Contents

Chapter 2

Basics of Optimization Theory

Chapter 1 investigated explicit optimal design problems and illustrated different approaches for obtaining optimality conditions. Terminology and results utilized in optimization theory were also used. This chapter presents a systematic discussion of optimization theory.

The stage of this chapter is a finite-dimensional vector space. In other words, the linear spaces of the design and state variables are assumed to be of finite dimension. Later in this book, optimization problems will be constructed on function spaces and methods for their solution will be considered. However, many of the concepts and results of this chapter can also be used in the function space setting. In this sense, the content of this chapter can be seen as forming the foundation of this book. In other words, the extent of the reliability of this book is dependent on the content of this chapter. For this reason, although the details become somewhat abstracted, concepts will be summarized in the format of definitions and theorems. Here, in order to tie the abstract notions together with concrete ideas, our discussions will be interlaced with examples related to the simple spring systems that the reader is already familiar with.

2.1 Definition of Optimization Problems

Considering the problems presented in Chap. 1, let us first define the optimization problems that will be the target of this chapter's discussions. In Problem 1.2.2, the cross-section was set as $\boldsymbol{a} \in X = \mathbb{R}^n$ and the displacement was $\boldsymbol{u} \in U = \mathbb{R}^n$. These were referred to as the design and state variables, respectively, where X and U represented their linear spaces. Let us now define several optimization problems which include this one.

With respect to the linear spaces, we will refrain from using their symbols in ways which are not observed in other chapters. In Chap. 1, X and U represented linear spaces containing the design and state variables. In Chap. 2, design and state variables are collectively referred to as design variables, and X represents the linear space of the design variables. That is to say, with respect to the variables of Chap. 1, we define $\boldsymbol{x} = \left(\boldsymbol{a}^\top, \boldsymbol{u}^\top\right)^\top \in X$. The definitions must be changed in this manner because design and state variables are not distinguished from each other in standard optimization problems (all variables are treated as design variables).

Next, let us define an optimization problem while considering its relationship with a problem from Chap. 1. In Problem 1.2.2, setting $\boldsymbol{x} = \left(\boldsymbol{a}^\top, \boldsymbol{u}^\top\right)^\top \in \mathbb{R}^{2n}$ where $n \in \mathbb{N}$, we had the equality constraint $\boldsymbol{h}(\boldsymbol{x}) = \boldsymbol{K}(\boldsymbol{a})\,\boldsymbol{u} - \boldsymbol{p} = \boldsymbol{0}_{\mathbb{R}^n}$. If $2n$ is replaced with $d \in \mathbb{N}$, an optimization problem of the following type is obtained.

Problem 2.1.1 (Optimization problem) Let $X = \mathbb{R}^d$ and assume that $f_0, f_1, \cdots, f_m : X \to \mathbb{R}$ are given. Also assume that $\boldsymbol{h} = (h_1, \ldots, h_n)^\top : X \to \mathbb{R}^n$ with respect to $n < d$ is given. Find $\boldsymbol{x}$ satisfying

$$\min_{\boldsymbol{x} \in X} \left\{ f_0(\boldsymbol{x}) \mid f_1(\boldsymbol{x}) \le 0, \ldots, f_m(\boldsymbol{x}) \le 0,\ \boldsymbol{h}(\boldsymbol{x}) = \boldsymbol{0}_{\mathbb{R}^n} \right\}.$$

□

Moreover, an optimization problem without equality constraint can be obtained from Problem 1.2.2 by regarding $\boldsymbol{a} \in X = \mathbb{R}^n$ as the design variable, and $\tilde{f}_i(\boldsymbol{a}) = f_i(\boldsymbol{a}, \boldsymbol{u}(\boldsymbol{a}))$. If $\boldsymbol{a} \in X = \mathbb{R}^n$ is rewritten as $\boldsymbol{x} \in X = \mathbb{R}^d$, and $\tilde{f}_i(\boldsymbol{a})$ is replaced by $f_i(\boldsymbol{x})$, then Problem 1.2.2 becomes an optimization problem as follows:

Problem 2.1.2 (Optimization problem) Let $X = \mathbb{R}^d$ and suppose that $f_0, f_1, \cdots, f_m : X \to \mathbb{R}$ are given. Find $\boldsymbol{x}$ satisfying

$$\min_{\boldsymbol{x} \in X} \left\{ f_0(\boldsymbol{x}) \mid f_1(\boldsymbol{x}) \le 0, \ldots, f_m(\boldsymbol{x}) \le 0 \right\}.$$

□

Furthermore, let the set of admissible design variables (also referred to as the feasible set) be

$$S = \left\{ \boldsymbol{x} \in X \mid f_1(\boldsymbol{x}) \le 0,\ \cdots,\ f_m(\boldsymbol{x}) \le 0 \right\}. \tag{2.1.1}$$

In this case, Problem 2.1.2 is equivalent to the following problem.

Problem 2.1.3 (Optimization problem) Let $X = \mathbb{R}^d$ and suppose that $f_0, f_1, \cdots, f_m : X \to \mathbb{R}$ are given. Let S be given by Eq. (2.1.1). Find $\boldsymbol{x}$ satisfying

$$\min_{\boldsymbol{x} \in S} f_0(\boldsymbol{x}).$$

□

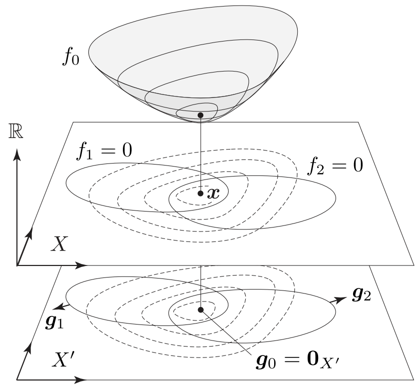


Fig. 2.1: The minimum when all constraints are inactive.

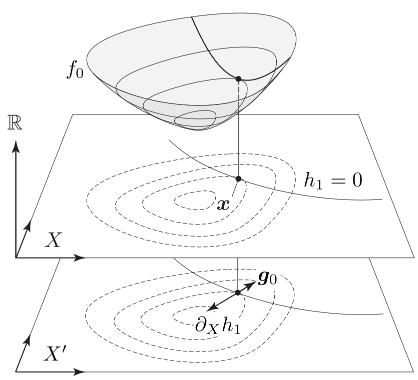


Fig. 2.2: The minimum when an equality constraint is active.

In this chapter, let us look at conditions that are satisfied by minimizers of Problems 2.1.1, 2.1.2, and 2.1.3. Before beginning this topic, we would like to draw attention to a few definitions that will be used from here on. In this chapter, f_0 is called the objective function, $\boldsymbol{h}$ is called an equality constraint function, and $f_1, \cdots$ and f_m denote inequality constraint functions. Two points are worth noting here.

The first is a cautionary remark regarding the direction of the inequality in the inequality constraint and its relationship to the optimization of the objective function. In particular, the maximization of f_0 is equivalent to the minimization of $-f_0$, and so we can so f_0 can be limited to minimization. Moreover, without loss of generality, $f_1, \ldots, f_m$ can be restricted to be non-positive.

The second remark regards the fact that for each $i \in \{1, \ldots, n\}$ the equality constraint $h_i = 0$ is equivalent to imposing two simultaneous inequality constraints: $h_i \leq 0$ and $-h_i \leq 0$. Here, by replacing $h_i = 0$ in Problem 2.1.1 with $h_i \leq 0$ and $-h_i \leq 0$, Problem 2.1.1 can be reformulated as Problem 2.1.2. However in this chapter, we will take a detailed look at the relationship formed

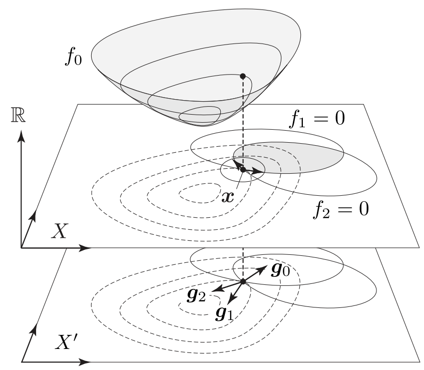


Fig. 2.3: The minimum when an inequality constraint is active.

at the minimum of Problem 2.1.1 when the equality constraints are specified separately. The reason for this is as follows. In an optimal design problem, state equations always appear as equality constraints. Later on, these will become partial differential equations of boundary value type. In this case, the method for treating equality constraints shown in this chapter (the Lagrange multiplier or adjoint variable method) will be the guiding principle when considering equality constraints in the function space setting. Details related to this will be shown in Chap. 7.

Let us illustrate the optimization problems considered in this chapter in figures. Examples of minimizers in optimization problems when $X = \mathbb{R}^2$ are shown in Figs. 2.1–2.3. Here, $\boldsymbol{g}_0$, $\boldsymbol{g}_1$, $\boldsymbol{g}_2$ and $\partial_X h_1$ denote the gradient (Definition 2.4.1) with respect to an arbitrary variation of f_0, f_1, f_2, and h_1 at $\boldsymbol{x} \in X$. The space to which these gradients belong is referred to as the dual space of X and is denoted by X' (Definition 4.4.5). However, since $X' = X$ in a finite-dimensional vector space, we can assume that $X' = \mathbb{R}^2$. When this figure is used in Chap. 7, X' is treated as a different vector space than X. Later on, whenever defining optimization problems, the variables and functions which appear should be referenced to these figures in order to understand the situation.

2.2 Classification of Optimization Problems

Next, in order to present a method for classifying optimization problems, let us focus on the properties of the functions used in Problems 2.1.1–2.1.3.

If $f_0, \ldots, f_m$ and $h_1, \ldots, h_n$ are all linear functions in Problem 2.1.1, or when $f_0, \ldots, f_m$ are all linear functions in Problems 2.1.2 and 2.1.3, then these problems are referred to as linear optimization problems or linear programming problems. Figure 2.4 shows the setting of a linear optimization problem when $X = \mathbb{R}^2$. Regarding the solution of linear optimization problems, methods such as the simplex method, which uses properties of linear functions, and

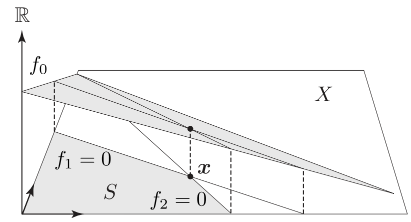


Fig. 2.4: The minimum point in a linear optimization problem.

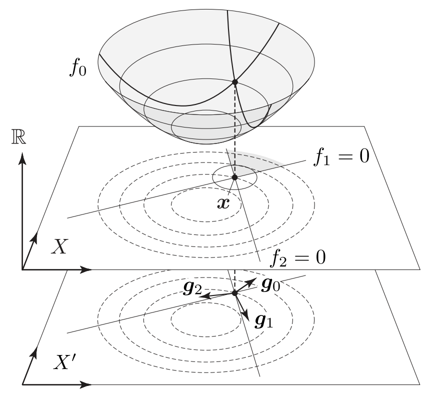


Fig. 2.5: Minimum point in a quadratic optimization problem.

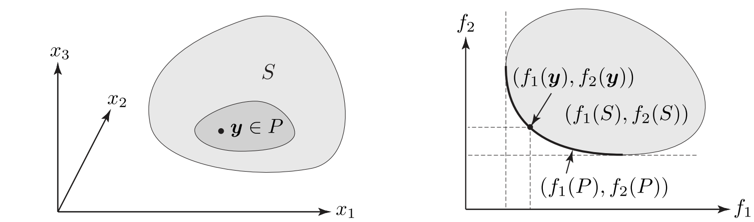
the dual interior point method are well known. There are even cases when non-linear optimization problems can be solved after being changed into a linear optimization problem via successive linear approximation. However, the details will be omitted in this book since they will not be directly used.

On the other hand, in Problem 2.1.1, if some function within $f_0, \dots, f_m$ or $h_1, \dots, h_n$ is not linear, or if some function from $f_0, \dots, f_m$ in Problem 2.1.2 or Problem 2.1.3 is not a linear, then these problems are referred to as non-linear optimization problems or as non-linear programming problems.

Moreover, when f_0 is a quadratic function and each of $h_1, \dots, h_n$ and $f_1, \dots, f_m$ are linear functions, or when f_0 in Problem 2.1.2 and Problem 2.1.3 is a quadratic function, and $f_1, \dots, f_m$ are all linear functions, these problems are called quadratic optimization problems or quadratic programming problems. Figure 2.5 demonstrates a quadratic optimization problem when $X = X' = \mathbb{R}^2$.

Furthermore, when $f_0, \dots, f_m$ are convex functions (Definition 2.4.3) and $h_1, \cdots, h_n$ are linear in Problem 2.1.1, or $f_0, \dots, f_m$ are convex functions in Problem 2.1.2 or Problem 2.1.3, these problems are called convex optimization problems or convex programming problems.

Here we would like to consider a problem which can be a source of some confusion. As can be understood from Section 1.1.7, Problem 1.1.4 is a convex optimization problem. This is because when Problem 1.1.4 is rewritten in the



(a) Linear space of design variables (b) Linear space of cost functions

Fig. 2.6: A set of Pareto solutions, P.

form of Problem 2.1.2, the Hesse matrix $\boldsymbol{H}_0$ of $\tilde{f}_0$ is positive definite (Theorem 2.4.6) and f_1 is a linear function with respect to the design variable (Theorem 2.4.4). However, Problem 1.1.4 does not look like a convex optimization problem when it is rewritten in the form of Problem 2.1.1.

This is because when we set $\boldsymbol{x} = \left(\boldsymbol{a}^\top, \boldsymbol{u}^\top\right)^\top$ and $\boldsymbol{h}(\boldsymbol{x}) = \boldsymbol{K}(\boldsymbol{a})\,\boldsymbol{u} - \boldsymbol{p} = \boldsymbol{0}_{\mathbb{R}^n}$ in Problem 2.1.1, $\boldsymbol{h}(\boldsymbol{x})$ is not a linear function of $\boldsymbol{x}$. Therefore it doesn't look like a convex optimization problem. As just described, optimization problems are still convex when they are obtained by rewriting a problem which includes equality constraints into a form without the equality constraints.

Also, although the problem formulation is different from Problems 2.1.1–2.1.3, optimization problems equipped with multiple objective functions are called multi-objective optimization problems. For example, if S denotes a subset of $X = \mathbb{R}^d$ and $f_1, \ldots, f_m : X \to \mathbb{R}$ are cost functions, then the problem becomes one in which we seek $\boldsymbol{x}$ to satisfy

$$\min_{\boldsymbol{x}\in S} f_1(\boldsymbol{x}), \ \cdots, \ \min_{\boldsymbol{x}\in S} f_m(\boldsymbol{x}).$$

We remark that minimizers need not exist for problems of this type and that, when the minimizer does not exist, the next best choice to use is the set of so-called Pareto solutions. Pareto solutions are defined as a set $P \subset S$ that satisfies the following conditions (see Fig. 2.6). Given an element $\boldsymbol{y}$ of P, there does not exist an $\boldsymbol{x} \in S$ such that the following holds for all $i \in \{1, \ldots, m\}$:

$$f_i(\boldsymbol{x}) \le f_i(\boldsymbol{y}).$$

Moreover, for each fixed $i \in \{1, \ldots, m\}$ there does not an exist $\boldsymbol{x} \in S$ satisfying

$$f_i(\boldsymbol{x}) < f_i(\boldsymbol{y})$$

for all $\boldsymbol{y} \in P$. In order to select a point from a set of Pareto solutions, a selection criterion based on a concrete value system is needed. Nevertheless, discussions surrounding such selection criteria will be avoided and multi-purpose optimization problems will not be considered in this book.

Furthermore, when the set of admissible design variables S is a set of discrete points (such as the integers) in Problem 2.1.3, this type of problem is referred to as a discrete optimization problem or a discrete programming problem. These

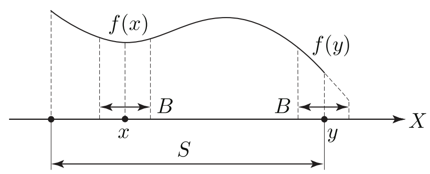


Fig. 2.7: A local minimizer x and the global minimizer y of function f.

problems display a property that is referred to as NP-hard, and exact solutions cannot be easily found. Moreover, special schemes are needed in order to obtain approximate solutions. These problems will also not be examined in this book.

2.3 Existence of a Minimum Point

Having defined optimization problems, let us now consider conditions under which minimizers exist in our problems. Although the following may seem obvious, failure to acknowledge such observations may lead to defining optimization problems for which no minimum is obtained.

Let us first note the difference between a local minimum point and a minimum point.

Definition 2.3.1 (Local and global minimizers) Let $X = \mathbb{R}^d$ and assume that S is non-empty subset of X. Also let $f : S \to \mathbb{R}$. When a neighborhood (a convex open set) B of $\boldsymbol{x} \in S$ exists and the following holds with respect to an arbitrary $\boldsymbol{y} \in B$:

$$f(\boldsymbol{x}) \leq f(\boldsymbol{y}),$$

then we say that $f(\boldsymbol{x})$ obtains a local minimum value at $\boldsymbol{x}$, and that $\boldsymbol{x}$ is a local minimizer. When the above inequality holds with respect to an arbitrary $\boldsymbol{y} \in S$, then we say that $f(\boldsymbol{x})$ obtains its minimum value at $\boldsymbol{x}$, and that $\boldsymbol{x}$ is the global minimizer. □

Figure 2.7 shows a local minimum x and the global minimum y of a function f when $X = \mathbb{R}$ and $S \subset X$ is a bounded closed set. Definitions of terminology such as neighborhood and open set can be found in Section A.1.1. When defining global minimizers as in Definition 2.3.1, the well-known Weierstrass's theorem gives sufficient conditions for their existence (cf. [10, Theorem 13, p. 27], [1, Section 22.6, p. 154], or [9, Theorem 4.16, p. 89]).

Theorem 2.3.2 (Weierstrass's Theorem) Let S be a bounded closed subset of $X = \mathbb{R}^d$, and $f_0 : S \to \mathbb{R}$ be a continuous function in Problem 2.1.3. Then there exists a global minimizer of f_0 in S. □

Note that continuous functions are defined in Section A.1.2, and that Theorem 2.3.2 still holds when continuity is replaced by lower semi-continuity

(Section A.1.2). However, given that lower semi-continuity will not be required in our future developments, this extension is omitted.

Let us take a look at cases where global minimizers fail to exist when S is not a bounded closed set in Problem 2.1.3. In Problem 1.1.4, the following assumption was made:

$$S = \left\{ \boldsymbol{a} \in X = \mathbb{R}^2 \;\middle|\; \boldsymbol{a} \geq \boldsymbol{a}_0,\ f_1(\boldsymbol{a}) = l(a_1 + a_2) - c_1 \leq 0 \right\}.$$

This set is bounded and closed. However, if this is replaced by

$$S = \left\{ \boldsymbol{a} \in X = \mathbb{R}^2 \;\middle|\; \boldsymbol{a} > \boldsymbol{0}_{\mathbb{R}^2},\ f_1(\boldsymbol{a}) = l(a_1 + a_2) - c_1 \leq 0 \right\}$$

then it is no longer a bounded closed set. For example, when $p_1 \neq 0$ and $p_2 = 0$, it follows that $a_1 = c_1/2l$ and $a_2 = 0$ express the minimum of f_0. However, $\boldsymbol{a}$ is not included in S hence there are no minimizers within S.

Moreover, when the underlying function is discontinuous, or doesn't uniquely determine its values, there is no guarantee that a minimum value will exist. None of the functions looked at so far has these qualities. However, if care is not taken, functional optimization problems may well result in having to deal with functions whose values are not uniquely defined. In Chap. 4, the linear space in which the design variables are defined is continuous (complete), and conditions under which the cost function are continuous will be considered.

2.4 Differentiation and Convex Functions

Before addressing the optimization problem, let us look at the basic methods of differentiation used in optimization theory, including the definition of a convex functions. We will use the following definition for the derivative of a function f.

Definition 2.4.1 (Gradient and Hesse matrix) Let $X = \mathbb{R}^d$ and suppose a function $f : B \to \mathbb{R}$ is defined in the neighborhood $B \subset X$ of $\boldsymbol{x} \in X$. When $\boldsymbol{y} = (y_1, \ldots, y_d)^\top \in X$ is arbitrary and

$$\begin{aligned}
\partial_X f(\boldsymbol{x}) &= \begin{pmatrix} \lim_{y_1 \to 0} \left(f\left(\boldsymbol{x} + (y_1, 0, \ldots, 0)^\top\right) - f(\boldsymbol{x}) \right) / y_1 \\ \vdots \\ \lim_{y_d \to 0} \left(f\left(\boldsymbol{x} + (0, \ldots, y_d)^\top\right) - f(\boldsymbol{x}) \right) / y_d \end{pmatrix} \\
&= \begin{pmatrix} \partial f / \partial x_1 \\ \vdots \\ \partial f / \partial x_d \end{pmatrix} (\boldsymbol{x}) = \boldsymbol{g}(\boldsymbol{x})
\end{aligned}$$

is an element of $X' = \mathbb{R}^d$, then f is said to be differentiable at $\boldsymbol{x}$, and

$$f'(\boldsymbol{x})[\boldsymbol{y}] = \boldsymbol{g}(\boldsymbol{x}) \cdot \boldsymbol{y}$$

is called the derivative, or the total derivative, of f at $\boldsymbol{x}$ and $\boldsymbol{g}(\boldsymbol{x})$ is the gradient of f at $\boldsymbol{x}$. Likewise, when we can resolve

$$\partial_X \partial_X^\top f(\boldsymbol{x}) = \begin{pmatrix} \partial^2 f/(\partial x_1 \partial x_1) & \dots & \partial^2 f/(\partial x_1 \partial x_d) \\ \vdots & \ddots & \vdots \\ \partial^2 f/(\partial x_d \partial x_1) & \dots & \partial^2 f/(\partial x_d \partial x_d) \end{pmatrix} (\boldsymbol{x}) = \boldsymbol{H}(\boldsymbol{x})$$

as an element of $\mathbb{R}^{d\times d}$, then f is said to be second-order differentiable at $\boldsymbol{x}$. Moreover,

$$f''(\boldsymbol{x})[\boldsymbol{y}_1, \boldsymbol{y}_2] = \boldsymbol{y}_2 \cdot (\boldsymbol{H}(\boldsymbol{x})\, \boldsymbol{y}_1)$$

is referred to as the second-order derivative of f at $\boldsymbol{x}$ with respect to arbitrary variations $\boldsymbol{y}_1, \boldsymbol{y}_2 \in X$ from $\boldsymbol{x}$, and $\boldsymbol{H}(\boldsymbol{x})$ is referred to as the Hesse matrix. □

In this book, the set of functions $f : X \to \mathbb{R}$ whose first $k \in \{0, 1, 2, \cdots\}$ derivatives are continuous over X will be denoted by $C^k(X; \mathbb{R})$ (Definition 4.2.2). Moreover, for simplicity of notation, $\partial_X f$, $\partial_X f_0$, ... , $\partial_X f_m$ will be denoted by $\boldsymbol{g}$, $\boldsymbol{g}_0$, ... , $\boldsymbol{g}_m$ respectively, and $\partial_X \partial_X^\top f$, $\partial_X \partial_X^\top f_0$, ... , $\partial_X \partial_X^\top f_m$ will be denoted by $\boldsymbol{H}$, $\boldsymbol{H}_0$, ... , $\boldsymbol{H}_m$ respectively. Also, when $\boldsymbol{x}$ is an element of X, we note that $\partial_X f$ will also be written as $f_{\boldsymbol{x}}$. When considering partial differential equations, etc., we remark that $\partial_X f$ will be expressed by $\boldsymbol{\nabla} f$. Various types of derivatives will be defined going forward, so methods for their expression will be needed. Definitions will be given in each situation to avoid confusion.

