u}}, \hat{p}, \hat{\mathbf{v}}_0, \hat{q}_0) \in X \times (U \times P)^2$ of $(\theta, \mathbf{u}, p, \mathbf{v}_0, q_0)$ is

$$\begin{aligned} \mathcal{L}_0'(\theta, \mathbf{u}, p, \mathbf{v}_0, q_0) [\vartheta, \hat{\mathbf{u}}, \hat{p}, \hat{\mathbf{v}}_0, \hat{q}_0] &= \mathcal{L}_{0\theta}(\theta, \mathbf{u}, p, \mathbf{v}_0, q_0) [\vartheta] + \mathcal{L}_{0\mathbf{u}p}(\theta, \mathbf{u}, p, \mathbf{v}_0, q_0) [\hat{\mathbf{u}}, \hat{p}] \\ &\quad + \mathcal{L}_{0\mathbf{v}_0q_0}(\theta, \mathbf{u}, p, \mathbf{v}_0, q_0) [\hat{\mathbf{v}}_0, \hat{q}_0]. \end{aligned} \quad (8.10.12)$$

Each term is considered below.

The third term on the right-hand side of Eq. (8.10.12) becomes

$$\begin{aligned} \mathcal{L}_{0\mathbf{v}_0q_0}(\theta, \mathbf{u}, p, \mathbf{v}_0, q_0) [\hat{\mathbf{v}}_0, \hat{q}_0] &= \mathcal{L}_{S\mathbf{v}_0q_0}(\theta, \mathbf{u}, p, \mathbf{v}_0, q_0) [\hat{\mathbf{v}}_0, \hat{q}_0] \\ &= -\mathcal{L}_S(\theta, \mathbf{u}, p, \hat{\mathbf{v}}_0, \hat{q}_0). \end{aligned} \quad (8.10.13)$$

Equation (8.10.13) is a Lagrange function of the state determination problem (Problem 8.10.2). Hence, if (\mathbf{u}, p) is the weak solution of the state determination problem, the third term on the right-hand side of Eq. (8.10.12) vanishes.

Moreover, the second term on the right-hand side of Eq. (8.10.12) becomes

$$\mathcal{L}_{0\mathbf{u}p}(\theta, \mathbf{u}, p, \mathbf{v}_0, q_0) [\hat{\mathbf{u}}, \hat{p}]$$

$$\begin{aligned}
&= \int_D \left\{ \mu \left(\nabla \hat{\mathbf{u}}^\top \right) \cdot \left(\nabla \mathbf{v}_0^\top \right) + \psi(\phi(\theta)) \hat{\mathbf{u}} \cdot \mathbf{v}_0 - \hat{p} \nabla \cdot \mathbf{v}_0 \right. \\
&\quad \left. - \mathbf{b} \cdot \hat{\mathbf{u}} - q_0 \nabla \cdot \hat{\mathbf{u}} \right\} dx \\
&\quad - \int_{\partial D} \left\{ \hat{\mathbf{u}} \cdot (\mu \partial_\nu \mathbf{v}_0 - q_0 \boldsymbol{\nu}) + (\mathbf{v}_0 - \mathbf{u}_D) \cdot (\mu \partial_\nu \hat{\mathbf{u}} - \hat{p} \boldsymbol{\nu}) \right\} d\gamma \\
&= -\mathcal{L}_S(\theta, \mathbf{v}_0, q_0, \hat{\mathbf{u}}, \hat{p})
\end{aligned} \tag{8.10.14}$$

with respect to an arbitrary variation $(\hat{\mathbf{u}}, \hat{p}) \in U \times P$ of (\mathbf{u}, p) . Hence, when the [self-adjoint relationship](#)

$$(\mathbf{u}, p) = (\mathbf{v}_0, q_0) \tag{8.10.15}$$

holds, the second term on the right-hand side of Eq. (8.10.12) becomes zero.

Furthermore, the first term on the right-hand side of Eq. (8.10.12) becomes

$$\mathcal{L}_{0\theta}(\theta, \mathbf{u}, p, \mathbf{v}_0, q_0)[\vartheta] = \int_D \psi'(\phi(\theta)) \phi'(\theta) \mathbf{u} \cdot \mathbf{v}_0 \vartheta \, dx. \tag{8.10.16}$$

Therefore, suppose (\mathbf{u}, p) is a weak solution of Problem 8.10.2 and that the self-adjoint relationship Eq. (8.10.15) holds. If $f_0(\theta, \mathbf{u}, p)$ in this case is written as $\tilde{f}_0(\theta)$, the equation

$$\tilde{f}'_0(\theta)[\vartheta] = \mathcal{L}_{0\theta}(\theta, \mathbf{u}, p, \mathbf{v}_0, q_0)[\vartheta] = \langle g_0, \vartheta \rangle \tag{8.10.17}$$

holds, where

$$g_0 = \psi' \phi' \mathbf{u} \cdot \mathbf{u}. \tag{8.10.18}$$

When using $\psi(\phi)$ of Eq. (8.10.3), we get

$$\psi'(\phi) = -\psi_1 \frac{\alpha(1+\alpha)}{(\phi+\alpha)^2}. \tag{8.10.19}$$

On the other hand, with respect to $f_1(\theta)$,

$$f'_1(\theta)[\vartheta] = \int_D \phi' \vartheta \, dx \tag{8.10.20}$$

holds with respect to an arbitrary $\vartheta \in X$.

Based on the results above, the function space containing g_0 of Eq. (8.10.18) is included in $W^{1,q_R}(D; \mathbb{R}) \subset X'$ which is smoother than the result of Theorem 8.5.2. From the fact that $W^{1,q_R}(D; \mathbb{R}) \subset C^0(D; \mathbb{R})$, it is thought that even without applying the H^1 gradient method, a numerically unstable phenomenon will not be generated. However, in order for the search vector ϑ_g to guarantee $C^{0,1}$ class, the H^1 gradient method is required.