2.4.1 Taylor's Theorem

Used in all kinds of situations hereafter, Taylor's theorem is shown below.

Theorem 2.4.2 (Taylor's theorem) Let $X = \mathbb{R}^d$. Suppose that a function $f \in C^2(B; \mathbb{R})$ is defined in a neighborhood B of $\boldsymbol{a} \in X$. If $\boldsymbol{y} = \boldsymbol{b} - \boldsymbol{a}$ with respect to an arbitrary $\boldsymbol{b} \in B$, then there exists $\theta \in (0, 1)$ satisfying

$$f(\boldsymbol{b}) = f(\boldsymbol{a}) + \boldsymbol{g}(\boldsymbol{a}) \cdot \boldsymbol{y} + \frac{1}{2!} \boldsymbol{y} \cdot (\boldsymbol{H}(\boldsymbol{a} + \theta \boldsymbol{y})\, \boldsymbol{y}). \tag{2.4.1}$$

□

Proof First assume that $X = \mathbb{R}$. Let $\boldsymbol{a}$, $\boldsymbol{b}$ and $\boldsymbol{y}$ in this case be denoted by a, b and y respectively. Given $x \in B$, let

$$h(x) = f(b) - \left\{ f(x) + f'(x)(b - x) + k(b - x)^2 \right\},$$

where we have written $\mathrm{d}f/\mathrm{d}x$ as f'. Moreover, the constant k is determined such that

$$h(a) = h(b) = 0.$$

We obtain

$$h'(x) = -f'(x) - f''(x)(b - x) + f'(x) + 2k(b - x)$$

$$= -f''(x)(b-x) + 2k(b-x).$$

By Rolle's theorem (the mean value theorem when $h(a) = h(b)$), there exists c in (a, b) satisfying

$$h'(c) = 0.$$

Hence, we can write $c = a + \theta y$ and obtain

$$k = \frac{1}{2} f''(a + \theta y).$$

Substituting this result into $h(a) = 0$ yields the result of the theorem.

Next let $X = \mathbb{R}^2$. Consider the following function of $t \in \mathbb{R}$ with respect to an arbitrary $\boldsymbol{a} = (a_1, a_2)^\top$ and $\boldsymbol{y} = (y_1, y_2)^\top$:

$$\begin{aligned}\phi(t) &= f(\boldsymbol{a} + t\boldsymbol{y}) \\ &= f(\boldsymbol{a}) + t\left(y_1 \frac{\partial}{\partial x_1} + y_2 \frac{\partial}{\partial x_2}\right) f(\boldsymbol{a}) + \frac{t^2}{2}\left(y_1 \frac{\partial}{\partial x_1} + y_2 \frac{\partial}{\partial x_2}\right)^2 f(\boldsymbol{a} + \theta \boldsymbol{y}).\end{aligned}$$

By Taylor expanding $\phi(t)$ around $t = 0$ (as a function of one variable, $X = \mathbb{R}$) the value of $\phi(1)$ can be written as

$$\begin{aligned}\phi(1) &= f(\boldsymbol{b}) \\ &= f(\boldsymbol{a}) + \left(y_1 \frac{\partial}{\partial x_1} + y_2 \frac{\partial}{\partial x_2}\right) f(\boldsymbol{a}) \\ &\quad + \frac{1}{2}\left(y_1 \frac{\partial}{\partial x_1} + y_2 \frac{\partial}{\partial x_2}\right)^2 f(\boldsymbol{a} + \theta \boldsymbol{y}) \\ &= f(\boldsymbol{a}) + \left\{\begin{pmatrix} \dfrac{\partial}{\partial x_1} & \dfrac{\partial}{\partial x_2} \end{pmatrix} f(\boldsymbol{a})\right\} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} \\ &\quad + \frac{1}{2}\begin{pmatrix} y_1 & y_2 \end{pmatrix} \left\{\begin{pmatrix} \dfrac{\partial}{\partial x_1} \\ \dfrac{\partial}{\partial x_2} \end{pmatrix} \begin{pmatrix} \dfrac{\partial}{\partial x_1} & \dfrac{\partial}{\partial x_2} \end{pmatrix} f(\boldsymbol{a} + \theta \boldsymbol{y})\right\} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}.\end{aligned}$$

When $X = \mathbb{R}^d$, the above equation becomes Eq. (2.4.1). □

Taylor's theorem can also be expressed with respect to arbitrary derivative orders. However, our expression stops at the second-order derivative of the function because the notation for higher-order differentials defined in $\mathbb{R}^d$ have not been defined. This notation will be presented in Definition 4.2.2. Moreover, we also refer to terms such as $\boldsymbol{y} \cdot (\boldsymbol{H}(\boldsymbol{a} + \theta \boldsymbol{y})\boldsymbol{y})/2!$ containing θ as remainder terms. Also, we will make use of the Bachmann–Landau small-o symbol in this book. This allows us to write Eq. (2.4.1) also as

$$f(\boldsymbol{a} + \boldsymbol{y}) = f(\boldsymbol{a}) + \boldsymbol{g}(\boldsymbol{a}) \cdot \boldsymbol{y} + \frac{1}{2!}\boldsymbol{y} \cdot (\boldsymbol{H}(\boldsymbol{a})\boldsymbol{y}) + o\left(\|\boldsymbol{y}\|_{\mathbb{R}^d}^2\right), \tag{2.4.2}$$

where $o(\epsilon)$ is defined to be a function such that $\lim_{\epsilon \to 0} o(\epsilon)/\epsilon = 0$. This equation is referred to as a Taylor expansion of f around $\boldsymbol{a}$.

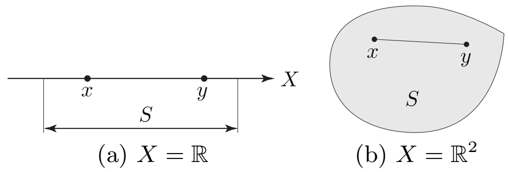


Fig. 2.8: S as a convex subset of the linear space X.

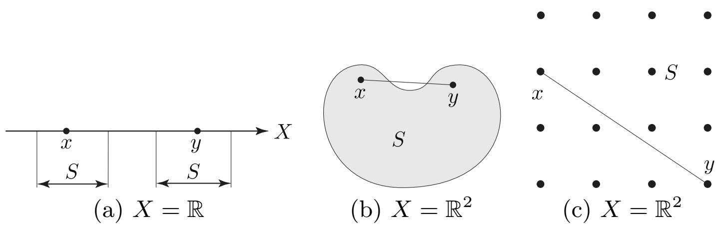


Fig. 2.9: S as a non-convex subset of the linear space X.

2.4.2 Convex Functions

Next let us take a look at a few basic definitions and results regarding convex functions. As we will show in Theorem 2.5.6, local and global minimizers coincide in the case of convex optimization problems. For this reason, convexity of functions is an important and useful property in optimization theory. The definition of a convex function is as follows.

Definition 2.4.3 (Convex functions) Let $X = \mathbb{R}^d$ and S be a non-empty subset of X. A function $f : S \to \mathbb{R}$ is said to be convex if the following holds for arbitrary $\boldsymbol{x}, \boldsymbol{y} \in S$ and $\theta \in (0, 1)$:

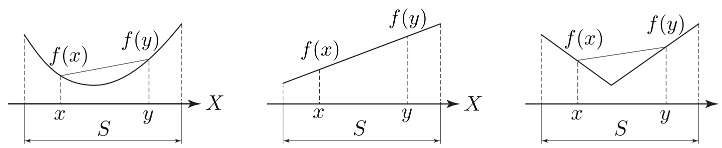
$$(1 - \theta)\, \boldsymbol{x} + \theta \boldsymbol{y} \in S, \tag{2.4.3}$$

$$f\left((1 - \theta)\, \boldsymbol{x} + \theta \boldsymbol{y}\right) \leq (1 - \theta)\, f(\boldsymbol{x}) + \theta f(\boldsymbol{y}). \tag{2.4.4}$$

When the direction of the inequality is reversed, f is called a concave function. □

Equations (2.4.3) and (2.4.4) are conditions which signify the convexity of a set and the convexity of a function, respectively. Figures 2.8 and 2.9 illustrate the case of convex and non-convex S. Moreover, if S is a set of integer-valued vectors (such as in Fig. 2.9 (c)), the optimization problem becomes a discrete programming problem. A difficulty regarding these problems can be thought to lie in the fact that, when the admissible set consists of such vectors, points at which the gradient of the cost function are $\mathbf{0}_X$ need not be included in the admissible set. Figure 2.10 shows an example when f is a convex function. We also note that, even if the derivative is non-continuous, convexity can still hold.

If a convex function is first-order differentiable, the following results can be obtained.



(a) $f \in C^1(S;\mathbb{R})$ (b) f : linear function (c) $f \in C^0(S;\mathbb{R})$

Fig. 2.10: Examples of convex functions ($X = \mathbb{R}$).

Theorem 2.4.4 (Convexity and first-order differentiation) Suppose $f \in C^1(S;\mathbb{R})$ and let $S \subseteq X$ be an open convex set of $X = \mathbb{R}^d$. A necessary and sufficient condition for f to be a convex function is for the following inequality to hold for arbitrary $\boldsymbol{x}, \boldsymbol{y} \in S$:

$$\boldsymbol{g}(\boldsymbol{x}) \cdot (\boldsymbol{y} - \boldsymbol{x}) \leq f(\boldsymbol{y}) - f(\boldsymbol{x}). \tag{2.4.5}$$

□

Proof We will first show the necessity (that Eq. (2.4.5) holds when f is a convex function). Since f is a convex function, one has

$$f((1-\theta)\boldsymbol{x} + \theta\boldsymbol{y}) = f(\boldsymbol{x} + \theta(\boldsymbol{y} - \boldsymbol{x})) \leq f(\boldsymbol{x}) + \theta(f(\boldsymbol{y}) - f(\boldsymbol{x})),$$

where $\boldsymbol{x}, \boldsymbol{y} \in S$ and $\theta \in (0,1)$ are arbitrary. Hence, it follows that

$$\frac{f(\boldsymbol{x} + \theta(\boldsymbol{y} - \boldsymbol{x})) - f(\boldsymbol{x})}{\theta} \leq f(\boldsymbol{y}) - f(\boldsymbol{x}). \tag{2.4.6}$$

When $\theta \to 0$, we obtain Eq. (2.4.5).

Next we will show the sufficiency (that is, if Eq. (2.4.5) holds, then f is a convex function). If we let $\boldsymbol{x} = (1-\theta)\boldsymbol{z} + \theta\boldsymbol{w}$ and $\boldsymbol{y} = \boldsymbol{z}$, then Eq. (2.4.5) becomes

$$f(\boldsymbol{z}) - f(\boldsymbol{x}) \geq \boldsymbol{g}(\boldsymbol{x}) \cdot (\boldsymbol{z} - \boldsymbol{x}). \tag{2.4.7}$$

Similarly, if $\boldsymbol{x} = (1-\theta)\boldsymbol{z} + \theta\boldsymbol{w}$ and $\boldsymbol{y} = \boldsymbol{w}$, Eq. (2.4.5) becomes

$$f(\boldsymbol{w}) - f(\boldsymbol{x}) \geq \boldsymbol{g}(\boldsymbol{x}) \cdot (\boldsymbol{w} - \boldsymbol{x}). \tag{2.4.8}$$

Multiplying Eq. (2.4.7) by $(1-\theta)$, and Eq. (2.4.8) by θ and taking their sum yields:

$$(1-\theta) f(\boldsymbol{z}) + \theta f(\boldsymbol{w}) - f(\boldsymbol{x}) \geq \boldsymbol{g}(\boldsymbol{x}) \cdot \{(1-\theta)\boldsymbol{z} + \theta\boldsymbol{w} - \boldsymbol{x}\} = 0.$$

In other words, since S is a convex set, we obtain the convexity of f:

$$(1-\theta) f(\boldsymbol{z}) + \theta f(\boldsymbol{w}) \geq f((1-\theta)\boldsymbol{z} + \theta\boldsymbol{w}).$$

□

Figure 2.11 illustrates the content of Theorem 2.4.4.

Additionally, properties of Hesse matrices can be obtained when convex functions are second-order differentiable. In order to derive the result, let us define the notion of a positive definite real symmetric matrix.

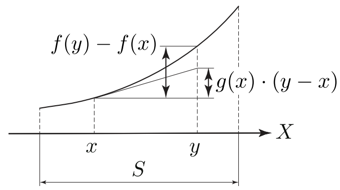


Fig. 2.11: Convexity and the first-order derivative ($X = \mathbb{R}$).

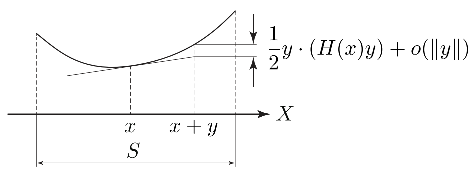


Fig. 2.12: Convexity and the second-order derivative ($X = \mathbb{R}$).

Definition 2.4.5 (Positive definite real symmetric matrix) Let $\boldsymbol{A} = \boldsymbol{A}^\top \in \mathbb{R}^{d\times d}$. Then $\boldsymbol{A}$ is said to be positive definite if there exists $\alpha > 0$ satisfying

$$\boldsymbol{x}\cdot(\boldsymbol{A}\boldsymbol{x}) \geq \alpha \|\boldsymbol{x}\|^2_{\mathbb{R}^d},$$

for all $\boldsymbol{x} \in \mathbb{R}^d$. When there only exists $\alpha \geq 0$ satisfying the above, then $\boldsymbol{A}$ is said to be semi-positive definite. Similarly, when $\alpha > 0$ exists and

$$\boldsymbol{x}\cdot(\boldsymbol{A}\boldsymbol{x}) \leq -\alpha \|\boldsymbol{x}\|^2_{\mathbb{R}^d},$$

for all $\boldsymbol{x} \in \mathbb{R}^d$, then $\boldsymbol{A}$ is said to be negative definite. In the case that there only exists $\alpha \geq 0$ satisfying the above, we say that $\boldsymbol{A}$ is semi-negative definite.
□

If $\boldsymbol{A}$ in Definition 2.4.5 is positive definite, then its eigenvalues are all positive and α is equal to their minimum value. Moreover, if $\boldsymbol{A}$ is negative definite, then all its eigenvalues are negative and $-\alpha$ is equal to their maximum value. The reader is encouraged to confirm these facts in Exercise **2.1**.

When a convex function is second-order differentiable, these definitions can be used to formulate the following result (illustrated in Fig. 2.12).

Theorem 2.4.6 (Convexity and second-order differentiation) Let $X = \mathbb{R}^d$, $S \subseteq X$ be an open convex set and $f \in C^2(S;\mathbb{R})$. Then the necessary and sufficient condition for f to be a convex function is that the Hesse matrix $\boldsymbol{H}(\boldsymbol{x})$ is semi-positive definite with respect to arbitrary $\boldsymbol{x} \in S$. □

Proof We will first show necessity. Since f is a convex function, Eq. (2.4.6) holds for arbitrary $\boldsymbol{x}, \boldsymbol{y} \in S$ and $\theta \in (0,1)$. Since $f \in C^2(S;\mathbb{R})$, given $\boldsymbol{x}, \boldsymbol{y} \in S$ there exists

$\vartheta \in (0, 1)$ such that the right-hand-side of Eq. (2.4.6) can be written as

$$f(\boldsymbol{y}) - f(\boldsymbol{x}) = \boldsymbol{g}(\boldsymbol{x}) \cdot (\boldsymbol{y} - \boldsymbol{x}) + \frac{1}{2}(\boldsymbol{y} - \boldsymbol{x}) \cdot \{\boldsymbol{H}((1 - \vartheta)\boldsymbol{x} + \vartheta\boldsymbol{y})(\boldsymbol{y} - \boldsymbol{x})\}. \tag{2.4.9}$$

Writing $\theta = \vartheta$, the left-hand side of Eq. (2.4.6) can be expressed as

$$\begin{aligned} &\frac{f(\boldsymbol{x} + \vartheta(\boldsymbol{y} - \boldsymbol{x})) - f(\boldsymbol{x})}{\vartheta} \\ &\quad = \boldsymbol{g}(\boldsymbol{x}) \cdot (\boldsymbol{y} - \boldsymbol{x}) + \frac{1}{2}\vartheta(\boldsymbol{y} - \boldsymbol{x}) \cdot \{\boldsymbol{H}((1 - \vartheta)\boldsymbol{x} + \vartheta\boldsymbol{y})(\boldsymbol{y} - \boldsymbol{x})\}. \end{aligned} \tag{2.4.10}$$

Therefore, substituting Eq. (2.4.9) and Eq. (2.4.10) into Eq. (2.4.6) when $\theta = \vartheta$ we obtain:

$$(1 - \vartheta)(\boldsymbol{y} - \boldsymbol{x}) \cdot \{\boldsymbol{H}((1 - \vartheta)\boldsymbol{x} + \vartheta\boldsymbol{y})(\boldsymbol{y} - \boldsymbol{x})\} \geq 0.$$

When $\vartheta \to 0$, $\boldsymbol{H}(\boldsymbol{x})$ is semi-positive definite.

Next let us show sufficiency. Given $\boldsymbol{x}, \boldsymbol{y} \in S$ there exists $\vartheta \in (0, 1)$ such that Eq. (2.4.9) is satisfied. Since $\boldsymbol{H}((1 - \vartheta)\boldsymbol{x} + \vartheta\boldsymbol{y})$ is semi-positive definite, the second term on the right-hand side of Eq. (2.4.9) is non-zero, and thus

$$f(\boldsymbol{y}) - f(\boldsymbol{x}) \geq \boldsymbol{g}(\boldsymbol{x}) \cdot (\boldsymbol{y} - \boldsymbol{x}).$$

From Theorem 2.4.4 it follows that f is a convex function. □

2.4.3 Exercises in Differentiation and Convex Functions

Let us make use of the previous theorems involving differentiation and convex functions in relation to simple problems from mechanics. Let us first confirm that the potential energy in the one-degree-of-freedom spring system considered in Exercise 1.1.1 is positive definite.

Exercise 2.4.7 (Potential energy of a 1DOF spring system) The potential energy in a one-degree-of-freedom spring system (such as is shown in Fig. 1.1.2) is given by

$$\pi(u) = \int_0^u (kv - p)\, \mathrm{d}v = \frac{1}{2}ku^2 - pu.$$

Show that π is a convex function. □

Answer With respect to π, we obtain

$$\frac{\mathrm{d}^2\pi}{\mathrm{d}u^2} = k > 0.$$

By Theorem 2.4.6, π is a convex function. □

Let us also confirm that the potential energy of a two-degree-of-freedom spring system is a convex function.

Exercise 2.4.8 (Potential energy of a 2DOF spring system) The potential energy of a two-degree-of-freedom spring system (such as is shown in Fig. 1.1.3) is given by

$$\pi(\boldsymbol{u}) = \frac{1}{2}k_1 u_1^2 + \frac{1}{2}k_2 (u_2 - u_1)^2 - (p_1 u_1 + p_2 u_2).$$

Show that π is a convex function. □

Answer The Hesse matrix of π is

$$\boldsymbol{H} = \begin{pmatrix} k_1 + k_2 & -k_2 \\ -k_2 & k_2 \end{pmatrix}.$$

The eigenvalues of $\boldsymbol{H}$ are λ satisfying

$$\det \begin{vmatrix} k_1 + k_2 - \lambda & -k_2 \\ -k_2 & k_2 - \lambda \end{vmatrix} = 0,$$

which leads to

$$\lambda_1, \lambda_2 = \frac{k_1 + 2k_2 \pm \sqrt{(k_1 + 2k_2)^2 - 4k_1 k_2}}{2}.$$

It follows that λ_1 and λ_2 are greater than zero whenever $k_1, k_2 > 0$. Therefore, since all of its eigenvalues are positive, $\boldsymbol{H}$ is positive definite (Theorem A.2.1). By Theorem 2.4.6, π is a convex function. □

Let us finish this section by taking a look at an example involving a familiar function which is not convex.

Exercise 2.4.9 (Area of a rectangle) Let $x_1 \in \mathbb{R}$ and $x_2 \in \mathbb{R}$ denote the length and width of a rectangle. Show that the area $f(\boldsymbol{x}) = x_1 x_2$ is not a convex function. □

Answer Upon substituting $\boldsymbol{x} = (1, 0)^\top$ and $\boldsymbol{y} = (0, 1)^\top$ into Eq. (2.4.4), we obtain

$$\begin{aligned} f((1-\theta)\boldsymbol{x} + \theta\boldsymbol{y}) &= \{(1-\theta)x_1 + \theta y_1\}\{(1-\theta)x_2 + \theta y_2\} = (1-\theta)\theta \\ &\geq (1-\theta) f(\boldsymbol{x}) + \theta f(\boldsymbol{y}) = 0. \end{aligned}$$

Therefore, f is not a convex function (see Fig. 2.13). □

2.5 Unconstrained Optimization Problems

We will now consider various cases of Problems 2.1.1–2.1.3 and look at foundational theorems of optimization theory. We will first consider the case when there are no constraints. This can be thought of as the case where all of the constraints are inactive. Namely, in Problem 2.1.3, that the minimum point is an interior point of $S \subseteq X = \mathbb{R}^d$. In this section, we will assume that S is an open set and denote f_0 by f in order to consider the following problem.

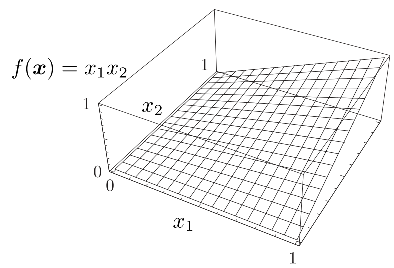


Fig. 2.13: The function $f(\boldsymbol{x}) = x_1 x_2$.

Problem 2.5.1 (Unconstrained optimization problems) Let $X = \mathbb{R}^d$ and S be an open subset of X. When $f : S \to \mathbb{R}$ is given, find $\boldsymbol{x}$ satisfying

$$\min_{\boldsymbol{x} \in S} f(\boldsymbol{x}).$$

□

2.5.1 A Necessary Condition for Local Minimizers

The conditions satisfied when $\boldsymbol{x} \in S$ is a local minimizer are referred to as necessary conditions for local minimization. When f is first-order differentiable, its derivative is defined and we obtain the following result expressing necessary conditions satisfied by local minimizers.

Theorem 2.5.2 (Necessary conditions for local minimizers) Let $f \in C^1(S; \mathbb{R})$ in Problem 2.5.1. If $\boldsymbol{x} \in S$ is a local minimizer, then

$$\boldsymbol{g}(\boldsymbol{x}) = \boldsymbol{0}_{\mathbb{R}^d}. \tag{2.5.1}$$

Equivalently, for all $\boldsymbol{y} \in X$

$$\boldsymbol{g}(\boldsymbol{x}) \cdot \boldsymbol{y} = 0. \tag{2.5.2}$$

□

Proof Suppose for contradiction that $\boldsymbol{g}(\boldsymbol{x}) \neq \boldsymbol{0}_{\mathbb{R}^d}$. If we set $\boldsymbol{y} = -\boldsymbol{g}(\boldsymbol{x})$, then $\boldsymbol{g}(\boldsymbol{x}) \cdot \boldsymbol{y} = -\|\boldsymbol{g}(\boldsymbol{x})\|_{\mathbb{R}^d}^2 < 0$. Since $\boldsymbol{g}$ is continuous, there exists t_1 such that

$$\boldsymbol{g}(\boldsymbol{x} + t\boldsymbol{y}) \cdot \boldsymbol{y} < 0$$

for all $t \in [0, t_1]$. By the mean value theorem, given $t \in (0, t_1]$ there exists $\theta \in (0, 1)$ such that

$$f(\boldsymbol{x} + t\boldsymbol{y}) = f(\boldsymbol{x}) + t\boldsymbol{g}(\boldsymbol{x} + \theta t\boldsymbol{y}) \cdot \boldsymbol{y}.$$

Since $\theta t \in (0, t_1)$ we have $\boldsymbol{g}(\boldsymbol{x} + \theta t\boldsymbol{y}) \cdot \boldsymbol{y} < 0$. Substituting this relation into the above equation yields a contradiction $f(\boldsymbol{x} + t\boldsymbol{y}) < f(\boldsymbol{x})$. □

Theorem 2.5.2, signifies that vector equalities (such as Eq. (2.5.1)) are equivalent to the condition that the inner product with any arbitrary vector (such as in Eq. (2.5.2)) is 0. Equivalence is obtained because Eq. (2.5.2) is required to hold for all $\boldsymbol{y} \in X$. Such expressions involving arbitrary vectors will appear frequently in this book, and it is thus important for the reader to understand this notion here.

If f is second-order differentiable, its Hesse matrix can be defined and the following results can be obtained.

Theorem 2.5.3 (2nd-order necessary condition for a local minimizer) Consider Problem 2.5.1 and let $f \in C^2(S;\mathbb{R})$. If $\boldsymbol{x} \in S$ is a local minimizer, then the Hesse matrix $\boldsymbol{H}(\boldsymbol{x})$ is semi-positive definite. □

Proof If $\boldsymbol{x}$ is a local minimizer, then by Definition 2.3.1 there exists a neighborhood $B \subset S$ of $\boldsymbol{x}$ such that the following holds for all $\boldsymbol{y} \in B$:

$$f(\boldsymbol{y}) - f(\boldsymbol{x}) \geq 0.$$

Additionally, since $\boldsymbol{x}$ is a local minimum, it follows from Taylor's theorem that

$$f(\boldsymbol{y}) - f(\boldsymbol{x}) = \frac{1}{2}(\boldsymbol{y}-\boldsymbol{x}) \cdot \{\boldsymbol{H}(\boldsymbol{x})(\boldsymbol{y}-\boldsymbol{x})\} + o\left(\|\boldsymbol{y}-\boldsymbol{x}\|_{\mathbb{R}^d}^2\right).$$

If $\boldsymbol{z} \in X$ is arbitrary and we multiply both sides of the above by $2\boldsymbol{z}/\|\boldsymbol{y}-\boldsymbol{x}\|_{\mathbb{R}^d}^2$ and take $\boldsymbol{y} \to \boldsymbol{x}$, then we obtain

$$\boldsymbol{z} \cdot (\boldsymbol{H}(\boldsymbol{x})\boldsymbol{z}) \geq 0.$$

□

2.5.2 Sufficient Conditions for Local Minimizers

Next, let us take a look at conditions guaranteeing when $\boldsymbol{x} \in S$ is a local minimum. In order to do so, we now give the definition of a stationary point.

Definition 2.5.4 (Stationary Point) Let $S \subseteq X$ be an open set and $\boldsymbol{x}$ an element of S. When

$$\boldsymbol{g}(\boldsymbol{x}) = \boldsymbol{0}_{\mathbb{R}^d}$$

we say that $\boldsymbol{x}$ is a stationary point. □

If f is second-order differentiable, then the following sufficient condition for attaining a local minimum can be obtained.

Theorem 2.5.5 (2nd-order sufficient condition for a local minimizer) Consider Problem 2.5.1 and let $f \in C^2(S;\mathbb{R})$. If $\boldsymbol{x} \in S$ is a stationary point and the Hesse matrix $\boldsymbol{H}(\boldsymbol{x})$ is positive definite, then $\boldsymbol{x}$ is a local minimizer. □

Proof Let $B \subset S$ be a neighborhood around a stationary point $\boldsymbol{x}$. Given $\boldsymbol{x}+\boldsymbol{y} \in B$ there exists $\theta \in (0,1)$ such that

$$f(\boldsymbol{x}+\boldsymbol{y}) - f(\boldsymbol{x}) = \frac{1}{2}\boldsymbol{y} \cdot (\boldsymbol{H}(\boldsymbol{x}+\theta\boldsymbol{y})\,\boldsymbol{y}).$$

Since $\boldsymbol{H}(\boldsymbol{x}+\theta\boldsymbol{y})$ is positive definite, the result follows:

$$f(\boldsymbol{x}+\boldsymbol{y}) > f(\boldsymbol{x}).$$

□

2.5.3 Sufficient Conditions for Global Minimizers

The previous section established conditions satisfied by local minimizers. Let us now take a look at conditions established in the case of global minimizers. In particular, if Problem 2.5.1 is a convex optimization problem, then the following result can be obtained.

Theorem 2.5.6 (Sufficient conditions for a global minimizer) In Problem 2.5.1, let $S \subseteq X$ be a non-empty open convex set and $f : S \to \mathbb{R}$ be a convex function. If $\boldsymbol{x} \in S$ is a local minimizer, then $\boldsymbol{x}$ yields the minimum over S. □

Proof If $\boldsymbol{x}$ is a local minimizer, then there exists a neighborhood $B \subset S$ around $\boldsymbol{x}$ such that $\boldsymbol{x}$ yields the minimum value over B. If we suppose that there exists another minimizer $\boldsymbol{y} \in S$ which is different from $\boldsymbol{x}$, then for sufficiently small $\theta \in (0,1)$ we can find $\boldsymbol{z} \in B$ such that

$$(1-\theta) f(\boldsymbol{x}) + \theta f(\boldsymbol{y}) \geq f((1-\theta)\,\boldsymbol{x} + \theta\boldsymbol{y}) = f(\boldsymbol{z}).$$

This is contrary to the fact that $\boldsymbol{x}$ is a local minimizer. Hence, $\boldsymbol{x}$ is the only local minimizer. □

2.5.4 Example of Unconstrained Optimization Problem

As in the previous section, let us now confirm the results thus far in relation to unconstrained problems involving systems of springs. Let us first consider a one-degree-of-freedom spring system.

Exercise 2.5.7 (Force equilibrium equation in a 1DOF spring system) Show that if u satisfies the force equilibrium equation of the one-degree-of-freedom spring system shown in Fig. 1.1.2, then it minimizes the potential energy π in Exercise 2.4.7. □

Answer By Exercise 2.4.7, π is a convex function. If u satisfies the force equilibrium equation, then by Theorem 2.5.5 it is a local minimizer. By Theorem 2.5.6, it is also a global minimizer. □

Next, let us treat a system involving multiple degrees-of-freedom.

Exercise 2.5.8 (Force equilibrium equation in a 2DOF spring system) Show that if $\boldsymbol{u}$ satisfies the force equilibrium equation of the two-degree-of-freedom spring system shown in Fig. 1.1.3, then it minimizes the potential energy π in Exercise 2.4.8. □

Answer By Exercise 2.4.8, π is a convex function. If $\boldsymbol{u}$ satisfies the force equilibrium equation, then by Theorem 2.5.5 it is a local minimizer. By Theorem 2.5.6, it is also a global minimizer. □

2.5.5 Considerations Relating to the Solutions of Unconstrained Optimization Problems

Combining the results from this section with results which will be shown later allows us to conclude the following about solutions of the unconstrained optimization problem (Problem 2.5.1).

(1) By Theorem 2.5.2, if a point is a local minimizer, it is also a stationary point. Hence stationary points are candidates for local minimizers.

(2) If after obtaining a stationary point $\boldsymbol{x}$ the Hesse matrix $\boldsymbol{H}(\boldsymbol{x})$ is found to be positive definite, then by Theorem 2.5.5 $\boldsymbol{x}$ can be deemed to be a local minimizer.

(3) If f is a convex function, any stationary point $\boldsymbol{x}$ which is also a local minimizer is necessarily a global minimizer by Theorem 2.5.6.

(4) When the convexity of f is unknown, local minimizers can be sought using various trial points and optimization methods developed in Chap. 3, amongst which the global minimizer can be found.

2.6 Optimization Problems with Equality Constraints

We will now consider Problem 2.1.1 in the case where the equality constraint $\boldsymbol{h}(\boldsymbol{x}) = \boldsymbol{0}_{\mathbb{R}^n}$ is active but all inequality constraints are inactive. As explained at the start of Sect. 2.1, this problem corresponds to the case where the cross-section $\boldsymbol{a}$ and displacement $\boldsymbol{u}$ of Problem 1.2.2 are $\boldsymbol{x} = \left(\boldsymbol{a}^\top, \boldsymbol{u}^\top\right)^\top$, and where the cost function $f_0(\boldsymbol{u}) = \boldsymbol{p} \cdot \boldsymbol{u}$ is written as $f_0(\boldsymbol{x})$ and the state equation $\boldsymbol{K}(\boldsymbol{a})\,\boldsymbol{u} - \boldsymbol{p} = \boldsymbol{0}_{\mathbb{R}^n}$ is expressed as an equality constraint $\boldsymbol{h}(\boldsymbol{x}) = \boldsymbol{0}_{\mathbb{R}^n}$.

In the case that $n < d$ equality constraints are given, it is considered that n elements become dependent variables. Therefore, putting $\boldsymbol{u} \in U = \mathbb{R}^n$ and $\boldsymbol{\xi} \in \Xi = \mathbb{R}^{d-n}$ for the remaining elements, we can write $\boldsymbol{x} = \left(\boldsymbol{\xi}^\top, \boldsymbol{u}^\top\right)^\top \in X = \Xi \times U$. In optimum design problems, $\boldsymbol{\xi}$ is called the design variable. In this section, while being careful that $X = \Xi \times U$, let us consider the following problem. Since $f_1, \ldots, f_m$ do not appear in this section, we denote f_0 by f.

Problem 2.6.1 (Optimization problems with equality constraints) Let $X = \mathbb{R}^d$. If $f : X \to \mathbb{R}$ and $\boldsymbol{h} = (h_1, \ldots, h_n)^\top : X \to \mathbb{R}^n$ are given with $n < d$, find $\boldsymbol{x}$ satisfying

$$\min_{\boldsymbol{x} \in X} \{ f(\boldsymbol{x}) \mid \boldsymbol{h}(\boldsymbol{x}) = \boldsymbol{0}_{\mathbb{R}^n} \}.$$

□

2.6.1 A Necessary Condition for Local Minimizers

Let us consider a relationship that is established when $\boldsymbol{x}$ is a local minimizer of Problem 2.6.1. Figure 2.14 illustrates a local minimum when $X = \mathbb{R}^2$ and $n = 1$. Let us consider this figure in order to describe the relationship that is established at local minimums and then consider the general case.

Let $\boldsymbol{x}$ in Fig. 2.14 designate a local minimum. That is, if we let B_X denote a neighborhood of $\boldsymbol{x}$ and move $\boldsymbol{x}$ to $\boldsymbol{x} + \boldsymbol{y} \in B_X$ while satisfying the equality constraint $h_1(\boldsymbol{x} + \boldsymbol{y}) = 0$, then $f(\boldsymbol{x}) \leq f(\boldsymbol{x} + \boldsymbol{y})$. Here it is assumed that f and h_1 are elements of $C^1(B_X; \mathbb{R})$. Then $\partial_X f = \boldsymbol{g}$ and $\partial_X h_1$ can be defined and the following relationships hold:

(1) $\boldsymbol{y}$ and $\partial_X h_1$ are orthogonal,

(2) $\boldsymbol{y}$ and $\boldsymbol{g}$ are orthogonal.

Relationship (1) expresses that the constraint is satisfied along the direction $\boldsymbol{y}$ of a point that satisfies the constraint. In fact, we have

$$h_1(\boldsymbol{x} + \boldsymbol{y}) = h_1(\boldsymbol{x}) + \partial_X h_1 \cdot \boldsymbol{y} + o(\|\boldsymbol{y}\|_{\mathbb{R}^d}),$$

and if $h_1(\boldsymbol{x} + \boldsymbol{y}) = h_1(\boldsymbol{x})$ at a point $\boldsymbol{x} + \boldsymbol{y} \in B_X$ of a neighborhood of $\boldsymbol{x}$, then $\partial_X h_1 \cdot \boldsymbol{y} = 0$. On the other hand, (2) states that the value of the cost function does not change even when it is moved in the direction of the constraint. This relationship is the same as in Eq. (2.5.2), where the variation in the direction of the cost function is limited to $\boldsymbol{y}$ in Theorem 2.5.2. Let us now generalize these relationships and consider necessary conditions relating local minimizers of optimization problems with equality constraints.

We begin by generalizing relationship (1). Let the admissible set be

$$V = \{ \boldsymbol{x} \in X \mid \boldsymbol{h}(\boldsymbol{x}) = \boldsymbol{0}_{\mathbb{R}^n} \}. \tag{2.6.1}$$

Figure 2.14 shows a curve of points satisfying $h_1 = 0$, where a neighborhood of $\boldsymbol{x} \in V$ is denoted by $B_X \subset X$. When $\boldsymbol{h} \in C^1(B_X; \mathbb{R}^n)$,

$$T_V(\boldsymbol{x}) = \{ \boldsymbol{y} \in X \mid \boldsymbol{h}_{\boldsymbol{x}^\top}(\boldsymbol{x}) \boldsymbol{y} = \boldsymbol{0}_{\mathbb{R}^n} \} \tag{2.6.2}$$

is called the feasible direction set or the tangent plane at $\boldsymbol{x}$. Here, $\boldsymbol{h}_{\boldsymbol{x}^\top} = (\partial h_i / \partial x_j) = (\partial_X h_1, \ldots, \partial_X h_n)^\top \in \mathbb{R}^{n \times d}$ corresponds to the Jacobi matrix of $\boldsymbol{h}$ with respect to $\boldsymbol{x}$. The rank of this matrix is n (in other words, $\partial_X h_1, \ldots,$

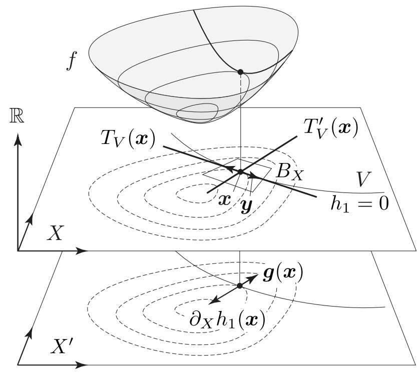


Fig. 2.14: A local minimizer of an optimization problem under an equality constraint ($X = \mathbb{R}^2$, $n = 1$).

$\partial_X h_n$ are all linearly independent) and we remark that the tangent to the curve $h_1 = 0$ at $\boldsymbol{x}$ is denoted by $T_V(\boldsymbol{x})$ in Fig. 2.14.

The cases of $n = 1$ and $n = 2$ are easy to imagine when $X = \mathbb{R}^3$. Figure 2.15 shows $T_V(\boldsymbol{x})$ in these cases. When $n = 1$, the set of points V satisfying $h_1 = 0$ forms a surface and $T_V(\boldsymbol{x})$ is the tangent plane at $\boldsymbol{x}$ to this surface. When $n = 2$, the set of points V simultaneously satisfying $h_1 = 0$ and $h_2 = 0$ is a curve and $T_V(\boldsymbol{x})$ is its tangent at $\boldsymbol{x}$. When $n = 2$, the fact that the rank of $\boldsymbol{h}_{\boldsymbol{x}^\top}(\boldsymbol{x}) = (\partial_X h_1(\boldsymbol{x}), \partial_X h_2(\boldsymbol{x}))^\top$ is $n = 2$ indicates that $\partial_X h_1(\boldsymbol{x})$ and $\partial_X h_2(\boldsymbol{x})$ face different directions. Based on Eq. (2.6.2), the definitions of the null space and the image space (also referred to as the kernel space and the range space in Section A.3, respectively) allow one to write:

$$T_V(\boldsymbol{x}) = \operatorname{Ker} \boldsymbol{h}_{\boldsymbol{x}^\top}(\boldsymbol{x}).$$

The generalization of condition (2) is as follows. Condition (2) expresses that $\boldsymbol{g}$ is orthogonal to all of the vectors contained in $T_V(\boldsymbol{x})$. We let

$$T'_V(\boldsymbol{x}) = (T_V(\boldsymbol{x}))' = \{\boldsymbol{z} \in X' \mid \boldsymbol{z} \cdot \boldsymbol{y} = 0 \text{ for all } \boldsymbol{y} \in T_V(\boldsymbol{x})\}. \tag{2.6.3}$$

and call $T'_V(\boldsymbol{x})$ the dual set or the dual plane of $T_V(\boldsymbol{x})$. Then, if f and $\boldsymbol{h}$ are first-order differentiable and T'_V can be evaluated, one can obtain the following result.

Theorem 2.6.2 (1st-order necessary conditions for a local minimizer) Let $f \in C^1(X;\mathbb{R})$ and $\boldsymbol{h} \in C^1(X;\mathbb{R}^n)$ in Problem 2.6.1 and $\partial_X h_1(\boldsymbol{x})$, ... , $\partial_X h_n(\boldsymbol{x})$ be linearly independent at $\boldsymbol{x} \in V$. Then if $\boldsymbol{x}$ is a local minimizer

$$\boldsymbol{g}(\boldsymbol{x}) \cdot \boldsymbol{y} = 0 \tag{2.6.4}$$

for all $\boldsymbol{y} \in T_V(\boldsymbol{x})$. Moreover,

$$\boldsymbol{g}(\boldsymbol{x}) \in T'_V(\boldsymbol{x}). \tag{2.6.5}$$

□

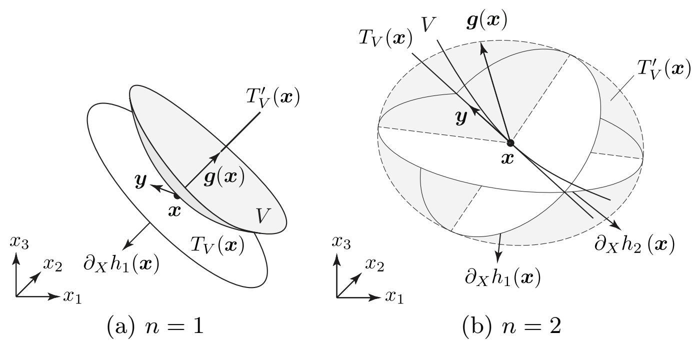


Fig. 2.15: Local minimizers in optimization problems with equality constraints ($X = \mathbb{R}^3$ and $X' = \mathbb{R}^3$ are superimposed).

Proof If we let $\boldsymbol{y} \in T_V(\boldsymbol{x})$ be arbitrary and suppose that $\boldsymbol{g}(\boldsymbol{x}) \cdot \boldsymbol{y} \neq 0$, then there exists $\boldsymbol{y}$ such that $\boldsymbol{g} \cdot \boldsymbol{y} < 0$. Then a contradiction similar to Theorem 2.5.2 can be obtained and Equation (2.6.5) is equivalent to Eq. (2.6.4) by the definition of $T'_V(\boldsymbol{x})$. □

2.6.2 The Lagrange Multiplier Method

Formulated using arbitrary $\boldsymbol{y} \in T_V(\boldsymbol{x})$ or $T'_V(\boldsymbol{x})$, Theorem 2.6.2 expresses a condition that is established when $\boldsymbol{x} \in V$ is a local minimizer. Nevertheless, even if the theorem's meaning is easy to understand, its evaluation is not necessarily so simple. For this reason, let us consider a method which does not make use of arbitrary $\boldsymbol{y} \in T_V(\boldsymbol{x})$ or $T'_V(\boldsymbol{x})$.

Before making a generalization, let us confirm the fundamental relationship illustrated in Fig. 2.14. Here we assume that both f and h_1 belong to $C^1(B_X; \mathbb{R})$. We also remark that $\boldsymbol{g}$ is orthogonal to $\boldsymbol{y} \in T_V(\boldsymbol{x})$ and that $\boldsymbol{y} \in T_V(\boldsymbol{x})$ is also orthogonal to $\partial_X h_1$. This relationship is equivalent to the fact that $\boldsymbol{g}$ and $\partial_X h_1$ are oriented in the same direction. This relationship asserts that there exists $\lambda_1 \in \mathbb{R}$ satisfying the following:

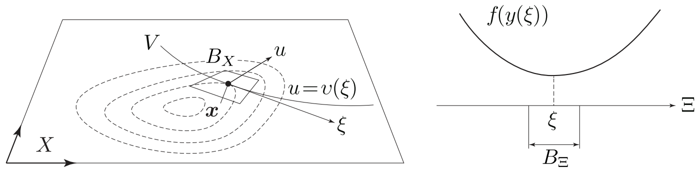
$$\boldsymbol{g} + \lambda_1 \partial_X h_1 = \boldsymbol{0}_{\mathbb{R}^2}. \tag{2.6.6}$$

In particular, λ_1 satisfying Eq. (2.6.6) cannot exist when $\boldsymbol{g}$ and $\partial_X h_1$ are non-zero vectors pointing in different directions. The reader is invited to confirm that when two vectors $\boldsymbol{a}, \boldsymbol{b} \in \mathbb{R}^d$ are fixed and have different directions, that there does not exist a $\lambda \in \mathbb{R}$ satisfying $\boldsymbol{a} + \lambda \boldsymbol{b} = \boldsymbol{0}_{\mathbb{R}^d}$.