8.10.4 Second-Order θ -Derivatives of Cost Functions

Furthermore, the second-order θ -derivatives of the cost functions of the mean flow resistance f_0 and constraint function f_1 with respect to the domain measure of flow field can be obtained. Based on the procedures looked at in Sect. 8.5.2, let us also look here at obtaining the second-order θ derivatives of f_0 and f_1 .

Firstly, let us think about the second-order θ -derivative of f_0 . With respect to Hypothesis 8.5.4 (1), \mathbf{b} is assumed not to be a function of θ . The relationship corresponding to Hypothesis 8.5.4 (2) is satisfied here.

The Lagrange function \mathcal{L}_0 of f_0 is defined in Eq. (8.10.11). Viewing (θ, \mathbf{u}, p) as a design variable, its admissible set and admissible direction is set as

$$\begin{aligned} S &= \{ (\theta, \mathbf{u}, p) \in \mathcal{D} \times \mathcal{S} \times \mathcal{Q} \mid \\ &\quad \mathcal{L}_S(\theta, \mathbf{u}, p, \mathbf{v}, q) = 0 \text{ for all } (\mathbf{v}, q) \in U \times P \}, \\ T_S(\theta, \mathbf{u}, p) &= \{ (\vartheta, \hat{\mathbf{v}}, \hat{\pi}) \in X \times U \times P \mid \\ &\quad \mathcal{L}_{S\theta\mathbf{u}p}(\theta, \mathbf{u}, p, \mathbf{v}, q) [\vartheta, \hat{\mathbf{v}}, \hat{\pi}] = 0 \text{ for all } (\mathbf{v}, \hat{\pi}) \in U \times P \}. \end{aligned}$$

The second-order θ -derivative of \mathcal{L}_0 with respect to arbitrary variations $(\vartheta_1, \hat{\mathbf{v}}_1, \hat{\pi}_1), (\vartheta_2, \hat{\mathbf{v}}_2, \hat{\pi}_2) \in T_S(\theta, \mathbf{u}, p)$ becomes

$$\begin{aligned} &\mathcal{L}_{0(\theta, \mathbf{u}, p)(\theta, \mathbf{u}, p)}(\theta, \mathbf{u}, p, \mathbf{v}_0, q_0) [(\vartheta_1, \hat{\mathbf{v}}_1, \hat{\pi}_1), (\vartheta_2, \hat{\mathbf{v}}_2, \hat{\pi}_2)] \\ &= \mathcal{L}_{0\theta\theta}(\theta, \mathbf{u}, p, \mathbf{v}_0, q_0) [\vartheta_1, \vartheta_2] + \mathcal{L}_{0\theta\mathbf{u}p}(\theta, \mathbf{u}, p, \mathbf{v}_0, q_0) [\vartheta_1, \hat{\mathbf{v}}_2, \hat{\pi}_2] \\ &\quad + \mathcal{L}_{0\theta\mathbf{u}p}(\theta, \mathbf{u}, \mathbf{v}_0) [\vartheta_2, \hat{\mathbf{v}}_1, \hat{\pi}_1] + \mathcal{L}_{0\mathbf{u}p\mathbf{u}p}(\theta, \mathbf{u}, \mathbf{v}_0) [\hat{\mathbf{v}}_1, \hat{\pi}_1, \hat{\mathbf{v}}_2, \hat{\pi}_2]. \end{aligned} \tag{8.10.21}$$

Each term on the right-hand side of Eq. (8.10.21) becomes

$$\begin{aligned} &\mathcal{L}_{0\theta\theta}(\theta, \mathbf{u}, p, \mathbf{v}_0, q_0) [\vartheta_1, \vartheta_2] \\ &= \int_D \left\{ \psi''(\phi(\theta)) (\phi'(\theta))^2 + \psi'(\phi(\theta)) \phi''(\theta) \right\} \mathbf{u} \cdot \mathbf{v}_0 \vartheta_1 \vartheta_2 \, dx, \end{aligned} \tag{8.10.22}$$

$$\mathcal{L}_{0\theta\mathbf{u}p}(\theta, \mathbf{u}, p, \mathbf{v}_0, q_0) [\vartheta_1, \hat{\mathbf{v}}_2, \hat{\pi}_2] = \int_D \psi'(\phi(\theta)) \phi'(\theta) \hat{\mathbf{v}}_2 \cdot \mathbf{v}_0 \vartheta_1 \, dx, \tag{8.10.23}$$

$$\mathcal{L}_{0\theta\mathbf{u}p}(\theta, \mathbf{u}, p, \mathbf{v}_0, q_0) [\vartheta_2, \hat{\mathbf{v}}_1, \hat{\pi}_1] = \int_D \psi'(\phi(\theta)) \phi'(\theta) \hat{\mathbf{v}}_1 \cdot \mathbf{v}_0 \vartheta_2 \, dx, \tag{8.10.24}$$

$$\mathcal{L}_{0\mathbf{u}p\mathbf{u}p}(\theta, \mathbf{u}, p, \mathbf{v}_0, q_0) [\hat{\mathbf{v}}_1, \hat{\pi}_1, \hat{\mathbf{v}}_2, \hat{\pi}_2] = 0. \tag{8.10.25}$$

Here, the fact that $\mathbf{u} - \mathbf{u}_D, \mathbf{v}_0 - \mathbf{u}_D, \hat{\mathbf{v}}_1$ and $\hat{\mathbf{v}}_2$ become $\mathbf{0}_{\mathbb{R}^d}$ on ∂D was used. In this case, with respect to arbitrary variation $(\vartheta_j, \hat{\mathbf{v}}_j, \hat{\pi}_j) \in T_S(\theta, \mathbf{u}, p)$ for $j \in \{1, 2\}$, the Fréchet partial derivative of the Lagrange function \mathcal{L}_S of the state determination problem establishes the equation

$$\begin{aligned} &\mathcal{L}_{S\theta\mathbf{u}p}(\theta, \mathbf{u}, p, \mathbf{v}, q) [\vartheta, \hat{\mathbf{v}}, \hat{\pi}] \\ &= \int_D \left\{ -\mu (\nabla \hat{\mathbf{v}}^\top) \cdot (\nabla \mathbf{v}^\top) - \psi'(\phi(\theta)) \phi'(\theta) \mathbf{u} \cdot \mathbf{v} \vartheta \right. \end{aligned}$$

$$\begin{aligned}
& -\psi(\phi(\theta)) \hat{\mathbf{v}} \cdot \mathbf{v} + \hat{\pi} \nabla \cdot \mathbf{v} + q \nabla \cdot \hat{\mathbf{v}} \} dx \\
& = 0
\end{aligned} \tag{8.10.26}$$

with respect to an arbitrary $(\mathbf{v}, q) \in U \times P$. Here, the fact that \mathbf{v} and $\hat{\mathbf{v}}$ are $\mathbf{0}_{\mathbb{R}^d}$ on Γ_D as well as Eq. (8.10.5) were used.

Here, the next assumption is set up. At a local minimum point of a mean flow resistance minimization problem (Problem 8.10.3), it is thought that the fluid content $\phi(\theta)$ converges to 0 and 1, and the terms introduced in order to provide flow resistance becomes sufficiently small in actual flow field of $\phi(\theta) \approx 1$. Hence, in Eq. (8.10.26), it is assumed that

$$\int_D \left\{ -\mu \left(\nabla \hat{\mathbf{v}}_j^\top \right) \cdot \left(\nabla \mathbf{v}^\top \right) + \hat{\pi}_j \nabla \cdot \mathbf{v} + q \nabla \cdot \hat{\mathbf{v}}_j \right\} dx = 0 \tag{8.10.27}$$

is established. In this case, the condition

$$\hat{\mathbf{v}}_j = -\frac{\psi'(\phi(\theta)) \phi'(\theta)}{\psi(\phi(\theta))} \vartheta_j \mathbf{u} \quad \text{in } D \tag{8.10.28}$$

can be obtained. Hence, substituting $(\hat{\mathbf{v}}_j, \hat{\pi}_j)$ into $(\hat{\mathbf{v}}_1, \hat{\pi}_1)$ in Eq. (8.10.24) and $(\hat{\mathbf{v}}_2, \hat{\pi}_2)$ in Eq. (8.10.23), then

$$\begin{aligned}
& \mathcal{L}_{0\theta up}(\theta, \mathbf{u}, \mathbf{v}_0) [\vartheta_1, \hat{\mathbf{v}}_2, \hat{\pi}_2] \\
& = \mathcal{L}_{0\theta up}(\theta, \mathbf{u}, p, \mathbf{v}_0, q_0) [\vartheta_2, \hat{\mathbf{v}}_1, \hat{\pi}_1] \\
& = \int_D -\frac{(\psi'(\phi(\theta)) \phi'(\theta))^2}{\psi(\phi(\theta))} \mathbf{u} \cdot \mathbf{v}_0 \vartheta_1 \vartheta_2 \, dx
\end{aligned} \tag{8.10.29}$$

is obtained.

Summarizing the results above, by substituting Eq. (8.10.29) and Eq. (8.10.22) into Eq. (8.10.21), the second-order θ -derivative of mean flow resistance f_0 becomes

$$\begin{aligned}
h_0(\vartheta_1, \vartheta_2) & = \int_D \left\{ \psi''(\phi')^2 + \psi' \phi'' - 2 \frac{(\psi' \phi')^2}{\psi} \right\} \mathbf{u} \cdot \mathbf{v}_0 \vartheta_1 \vartheta_2 \, dx \\
& = \int_D \psi_1 \beta(\alpha, \theta) \mathbf{u} \cdot \mathbf{v}_0 \vartheta_1 \vartheta_2 \, dx.
\end{aligned} \tag{8.10.30}$$

In the above equation, $\psi'(\phi)$ becomes Eq. (8.10.19) and

$$\psi''(\phi) = \frac{2\alpha(1+\alpha)}{(\phi+\alpha)^3}. \tag{8.10.31}$$

When Eq. (8.1.1) is used in $\phi(\theta)$, $\phi'(\theta)$ and $\phi''(\theta)$ are given by Eq. (8.5.7) and Eq. (8.9.27), respectively. Moreover, if $\phi(\theta)$ is given by Eq. (8.1.2), these are given by Eq. (8.5.8) and Eq. (8.9.28), respectively. Figure 8.19 shows the graph of $\beta(\alpha, \theta)$. From $\beta(\alpha, \theta) < 0$ and the self-adjoint relationship $\mathbf{u} \cdot \mathbf{v}_0 = \mathbf{u} \cdot \mathbf{u} > 0$, it can be confirmed that $h_0(\cdot, \cdot)$ is not coercive.

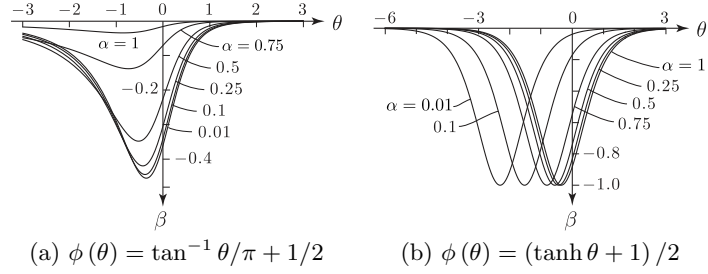


Fig. 8.19: Coefficient functions $\beta(\alpha, \theta)$ at second-order θ -derivative of mean flow resistance.