Now let us generalize Eq. (2.6.6). At first, we will generalize the condition:

- $\boldsymbol{y} \in T_V(\boldsymbol{x})$ and $\boldsymbol{g}$ are orthogonal.

This condition can be obtained from the condition that the gradient of cost function f becomes zero when the variable $\boldsymbol{x}$ moves to the direction where the equality constraints are satisfied. Let V denote the admissible set in Eq. (2.6.1) and assume that the following conditions are satisfied:



(a) ξ–u coordinate system (b) ξ coordinate system

Fig. 2.16: A set satisfying an equality constraint and the ξ–u local coordinate system.

Hypothesis 2.6.3 (Implicit function theorem assumptions) Let $d > n$ and $X = \mathbb{R}^d = \Xi \times \mathbb{R}^n$. Also assume that $\boldsymbol{h} : X \to \mathbb{R}^n$ satisfies the following conditions in a neighborhood $B_X = B_\Xi \times B_{\mathbb{R}^n}$ of $\boldsymbol{x} = \left(\boldsymbol{\xi}_0^\top, \boldsymbol{u}_0^\top\right)^\top$:

(1) $\boldsymbol{h}(\boldsymbol{x}) = \boldsymbol{0}_{\mathbb{R}^n}$ (in other words $\boldsymbol{x} \in V$),

(2) $\boldsymbol{h} \in C^0(B_X; \mathbb{R}^n)$,

(3) $\boldsymbol{h}(\boldsymbol{\xi}, \cdot)$ belongs to $C^1(B_{\mathbb{R}^n}; \mathbb{R}^n)$ whenever $\tilde{\boldsymbol{x}} = \left(\boldsymbol{\xi}^\top, \boldsymbol{u}^\top\right)^\top \in B_\Xi \times B_{\mathbb{R}^n}$,

(4) the Jacobi matrix $\boldsymbol{h}_{\boldsymbol{u}^\top}(\boldsymbol{x})$ is invertible at $\boldsymbol{x}$.

□

By the implicit function theorem (Theorem A.4.1), there exists a neighborhood (a convex open set) $U_\Xi \times U_{\mathbb{R}^n} \subset B_\Xi \times B_{\mathbb{R}^n}$ and a continuous function $\boldsymbol{\upsilon} : U_\Xi \to U_{\mathbb{R}^n}$ (the letter $\boldsymbol{\upsilon}$ is a bold Greek upsilon) and $\boldsymbol{h}(\boldsymbol{x}) = \boldsymbol{0}_{\mathbb{R}^n}$ is equivalent to

$$\boldsymbol{u} = \boldsymbol{\upsilon}(\boldsymbol{\xi}). \tag{2.6.7}$$

Together with the ξ–u local coordinate system, Figure 2.16 also shows a set satisfying the equality constraint when $X = \mathbb{R}^2$ and $n = 1$.

If we set

$$\tilde{\boldsymbol{x}}(\boldsymbol{\xi}) = \left(\boldsymbol{\xi}^\top, \boldsymbol{\upsilon}^\top(\boldsymbol{\xi})\right)^\top,$$

then $\tilde{\boldsymbol{x}}(\boldsymbol{\xi}) \in V$ and $\boldsymbol{\xi}$ is called the local coordinate of V.

Furthermore, a generalization of

- $\boldsymbol{y} \in T_V(\boldsymbol{x})$ and $\partial_X h_1$ are orthogonal.

can be obtained from the conditions that the variable $\boldsymbol{x}$ satisfies the equality conditions. Let $\tilde{f}(\boldsymbol{\xi}) = f(\tilde{\boldsymbol{x}}(\boldsymbol{\xi}))$. If $f \in C^1(B_X; \mathbb{R}^n)$, then when $\boldsymbol{\xi} \in B_\Xi$ and $\boldsymbol{x} = \tilde{\boldsymbol{x}}(\boldsymbol{\xi}) \in B_X$ are local minimizers one has:

$$\partial_\Xi \tilde{f}(\boldsymbol{\xi}) = \left(\frac{\partial \tilde{\boldsymbol{x}}}{\partial \boldsymbol{\xi}^\top}(\boldsymbol{\xi})\right)^\top \frac{\partial f}{\partial \boldsymbol{x}}(\boldsymbol{x}) = \left(\tilde{\boldsymbol{x}}_{\boldsymbol{\xi}^\top}(\boldsymbol{x})\right)^\top \boldsymbol{g}(\boldsymbol{x}) = \boldsymbol{0}_{\mathbb{R}^{d-n}}. \tag{2.6.8}$$

The definitions of the null and image spaces allow us to rewrite this relationship as

$$\boldsymbol{g}(\boldsymbol{x}) \in T_V'(\boldsymbol{x}) = \mathrm{Ker}\,\left(\tilde{\boldsymbol{x}}_{\boldsymbol{\xi}^\top}(\boldsymbol{x})\right)^\top. \tag{2.6.9}$$

On the other hand, differentiating both sides of $\boldsymbol{h}(\boldsymbol{x}) = \boldsymbol{h}(\tilde{\boldsymbol{x}}(\boldsymbol{\xi})) = \boldsymbol{0}_{\mathbb{R}^n}$ with respect to $\boldsymbol{\xi}$ yields

$$\frac{\partial \boldsymbol{h}}{\partial \boldsymbol{x}^\top}(\boldsymbol{x}) \frac{\partial \tilde{\boldsymbol{x}}}{\partial \boldsymbol{\xi}^\top}(\boldsymbol{\xi}) = \boldsymbol{h}_{\boldsymbol{x}^\top}(\boldsymbol{x})\,\tilde{\boldsymbol{x}}_{\boldsymbol{\xi}^\top}(\boldsymbol{x}) = \boldsymbol{0}_{\mathbb{R}^{n\times(d-n)}}. \tag{2.6.10}$$

According to the definitions of the null and image spaces, since the image space of $\tilde{\boldsymbol{x}}_{\boldsymbol{\xi}^\top}(\boldsymbol{x})$ is the null space of $\boldsymbol{h}_{\boldsymbol{x}^\top}(\boldsymbol{x})$, we can write

$$T_V(\boldsymbol{x}) = \mathrm{Ker}\,\boldsymbol{h}_{\boldsymbol{x}^\top}(\boldsymbol{x}) = \mathrm{Im}\,\tilde{\boldsymbol{x}}_{\boldsymbol{\xi}^\top}(\boldsymbol{x}). \tag{2.6.11}$$

These relationships lead us to the following necessary condition for attaining a local minimizer without using $T_V(\boldsymbol{x})$ or $T_V'(\boldsymbol{x})$.

Theorem 2.6.4 (1st-order necessary condition for local minimizers) Consider Problem 2.6.1 with $f \in C^1(X;\mathbb{R})$ and $\boldsymbol{h} \in C^1(X;\mathbb{R}^n)$. Let $\partial_X h_1(\boldsymbol{x})$, $\dots$, $\partial_X h_n(\boldsymbol{x})$ be linearly independent at $\boldsymbol{x} \in X$. If $\boldsymbol{x}$ is a local minimizer, then there exists $\boldsymbol{\lambda} \in \mathbb{R}^n$ satisfying

$$\boldsymbol{g}(\boldsymbol{x}) + \partial_X \boldsymbol{h}^\top(\boldsymbol{x})\,\boldsymbol{\lambda} = \boldsymbol{0}_{\mathbb{R}^d}, \tag{2.6.12}$$

$$\boldsymbol{h}(\boldsymbol{x}) = \boldsymbol{0}_{\mathbb{R}^n}. \tag{2.6.13}$$

□

Proof By assumption, Hypothesis 2.6.3 holds at $\boldsymbol{x}$. If $\boldsymbol{x}$ is a local minimizer of Problem 2.6.1, then Eq. (2.6.9) holds. Furthermore, if Eq. (2.6.11) is used, then we have

$$\boldsymbol{g}(\boldsymbol{x}) \in T_V'(\boldsymbol{x}) = (T_V(\boldsymbol{x}))^\perp = \left(\mathrm{Im}\,\tilde{\boldsymbol{x}}_{\boldsymbol{\xi}^\top}(\boldsymbol{x})\right)^\perp = \left(\mathrm{Ker}\,\boldsymbol{h}_{\boldsymbol{x}^\top}(\boldsymbol{x})\right)^\perp$$

and Lemma A.3.1 (relating the orthogonal complement of the null and image spaces) yields

$$\boldsymbol{g}(\boldsymbol{x}) \in \left(\mathrm{Ker}\,\boldsymbol{h}_{\boldsymbol{x}^\top}(\boldsymbol{x})\right)^\perp = \mathrm{Im}\,\left(\boldsymbol{h}_{\boldsymbol{x}^\top}(\boldsymbol{x})\right)^\top = \mathrm{Im}\,(\partial_X h_1, \dots, \partial_X h_n).$$

This relationship is equivalent to Eq. (2.6.12). Moreover, Eq. (2.6.13) holds whenever $\boldsymbol{x}$ is a local minimizer of Problem 2.6.1. □

The relation shown at the last part of the proof in Theorem 2.6.4 is a generalization of Eq. (2.6.6). In other words, $\boldsymbol{g}(\boldsymbol{x})$ can be given as a linear combination of $\partial_X h_1, \dots, \partial_X h_n$. In Theorem 2.6.4, the vector $\boldsymbol{\lambda} = (\lambda_1, \dots, \lambda_n)^\top \in \mathbb{R}^n$ is called a Lagrange multiplier with respect to the equality constraint $\boldsymbol{h}(\boldsymbol{x}) = \boldsymbol{0}_{\mathbb{R}^n}$. Furthermore, Eq. (2.6.12) and Eq. (2.6.13) are called the first-order necessary conditions for the existence of local minimizers under the Lagrange method. The reason for this is because the following relationship holds. The Lagrange function for the optimization problem of Problem 2.6.1 is defined as

$$\mathscr{L}(\boldsymbol{x}, \boldsymbol{\lambda}) = f(\boldsymbol{x}) + \boldsymbol{\lambda} \cdot \boldsymbol{h}(\boldsymbol{x}). \tag{2.6.14}$$

The derivative of $\mathscr{L}$ with respect to an arbitrary variation $\left(\boldsymbol{y}, \hat{\boldsymbol{\lambda}}\right) \in X \times \mathbb{R}^n$ of $(\boldsymbol{x}, \boldsymbol{\lambda})$ is

$$\begin{aligned}\mathscr{L}'(\boldsymbol{x}, \boldsymbol{\lambda})\left[\boldsymbol{y}, \hat{\boldsymbol{\lambda}}\right] &= f'(\boldsymbol{x})[\boldsymbol{y}] + \boldsymbol{\lambda} \cdot \left(\partial_{\boldsymbol{x}^\top} \boldsymbol{h}(\boldsymbol{x})\, \boldsymbol{y}\right) + \hat{\boldsymbol{\lambda}} \cdot \boldsymbol{h}(\boldsymbol{x}) \\ &= \boldsymbol{g}(\boldsymbol{x}) \cdot \boldsymbol{y} + \left(\partial_X \boldsymbol{h}^\top(\boldsymbol{x})\, \boldsymbol{\lambda}\right) \cdot \boldsymbol{y} + \hat{\boldsymbol{\lambda}} \cdot \boldsymbol{h}(\boldsymbol{x}). \end{aligned} \tag{2.6.15}$$

Eq. (2.6.12) and Eq. (2.6.13) of Theorem 2.6.4 are equivalent to the first-order necessary (stationary) condition for the existence of a local minimizer of the Lagrange function, $\mathscr{L}'(\boldsymbol{x}, \boldsymbol{\lambda})\left[\boldsymbol{y}, \hat{\boldsymbol{\lambda}}\right] = 0$ for all $\left(\boldsymbol{y}, \hat{\boldsymbol{\lambda}}\right) \in X \times \mathbb{R}^n$.

We can thus consider using the solution of the following problem as a method for producing candidate solutions to Problem 2.6.1. This method is called the Lagrange multiplier method for optimization problems under an equality constraint.

Problem 2.6.5 (Lagrange multiplier method for equality constraints) With respect to Problem 2.6.1, let $\mathscr{L}(\boldsymbol{x}, \boldsymbol{\lambda})$ be given by Eq. (2.6.14). Find $(\boldsymbol{x}, \boldsymbol{\lambda})$ satisfying the stationary condition of $\mathscr{L}(\boldsymbol{x}, \boldsymbol{\lambda})$:

$$\partial_X \mathscr{L}(\boldsymbol{x}, \boldsymbol{\lambda}) = \boldsymbol{g}(\boldsymbol{x}) + \partial_X \boldsymbol{h}^\top(\boldsymbol{x})\, \boldsymbol{\lambda} = \mathbf{0}_{\mathbb{R}^d}, \tag{2.6.16}$$

$$\frac{\partial \mathscr{L}}{\partial \boldsymbol{\lambda}}(\boldsymbol{x}, \boldsymbol{\lambda}) = \boldsymbol{h}(\boldsymbol{x}) = \mathbf{0}_{\mathbb{R}^n}. \tag{2.6.17}$$

□

The Lagrange multiplier method will be used in various scenarios going forward. Please note that this method expresses conditions satisfied at local minimizers of Problem 2.6.1, and that it does not directly solve Problem 2.6.1.

Next, let us look at the physical meaning of Lagrange multipliers. Equation (2.6.16) can be written as

$$\lambda_i = -\frac{\left(\boldsymbol{g}(\boldsymbol{x}) + \sum_{j \in \{1,\ldots,n\},\ j \neq i} \lambda_j \partial_X h_j(\boldsymbol{x})\right) \cdot \boldsymbol{y}}{\partial_X h_i(\boldsymbol{x}) \cdot \boldsymbol{y}}, \tag{2.6.18}$$

where $\boldsymbol{y} \in X$ is arbitrary. When f and $h_1, \ldots, h_n$ are mechanical quantities, λ_i is also a mechanical quantity with units f/h_i. In fact, in Problem 1.1.4, the equality constraint $\boldsymbol{K}(\boldsymbol{a})\, \boldsymbol{u} = \boldsymbol{p}$ has the unit of force [N], $f_0 = \boldsymbol{p} \cdot \boldsymbol{u}$ has the unit of work [Nm], and $\boldsymbol{v}_0$ (introduced as a Lagrange multiplier (adjoint variable) with respect to a state equation) has the unit of displacement [m = Nm/N]. The physical meaning of the Lagrange multiplier method for optimization problems with inequality constraints is also the same. In Problem 1.1.4, f_1 and f_0 had the units of volume [m^3] and work [Nm], respectively. The Lagrange multiplier λ_1 thus has the unit of energy density [N/m^2 = Nm/m^3].

The cost function in Theorem 2.6.4 was assumed to be first-order differentiable. If it is further assumed to be twice differentiable, then the following results can be obtained. Hereafter, we will write the Hesse matrix with respect to variation of $\boldsymbol{x}$ of the Lagrange function by $\partial_X \partial_X^\top \mathscr{L}(\boldsymbol{x}, \boldsymbol{\lambda}) = \boldsymbol{H}_{\mathscr{L}}(\boldsymbol{x}, \boldsymbol{\lambda}) \in \mathbb{R}^{d \times d}$.

Theorem 2.6.6 (2nd-order necessary condition) Let $f \in C^2(X; \mathbb{R})$ and $\boldsymbol{h} \in C^2(X; U)$ in Problem 2.6.1. Also let $\partial_X h_1(\boldsymbol{x}), \ldots, \partial_X h_n(\boldsymbol{x})$ be linearly independent at $\boldsymbol{x} \in V$. If $\boldsymbol{x}$ is a local minimizer

$$\boldsymbol{y} \cdot (\boldsymbol{H}_{\mathscr{L}}(\boldsymbol{x}, \boldsymbol{\lambda}) \boldsymbol{y}) \geq 0$$

for arbitrary $\boldsymbol{y} \in T_V(\boldsymbol{x})$. □

Proof Calculations similar to Eq. (2.6.8) yield

$$\begin{aligned} \frac{\partial^2 \tilde{f}}{\partial \boldsymbol{\xi} \partial \boldsymbol{\xi}^\top}(\boldsymbol{\xi}) &= \left(\frac{\partial \boldsymbol{y}}{\partial \boldsymbol{\xi}^\top}(\boldsymbol{\xi}) \right)^\top \frac{\partial^2 f}{\partial \boldsymbol{x} \partial \boldsymbol{x}^\top}(\boldsymbol{x}) \frac{\partial \boldsymbol{y}}{\partial \boldsymbol{\xi}^\top}(\boldsymbol{\xi}) \\ &= \left(\boldsymbol{y}_{\boldsymbol{\xi}^\top}(\boldsymbol{x}) \right)^\top \partial_X \partial_X^\top f(\boldsymbol{x}) \, \boldsymbol{y}_{\boldsymbol{\xi}^\top}(\boldsymbol{x}) \in \mathbb{R}^{(d-n) \times (d-n)}. \end{aligned}$$

If $\boldsymbol{x}$ is a local minimizer, $\partial^2 \tilde{f} / \partial \boldsymbol{\xi} \partial \boldsymbol{\xi}^\top(\boldsymbol{\xi})$ is positive definite and Eq. (2.6.10) yields

$$\begin{aligned} &\left(\frac{\partial \boldsymbol{y}}{\partial \boldsymbol{\xi}^\top}(\boldsymbol{\xi}) \right)^\top \frac{\partial h_i}{\partial \boldsymbol{x} \partial \boldsymbol{x}^\top}(\boldsymbol{y}) \frac{\partial \boldsymbol{y}}{\partial \boldsymbol{\xi}^\top}(\boldsymbol{\xi}) \\ &\quad = \left(\boldsymbol{y}_{\boldsymbol{\xi}^\top}(\boldsymbol{x}) \right)^\top \partial_X \partial_X^\top h_i(\boldsymbol{x}) \, \boldsymbol{y}_{\boldsymbol{\xi}^\top}(\boldsymbol{x}) = \boldsymbol{0}_{\mathbb{R}^{(d-n) \times (d-n)}}. \end{aligned}$$

Since $\mathscr{L}(\boldsymbol{x}, \boldsymbol{\lambda}) = f(\boldsymbol{x}) + \boldsymbol{\lambda} \cdot \boldsymbol{h}(\boldsymbol{x})$, the theorem is established. □

Based on Theorem 2.6.6, when $\boldsymbol{x}$ is a local minimizer the Lagrange function $\mathscr{L}(\boldsymbol{x}, \boldsymbol{\lambda})$ can be interpreted as a quadratic approximation of $\tilde{f}(\boldsymbol{\xi})$ in the tangent plane $T_V(\boldsymbol{x})$. In fact, if $\boldsymbol{x}$ is a local minimizer, $\partial \tilde{f} / \partial \boldsymbol{\xi} = \boldsymbol{0}_{\mathbb{R}^{d-n}}$ and the proof of Theorem 2.6.6 leads to

$$\begin{aligned} \frac{\partial^2 \tilde{f}}{\partial \boldsymbol{\xi} \partial \boldsymbol{\xi}^\top}(\boldsymbol{\xi}) &= \left(\boldsymbol{y}_{\boldsymbol{\xi}^\top}(\boldsymbol{x}) \right)^\top \partial_X \partial_X^\top \left(f(\boldsymbol{x}) + \sum_{i \in \{1, \ldots, n\}} \lambda_i h_i \right) \boldsymbol{y}_{\boldsymbol{\xi}^\top}(\boldsymbol{x}) \\ &= \left(\boldsymbol{y}_{\boldsymbol{\xi}^\top}(\boldsymbol{x}) \right)^\top \partial_X \partial_X^\top \mathscr{L}(\boldsymbol{x}, \boldsymbol{\lambda}) \, \boldsymbol{y}_{\boldsymbol{\xi}^\top}(\boldsymbol{x}). \end{aligned}$$

Therefore, if $\boldsymbol{\eta} \in \mathbb{R}^{d-n}$ is arbitrary and we set $\boldsymbol{y} = \boldsymbol{y}_{\boldsymbol{\xi}^\top}(\boldsymbol{x}) \boldsymbol{\eta} \in T_V(\boldsymbol{x})$ then

$$\tilde{f}(\boldsymbol{\xi} + \boldsymbol{\eta}) = \mathscr{L}(\boldsymbol{x}, \boldsymbol{\lambda}) + \boldsymbol{y}^\top \partial_X \partial_X^\top \mathscr{L}(\boldsymbol{x}, \boldsymbol{\lambda}) \, \boldsymbol{y} + o\left(\|\boldsymbol{y}\|_X^2 \right).$$

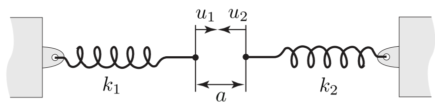


Fig. 2.17: Spring combination problem.

2.6.3 Sufficient Conditions for Local Minimizers

Regarding sufficient conditions for attaining local minimizers, the following results can be obtained.

Theorem 2.6.7 (2nd-order sufficient conditions) Let $f \in C^2(X;\mathbb{R})$ and $\boldsymbol{h} \in C^2(X;U)$ in Problem 2.6.5. Also let $\partial_X h_1(\boldsymbol{x}), \ldots, \partial_X h_n(\boldsymbol{x})$ be linearly independent at $\boldsymbol{x} \in X$. If $\boldsymbol{x}$ solves Problem 2.6.5, and if there exists a $(\boldsymbol{x}, \boldsymbol{\lambda})$ satisfying

$$\boldsymbol{y} \cdot (\boldsymbol{H}_{\mathscr{L}}(\boldsymbol{x}, \boldsymbol{\lambda})\, \boldsymbol{y}) > 0$$

for arbitrary $\boldsymbol{y} \in T_V(\boldsymbol{x})$, then $\boldsymbol{x}$ is a local minimizer of Problem 2.6.1. □

Proof Apply the proof of Theorem 2.5.5 to $\tilde{f}$. □

2.6.4 An Optimization Problem with an Equality Constraint

Let us consider a spring system and apply the Lagrange multiplier method to solve an optimization problem with an equality constraint.

Exercise 2.6.8 (A combined spring problem) Consider the two-degree-of-freedom spring system shown in Fig. 2.17 and let k_1 and k_2 be positive real constants representing the rigidity of the springs. Also let a be a positive real constant expressing the gap (length) of the spring. Find the displacement $\boldsymbol{u} = (u_1, u_2)^\top \in \mathbb{R}^2$ at which the potential energy is minimized when the springs are combined. In other words, find $\boldsymbol{u}$ satisfying

$$\min_{\boldsymbol{u} \in \mathbb{R}^2} \left\{ f(\boldsymbol{u}) = \frac{1}{2} k_1 u_1^2 + \frac{1}{2} k_2 u_2^2 \;\middle|\; h_1(\boldsymbol{u}) = a - (u_1 + u_2) = 0 \right\}.$$

□

Answer Let us first solve the problem using the substitution method. If we let $u_2 = a - u_1$, then we can write

$$f(\boldsymbol{u}) = \bar{f}(u_1) = \frac{1}{2} k_1 u_1^2 + \frac{1}{2} k_2 (a - u_1)^2.$$

Since

$$\frac{\mathrm{d}\bar{f}}{\mathrm{d}u_1}(u_1) = k_1 u_1 - k_2 (a - u_1) = (k_1 + k_2) u_1 - k_2 a = 0,$$

the stationary point of $\bar{f}$ becomes

$$u_1 = \frac{k_2}{k_1 + k_2} a, \quad u_2 = a - u_1 = \frac{k_1}{k_1 + k_2} a.$$

Furthermore, since

$$\frac{\mathrm{d}^2 \bar{f}}{\mathrm{d}u_1^2}(u_1) = k_1 + k_2 > 0,$$

$(u_1, u_2)^\top$ is a minimizer.