On the other hand, the second-order θ -derivative of $f_1(\theta)$ becomes Eq. (8.9.26). The graph of $\phi''(\theta)$ is shown in Fig. 8.13.

In this way, the second-order θ -derivative of the cost function f_0 in mean flow resistance minimization problem is not coercive and the second-order θ -derivative of the constraint function f_1 does not become coercive either. Hence, if the Newton method (Problem 8.6.6) is to be used with respect to a mean flow resistance minimization problem, there is a need to use an appropriate bilinear form $a_X(\vartheta_{gi}, \psi)$ to capture coerciveness.

8.10.5 Second-Order θ -Derivative of Cost Function Using Lagrange Multiplier Method

When the Lagrange multiplier method is used to obtain the second-order θ -derivative of the mean flow resistance f_0 , it becomes as follows. Using the same discussion as Section 7.5.4, we fix ϑ_1 and define the Lagrange function for $\hat{f}'_0(\theta)[\vartheta_1] = \langle g_0, \vartheta_1 \rangle$ in Eq. (8.10.17) by

$$\mathcal{L}_{10}(\theta, \mathbf{u}, p, \mathbf{w}_0, r_0) = \langle g_0, \vartheta_1 \rangle - \mathcal{L}_S(\theta, \mathbf{u}, p, \mathbf{w}_0, r_0), \quad (8.10.32)$$

where \mathcal{L}_S is given by Eq. (8.10.8), and $(\mathbf{w}_0, r_0) \in U \times P$ is the adjoint variable provided for (\mathbf{u}, p) in \mathbf{g}_0 .

With respect to arbitrary variations $(\vartheta_2, \hat{\mathbf{u}}, \hat{p}, \hat{\mathbf{w}}_0, \hat{r}_0) \in X \times (U \times P)^2$ of $(\theta, \mathbf{u}, p, \mathbf{w}_0, r_0)$, the Fréchet derivative of \mathcal{L}_{10} is written as

$$\begin{aligned} \mathcal{L}'_{10}(\theta, \mathbf{u}, p, \mathbf{w}_0, r_0)[\vartheta_2, \hat{\mathbf{u}}, \hat{p}, \hat{\mathbf{w}}_0, \hat{r}_0] \\ = \mathcal{L}_{10\theta}(\theta, \mathbf{u}, p, \mathbf{w}_0, r_0)[\vartheta_2] + \mathcal{L}_{10\mathbf{u}p}(\theta, \mathbf{u}, p, \mathbf{w}_0, r_0)[\hat{\mathbf{u}}, \hat{p}] \\ + \mathcal{L}_{10\mathbf{w}_0r_0}(\theta, \mathbf{u}, p, \mathbf{w}_0, r_0)[\hat{\mathbf{w}}_0, \hat{r}_0]. \end{aligned} \quad (8.10.33)$$

The third term on the right-hand side of Eq. (8.10.33) vanishes if (\mathbf{u}, p) is the solution of the state determination problem.

The second term on the right-hand side of Eq. (8.10.33) is

$$\mathcal{L}_{10\mathbf{u}p}(\theta, \mathbf{u}, p, \mathbf{w}_0, r_0)[\hat{\mathbf{u}}, \hat{p}]$$

$$\begin{aligned}
&= \int_D \left\{ 2\psi' \phi' \mathbf{u} \cdot \hat{\mathbf{u}} \vartheta_1 + \mu (\nabla \mathbf{w}_0^\top) \cdot (\nabla \hat{\mathbf{u}}^\top) + \psi(\phi(\theta)) \mathbf{w}_0 \cdot \hat{\mathbf{u}} \right. \\
&\quad \left. - \hat{p} \nabla \cdot \mathbf{w}_0 - r_0 \nabla \cdot \hat{\mathbf{u}} \right\} dx. \tag{8.10.34}
\end{aligned}$$

Here, the condition that Eq. (8.10.34) is zero for arbitrary $(\hat{\mathbf{u}}, \hat{p}) \in U \times P$ is equivalent to setting (\mathbf{w}_0, r_0) to be the solution of the following adjoint problem.

Problem 8.10.4 (Adjoint problem of (\mathbf{w}_0, r_0) with respect to $\langle g_0, \vartheta_1 \rangle$)

Under the assumption of Problem 8.10.2, let $\vartheta_1 \in X$ be given. Find $(\mathbf{w}_0, r_0) = (\mathbf{w}_0(\vartheta_1), r_0(\vartheta_1)) \in U \times P$ satisfying

$$\begin{aligned}
-\nabla^\top (\mu \nabla \mathbf{w}_0^\top) + \psi \mathbf{w}_0^\top + \nabla^\top r_0 &= -2\psi' \phi' \mathbf{v}_0^\top \vartheta_1 \quad \text{in } D, \\
\nabla \cdot \mathbf{w}_0 &= 0 \quad \text{in } D, \\
\mathbf{w}_0 &= \mathbf{0}_{\mathbb{R}^d} \quad \text{on } \partial D, \\
\int_D r_0 \, dx &= 0.
\end{aligned}$$

□

Finally, the first term on the right-hand side of Eq. (8.10.33) becomes

$$\begin{aligned}
&\mathcal{L}_{10\theta}(\theta, \mathbf{u}, p, \mathbf{w}_0, r_0)[\vartheta_2] \\
&= \int_D \left\{ \left(\psi''(\phi')^2 + \psi' \phi'' \right) \mathbf{u} \cdot \mathbf{u} \vartheta_1 + \psi' \phi' \mathbf{u} \cdot \mathbf{w}_0(\vartheta_1) \right\} \vartheta_2 \, dx.
\end{aligned}$$