Next, let us solve the same problem using the Lagrange multiplier method. Let the Lagrange function be

$$\mathscr{L}(\boldsymbol{u}, \lambda) = \frac{1}{2} k_1 u_1^2 + \frac{1}{2} k_2 u_2^2 + \lambda (a - u_1 - u_2).$$

The stationary condition for $\mathscr{L}(\boldsymbol{u}, \lambda)$ becomes

$$\begin{pmatrix} \mathscr{L}_{u_1} \\ \mathscr{L}_{u_2} \\ \mathscr{L}_{\lambda} \end{pmatrix} = \begin{pmatrix} k_1 u_1 - \lambda \\ k_2 u_2 - \lambda \\ a - u_1 - u_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix},$$

which can be written

$$\begin{pmatrix} k_1 & 0 & -1 \\ 0 & k_2 & -1 \\ 1 & 1 & 0 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ \lambda \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ a \end{pmatrix}.$$

The solution of the above is readily obtained:

$$\begin{pmatrix} u_1 \\ u_2 \\ \lambda \end{pmatrix} = \frac{1}{k_1 + k_2} \begin{pmatrix} 1 & -1 & k_2 \\ -1 & 1 & k_1 \\ -k_2 & -k_1 & k_1 k_2 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ a \end{pmatrix} = \begin{pmatrix} \dfrac{k_2}{k_1 + k_2} a \\ \dfrac{k_1}{k_1 + k_2} a \\ \dfrac{k_1 k_2}{k_1 + k_2} a \end{pmatrix}.$$

We remark that $\boldsymbol{u}$ agrees with the results from the substitution method and that $\lambda = k_1 u_1 = k_2 u_2$ carries the meaning of an internal force.

Moreover, the Hesse matrix of the Lagrange function with respect to variation of $\boldsymbol{u} \in U = \mathbb{R}^2$ is positive definite and independent of $\boldsymbol{u}$ and λ:

$$\partial_U \partial_U^\top \mathscr{L}(\boldsymbol{u}, \lambda) = \boldsymbol{H}_{\mathscr{L}}(\boldsymbol{u}, \lambda) = \begin{pmatrix} k_1 & 0 \\ 0 & k_2 \end{pmatrix}.$$

By Theorem 2.6.7, $\boldsymbol{u}$ is a local minimizer. In fact, by Corollary 2.7.10 of Theorem 2.7.9 (shown later), it can be shown that $\boldsymbol{u}$ is a global minimizer. □

2.6.5 Direct Differentiation and Adjoint Variable Methods

So far we have investigated necessary and sufficient conditions for the existence of local minimizers with respect to optimization problems under equality constraints (Problem 2.6.1). Let us now replace Problem 2.6.1 with the format of the optimization problem presented in Chap. 1 and look at methods for calculating the derivative of the cost function with respect to variation of the design variable. Chapter 1 referred to these as the direct differentiation method and the adjoint variable method, where only their procedures were considered. Hence we will now define these methods and show the equivalence of the adjoint variable method and the Lagrange multiplier method.

The state determination problem of the optimal design problem presented in Chap. 1 corresponds to an equality constraint. Here, the state determination problem will be defined as follows.

Problem 2.6.9 (Linear system problem) Let $\Xi = \mathbb{R}^{d-n}$ and $U = \mathbb{R}^n$. Assume that $\boldsymbol{K} : \Xi \to \mathbb{R}^{n \times n}$ and $\boldsymbol{b} : \Xi \to \mathbb{R}^n$ are given. When $\boldsymbol{\xi} \in \Xi$, find $\boldsymbol{u} \in U$ satisfying

$$\boldsymbol{K}(\boldsymbol{\xi})\,\boldsymbol{u} = \boldsymbol{b}(\boldsymbol{\xi})\,. \tag{2.6.19}$$

□

An optimization problem where a state determination problem such as the previous imparts an equality constraint is defined as follows.

Problem 2.6.10 (Optimization problem with an equality constraint) In Problem 2.6.9, let $\boldsymbol{K} \in C^1(\Xi; \mathbb{R}^{n \times n})$ and $\boldsymbol{b} \in C^1(\Xi; \mathbb{R}^n)$. When $f \in C^1(\Xi \times U; \mathbb{R})$ is given, find $(\boldsymbol{\xi}, \boldsymbol{u})$ which satisfies

$$\min_{(\boldsymbol{\xi}, \boldsymbol{u}) \in \Xi \times U} \{ f(\boldsymbol{\xi}, \boldsymbol{u}) \mid \text{Problem 2.6.9} \}\,.$$

□

Before beginning our explanation, we remark that the derivative of a cost functional (referred to as the cross-sectional derivative in Chap. 1) with respect to variation of a design variable is defined differently than $\boldsymbol{g}(\boldsymbol{x})$ from Sect. 2.6. In fact, in Eq. (2.6.8), the derivative of $\tilde{f}(\boldsymbol{\xi}) = f(\boldsymbol{\xi}, \boldsymbol{v}(\boldsymbol{\xi}))$ with respect to $\boldsymbol{\xi} \in \Xi$ was written $\partial_\Xi \tilde{f}(\boldsymbol{\xi}) = \left(\boldsymbol{y}_{\boldsymbol{\xi}^\top}(\boldsymbol{x})\right)^\top \boldsymbol{g}(\boldsymbol{x})$, where $\boldsymbol{g}(\boldsymbol{x})$ was used to refer to $\partial_X f \in \mathbb{R}^d$. On the other hand, $\partial_\Xi \tilde{f}_0 \in \mathbb{R}^{d-n}$ was written as $\boldsymbol{g}_0$ in Chap. 1. Here, in keeping with the notation in Chap. 2, we will write $\tilde{\boldsymbol{g}} = \partial_\Xi \tilde{f}$.

Let us begin by defining the direct differentiation method. If f, $\boldsymbol{K}$ and $\boldsymbol{b}$ are first-order differentiable, then

$$\tilde{\boldsymbol{g}} = \partial_\Xi \tilde{f}(\boldsymbol{\xi}) = \frac{\partial f}{\partial \boldsymbol{\xi}}(\boldsymbol{\xi}, \boldsymbol{u}) + \left(\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{\xi}^\top}(\boldsymbol{\xi})\right)^\top \frac{\partial f}{\partial \boldsymbol{u}}(\boldsymbol{\xi})\,. \tag{2.6.20}$$

On the other hand, the column vector resulting from the partial derivatives of Eq. (2.6.19) with respect to $\xi_1, \ldots, \xi_{d-n}$ can be written in a matrix fashion:

$$\frac{\partial \boldsymbol{K}}{\partial \boldsymbol{\xi}^\top}\boldsymbol{u} + \boldsymbol{K}\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{\xi}^\top} = \frac{\partial \boldsymbol{b}}{\partial \boldsymbol{\xi}^\top}.$$

In other words we set

$$\frac{\partial \boldsymbol{K}}{\partial \boldsymbol{\xi}^\top}\boldsymbol{u} = \left(\frac{\partial \boldsymbol{K}}{\partial \xi_1}\boldsymbol{u}, \dots, \frac{\partial \boldsymbol{K}}{\partial \xi_{d-n}}\boldsymbol{u}\right) \in \mathbb{R}^{n\times(d-n)}. \tag{2.6.21}$$

Therefore

$$\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{\xi}^\top} = \boldsymbol{K}^{-1}\left(\frac{\partial \boldsymbol{b}}{\partial \boldsymbol{\xi}^\top} - \frac{\partial \boldsymbol{K}}{\partial \boldsymbol{\xi}^\top}\boldsymbol{u}\right). \tag{2.6.22}$$

The right-hand side of the above equation can be calculated and substituted into Eq. (2.6.20) to obtain $\tilde{\boldsymbol{g}}$. This method is referred to as the direct differentiation method. Here we view $\partial f/\partial \boldsymbol{\xi}$, $\partial f/\partial \boldsymbol{u}$, $\partial \boldsymbol{K}/\partial \boldsymbol{\xi}^\top$ and $\partial \boldsymbol{b}/\partial \boldsymbol{\xi}^\top$ as being analytically computable.

In contrast, the adjoint variable method is defined below. First of all, the adjoint problem with respect to f is defined as follows.

Problem 2.6.11 (Adjoint problem with respect to f) Let $\boldsymbol{K}$ and f be given with respect to $\boldsymbol{\xi} \in \Xi$ in Problem 2.6.10. Find $\boldsymbol{v} \in U$ satisfying

$$\boldsymbol{K}^\top \boldsymbol{v} = \frac{\partial f}{\partial \boldsymbol{u}}. \tag{2.6.23}$$

□

The solution $\boldsymbol{v}$ of Problem 2.6.11 is called an adjoint variable. Combining Eq. (2.6.22) and Eq. (2.6.23) yields

$$\left(\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{\xi}^\top}\right)^\top \frac{\partial f}{\partial \boldsymbol{u}} = \left(\frac{\partial \boldsymbol{b}}{\partial \boldsymbol{\xi}^\top} - \frac{\partial \boldsymbol{K}}{\partial \boldsymbol{\xi}^\top}\boldsymbol{u}\right)^\top \boldsymbol{K}^{-\top}\boldsymbol{K}^\top \boldsymbol{v} = \left(\frac{\partial \boldsymbol{b}}{\partial \boldsymbol{\xi}^\top} - \frac{\partial \boldsymbol{K}}{\partial \boldsymbol{\xi}^\top}\boldsymbol{u}\right)^\top \boldsymbol{v}. \tag{2.6.24}$$

Substituting Eq. (2.6.24) into Eq. (2.6.20) gives

$$\tilde{\boldsymbol{g}} = \frac{\partial f}{\partial \boldsymbol{\xi}} + \left(\frac{\partial \boldsymbol{b}}{\partial \boldsymbol{\xi}^\top} - \frac{\partial \boldsymbol{K}}{\partial \boldsymbol{\xi}^\top}\boldsymbol{u}\right)^\top \boldsymbol{v} \in \mathbb{R}^{d-n}. \tag{2.6.25}$$

The method of calculating $\tilde{\boldsymbol{g}}$ by solving Problem 2.6.11 for $\boldsymbol{v}$ and using Eq. (2.6.25) is called the adjoint variable method. In this approach, the definition of the Lagrange function is not required. Nevertheless, it can be shown that the Lagrange multiplier method yields the same results as the adjoint variable method.

To see this, let $\boldsymbol{v} \in \mathbb{R}^n$ be a Lagrange multiplier with respect to an equality constraint (state equation) and define the Lagrange function as

$$\mathscr{L}(\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v}) = f(\boldsymbol{\xi}, \boldsymbol{u}) + \boldsymbol{v} \cdot (\boldsymbol{b}(\boldsymbol{\xi}) - \boldsymbol{K}(\boldsymbol{\xi})\boldsymbol{u}).$$

Stationary conditions of $\mathscr{L}(\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v})$ with respect to $\boldsymbol{u}$ and $\boldsymbol{v}$ are

$$\frac{\partial \mathscr{L}}{\partial \boldsymbol{u}}(\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v}) = \frac{\partial f}{\partial \boldsymbol{u}} - \boldsymbol{K}^\top \boldsymbol{v} = \boldsymbol{0}_{\mathbb{R}^n},$$

$$\frac{\partial \mathscr{L}}{\partial \boldsymbol{v}}(\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v}) = \boldsymbol{b} - \boldsymbol{K}\boldsymbol{u} = \boldsymbol{0}_{\mathbb{R}^n}.$$

These agree with Eq. (2.6.23) and Eq. (2.6.19). Moreover, the partial derivative of $\mathscr{L}$ with respect to $\boldsymbol{\xi}$ is consistent with Eq. (2.6.25):

$$\frac{\partial \mathscr{L}}{\partial \boldsymbol{\xi}}(\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v}) = \frac{\partial f}{\partial \boldsymbol{\xi}} + \left(\frac{\partial \boldsymbol{b}}{\partial \boldsymbol{\xi}^\top} - \frac{\partial \boldsymbol{K}}{\partial \boldsymbol{\xi}^\top}\boldsymbol{u}\right)^\top \boldsymbol{v} = \tilde{\boldsymbol{g}}.$$

From this we see that the Lagrange multiplier method and the adjoint variable method are equivalent. Moreover, the adjoint variable is the same as the Lagrange multiplier.

Moreover, writing the Hessian $\partial_\Xi \partial_\Xi^\top \tilde{f}$ of $\tilde{f}(\boldsymbol{\xi})$ as $\tilde{\boldsymbol{H}}$, let us use the Lagrange multiplier method to obtain the $\tilde{\boldsymbol{H}}$. We define the Lagrange function with respect to $\tilde{f}'(\boldsymbol{\xi})[\boldsymbol{\eta}_1] = \tilde{\boldsymbol{g}} \cdot \boldsymbol{\eta}_1$ based on the definition of a Fréchet derivative (Definition 4.5.4) by

$$\begin{aligned} &\mathscr{L}_{\mathrm{I}}(\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}, \boldsymbol{z}) \\ &\quad = \tilde{\boldsymbol{g}}(\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v}) \cdot \boldsymbol{\eta}_1 + \boldsymbol{w} \cdot (\boldsymbol{b}(\boldsymbol{\xi}) - \boldsymbol{K}(\boldsymbol{\xi})\boldsymbol{u}) + \boldsymbol{z} \cdot \left(\frac{\partial f}{\partial \boldsymbol{u}} - \boldsymbol{K}^\top \boldsymbol{v}\right), \end{aligned} \tag{2.6.26}$$

where $\boldsymbol{w} \in U$ and $\boldsymbol{z} \in U$ are the adjoint variables provided for $\boldsymbol{u}$ and $\boldsymbol{v}$ in $\tilde{\boldsymbol{g}}(\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v})$. $\boldsymbol{\eta}_1 \in \Xi$ is assumed to be a constant vector in $\mathscr{L}_{\mathrm{I}}$. The $\mathscr{L}_{\mathrm{I}}$ in Eq. (2.6.26) corresponds to $\mathscr{L}_{\mathrm{I}0}$ in Eq. (1.1.43) with respect to the mean compliance in Chap. 1. When we generalize the argument in Chap. 1, it becomes as follows.

With respect to arbitrary variations $(\boldsymbol{\eta}_2, \hat{\boldsymbol{u}}, \hat{\boldsymbol{v}}, \hat{\boldsymbol{w}}, \hat{\boldsymbol{z}}) \in \Xi \times U^4$ of $(\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}, \boldsymbol{z})$, the derivative of $\mathscr{L}_{\mathrm{I}}$ is written as

$$\begin{aligned} &\mathscr{L}_{\mathrm{I}}'(\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}, \boldsymbol{z})[\boldsymbol{\eta}_2, \hat{\boldsymbol{u}}, \hat{\boldsymbol{v}}, \hat{\boldsymbol{w}}, \hat{\boldsymbol{z}}] \\ &\quad = \mathscr{L}_{\mathrm{I}\boldsymbol{\xi}}(\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}, \boldsymbol{z})[\boldsymbol{\eta}_2] + \mathscr{L}_{\mathrm{I}\boldsymbol{u}}(\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}, \boldsymbol{z})[\hat{\boldsymbol{u}}] \\ &\qquad + \mathscr{L}_{\mathrm{I}\boldsymbol{v}}(\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}, \boldsymbol{z})[\hat{\boldsymbol{v}}] + \mathscr{L}_{\mathrm{I}\boldsymbol{w}}(\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}, \boldsymbol{z})[\hat{\boldsymbol{w}}] \\ &\qquad + \mathscr{L}_{\mathrm{I}\boldsymbol{z}}(\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}, \boldsymbol{z})[\hat{\boldsymbol{z}}]. \end{aligned} \tag{2.6.27}$$

The fourth term on the right-hand side of Eq. (2.6.27) vanishes if $\boldsymbol{u}$ is the solution of the state determination problem. If $\boldsymbol{v}$ can be determined as the solution of the adjoint problem, the fifth term of Eq. (2.6.27) also vanishes. Moreover, the second term on the right-hand side of Eq. (2.6.27) is

$$\begin{aligned} &\mathscr{L}_{\mathrm{I}\boldsymbol{u}}(\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}, \boldsymbol{z})[\hat{\boldsymbol{u}}] \\ &\quad = \tilde{\boldsymbol{g}}_{\boldsymbol{u}^\top}(\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v})[\hat{\boldsymbol{u}}] \cdot \boldsymbol{\eta}_1 - \boldsymbol{w} \cdot (\boldsymbol{K}(\boldsymbol{\xi})\hat{\boldsymbol{u}}) \\ &\quad = \hat{\boldsymbol{u}} \cdot \left(\tilde{\boldsymbol{g}}_{\boldsymbol{u}}^\top(\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v})[\boldsymbol{\eta}_1] - \boldsymbol{K}^\top(\boldsymbol{\xi})\boldsymbol{w}\right). \end{aligned} \tag{2.6.28}$$

Here, the condition that Eq. (2.6.28) is zero for arbitrary $\hat{\boldsymbol{u}} \in U$ becomes an adjoint problem to determine $\boldsymbol{w}$. The third term on the right-hand side of Eq. (2.6.27) is

$$\mathscr{L}_{\mathrm{I}\boldsymbol{v}}(\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}, \boldsymbol{z})[\hat{\boldsymbol{v}}]$$

$$
\begin{aligned}
&= \tilde{\boldsymbol{g}}_{\boldsymbol{v}^\top}(\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v})[\hat{v}] \cdot \boldsymbol{\eta}_1 - \boldsymbol{z} \cdot \left(\boldsymbol{K}^\top(\boldsymbol{\xi})\,\hat{\boldsymbol{v}}\right) \\
&= \hat{\boldsymbol{v}} \cdot \left(\tilde{\boldsymbol{g}}_{\boldsymbol{v}}^\top(\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v})[\boldsymbol{\eta}_1] - \boldsymbol{K}(\boldsymbol{\xi})\,\boldsymbol{z}\right).
\end{aligned} \tag{2.6.29}
$$

Here, the condition that Eq. (2.6.29) is zero for arbitrary $\hat{\boldsymbol{v}} \in U$ corresponds to the adjoint problem for $\boldsymbol{z}$.

Finally, the first term on the right-hand side of Eq. (2.6.27) becomes

$$
\begin{aligned}
&\mathscr{L}_{\mathrm{I}\boldsymbol{\xi}}(\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}, \boldsymbol{z})[\boldsymbol{\eta}_2] \\
&\quad = -\left\{\boldsymbol{w}^\top \begin{pmatrix} \dfrac{\partial \boldsymbol{K}(\boldsymbol{\xi})}{\partial \xi_1}\boldsymbol{u} & \dots & \dfrac{\partial \boldsymbol{K}(\boldsymbol{\xi})}{\partial \xi_{d-n}}\boldsymbol{u} \end{pmatrix}\right. \\
&\qquad \left. + \boldsymbol{z}^\top \begin{pmatrix} \dfrac{\partial \boldsymbol{K}^\top(\boldsymbol{\xi})}{\partial \xi_1}\boldsymbol{v} & \dots & \dfrac{\partial \boldsymbol{K}^\top(\boldsymbol{\xi})}{\partial \xi_{d-n}}\boldsymbol{v} \end{pmatrix}\right\}\boldsymbol{\eta}_2.
\end{aligned}
$$

Here, $\boldsymbol{u}$, $\boldsymbol{v}$, $\boldsymbol{w}(\boldsymbol{\eta}_1)$ and $\boldsymbol{z}(\boldsymbol{\eta}_1)$ are assumed to be determined by the conditions above, respectively. If we denote $f(\boldsymbol{\xi}, \boldsymbol{u})$ here by $\tilde{f}(\boldsymbol{\xi})$, we have the relation:

$$
\mathscr{L}_{\mathrm{I}\boldsymbol{\xi}}(\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}, \boldsymbol{z})[\boldsymbol{\eta}_2] = \tilde{f}''(\boldsymbol{\xi})[\boldsymbol{\eta}_1, \boldsymbol{\eta}_2] = \tilde{\boldsymbol{g}}_{\mathrm{H}}(\boldsymbol{\xi}, \boldsymbol{\eta}_1) \cdot \boldsymbol{\eta}_2, \tag{2.6.30}
$$

where the Hesse gradient $\tilde{\boldsymbol{g}}_{\mathrm{H}}$ of $\tilde{f}$ is given by

$$
\begin{aligned}
\tilde{\boldsymbol{g}}_{\mathrm{H}}(\boldsymbol{\xi}, \boldsymbol{\eta}_1) = -&\left\{\boldsymbol{w}^\top(\boldsymbol{\eta}_1) \begin{pmatrix} \dfrac{\partial \boldsymbol{K}(\boldsymbol{\xi})}{\partial \xi_1}\boldsymbol{u} & \dots & \dfrac{\partial \boldsymbol{K}(\boldsymbol{\xi})}{\partial \xi_{d-n}}\boldsymbol{u} \end{pmatrix}\right. \\
&\left. + \boldsymbol{z}^\top(\boldsymbol{\eta}_1) \begin{pmatrix} \dfrac{\partial \boldsymbol{K}^\top(\boldsymbol{\xi})}{\partial \xi_1}\boldsymbol{v} & \dots & \dfrac{\partial \boldsymbol{K}^\top(\boldsymbol{\xi})}{\partial \xi_{d-n}}\boldsymbol{v} \end{pmatrix}\right\}^\top.
\end{aligned} \tag{2.6.31}
$$

2.6.6 Considerations Relating to the Solution of Optimization Problems with Equality Constraints

Combining the results obtained in this section with a few shown later on allows us to conclude the following about the solution of optimization problems under equality constraints (Problem 2.6.1):

(1) By Theorem 2.6.4, the solution of the Lagrange multiplier method $(\boldsymbol{x}, \boldsymbol{\lambda})$ (Problem 2.6.5) satisfies the necessary conditions for a local minimizer. Such $\boldsymbol{x}$'s are candidates for local minimizers.