Here, (\mathbf{u}, p) and $(\mathbf{w}_0(\vartheta_1), r_0(\vartheta_1))$ are assumed to be the weak solutions of Problems 8.10.2 and 8.10.4, respectively. If we denote $f_i(\theta, \mathbf{u}, p)$ here by $\tilde{f}_i(\theta)$, we have the relation:

$$\begin{aligned}
\mathcal{L}_{10\theta}(\theta, \mathbf{u}, p, \mathbf{w}_0(\vartheta_1), r_0)[\vartheta_2] &= \tilde{f}_0''(\theta)[\vartheta_1, \vartheta_2] \\
&= \langle g_{H0}(\theta, \vartheta_1), \vartheta_2 \rangle, \tag{8.10.35}
\end{aligned}$$

where the Hesse gradient g_{H0} of the mean flow resistance is given by

$$g_{H0}(\theta, \vartheta_1) = \left(\psi''(\phi')^2 + \psi' \phi'' \right) \mathbf{u} \cdot \mathbf{u} \vartheta_1 + \psi' \phi' \mathbf{u} \cdot \mathbf{w}_0(\vartheta_1). \tag{8.10.36}$$

If the same relation with Eq. (8.10.27) is satisfied in Problem 8.10.4,

$$\mathbf{w}_0(\vartheta_1) = -\frac{\psi' \phi'}{\psi} \mathbf{v}_0 \vartheta_1 \tag{8.10.37}$$

holds. Substituting Eq. (8.10.37) into Eq. (8.10.36), it can be confirmed that Eq. (8.10.35) accords with Eq. (8.10.30).

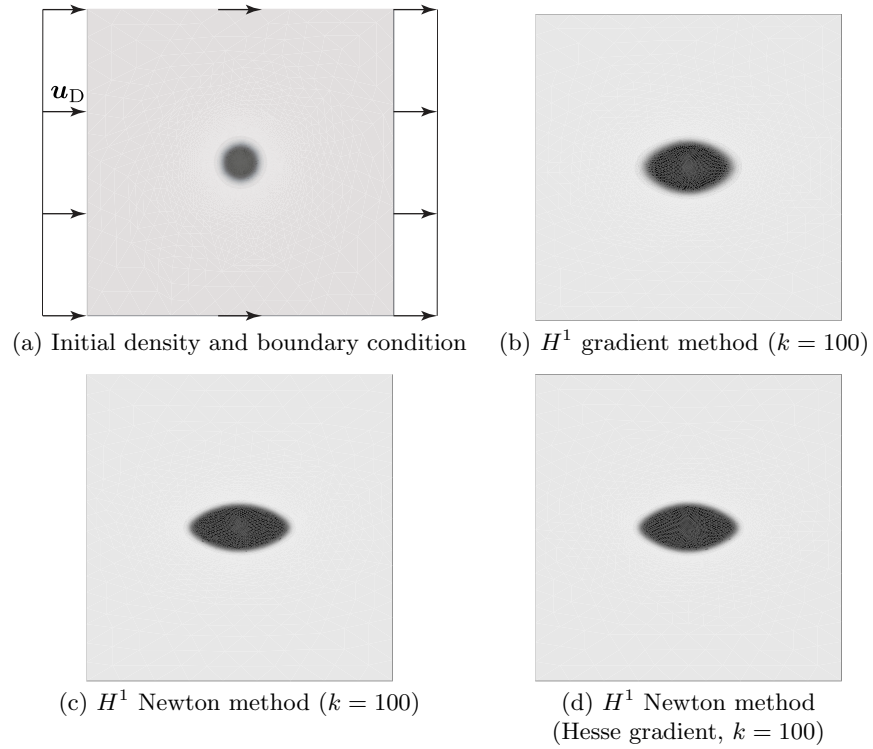


Fig. 8.20: Numerical example of mean flow resistance minimization: densities (black and white are inverted).

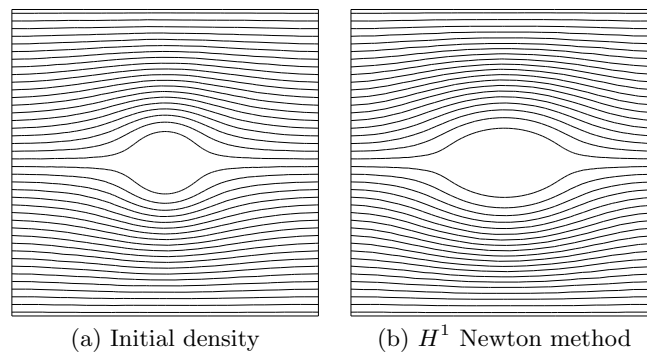


Fig. 8.21: Numerical example of mean flow resistance minimization problem: streamlines

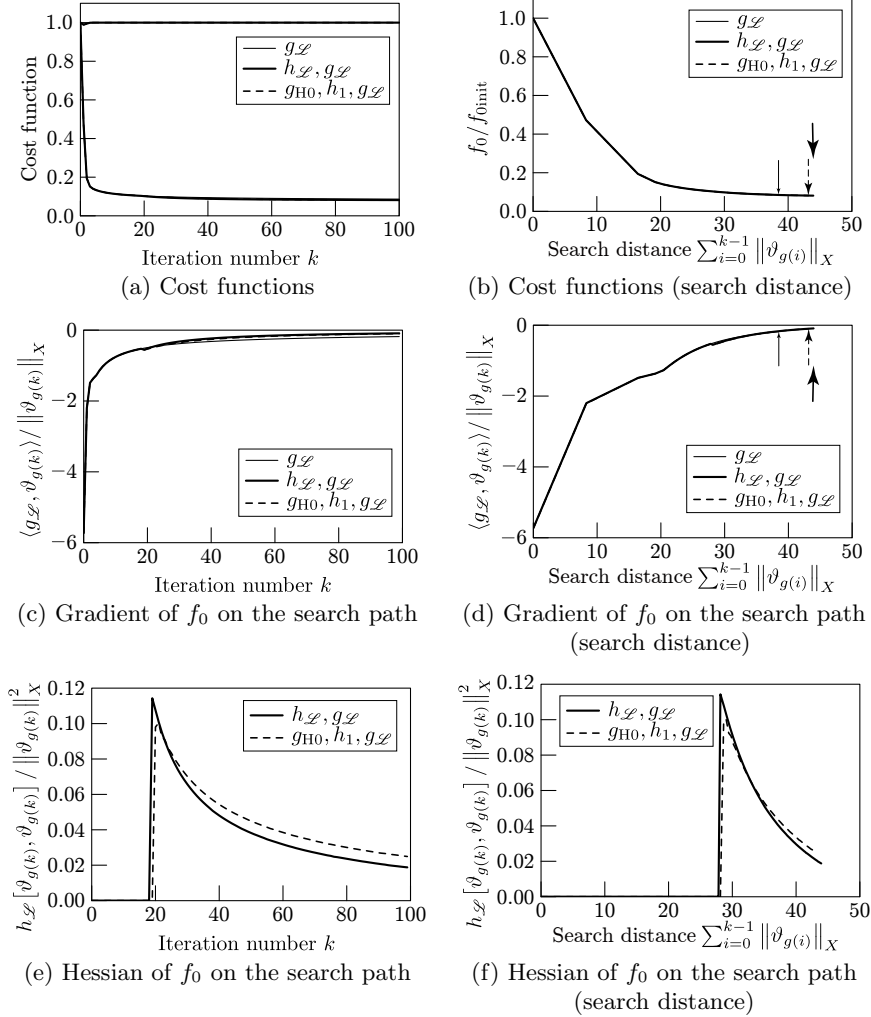


Fig. 8.22: Numerical example of mean flow resistance minimization: cost functions and gradients and Hessians of f_0 on the search path ($g_{\mathcal{L}}$: H^1 gradient method, $h_{\mathcal{L}}, g_{\mathcal{L}}$: H^1 Newton method, $g_{\text{H0}}, h_1, g_{\mathcal{L}}$: H^1 Newton method using Hesse gradient).

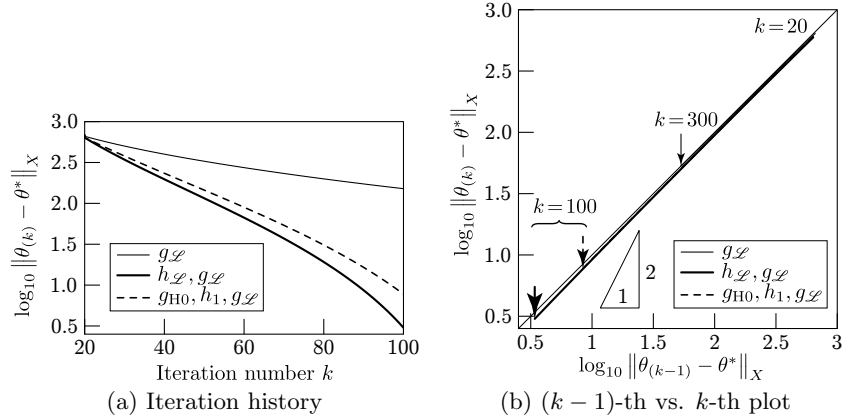


Fig. 8.23: Numerical example of mean flow resistance minimization problem: distance $\|\theta^{(k)} - \theta^*\|_X$ from an approximate minimum point θ^* ($g_{\mathcal{L}}$: the gradient method, $h_{\mathcal{L}}, g_{\mathcal{L}}$: the Newton method, $g_{H0}, h_1, g_{\mathcal{L}}$: the Newton method using the Hesse gradient).

8.10.6 Numerical Example

The results of mean flow resistance minimization for a two-dimensional Stokes flow field around an isolated object are shown in Figs. 8.20 to 8.23. The boundary condition of a state determination problem is assumed on the outer boundary with a uniform flow field in the horizontal direction as shown in Fig. 8.20 (a). With respect to the initial θ , a two-dimensional Gaussian distribution was assumed in order for it to be an element of the admissible set \mathcal{D} . Also in this example, a domain in which the density is constrained was not set. The programs were written using the programming language FreeFEM (<https://freefem.org/>) [16] using the finite element method. In the finite element analyses of the Stokes problem, triangular elements of the second order with respect to the velocity and of the first order with respect to the pressure were used. In the case using the H^1 Newton method, the routine of the H^1 Newton method was started at $k_N = 20$. For further details, we recommend the readers to also examine the exact codes in the programs.²

Figure 8.20 (b) to (d) show the densities obtained by the three methods (H^1 gradient method using $g_{\mathcal{L}} = g_0 + \lambda_1 g_1$, H^1 Newton method using $h_{\mathcal{L}} = h_0 + \lambda_1 h_1$ and $g_{\mathcal{L}}$, and the H^1 Newton method using $g_{H0}, h_1, g_{\mathcal{L}}$). In Fig. 8.21, the streamlines at the initial density and at the optimal density obtained from the H^1 Newton method are shown, respectively. The streamlines are defined as the contour lines of the flow function $\psi : \Omega(\phi) \rightarrow \mathbb{R}$ such that the flow speed \mathbf{u} is given by $(\partial\psi/\partial x_2, -\partial\psi/\partial x_1)^\top$.