(2) When $(\boldsymbol{x}, \boldsymbol{\lambda})$ is a solution of the Lagrange multiplier method (Problem 2.6.5) whose Hesse matrix $\partial_X \partial_X^\top \mathscr{L}(\boldsymbol{x}, \boldsymbol{\lambda}) = \boldsymbol{H}_{\mathscr{L}}(\boldsymbol{x}, \boldsymbol{\lambda})$ (with respect to variation of $\boldsymbol{x}$ of the Lagrange function) satisfies $\boldsymbol{y} \cdot (\boldsymbol{H}_{\mathscr{L}}(\boldsymbol{x}, \boldsymbol{\lambda})\,\boldsymbol{y}) > 0$ for arbitrary variations $\boldsymbol{y} \in T_V(\boldsymbol{x})$ satisfying the equality constraints, then $\boldsymbol{x}$ yields a local minimum by Theorem 2.6.7.

(3) Based on Corollary 2.7.10 of Theorem 2.7.9 shown later, when a convex optimization problem is subject to an equality constraint (Problem 2.6.1), the solution $\boldsymbol{x}$ of the Lagrange multiplier method is the minimizer.

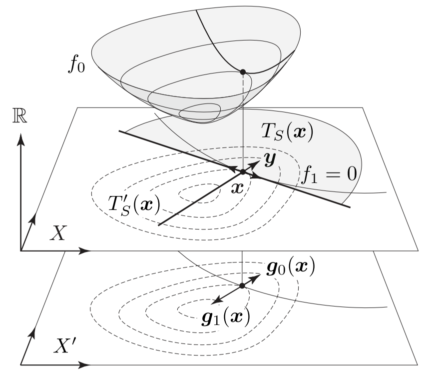


Fig. 2.18: A local minimizer of an optimization problem under an inequality constraint when $X = \mathbb{R}^2$ and $m = 1$.

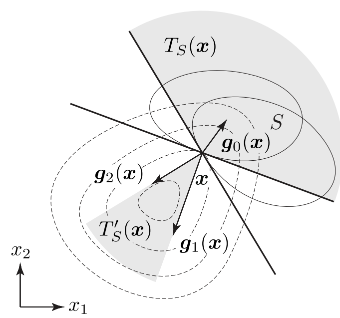
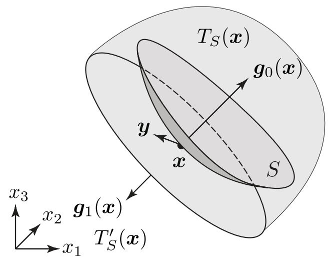


Fig. 2.19: A local minimizer of an optimization problem under an inequality constraint when $X = \mathbb{R}^2$ and $m = 2$.

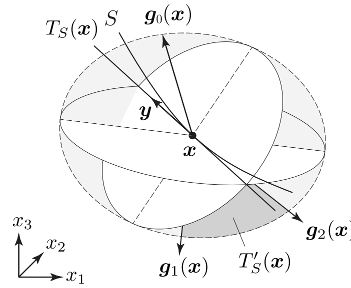
(4) Based on Corollary 2.7.3 of Theorem 2.7.2 (shown later), even when non-convex optimization problems include equality constraints (Problem 2.6.1), if $\tilde{f}$ is convex then the stationary point of $\tilde{f}$ (that is, the $\boldsymbol{x}$ for which $\tilde{\boldsymbol{g}} = \mathbf{0}_{\mathbb{R}^{d-n}}$) can be shown to yield the minimum.

2.7 Optimization Problems Under Inequality Constraints

Let us now change the constraint condition from an equality to an inequality. We will only consider the case when the inequalities are assumed to be such as those presented in Problem 2.1.2 and Problem 2.1.3. Figure 2.18 shows a local minimizer in the case $X = \mathbb{R}^2$ and $m = 1$. When $X = \mathbb{R}^2$ and $m = 2$, the situation is as shown in Fig. 2.19. Using these diagrams, let us first take a look at conditions established at local minimizers and then treat the general case.



(a) $m = 1$



(b) $m = 2$

Fig. 2.20: A local minimizer in an optimization problem with an inequality constraint ($X = \mathbb{R}^3$ and $X' = \mathbb{R}^3$ are shown superimposed.)

2.7.1 Necessary Conditions at Local Minimizers

We will begin with the case illustrated in Fig. 2.18, where one of the inequality constraints is active at the local minimizer $\boldsymbol{x}$. In this case, the following can be said:

(1) The directions $\boldsymbol{y}$ in which variations of $\boldsymbol{x}$ are permitted satisfy $\boldsymbol{g}_1 \cdot \boldsymbol{y} \leq 0$. These directions are shown in the semicircle region of the figure, where they are denoted by $T_S(\boldsymbol{x})$.

(2) If $\boldsymbol{x}$ is a local minimizer, then f_0 cannot fluctuate and should increase with respect to variations in all directions $\boldsymbol{y} \in T_S(\boldsymbol{x})$. This relationship indicates that $\boldsymbol{g}_0 \cdot \boldsymbol{y} \geq 0$ for all $\boldsymbol{y} \in T_S(\boldsymbol{x})$. Such directions $\boldsymbol{z}$ satisfying $\boldsymbol{z} \cdot \boldsymbol{y} \leq 0$ for all $\boldsymbol{y} \in T_S(\boldsymbol{x})$ are shown in the region $T'_S(\boldsymbol{x})$ of the digram.

(3) If $\boldsymbol{x}$ is a local minimizer, the fact that $\boldsymbol{g}_0 \cdot \boldsymbol{y} \geq 0$ holds for all $\boldsymbol{y} \in T_S(\boldsymbol{x})$ is equivalent to $-\boldsymbol{g}_0$ being included in $T'_S(\boldsymbol{x})$.

When two inequality constraints are active, the situation becomes as is shown in Fig. 2.19. The set of directions $T_S(\boldsymbol{x})$ in which variations from $\boldsymbol{x}$ are permissible is wedge-shaped because there are two inequality constraints which must be satisfied simultaneously. In response to this, $T'_S(\boldsymbol{x})$ is broader than when there is just one inequality constraint and its region becomes wedge-shaped. When $\boldsymbol{x}$ is a local minimizer, then $\boldsymbol{g}_0 \cdot \boldsymbol{y} \geq 0$ holds for all $\boldsymbol{y} \in T_S(\boldsymbol{x})$, as does the fact that $-\boldsymbol{g}_0$ is included in $T'_S(\boldsymbol{x})$. Figure 2.20 shows the state of a local minimizer when $X = \mathbb{R}^3$.

We now turn to generalizing the above observations. In Figs. 2.18–2.20, $T_S(\boldsymbol{x})$ and $T'_S(\boldsymbol{x})$ were defined using $\boldsymbol{g}_1$ and $\boldsymbol{g}_2$. Here we define $C_S(\boldsymbol{x})$ to be the set of admissible directions including $T_S(\boldsymbol{x})$, and conduct a similar discussion centering on $C_S(\boldsymbol{x})$ and $C'_S(\boldsymbol{x})$. Moreover, the relationships between $T_S(\boldsymbol{x})$ and $C_S(\boldsymbol{x})$ can be viewed equivalently when the conditions of Proposition 2.7.4 (presented later) are satisfied.

The set S of admissible design variables satisfying the inequality constraints are defined as in Eq. (2.1.1). Given $\boldsymbol{x} \in S$, the active constraints are indicated by the following set:

$$I_{\mathrm{A}}(\boldsymbol{x}) = \{\, i \in \{1, \ldots, m\} \mid f_i(\boldsymbol{x}) = 0\} = \left\{i_1, \ldots, i_{|I_{\mathrm{A}}(\boldsymbol{x})|}\right\}. \tag{2.7.1}$$

Considering the set of sequences $\{\boldsymbol{y}_k\}_{k \in \mathbb{N}} \in S$ converging to $\boldsymbol{x} \in S$ and having a direction $\boldsymbol{y}$, the set

$$C_S(\boldsymbol{x}) = \left\{ \boldsymbol{y} \in X \;\middle|\; \frac{\boldsymbol{y}}{\|\boldsymbol{y}\|} = \lim_{k \to \infty} \frac{\boldsymbol{y}_k - \boldsymbol{x}}{\|\boldsymbol{y}_k - \boldsymbol{x}\|} \text{ for } \boldsymbol{y} \neq \boldsymbol{0}_X \right\}$$

is called the feasible direction set or the tangential cone of S. The dual cone of $C_S(\boldsymbol{x})$ is the set:

$$C'_S(\boldsymbol{x}) = \{\, \boldsymbol{z} \in X' \mid \boldsymbol{z} \cdot \boldsymbol{y} \le 0 \text{ for all } \boldsymbol{y} \in C_S(\boldsymbol{x})\}.$$

Our next result follows easily from the above considerations when C'_S can be evaluated and f_0 is first-order differentiable.

Theorem 2.7.1 (1st-order necessary condition for local minimizers) Let $f_0 \in C^1(X; \mathbb{R})$ in Problem 2.1.2. If $\boldsymbol{x}$ is a local minimizer, then for arbitrary $\boldsymbol{y} \in C_S(\boldsymbol{x})$,

$$\boldsymbol{g}_0(\boldsymbol{x}) \cdot \boldsymbol{y} \ge 0. \tag{2.7.2}$$

Moreover,

$$-\boldsymbol{g}_0(\boldsymbol{x}) \in C'_S(\boldsymbol{x}). \tag{2.7.3}$$

□

Proof If we suppose $\boldsymbol{g}_0(\boldsymbol{x}) \cdot \boldsymbol{y} \neq 0$ for all $\boldsymbol{y} \in C_S(\boldsymbol{x})$, then there exists $\boldsymbol{y}$ such that $\boldsymbol{g}_0(\boldsymbol{x}) \cdot \boldsymbol{y} < 0$. The same contradiction as was obtained in the proof of Theorem 2.5.2 can then be obtained. Moreover, Eq. (2.7.3) is equivalent to Eq. (2.7.2). □

2.7.2 Necessary and Sufficient Conditions for Global Minimizers

If Problem 2.1.2 is a convex optimization problem and C'_S can be evaluated, then the following necessary and sufficient condition satisfied by global minimizers can be obtained.

Theorem 2.7.2 (1st-order necessary and sufficient condition) In Problem 2.1.2, let f_0 be an element of $C^1(X; \mathbb{R})$, $f_1, \ldots, f_m$ be elements of $C^0(X; \mathbb{R})$, and $f_0, \ldots, f_m$ be convex functions. Also let S be given by Eq. (2.1.1). Then the following condition is both necessary and sufficient for $\boldsymbol{x} \in S$ to be a global minimizer:

$$-\boldsymbol{g}_0(\boldsymbol{x}) \in C'_S(\boldsymbol{x}).$$

□

Proof Necessity follows directly from Theorem 2.7.1 and so we only show the sufficient condition. Let each member of the sequence $\{\beta_k\}_{k\in\mathbb{N}}$ satisfy $\beta_k \in (0,1)$ and $\beta_k \to 0$. Given $\boldsymbol{y} \in S$, construct $\{\boldsymbol{y}_k\}_{k\in\mathbb{N}}$ such that $\boldsymbol{y}_k = (1-\beta_k)\,\boldsymbol{x} + \beta_k \boldsymbol{y}$. Since S is convex, $\{\boldsymbol{y}_k\}_{k\in\mathbb{N}} \subseteq S$. By the definition of $C_S(\boldsymbol{x})$, it follows that $\boldsymbol{y} - \boldsymbol{x} \in C_S(\boldsymbol{x})$. Therefore, by the definition of $C_S'(\boldsymbol{x})$, and since $-\boldsymbol{g}_0(\boldsymbol{x}) \in C_S'(\boldsymbol{x})$,

$$-\boldsymbol{g}_0(\boldsymbol{x}) \cdot (\boldsymbol{y} - \boldsymbol{x}) \leq 0.$$

Since f_0 is a convex function, Theorem 2.4.4 implies that

$$\boldsymbol{g}_0(\boldsymbol{x}) \cdot (\boldsymbol{y} - \boldsymbol{x}) \leq f_0(\boldsymbol{y}) - f_0(\boldsymbol{x}).$$

Hence, $f_0(\boldsymbol{x}) \leq f_0(\boldsymbol{y})$. □

If the global minimizer occurs at an interior point of S, Theorem 2.7.2 is as follows (this result is equivalent to Theorem 2.5.6).

Corollary 2.7.3 (1st-order necessary and sufficient condition)
In Problem 2.1.2, let f_0 be $C^1(X;\mathbb{R})$ and $f_1, \ldots, f_m$ be convex functions belonging to $C^0(X;\mathbb{R})$. Let S be given by Eq. (2.1.1). Then the following is both necessary and sufficient for an internal point $\boldsymbol{x}$ of S to yield the global minimum in Problem 2.1.3:

$$\boldsymbol{g}_0(\boldsymbol{x}) = \boldsymbol{0}_{\mathbb{R}^d}.$$

□

Proof If $\boldsymbol{x}$ is an internal point of S, $C_S(\boldsymbol{x}) = X$. Hence, we obtain $C_S'(\boldsymbol{x}) = \{\boldsymbol{0}_{\mathbb{R}^d}\}$. Theorem 2.7.2 then implies $\boldsymbol{g}_0(\boldsymbol{x}) = \boldsymbol{0}_{\mathbb{R}^d}$. □

2.7.3 KKT Conditions

Conditions governing all $\boldsymbol{y}$ in $C_S(\boldsymbol{x})$ or C_S' were included in the necessary and sufficient conditions for the existence of local and global minimizers of Problem 2.1.2. However, checking such conditions is not necessarily easy. Therefore, as we did in the case of optimization problems with equality constraints, we will consider expressions using Lagrange functions here as well.

Let us first consider the situation shown in Fig. 2.18, where one inequality constraint is active. Since the inequality constraint condition is active, even if there is an equality constraint, $\boldsymbol{x}$ will yield a local minimum. Then Eq. (2.6.6) (which was used with an equality constraint) can be rewritten as

$$\boldsymbol{g}_0 + \lambda_1 \boldsymbol{g}_1 = \boldsymbol{0}_{\mathbb{R}^2}. \tag{2.7.4}$$

However, the range of admissible variations is enlarged in the presence of inequality constraints. Let us consider this in detail. Taking the inner product of Eq. (2.7.4) with an arbitrary $\boldsymbol{y} \in \mathbb{R}^2$ yields

$$\boldsymbol{g}_0 \cdot \boldsymbol{y} + \lambda_1 \boldsymbol{g}_1 \cdot \boldsymbol{y} = 0. \tag{2.7.5}$$

If $\boldsymbol{y}$ is a direction in which the inequality constraint is satisfied, then $\boldsymbol{g}_1 \cdot \boldsymbol{y} \leq 0$. Moreover, if $\boldsymbol{x}$ is a local minimizer, then the cost function remains constant or increases for such a $\boldsymbol{y}$ and we obtain $\boldsymbol{g}_0 \cdot \boldsymbol{y} \geq 0$. In order to simultaneously satisfy these two conditions, we require:

$$\lambda_1 \geq 0. \tag{2.7.6}$$

Moreover, the original inequality constraint is satisfied at the local minimizer

$$f_1 \leq 0. \tag{2.7.7}$$

Furthermore, when the inequality constraint is inactive ($f_1(\boldsymbol{x}) < 0$), since this situation is the same as when there are no inequality constraints, $\lambda_1 = 0$. On the other hand, when the inequality constraint is active ($f_1(\boldsymbol{x}) = 0$), Eq. (2.7.6) is established. These relationships are satisfied if

$$\lambda_1 f_1 = 0. \tag{2.7.8}$$

Eq. (2.7.4), Eq. (2.7.6), Eq. (2.7.8) and Eq. (2.7.7) are the conditions established at local minimizers when there is one active inequality constraint. These conditions correspond to the KKT conditions with $m = 1$ (described later).

Next we consider the case when two inequality constraints are active at a local minimizer, such as is shown in Fig. 2.19. In this case as well, imposing equality constraints is equivalent to the existence of certain $\lambda_1, \lambda_2 \in \mathbb{R}$ satisfying

$$\boldsymbol{g}_0 + \lambda_1 \boldsymbol{g}_1 + \lambda_2 \boldsymbol{g}_2 = \boldsymbol{0}_{\mathbb{R}^2}. \tag{2.7.9}$$

Let us rewrite Eq. (2.7.9) as

$$-\boldsymbol{g}_0 = \lambda_1 \boldsymbol{g}_1 + \lambda_2 \boldsymbol{g}_2. \tag{2.7.10}$$

If we fix $\boldsymbol{g}_1$ and $\boldsymbol{g}_2$ and take

$$\lambda_1 \geq 0, \quad \lambda_2 \geq 0, \tag{2.7.11}$$

then the vector on the right-hand side of Eq. (2.7.10) expresses the region drawn as $T'_S(\boldsymbol{x})$ in Fig. 2.19 (the definition of $T'_S(\boldsymbol{x})$ is given later as Eq. (2.7.15)). Eq. (2.7.10) is therefore a condition for which $C'_S(\boldsymbol{x})$ of Theorem 2.7.1 is rewritten as $T'_S(\boldsymbol{x})$. Moreover, at local minimizers the original inequality constraints are satisfied:

$$f_1 \leq 0, \quad f_2 \leq 0. \tag{2.7.12}$$

For the reasons explained above, the following equations hold at local minimizers:

$$\lambda_1 f_1 = 0, \quad \lambda_2 f_2 = 0. \tag{2.7.13}$$

Therefore, Eq. (2.7.9), Eq. (2.7.11), Eq. (2.7.13) and Eq. (2.7.12) are the conditions holding at local minimizers when two inequality constraints are active. These are the KKT conditions with $m = 2$ (described later).

In order to generalize the above results we now state a few required definitions and assumptions. Let a neighborhood of $\boldsymbol{x} \in S$ be denoted by $B_X \subset X$. Given $i \in I_{\mathrm{A}}(\boldsymbol{x})$ and $f_i \in C^1(B_X;\mathbb{R})$, let $\boldsymbol{g}_i(\boldsymbol{y})$ be linearly independent with respect to $\boldsymbol{y} \in B_X$. Then the linearized feasible direction set at $\boldsymbol{x}$ is the set

$$T_S(\boldsymbol{x}) = \{\boldsymbol{y} \in X \mid \boldsymbol{g}_i(\boldsymbol{x}) \cdot \boldsymbol{y} \leq 0 \text{ for all } i \in I_{\mathrm{A}}(\boldsymbol{x})\}.$$

Corresponding to the null space in the optimization problem with an equality constraint, $T_S(\boldsymbol{x})$ will be written as

$$T_S(\boldsymbol{x}) = \operatorname{Kco}\left(\boldsymbol{g}_{i_1}(\boldsymbol{x}), \ldots, \boldsymbol{g}_{i_k}(\boldsymbol{x})\right)^{\top}. \tag{2.7.14}$$

Moreover,

$$T_S'(\boldsymbol{x}) = \{\boldsymbol{z} \in X' \mid \boldsymbol{z} \cdot \boldsymbol{y} \leq 0 \text{ for all } \boldsymbol{y} \in T_S(\boldsymbol{x})\} \tag{2.7.15}$$

is called the dual cone of $T_S(\boldsymbol{x})$.

Let us now take a look at the difference between $T_S(\boldsymbol{x})$ and $C_S(\boldsymbol{x})$. We note that $T_S(\boldsymbol{x})$ is a closed convex polyhedral cone, but that $C_S(\boldsymbol{x})$ need not share this property [4]. For example, when

$$S = \left\{\boldsymbol{y} \in \mathbb{R}^2 \,\middle|\, f_1 = -y_1^2 + y_1^3 + y_2^2 \leq 0,\ f_2 = -y_1 - y_2 \leq 0\right\}, \tag{2.7.16}$$

we obtain

$$\begin{aligned} C_S(\mathbf{0}_{\mathbb{R}^2}) &= \left\{\boldsymbol{y} \in \mathbb{R}^2 \,\middle|\, y_1 + y_2 \geq 0,\ y_1 - y_2 \geq 0\right\} \\ &\qquad \cup \left\{\boldsymbol{y} \in \mathbb{R}^2 \,\middle|\, y_1 + y_2 = 0\right\}, \\ C_S'(\mathbf{0}_{\mathbb{R}^2}) &= \left\{\alpha(-1,-1)^{\top} \in \mathbb{R}^2 \,\middle|\, \alpha \geq 0\right\}. \end{aligned}$$

Figure 2.21 shows $C_S(\mathbf{0}_{\mathbb{R}^2})$ which is clearly not a closed convex polyhedral cone. In general, given $\boldsymbol{x} \in S$ we have

$$C_S(\boldsymbol{x}) \subseteq T_S(\boldsymbol{x}).$$

For example, when S is given by Eq. (2.7.16), we obtain

$$\begin{aligned} T_S(\mathbf{0}_{\mathbb{R}^2}) &= \left\{\boldsymbol{y} \in \mathbb{R}^2 \,\middle|\, y_1 + y_2 \geq 0\right\}, \\ T_S'(\mathbf{0}_{\mathbb{R}^2}) &= \left\{\alpha(-1,-1)^{\top} \in \mathbb{R}^2 \,\middle|\, \alpha \geq 0\right\}. \end{aligned}$$

Sufficient conditions for establishing the equality $T_S(\boldsymbol{x}) = C_S(\boldsymbol{x})$ are called first-order constraint qualifications. Cottle's constraint qualification, shown next, is one such condition [5].

Proposition 2.7.4 (Cottle's constraint qualification) Let S be given by Eq. (2.1.1) in Problem 2.1.2. Also, let $\boldsymbol{x} \in S$ and $I_{\mathrm{A}}(\boldsymbol{x})$ be given by Eq. (2.7.1). When $\boldsymbol{g}_i(\boldsymbol{x})$ is linear for all $i \in I_{\mathrm{A}}(\boldsymbol{x})$, if there exists $\boldsymbol{y} \in X$ such that $\boldsymbol{g}_i(\boldsymbol{x}) \cdot \boldsymbol{y} \leq 0$, one has $T_S(\boldsymbol{x}) = C_S(\boldsymbol{x})$. In the case that some $\boldsymbol{g}_i(\boldsymbol{x})$ is nonlinear, if there exists $\boldsymbol{y} \in X$ such that $\boldsymbol{g}_i(\boldsymbol{x}) \cdot \boldsymbol{y} < 0$, one has $T_S(\boldsymbol{x}) = C_S(\boldsymbol{x})$. □

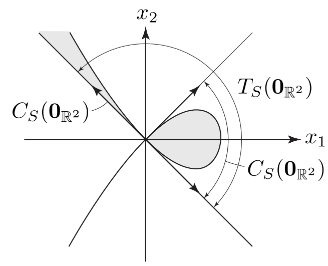


Fig. 2.21: An example when C_S is not a closed convex polyhedral cone: $C_S\left(\mathbf{0}_{\mathbb{R}^2}\right)$.

If linear constraint qualifications such as these are used, the conditions holding at local minimizers of Problem 2.1.2 can be expressed in the following way.