The graphs in Fig. 8.22 illustrate the histories of the cost functions as well as the gradients and Hessians of the objective function f_0 on the search path

²See Electronic supplementary material.

with respect to the iteration number k and the search distance $\sum_{i=0}^{k-1} \|\vartheta_{g(i)}\|_X$ on X . In this figure, $f_{0\text{init}}$ denotes the value of f_0 at the initial density. Also, the value of c_1 is taken to be the domain integral of the initial density (volume). The gradient of f_0 on the search path was calculated using the Lagrange function $\mathcal{L} = \mathcal{L}_0 + \lambda_1 f_1$ as $\langle g_0 + \lambda_1 g_1, \vartheta_{g(k)} \rangle / \|\vartheta_{g(k)}\|_X$. On the other hand, the Hessian of f_0 on the search path was computed via $h_{\mathcal{L}}[\vartheta_{g(k)}, \vartheta_{g(k)}] / \|\vartheta_{g(k)}\|_X^2$. In the case of the Newton method using the Hesse gradient, the ratio $(\langle g_{H0}, \vartheta_{g(k)} \rangle + \lambda_1 h_1[\vartheta_{g(k)}, \psi]) / \|\vartheta_{g(k)}\|_X^2$ was used to calculate the Hessian. The norm $\|\vartheta_{g(i)}\|_X$ of the i -th search vector is defined by Eq. (8.9.35). The computational times until $k = 100$ by PC were 10.839, 14.763 and 17.046 sec by the H^1 gradient method, the H^1 Newton method and the H^1 Newton method using the Hesse gradient, respectively.

Looking at the graphs in Fig. 8.22 (c), it also seems that the convergence speed with respect to the iteration number k is faster when the H^1 Newton method is applied than when the H^1 gradient method is used. However, this increase in convergence speed might have been due to the fact that c_{D1} and c_{D0} in Eq. (8.6.7) are set with smaller values that had made the step sizes larger. Meanwhile, we noticed that the search paths for the three methods are the same as evident from the three coinciding graphs plotted in Fig. 8.22 (d). Moreover, from Fig. 8.22 (d) and (f), it can be observed that the point of convergence is a local minimum and that both the first derivative and the Hessian eventually diminish to zero. The reason behind these observed behaviors of the methods is the same as the ones given at the end of Sect. 8.9.6. Moreover, in the case of the Stokes flow field, although $h_0(\cdot, \cdot)$ itself is not coercive as shown in Sect. 8.10.4, it can be confirmed that the point of convergence is a minimum point, since the Hessian of f_0 on the search path is positive valued.

In addition, Fig. 8.23 (a) shows the graphs of the distance $\|\theta_{(k)} - \theta^*\|_X$ from an approximate minimum point θ^* obtained by the three methods with respect to the iteration number k . The approximate minimum point θ^* was substituted with the numerical solution of θ when the iteration time is taken larger than the given value in the H^1 Newton method. From this figure, it can be confirmed that the convergence orders for the results via the H^1 Newton methods are higher compared to that of the first order. However, from Fig. 8.23 (b), plotting the k -th distance $\|\theta_{(k)} - \theta^*\|_X$ with respect to the $(k-1)$ -th distance, the convergence order of the H^1 Newton method is less than the second order but is greater than the first order. The reason behind this result is considered the same as that stated at the end of Sect. 8.9.6.

8.11 Summary

In Chap. 8, the problem for seeking optimal hole positions with respect to a domain, in which a boundary value problem of partial differential equation is defined, is constructed as topology optimization problem of θ -type and its solution was looked at in detail. The key points are as below:

- (1) If the characteristic function of a domain is chosen as a design variable, it is known that regularity is insufficient and an optimization problem cannot be constructed (beginning of Chap. 8).
- (2) If a density is chosen as the design variable, a topology optimization problem can be constructed (beginning of Chap. 8). However, the set of functions whose range is limited to $[0, 1]$ does not become a linear space. Hence, by choosing a function $\theta \in X = H^1(D; \mathbb{R})$ whose range is not constrained as the design variable and providing the density as a sigmoid function of θ , a topology optimization problem of θ -type can be constructed based on the framework of the abstract optimal design problem shown in Chap. 7 (Sect. 8.1).
- (3) When a Poisson problem is chosen as a state determination problem (Sect. 8.2), a topology optimization problem of θ -type will be constructed as Problem 8.3.2 (Sect. 8.3).
- (4) The θ -derivatives of cost functions can be obtained by the Lagrange multiplier method (Sect. 8.5.1). However, such θ -derivatives are not necessarily going to be in X (Remark 8.5.3). Moreover, the second-order θ -derivatives of cost functions can be sought by substituting in the θ -derivative of the solution of a state determination problem into the second-order θ -derivative of the Lagrange function (Sect. 8.5.2).
- (5) The descent vectors of cost functions can be obtained using the θ -derivatives of cost functions by a gradient method (H^1 gradient method) on $X = H^1(D; \mathbb{R})$ (Sect. 8.6.1). The solution of the H^1 gradient method is included in the admissible set apart from the singular points (Theorem 8.6.5). Furthermore, if the second-order θ -derivatives of cost functions can be calculated, the descent vectors of the cost functions can be sought via the H^1 Newton method (Sect. 8.6.2).
- (6) The solution to the topology optimization problem of θ -type can be constructed using the same framework as the gradient method with respect to a constrained problem and the Newton method with respect to a constrained problem shown in Chap. 3 (Sect. 8.7.1 and Sect. 8.7.2).
- (7) When the numerical solutions of a state determination problem, adjoint problem, and H^1 gradient method are to be sought via the finite element method, and a first-order finite element is used to seek the search vector ϑ_g , the error of the finite element solution reduces linearly with respect to the maximum diameter of the finite element (Theorem 8.8.5).
- (8) When a linear elastic problem is taken to be a state determination problem, and a mean compliance and a function for domain measure are chosen as object and constraint cost functions, the θ -derivatives and second-order θ -derivatives of the cost functions can be obtained (Sect. 8.9.3).

- (9) If the Stokes problem is taken to be a state determination problem, and a mean flow resistance minimization problem under a domain measure constraint is considered, the θ -derivatives and second-order θ -derivatives of the cost functions can be obtained (Sect. 8.10.3).

8.12 Practice Problems

- 8.1** When a θ -type Poisson problem (Problem 8.2.3) is made into a state determination problem, what would be the cost function such that the self-adjoint relationship holds? Moreover, show its θ -derivative.
- 8.2** Change the extended Poisson problem defined in Chap. 5 (Problem 5.1.3) to θ -type, and formulate a topology optimization problem of θ -type using the extended Poisson problem as a state determination problem, the object cost function such that the self-adjoint relationship holds, and the constraint cost function with respect to the domain measure. Moreover, show the KKT conditions with respect to that problem.
- 8.3** When many cost functions are defined and the maximum values of them have to be minimized, the β method is known as a way to construct an optimal design problem [39]. If the topology optimization problem of θ -type is rewritten with the β method, we obtain the following:

Problem 8.12.1 (The β method) Let \mathcal{D} and \mathcal{S} be Eq. (8.1.4) and Eq. (8.2.2), respectively, and $f_1, \dots, f_m : X \times \mathcal{S} \rightarrow \mathbb{R}$ be given as Eq. (8.3.1). Moreover, let $\beta \in \mathbb{R}$. In this case, obtain θ which satisfies:

$$\min_{(\theta, u - u_D) \in \mathcal{D} \times \mathcal{S}} \{\beta \mid f_1(\theta, u) \leq \beta, \dots, f_m(\theta, u) \leq \beta, \text{ Problem 8.2.3}\}.$$

□

Show the KKT conditions with respect to this problem. Moreover, show the method to determine the Lagrange multipliers when solving this problem using the H^1 gradient method (Sect. 8.7.1) with respect to a constrained problem.

(Supplement) The reason that the β method is preferred is shown as follows. Even if there are many cost functions, the Lagrange multipliers with respect to cost functions for which inequality constraints are not active are zero. Hence, there are no reasons to seek their θ -derivatives.

- 8.4** In Practice 1.2, the gradient \mathbf{g}_0 of mean compliance f_0 with respect to variation of cross-sectional area was sought by using the gradient of maximization problem of the potential energy with respect to variation of \mathbf{a} and the minimum condition of the potential energy with respect to variation of \mathbf{u} . With respect to the mean compliance minimization

problem (Problem 8.9.3) of a $d \in \{2, 3\}$ -dimensional linear elastic body, think about the problem using

$$\begin{aligned} \pi(\theta, \mathbf{u}) = & \int_D \left(\frac{1}{2} \phi^\alpha(\theta) \mathbf{S}(\mathbf{u}) \cdot \mathbf{E}(\mathbf{u}) - \mathbf{b}(\theta) \cdot \mathbf{u} \right) dx \\ & - \int_{\Gamma_N} \mathbf{p}_N \cdot \mathbf{u} \, d\gamma - \int_{\Gamma_D} (\mathbf{u} - \mathbf{u}_D) \cdot (\phi^\alpha(\theta) \mathbf{S}(\mathbf{v}_0) \boldsymbol{\nu}) \, d\gamma \end{aligned}$$

as the potential energy and seeking (θ, \mathbf{u}) that satisfies

$$\max_{\theta \in \mathcal{D}} \min_{\mathbf{u} \in U} \pi(\theta, \mathbf{u}).$$

In this case, show that the θ gradient when using \mathbf{u} satisfying $\min_{\mathbf{u} \in U} \pi$ is the same as half of g_0 in Eq. (8.9.14).

- 8.5** In Practice 1.8, the gradient g_0 of mean flow resistance f_0 with respect to variation of cross-sectional area was obtained using the gradient of minimization problem of a formal potential energy for a dissipative system with respect to variation of \mathbf{a} and maximum condition of the formal potential energy with respect to variation of \mathbf{p} . With respect to the mean flow resistance minimization problem (Problem 8.10.3) of $d \in \{2, 3\}$ -dimensional Stokes flow field,

$$\begin{aligned} \pi(\theta, \mathbf{u}, p) = & \int_D \left\{ \frac{1}{2} \mu (\nabla \mathbf{u}^\top) \cdot (\nabla \mathbf{u}^\top) + \frac{1}{2} \psi(\phi(\theta)) \mathbf{u} \cdot \mathbf{u} - p \nabla \cdot \mathbf{u} \right. \\ & \left. - \mathbf{b} \cdot \mathbf{u} \right\} dx - \int_{\partial D} (\mathbf{u} - \mathbf{u}_D) \cdot (\mu \partial_\nu \mathbf{u} - p \boldsymbol{\nu}) \, d\gamma \end{aligned}$$

is used to seek (θ, \mathbf{u}, p) which satisfies

$$\min_{\theta \in \mathcal{D}} \min_{\mathbf{u} \in U} \max_{p \in P} \pi(\theta, \mathbf{u}, p).$$

In this case, show that the θ gradient of π when using (\mathbf{u}, p) satisfying $\min_{\mathbf{u} \in U} \max_{p \in P} \pi$ is the same as half of g_0 in Eq. (8.10.17).

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