Theorem 2.7.5 (KKT conditions) In Problem 2.1.2, let $f_0, \ldots, f_m$ be elements of $C^1(X;\mathbb{R})$. Given $\boldsymbol{x} \in S$, let the linear constraint qualification be satisfied. If $\boldsymbol{x}$ is a local minimizer, then there exists $(\lambda_1, \ldots, \lambda_m)^\top \in \mathbb{R}^m$ satisfying

$$\boldsymbol{g}_0(\boldsymbol{x}) + \sum_{i\in\{1,\ldots,m\}} \lambda_i \boldsymbol{g}_i(\boldsymbol{x}) = \mathbf{0}_{\mathbb{R}^d}, \tag{2.7.17}$$

$$f_i(\boldsymbol{x}) \le 0 \quad \text{for } i \in \{1,\ldots,m\}, \tag{2.7.18}$$

$$\lambda_i f_i(\boldsymbol{x}) = 0 \quad \text{for } i \in \{1,\ldots,m\}, \tag{2.7.19}$$

$$\lambda_i \ge 0 \quad \text{for } i \in \{1,\ldots,m\}. \tag{2.7.20}$$

□

Proof Given arbitrary $\boldsymbol{t} = (t_1, \ldots, t_m)^\top \in \mathbb{R}^m$, the inequality constraint of Problem 2.1.2 can be written as

$$h_i(\boldsymbol{x}, t_i) = f_i(\boldsymbol{x}) + t_i^2 = 0 \quad \text{for } i \in \{1,\ldots,m\}. \tag{2.7.21}$$

Include $\boldsymbol{t}$ in the design variables and let the Lagrange function for Problem 2.1.2 be given by

$$\mathscr{L}(\boldsymbol{x}, \boldsymbol{t}, \boldsymbol{\lambda}) = f_0(\boldsymbol{x}) + \sum_{i\in\{1,\ldots,m\}} \lambda_i h_i(\boldsymbol{x}, t_i). \tag{2.7.22}$$

When $(\boldsymbol{x}, \boldsymbol{t})$ is a local minimizer of f_0 which satisfies the equality constraint Eq. (2.7.21), then by Theorem 2.6.4 the following hold:

$$\mathscr{L}_{\boldsymbol{x}}(\boldsymbol{x}, \boldsymbol{t}, \boldsymbol{\lambda}) = \boldsymbol{g}_0(\boldsymbol{x}) + \sum_{i\in\{1,\ldots,m\}} \lambda_i \boldsymbol{g}_i(\boldsymbol{x}) = \mathbf{0}_{\mathbb{R}^d}, \tag{2.7.23}$$

$$\mathscr{L}_{t_i}(\boldsymbol{x}, \boldsymbol{t}, \boldsymbol{\lambda}) = 2\lambda_i t_i = 0 \quad \text{for } i \in \{1,\ldots,m\}, \tag{2.7.24}$$

$$\mathscr{L}_{\lambda_i}(\boldsymbol{x}, \boldsymbol{t}, \boldsymbol{\lambda}) = f_i(\boldsymbol{x}) + t_i^2 = 0 \quad \text{for } i \in \{1,\ldots,m\}. \tag{2.7.25}$$

Equations Eq. (2.7.23) and Eq. (2.7.25) are equivalent to Eq. (2.7.17) and Eq. (2.7.18), respectively. Moreover, Eq. (2.7.19) can be obtained by multiplying both sides of Eq. (2.7.24) by t_i and using Eq. (2.7.21).

The fact that Eq. (2.7.20) holds can be confirmed as follows. If $\boldsymbol{x}$ is a local minimizer of Problem 2.1.2 and the linear constraint qualification is satisfied, then by Theorem 2.7.1, Eq. (2.7.14) and Farkas's lemma (Lemma A.3.2)

$$\begin{aligned}-\boldsymbol{g}_0(\boldsymbol{x}) \in C_S'(\boldsymbol{x}) = T_S'(\boldsymbol{x}) = (T_S(\boldsymbol{x}))' &= \left(\mathrm{Kco}\left(\boldsymbol{g}_{i_1}(\boldsymbol{x}), \ldots, \boldsymbol{g}_{i_k}(\boldsymbol{x})\right)^\top\right)' \\ &= \mathrm{Ico}\left(\boldsymbol{g}_{i_1}, \ldots, \boldsymbol{g}_{i_k}\right),\end{aligned}$$

where $i_i, \ldots, i_k \in I_\mathrm{A}(\boldsymbol{x})$. Here we have written

$$\mathrm{Ico}\left(\boldsymbol{g}_{i_1}, \ldots, \boldsymbol{g}_{i_k}\right) = \left\{ \left(\boldsymbol{g}_{i_1}, \ldots, \boldsymbol{g}_{i_k}\right)\boldsymbol{\lambda} \in X' \;\middle|\; \boldsymbol{\lambda} \geq \boldsymbol{0}_{\mathbb{R}^k} \right\},$$

where $\boldsymbol{\lambda} = (\lambda_{i_1}, \ldots, \lambda_{i_k})^\top$. Also $\lambda_i = 0$ when $i \notin I_\mathrm{A}(\boldsymbol{x})$. This relationship shows that Eq. (2.7.20) holds. □

Equations (2.7.17) to (2.7.20) are called the Karush–Kuhn–Tucker conditions. Equation (2.7.18) states that $\boldsymbol{x}$ satisfies the inequality constraints. Equation (2.7.19) is called a complementarity condition and has the effect of removing $\boldsymbol{g}_i$ from Eq. (2.7.17) by setting $\lambda_i = 0$ with respect to an inactive constraint $f_i(\boldsymbol{x}) < 0$. Finally, as described in the considerations used in Fig. 2.19, the conditions which combine Eq. (2.7.17) and Eq. (2.7.20) are those establishing when $-\boldsymbol{g}_0$ is contained in $T_S'(\boldsymbol{x})$, and are the conditions that allow one to rewrite $C_S'(\boldsymbol{x})$ (Theorem 2.7.1) as $T_S'(\boldsymbol{x})$. The variable $\boldsymbol{t}$ is called a slack variable.

Let us also define the Lagrange function approach for optimization problems under inequality constraints. Its relationship with the duality theorem (shown later) will be considered, and we set

$$\mathscr{L}(\boldsymbol{x}, \boldsymbol{\lambda}) = \begin{cases} f_0(\boldsymbol{x}) + \sum_{i \in \{1,\ldots,m\}} \lambda_i f_i(\boldsymbol{x}) & (\boldsymbol{\lambda} \geq \boldsymbol{0}_{\mathbb{R}^m}), \\ -\infty \quad (\boldsymbol{\lambda} \not\geq \boldsymbol{0}_{\mathbb{R}^m}). \end{cases} \tag{2.7.26}$$

Here, $\boldsymbol{\lambda} = (\lambda_1, \ldots, \lambda_m)^\top \in \mathbb{R}^m$ is a Lagrange multiplier and we remark that Eq. (2.7.17) and Eq. (2.7.18) can be rewritten in terms of $\mathscr{L}(\boldsymbol{x}, \boldsymbol{\lambda})$. The method of using solutions of the next problem as candidates for solutions to Problem 2.1.2 is called the Lagrange multiplier method for an optimization problem with an inequality constraint.

Problem 2.7.6 (Lagrange multiplier method for inequality constraints) Let $\mathscr{L}(\boldsymbol{x}, \boldsymbol{\lambda})$ be given by Eq. (2.7.26) in Problem 2.1.2. Find $(\boldsymbol{x}, \boldsymbol{\lambda})$ which satisfies the KKT conditions

$$\mathscr{L}_{\boldsymbol{x}}(\boldsymbol{x}, \boldsymbol{\lambda}) = \boldsymbol{g}_0(\boldsymbol{x}) + \sum_{i \in \{1,\ldots,m\}} \lambda_i \boldsymbol{g}_i(\boldsymbol{x}) = \boldsymbol{0}_{\mathbb{R}^d}, \tag{2.7.27}$$

$$\mathscr{L}_{\lambda_i}(\boldsymbol{x}, \boldsymbol{\lambda}) = f_i(\boldsymbol{x}) \leq 0 \quad \text{for } i \in \{1, \ldots, m\}, \tag{2.7.28}$$

$$\lambda_i f_i(\boldsymbol{x}) = 0 \quad \text{for } i \in \{1, \ldots, m\}, \tag{2.7.29}$$

$$\lambda_i \geq 0 \quad \text{for } i \in \{1, \ldots, m\}. \tag{2.7.30}$$

□

We can obtain the following necessary condition holding at local minimizers of Problem 2.1.2. With respect to $(\boldsymbol{x}, \boldsymbol{\lambda}) \in X \times \mathbb{R}^m$ satisfying the KKT conditions, in addition to $I_{\mathrm{A}}(\boldsymbol{x})$ and S of Eq. (2.7.1) and Eq. (2.1.1) respectively, we define

$$\bar{I}_{\mathrm{A}}(\boldsymbol{\lambda}) = \{ i \in \{1, \ldots, m\} \mid \lambda_i > 0 \}, \tag{2.7.31}$$

$$\bar{S} = S \cap \left\{ \boldsymbol{x} \in X \mid f_i(\boldsymbol{x}) = 0, \ i \in \bar{I}_{\mathrm{A}}(\boldsymbol{x}) \right\} \tag{2.7.32}$$

and $T_{\bar{S}}(\boldsymbol{x})$ as the feasible direction set of $\bar{S}$ at $\boldsymbol{x}$. Moreover, we write the Hesse matrix with respect to $\boldsymbol{x}$ of the Lagrange function $\mathscr{L}(\boldsymbol{x}, \boldsymbol{\lambda})$ by $\boldsymbol{H}_{\mathscr{L}}(\boldsymbol{x}, \boldsymbol{\lambda}) = \partial_X \partial_X^{\top} \mathscr{L}(\boldsymbol{x}, \boldsymbol{\lambda})$.

Theorem 2.7.7 (2nd-order necessary condition for local minimizers) Let $f_0, \ldots, f_m$ be elements of $C^2(X; \mathbb{R})$ in Problem 2.1.2. Given $\boldsymbol{x} \in X$, assume that $\boldsymbol{g}_i$ is linearly independent with respect to $i \in I_{\mathrm{A}}(\boldsymbol{x})$ and satisfies the linear constraint qualification. In this case, if $\boldsymbol{x}$ is a local minimizer of Problem 2.1.2, then the following holds for an arbitrary tangential vector $\boldsymbol{y} \in T_{\bar{S}}(\boldsymbol{x})$:

$$\boldsymbol{y} \cdot (\boldsymbol{H}_{\mathscr{L}}(\boldsymbol{x}, \boldsymbol{\lambda}) \boldsymbol{y}) \geq 0.$$

□

Proof Let $\{\boldsymbol{y}_k\}_{k \in \mathbb{N}} \in \bar{S}$ satisfy $\lambda_i f_i(\boldsymbol{y}_k) = 0$ for each $i \in \{1, \ldots, m\}$ and $\boldsymbol{t} / \|\boldsymbol{t}\|_{\mathbb{R}^d} = \lim_{k \to \infty} (\boldsymbol{y}_k - \boldsymbol{x}) / \|\boldsymbol{y}_k - \boldsymbol{x}\|_{\mathbb{R}^d}$. From the fact that $\boldsymbol{x}$ is a local minimizer, there exists a neighborhood B of $\boldsymbol{x}$ and $\theta \in (0, 1)$ such that

$$\begin{aligned} f_0(\boldsymbol{y}_k) - f_0(\boldsymbol{x}) &= \mathscr{L}(\boldsymbol{y}_k, \boldsymbol{\lambda}) - \mathscr{L}(\boldsymbol{x}, \boldsymbol{\lambda}) \\ &= \frac{1}{2} (\boldsymbol{y}_k - \boldsymbol{x}) \cdot \{ \boldsymbol{H}_{\mathscr{L}}(\boldsymbol{x} + \theta(\boldsymbol{y}_k - \boldsymbol{x}), \boldsymbol{\lambda}) (\boldsymbol{y}_k - \boldsymbol{x}) \} \geq 0 \end{aligned} \tag{2.7.33}$$

for arbitrary $\boldsymbol{y}_k \in B$. Multiplying both sides by $2\boldsymbol{t} / \|\boldsymbol{y}_k - \boldsymbol{x}\|_{\mathbb{R}^d}^2$ and taking $k \to \infty$ yields the result. □

2.7.4 Sufficient Conditions for Local Minimizers

The following sufficient conditions for yielding local minimizers Problem 2.1.2 can be obtained. $T_{\bar{S}}(\boldsymbol{x})$ denotes the linearized admissible direction set of $\bar{S}$ defined in Eq. (2.7.32) at $\boldsymbol{x}$.

Theorem 2.7.8 (2nd-order sufficient conditions for local minimizers) Let $f_0, \ldots, f_m$ be elements of $C^2(X; \mathbb{R})$ in Problem 2.1.2. Given $\boldsymbol{x} \in X$, let $\boldsymbol{g}_i$ be linearly independent with respect to $i \in I_{\mathrm{A}}(\boldsymbol{x})$ and satisfy the first-order constraint qualification. If there exists $(\boldsymbol{x}, \boldsymbol{\lambda})$ satisfying the KKT conditions and if

$$\boldsymbol{y} \cdot (\boldsymbol{H}_{\mathscr{L}} (\boldsymbol{x}, \boldsymbol{\lambda}) \boldsymbol{y}) > 0$$

for arbitrary $\boldsymbol{y} \in T_{\bar{S}} (\boldsymbol{x})$, then $\boldsymbol{x}$ is a local minimizer. □

Proof Eq. (2.7.33) is obtained when $(\boldsymbol{x}, \boldsymbol{\lambda})$ satisfies the KKT conditions. Since $\boldsymbol{H}_{\mathscr{L}} (\boldsymbol{x}, \boldsymbol{\lambda})$ is positive definite, $\boldsymbol{x}$ is a local minimizer. □

2.7.5 Sufficient Conditions for Global Minimizers Using the KKT Conditions

Sufficient conditions for global minimizers can be obtained when Problem 2.1.2 is a convex optimization problem.

Theorem 2.7.9 (1st-order sufficient conditions for global minimizers) In Problem 2.1.2, let $f_0, \ldots, f_m$ be convex functions from $C^1 (X; \mathbb{R})$. Given $\boldsymbol{x} \in X$, assume that $\boldsymbol{g}_i$ is linearly independent with respect to $i \in I_{\mathrm{A}} (\boldsymbol{x})$, that the linear constraint qualification is satisfied, and that $(\boldsymbol{x}, \boldsymbol{\lambda})$ satisfies the KKT conditions. If $\boldsymbol{x}$ satisfies these conditions, then it is a global minimizer. □

Proof Fix $\lambda_1, \ldots, \lambda_m$ satisfying the KKT conditions and let

$$\mathscr{L} (\boldsymbol{y}) = f_0 (\boldsymbol{y}) + \sum_{i \in \{1, \ldots, m\}} \lambda_i f_i (\boldsymbol{y}) .$$

By the KKT conditions, it follows that $\partial_X \mathscr{L} (\boldsymbol{x}) = \boldsymbol{0}_{\mathbb{R}^d}$. Since $\mathscr{L}$ is convex, Corollary 2.7.3 ensures that $\boldsymbol{x}$ minimizes $\mathscr{L}$. In other words, the following inequality holds for arbitrary $\boldsymbol{y} \in S$:

$$f_0 (\boldsymbol{x}) + \sum_{i \in \{1, \ldots, m\}} \lambda_i f_i (\boldsymbol{x}) \leq f_0 (\boldsymbol{y}) + \sum_{i \in \{1, \ldots, m\}} \lambda_i f_i (\boldsymbol{y}) .$$

The KKT conditions also imply that $\lambda_i f_i (\boldsymbol{x}) = 0$ and $\lambda_i \geq 0$ for each $i \in \{1, \ldots, m\}$. Therefore

$$f_0 (\boldsymbol{x}) \leq f_0 (\boldsymbol{y})$$

holds for arbitrary $\boldsymbol{y} \in S$. □

Theorem 2.7.9 can be used to obtain the following sufficient conditions for showing the existence of global minimizers of optimization problems under equality constraints (Problem 2.6.1).

Corollary 2.7.10 (1st-order sufficient conditions for global minimizers) Assume that f_0 is a convex function from $C^1 (X; \mathbb{R})$, that $\boldsymbol{h} \in C^1 (X; \mathbb{R}^n)$ is a linear function, and that $\partial_X h_1 (\boldsymbol{x}), \ldots, \partial_X h_n (\boldsymbol{x})$ are linearly independent at $\boldsymbol{x} \in X$ and satisfy the linear constraint qualifications. If $(\boldsymbol{x}, \boldsymbol{\lambda})$ is a solution of Problem 2.6.5, then it yields the minimum in Problem 2.6.1. □

Proof The equality constraint is equivalent to the following two inequalities:

$$\boldsymbol{h}(\boldsymbol{x}) \leq \mathbf{0}_{\mathbb{R}^n}, \quad -\boldsymbol{h}(\boldsymbol{x}) \leq \mathbf{0}_{\mathbb{R}^n}.$$

Let the Lagrange multipliers with respect to these be $\boldsymbol{\lambda}_+ = (\lambda_{+1}, \ldots, \lambda_{+n})^\top \in \mathbb{R}^n$, and $\boldsymbol{\lambda}_- = (\lambda_{-1}, \ldots, \lambda_{-n})^\top \in \mathbb{R}^n$. Since $h_1, \ldots, h_n$ are linear functions, they are also convex. This follows from the fact that

$$\partial_X h_i(\boldsymbol{x}) \cdot (\boldsymbol{y} - \boldsymbol{x}) = h_i(\boldsymbol{y}) - h_i(\boldsymbol{x})$$

for arbitrary $\boldsymbol{x} \in X$ and $\boldsymbol{y} \in X$ (Theorem 2.4.4). Hence, the optimization is convex optimization, including an inequality constraint. The KKT conditions can then be written as

$$\begin{aligned}
\mathscr{L}_{\boldsymbol{x}}(\boldsymbol{x}, \boldsymbol{\lambda}_+, \boldsymbol{\lambda}_-) &= \boldsymbol{g}_0(\boldsymbol{x}) + \partial_X \boldsymbol{h}^\top(\boldsymbol{x})(\boldsymbol{\lambda}_+ - \boldsymbol{\lambda}_-) = \mathbf{0}_{\mathbb{R}^d}, \\
\mathscr{L}_{\lambda_{+i}}(\boldsymbol{x}, \boldsymbol{\lambda}_+, \boldsymbol{\lambda}_-) &= h_i(\boldsymbol{x}) \leq 0 \quad \text{for } i \in \{1, \ldots, n\}, \\
\mathscr{L}_{\lambda_{-i}}(\boldsymbol{x}, \boldsymbol{\lambda}_+, \boldsymbol{\lambda}_-) &= -h_i(\boldsymbol{x}) \leq 0 \quad \text{for } i \in \{1, \ldots, n\}, \\
\lambda_{+i} h_i(\boldsymbol{x}) &= 0 \quad \text{for } i \in \{1, \ldots, n\}, \quad \lambda_{-i} h_i(\boldsymbol{x}) = 0 \quad \text{for } i \in \{1, \ldots, n\}, \\
\lambda_{+i} &\geq 0 \quad \text{for } i \in \{1, \ldots, n\}, \quad \lambda_{-i} \geq 0 \quad \text{for } i \in \{1, \ldots, n\}.
\end{aligned}$$

Writing $\boldsymbol{\lambda}_+ - \boldsymbol{\lambda}_- = \boldsymbol{\lambda}$, we see that $(\boldsymbol{x}, \boldsymbol{\lambda})$ is equivalent to the solution of Problem 2.6.5. □

2.7.6 Example of an Optimization Problem Under an Inequality Constraint

Let us now consider the KKT conditions in relation to the spring combination problem.

Exercise 2.7.11 (Spring combination problem) Consider Exercise 2.6.8 and find the global minimizer when the spring combination conditions are changed to inequalities. In other words, find $\boldsymbol{u}$ satisfying the following minimization problem:

$$\min_{\boldsymbol{u} \in \mathbb{R}^2} \left\{ f_0(\boldsymbol{u}) = \frac{1}{2} k_1 u_1^2 + \frac{1}{2} k_2 u_2^2 \;\middle|\; f_1(\boldsymbol{u}) = a - (u_1 + u_2) \leq 0 \right\}.$$

Also find $\boldsymbol{u}$ satisfying

$$\min_{\boldsymbol{u} \in \mathbb{R}^2} \left\{ f_0(\boldsymbol{u}) = \frac{1}{2} k_1 u_1^2 + \frac{1}{2} k_2 u_2^2 \;\middle|\; f_1(\boldsymbol{u}) = (u_1 + u_2) - a \leq 0 \right\}.$$

□

Answer When $f_1 = a - (u_1 + u_2) \leq 0$, if we let $\lambda \in \mathbb{R}$ be the Lagrange multiplier, then the Lagrange function becomes

$$\mathscr{L}(\boldsymbol{u}, \lambda) = \frac{1}{2} k_1 u_1^2 + \frac{1}{2} k_2 u_2^2 + \lambda (a - u_1 - u_2).$$

The stationary conditions of $\mathscr{L}(\boldsymbol{u}, \lambda)$ are the same as the results from Exercise 2.6.8, and when $k_1 > 0$, $k_2 > 0$ and $a > 0$ we obtain

$$u_1 = \frac{k_2}{k_1 + k_2} a > 0, \quad u_2 = \frac{k_1}{k_1 + k_2} a > 0, \quad \lambda = \frac{k_1 k_2}{k_1 + k_2} a > 0.$$

This result satisfies the KKT conditions. As investigated in Exercise 2.6.8, this problem is also a convex optimization problem and therefore, by Theorem 2.7.9, $\boldsymbol{u}$ yields the minimum.

On the other hand, when $f_1 = (u_1 + u_2) - a \leq 0$, the Lagrange function becomes

$$\mathscr{L}(\boldsymbol{u}, \lambda) = \frac{1}{2} k_1 u_1^2 + \frac{1}{2} k_2 u_2^2 + \lambda (u_1 + u_2 - a).$$

When $k_1 > 0$, $k_2 > 0$ and $a > 0$, the stationary conditions for $\mathscr{L}(\boldsymbol{u}, \lambda)$ are

$$u_1 = \frac{k_2}{k_1 + k_2} a > 0, \quad u_2 = \frac{k_1}{k_1 + k_2} a > 0, \quad \lambda = -\frac{k_1 k_2}{k_1 + k_2} a < 0.$$

Since $\lambda < 0$, this result does not satisfy the KKT conditions. Therefore, the coupled constraints can be viewed as inactive and we can set $\lambda = 0$. The problem can then be rewritten as

$$\min_{\boldsymbol{u} \in \mathbb{R}^2} \left\{ f_0(\boldsymbol{u}) = \frac{1}{2} k_1 u_1^2 + \frac{1}{2} k_2 u_2^2 \right\}.$$

Here, since

$$\boldsymbol{g}_0(\boldsymbol{u}) = \begin{pmatrix} k_1 & 0 \\ 0 & k_2 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix},$$

we obtain $\boldsymbol{u} = \boldsymbol{0}_{\mathbb{R}^2}$. □

2.7.7 Considerations Relating to the Solutions of Optimization Problems Under Inequality Constraints

The results of this section lead to the following observations regarding the solution of optimization problems under inequality constraints (Problem 2.1.2):

(1) By Theorem 2.7.5, the solution $(\boldsymbol{x}, \boldsymbol{\lambda})$ of the Lagrange multiplier method (Problem 2.7.6) satisfies a necessary condition for attaining a local minimum. Such $\boldsymbol{x}$ are candidates for local minimizers.

(2) When $(\boldsymbol{x}, \boldsymbol{\lambda})$ is the solution from the Lagrange multiplier method (Problem 2.7.6), if the Hesse matrix $\partial_X \partial_X^\top \mathscr{L}(\boldsymbol{x}, \boldsymbol{\lambda}) = \boldsymbol{H}_{\mathscr{L}}(\boldsymbol{x}, \boldsymbol{\lambda})$ of the Lagrange function with respect to $\boldsymbol{x}$ satisfies $\boldsymbol{y} \cdot (\boldsymbol{H}_{\mathscr{L}}(\boldsymbol{x}, \boldsymbol{\lambda}) \boldsymbol{y}) > 0$ for arbitrary $\boldsymbol{y} \in T_{\bar{S}}(\boldsymbol{x})$, then Theorem 2.7.8 implies that $\boldsymbol{x}$ is a local minimizer.

(3) When an optimization problem under an inequality constraint (Problem 2.1.2) is convex, Theorem 2.7.9 implies that the solution $\boldsymbol{x}$ from the Lagrange multiplier method yields the global minimum.

2.8 Optimization Problems Under Equality and Inequality Constraints

In optimal design problems, state equations are set using equality constraints, and cost function constraints are set through inequality constraints. The optimization problem defined at the beginning of Sect. 2.1 (Problem 2.1.1) was defined with this in mind. Keeping in mind its correspondence with optimal design problems, we write Problem 2.1.1 in the following way.

Problem 2.8.1 (Optimization under equality and inequality constraints) Given $d > n$, let $\Xi = \mathbb{R}^{d-n}$ and $U = \mathbb{R}^n$. When $\boldsymbol{K} : \Xi \to \mathbb{R}^{n \times n}$ and $\boldsymbol{b} : \Xi \to \mathbb{R}^n$ are given together with $f_0, f_1, \dots, f_m : \Xi \times U \to \mathbb{R}$, find $(\boldsymbol{\xi}, \boldsymbol{u})$ satisfying

$$\min_{(\boldsymbol{\xi},\boldsymbol{u}) \in \Xi \times U} \big\{ f_0(\boldsymbol{\xi}, \boldsymbol{u}) \mid \boldsymbol{h}(\boldsymbol{\xi}, \boldsymbol{u}) = -\boldsymbol{K}(\boldsymbol{\xi})\boldsymbol{u} + \boldsymbol{b}(\boldsymbol{\xi}) = \boldsymbol{0}_{\mathbb{R}^n}, \\ f_1(\boldsymbol{\xi}, \boldsymbol{u}) \le 0, \dots, f_m(\boldsymbol{\xi}, \boldsymbol{u}) \le 0 \big\}.$$

□

Consider Problem 2.8.1 and let the set of $(\boldsymbol{\xi}, \boldsymbol{u})$ satisfying the equality constraints be given by

$$V = \{(\boldsymbol{\xi}, \boldsymbol{u}) \in \Xi \times U \mid \boldsymbol{h}(\boldsymbol{\xi}, \boldsymbol{u}) = -\boldsymbol{K}(\boldsymbol{\xi})\boldsymbol{u} + \boldsymbol{b}(\boldsymbol{\xi}) = \boldsymbol{0}_{\mathbb{R}^n}\}.$$

For $i \in \{0, 1, \dots, m\}$ let

$$\tilde{f}_i(\boldsymbol{\xi}) = \{f_i(\boldsymbol{\xi}, \boldsymbol{u}) \mid (\boldsymbol{\xi}, \boldsymbol{u}) \in V\}. \tag{2.8.1}$$

Then the derivative of $\tilde{f}_i(\boldsymbol{\xi})$ with respect to $\boldsymbol{\xi}$ can be obtained:

$$\tilde{\boldsymbol{g}}_i = \frac{\partial f_i}{\partial \boldsymbol{\xi}} + \left(\frac{\partial \boldsymbol{b}}{\partial \boldsymbol{\xi}^\top} - \frac{\partial \boldsymbol{K}}{\partial \boldsymbol{\xi}^\top} \boldsymbol{u} \right)^\top \boldsymbol{v}_i \in \mathbb{R}^{d-n}, \tag{2.8.2}$$

The above is arrived at in the same manner as Eq. (2.6.25) from Sect. 2.6.5. Here, $\left(\partial \boldsymbol{K} / \partial \boldsymbol{\xi}^\top\right) \boldsymbol{u}$ is defined by Eq. (2.6.21) and $\boldsymbol{v}_i \in U$ is the solution of the equivalent adjoint problem to Eq. (2.6.23):

$$\boldsymbol{K}^\top \boldsymbol{v}_i = \frac{\partial f_i}{\partial \boldsymbol{u}}. \tag{2.8.3}$$

The functions $\tilde{\boldsymbol{g}}_0, \dots, \tilde{\boldsymbol{g}}_m$ obtained in this way are the derivatives with respect to $\boldsymbol{\xi}$ when the cost functions are taken to be $\tilde{f}_0(\boldsymbol{\xi}), \dots, \tilde{f}_m(\boldsymbol{\xi})$. These facts allow one to rewrite Problem 2.8.1 as follows.

Problem 2.8.2 (Optimization under inequality constraints) Let $\Xi = \mathbb{R}^{d-n}$ and $\tilde{f}_0, \tilde{f}_1, \dots, \tilde{f}_m : \Xi \to \mathbb{R}$ be given. Find $\boldsymbol{\xi}$ satisfying

$$\min_{\boldsymbol{\xi} \in \Xi} \left\{ \tilde{f}_0(\boldsymbol{\xi}) \;\middle|\; \tilde{f}_1(\boldsymbol{\xi}) \le 0, \dots, \tilde{f}_m(\boldsymbol{\xi}) \le 0 \right\}.$$

□

Let the Lagrange function with respect to Problem 2.8.2 be

$$\tilde{\mathscr{L}}(\boldsymbol{\xi}, \boldsymbol{\lambda}) = \tilde{f}_0(\boldsymbol{\xi}) + \sum_{i \in \{1,\ldots,m\}} \lambda_i \tilde{f}_i(\boldsymbol{\xi}). \tag{2.8.4}$$

Then the KKT conditions with respect to Problem 2.8.2 become

$$\tilde{\mathscr{L}}_{\boldsymbol{\xi}}(\boldsymbol{\xi}, \boldsymbol{\lambda}) = \tilde{\boldsymbol{g}}_0 + \sum_{i \in \{1,\ldots,m\}} \lambda_i \tilde{\boldsymbol{g}}_i = \mathbf{0}_{\mathbb{R}^{d-n}}, \tag{2.8.5}$$

$$\tilde{\mathscr{L}}_{\lambda_i}(\boldsymbol{\xi}, \boldsymbol{\lambda}) = \tilde{f}_i(\boldsymbol{\xi}) \le 0 \quad \text{for } i \in \{1,\ldots,m\}, \tag{2.8.6}$$

$$\lambda_i \tilde{f}_i(\boldsymbol{\xi}) = 0 \quad \text{for } i \in \{1,\ldots,m\}, \tag{2.8.7}$$

$$\lambda_i \ge 0 \quad \text{for } i \in \{1,\ldots,m\}. \tag{2.8.8}$$

Therefore, the Lagrange multiplier method for seeking candidates for local minimizers of Problem 2.8.2 can be expressed as follows.

Problem 2.8.3 (Lagrange multiplier method with inequality constraints) Let $\tilde{\mathscr{L}}(\boldsymbol{\xi}, \boldsymbol{\lambda})$ be given by Eq. (2.8.4) with respect to Problem 2.8.2. Find $(\boldsymbol{\xi}, \boldsymbol{\lambda})$ satisfying the KKT conditions (Eqs. (2.8.5)–(2.8.8)). □

Therefore the results of Theorems 2.7.5–2.7.8 can be obtained with respect to the solution $(\boldsymbol{\xi}, \boldsymbol{\lambda})$ of Problem 2.8.3. We will postpone our discussion of what these results say about the solution of optimization problems under equality and inequality constraints (Problem 2.8.1) until Sect. 2.8.2.

2.8.1 The Lagrange Multiplier Method for Optimization Problems Under Equality and Inequality Constraints

The conditions satisfied by the minimizer of Problem 2.8.1 are as described above. Let us now define the Lagrange function for Problem 2.8.1 and consider how it can be related to the Lagrange multiplier method for Problem 2.8.3. We remark that the content shown here was also shown in Chap. 1. The concepts are the same as those used in deriving derivatives of cost functionals with respect to design variables in the optimal design problems of Chap. 7 and beyond. The purpose of this section is to clarify the relationship of such concepts with the content of Chap. 2.

Let the Lagrange function with respect to Problem 2.8.1 be given by

$$\mathscr{L}(\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v}_0, \ldots, \boldsymbol{v}_m, \boldsymbol{\lambda}) = \mathscr{L}_0(\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v}_0) + \sum_{i \in \{1,\ldots,m\}} \lambda_i \mathscr{L}_i(\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v}_i), \tag{2.8.9}$$

where $\boldsymbol{\lambda} = (\lambda_1, \ldots, \lambda_m)^\top \in \mathbb{R}^m$ denotes the Lagrange multiplier with respect to $f_1 \le 0, \ldots, f_m \le 0$. Also, let

$$\mathscr{L}_i(\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v}_i) = f_i(\boldsymbol{\xi}, \boldsymbol{u}) + \mathscr{L}_{\mathrm{S}}(\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v}_i) \tag{2.8.10}$$

denote the Lagrange function with respect to $f_i(\boldsymbol{\xi}, \boldsymbol{u})$. Moreover, let the Lagrange function with respect to the equality constraint be given by

$$\mathscr{L}_{\mathrm{S}}(\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v}_i) = -\boldsymbol{v}_i \cdot (\boldsymbol{K}(\boldsymbol{\xi})\,\boldsymbol{u} - \boldsymbol{b}(\boldsymbol{\xi})), \tag{2.8.11}$$

and $\boldsymbol{v}_0, \ldots, \boldsymbol{v}_m$ be Lagrange multipliers (adjoint variables) defined for $f_0, \ldots, f_m$, respectively.

The function $\tilde{\boldsymbol{g}}_i$ from Eq. (2.8.2) is obtained as follows. The derivative (total differential) of $\mathscr{L}_i$ with respect to an arbitrary variation $(\boldsymbol{\eta}, \hat{\boldsymbol{u}}, \hat{\boldsymbol{v}}_i) \in \Xi \times U \times U$ of $(\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v}_i)$ is given by

$$\begin{aligned}\mathscr{L}_i'(\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v}_i)[\boldsymbol{\eta}, \hat{\boldsymbol{u}}, \hat{\boldsymbol{v}}_i] &= \mathscr{L}_{i\boldsymbol{\xi}}(\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v}_i)[\boldsymbol{\eta}] + \mathscr{L}_{i\boldsymbol{u}}(\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v}_i)[\hat{\boldsymbol{u}}] \\ &\quad + \mathscr{L}_{i\boldsymbol{v}_i}(\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v}_i)[\hat{\boldsymbol{v}}_i].\end{aligned} \tag{2.8.12}$$

The third term on the right-hand side of Eq. (2.8.12) becomes

$$\mathscr{L}_{i\boldsymbol{v}_i}(\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v}_i)[\hat{\boldsymbol{v}}_i] = -\hat{\boldsymbol{v}}_i \cdot (\boldsymbol{K}(\boldsymbol{\xi})\,\boldsymbol{u} - \boldsymbol{b}(\boldsymbol{\xi})) = \mathscr{L}_{\mathrm{S}}(\boldsymbol{\xi}, \boldsymbol{u}, \hat{\boldsymbol{v}}_i). \tag{2.8.13}$$

Equation (2.8.13) takes the value zero when $\boldsymbol{u}$ satisfies the equality constraint. The second term on the right-hand side of Eq. (2.8.12) is expressed as

$$\mathscr{L}_{i\boldsymbol{u}}(\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v}_i)[\hat{\boldsymbol{u}}] = -\hat{\boldsymbol{u}} \cdot \left(\boldsymbol{K}^{\top}(\boldsymbol{\xi})\,\boldsymbol{v}_i - \frac{\partial f_i}{\partial \boldsymbol{u}}\right). \tag{2.8.14}$$

Equation (2.8.14) also takes the value zero when $\boldsymbol{v}_i$ satisfies Eq. (2.8.3). The first term on the right-hand side of Eq. (2.8.12) is given by

$$\mathscr{L}_{i\boldsymbol{\xi}}(\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v}_i)[\boldsymbol{\eta}] = \left(\frac{\partial f_i}{\partial \boldsymbol{\xi}} + \left(\frac{\partial \boldsymbol{b}}{\partial \boldsymbol{\xi}^{\top}} - \frac{\partial \boldsymbol{K}}{\partial \boldsymbol{\xi}^{\top}}\boldsymbol{u}\right)^{\top} \boldsymbol{v}_i\right) \cdot \boldsymbol{\eta}. \tag{2.8.15}$$

The above results show that placing the equality constraint on $\boldsymbol{u}$ is equivalent to the condition that $\mathscr{L}_{i\boldsymbol{v}_i}(\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v}_i)[\hat{\boldsymbol{v}}_i] = 0$ for all $\hat{\boldsymbol{v}}_i \in U$, and that placing an adjoint equation on $\boldsymbol{v}_i$ is equivalent to $\mathscr{L}_{i\boldsymbol{u}}(\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v}_i)[\hat{\boldsymbol{u}}] = 0$ for all $\hat{\boldsymbol{u}} \in U$. These results also show that $\boldsymbol{u}$ and $\boldsymbol{v}_i$ can be used to obtain $\tilde{f}_i'(\boldsymbol{\xi})[\boldsymbol{\eta}]$ (the derivative of $\tilde{f}_i$) from $\mathscr{L}_{i\boldsymbol{\xi}}(\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v}_i)[\boldsymbol{\eta}] = \tilde{\boldsymbol{g}}_i \cdot \boldsymbol{\eta}$.

2.8.2 Considerations Regarding Optimization Problems Under Equality and Inequality Constraints

Based on the results obtained thus far, the following can be said with respect to the solution of optimization problems (Problem 2.8.1) under equality and inequality constraints:

(1) Let $\tilde{f}_0, \ldots, \tilde{f}_m$ be given by Eq. (2.8.1). Then an optimization problem under equality and inequality constraints (Problem 2.8.1) can be rewritten as an optimization problem under an inequality constraint (Problem 2.8.2).

(2) Let $i \in \{0, 1, \ldots, m\}$ and the Lagrange function of Problem 2.8.1 be given by $\mathscr{L}_i$ from Eq. (2.8.10). Then $\tilde{f}_i' (\boldsymbol{\xi}) [\boldsymbol{\eta}]$ (the derivative of $\tilde{f}_i$) can be obtained from $\mathscr{L}_{i\boldsymbol{\xi}} (\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v}_i) [\boldsymbol{\eta}] = \tilde{\boldsymbol{g}}_i \cdot \boldsymbol{\eta}$ by using $\boldsymbol{u}$ and $\boldsymbol{v}_i$ which satisfy the equality constraint and the adjoint equation, respectively (or, by using $\mathscr{L}_{i\boldsymbol{u}} (\boldsymbol{\xi}, \boldsymbol{u}, \boldsymbol{v}_i) [\hat{\boldsymbol{u}}] = 0$ with respect arbitrary $\hat{\boldsymbol{u}} \in U$).

(3) Let $(\boldsymbol{\xi}, \boldsymbol{\lambda})$ denote the solution of an optimization problem under an inequality constraint (Problem 2.8.2) which has been obtained via the Lagrange multiplier method (Problem 2.8.3) (details of the methodology are given in Chap. 3). When the Hesse matrix $\partial_\Xi \partial_\Xi^\top \tilde{\mathscr{L}} (\boldsymbol{\xi}, \boldsymbol{\lambda}) = \boldsymbol{H}_{\tilde{\mathscr{L}}} (\boldsymbol{\xi}, \boldsymbol{\lambda})$ with respect to $\boldsymbol{\xi}$ of the Lagrange function $\tilde{\mathscr{L}} (\boldsymbol{\xi}, \boldsymbol{\lambda})$ satisfies

$$\boldsymbol{\eta} \cdot \left(\boldsymbol{H}_{\tilde{\mathscr{L}}} (\boldsymbol{\xi}, \boldsymbol{\lambda}) \, \boldsymbol{\eta} \right) > 0$$

for all variations $\boldsymbol{\eta}$ belonging to

$$T_{\bar{S}} (\boldsymbol{\xi}) = \{ \boldsymbol{\eta} \in \Xi \mid \tilde{g}_i (\boldsymbol{\xi}) \cdot \boldsymbol{\eta} = 0 \quad \text{for all } i \in I_{\mathrm{A}} (\boldsymbol{\xi}) \},$$

then Theorem 2.7.8 implies that $\boldsymbol{\xi}$ is a local minimizer.

(4) When optimization problems include an inequality constraint (Problem 2.8.2) and are convex, Theorem 2.7.9 implies that the Lagrange multiplier method's solution $\boldsymbol{\xi}$ and the function $\boldsymbol{u}$ satisfying $\boldsymbol{h} (\boldsymbol{\xi}, \boldsymbol{u}) = \boldsymbol{0}_{\mathbb{R}^n}$ are global minimizers.

A one-dimensional linear elastic body and a one-dimensional steady Stokes flow field were used as examples of an optimization problem under inequality constraints in Chap. 1. These problems are convex optimization problems. Hence, if $\boldsymbol{a}$ satisfying the KKT conditions can be found, then it can be deemed to minimize the problems.

2.9 Duality Theorem

The KKT conditions used in Sect. 2.7 and Sect. 2.8 required that $f_0, \ldots, f_m$ be first-order differentiable. The duality theorem (shown next) allows one to replace first-order differentiability with convexity. Since this theorem is not directly used in this book the result will be stated without proof.

Let us define the constraint qualification as follows.

Definition 2.9.1 (Slater constraint qualification) In Problem 2.1.2, if there exists $\boldsymbol{y} \in S$ such that $\boldsymbol{f} (\boldsymbol{y}) < \boldsymbol{0}_{\mathbb{R}^m}$, then we say that the Slater constraint qualification is satisfied. □

The duality theorem is expressed as follows [4–6].

Theorem 2.9.2 (Duality theorem) Suppose that Problem 2.1.2 is a convex optimization problem and the Slater constraint qualification is satisfied. Let

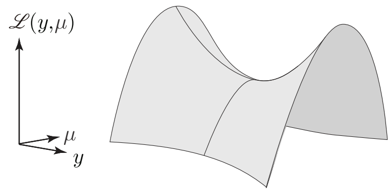


Fig. 2.22: Saddle point.

$\mathscr{L}(\boldsymbol{x},\boldsymbol{\lambda})$ be given by Eq. (2.7.26). Here, the necessary and sufficient condition for $\boldsymbol{x}\in X$ to yield the minimum is for there to exist $\boldsymbol{\lambda}\geq\mathbf{0}_{\mathbb{R}^m}$ such that the following holds for arbitrary $\boldsymbol{y}\in X$ and $\boldsymbol{\mu}\geq\mathbf{0}_{\mathbb{R}^m}$:

$$\mathscr{L}(\boldsymbol{x},\boldsymbol{\mu})\leq\mathscr{L}(\boldsymbol{x},\boldsymbol{\lambda})\leq\mathscr{L}(\boldsymbol{y},\boldsymbol{\lambda}). \tag{2.9.1}$$

□

A pair $(\boldsymbol{x},\boldsymbol{\lambda})$ which satisfies Eq. (2.9.1) describes a saddle point such as the one shown in Fig. 2.22. For this reason, the duality theorem is also referred to as the saddle point theorem.

2.9.1 Examples of the Duality Theorem

Let us make use of the duality theorem with respect to the following combined spring problem.

Exercise 2.9.3 (Spring combination problem) Consider Exercise 2.7.11 and show that the $\boldsymbol{u}$ satisfying

$$\min_{\boldsymbol{u}\in\mathbb{R}^2}\left\{f_0(\boldsymbol{u})=\frac{1}{2}k_1u_1^2+\frac{1}{2}k_2u_2^2\;\middle|\;f_1(\boldsymbol{u})=a-(u_1+u_2)\leq 0\right\}$$

is a saddle point of the Lagrange function. □

Answer Let $\boldsymbol{u}$ be the minimizer for this problem and $\boldsymbol{v}\in\mathbb{R}^2$ be arbitrary. Since $f_0(\boldsymbol{v})$ and $f_1(\boldsymbol{v})$ are convex functions, the optimization problem is convex. Moreover, from the fact that $f_1(\boldsymbol{v})<0$ when $(v_1,v_2)=(a/4,a/4)$, the Slater constraint qualification is satisfied. The Lagrange function for this problem is defined by

$$\mathscr{L}(\boldsymbol{v},\mu)=f_0(\boldsymbol{v})+\mu f_1(\boldsymbol{v})=\frac{1}{2}k_1v_1^2+\frac{1}{2}k_2v_2^2+\mu(a-v_1-v_2),$$

where $\mu\in\mathbb{R}$ is a Lagrange multiplier with respect to $f_1\leq 0$. For $\mu>0$, we have

$$\begin{aligned}\mathscr{L}(\boldsymbol{u},\mu)&=\inf_{\boldsymbol{v}\in\mathbb{R}^2}\mathscr{L}(\boldsymbol{v},\mu)=\mathscr{L}\left(\frac{\mu}{k_1},\frac{\mu}{k_2},\mu\right)=\mathscr{L}_S(\mu)\\&=\frac{1}{2}\frac{\mu^2}{k_1}+\frac{1}{2}\frac{\mu^2}{k_2}+\mu\left(a-\frac{\mu}{k_1}-\frac{\mu}{k_2}\right)=-\frac{1}{2}\left(\frac{1}{k_1}+\frac{1}{k_2}\right)\mu^2+a\mu.\end{aligned}$$

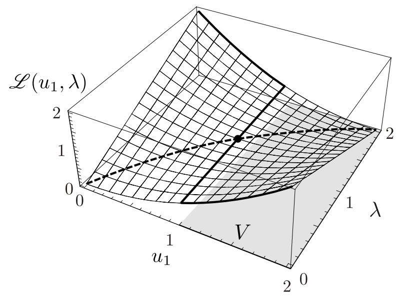


Fig. 2.23: The saddle point in Exercise 2.9.3.

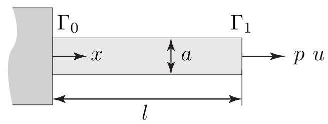


Fig. 2.24: One-dimensional elastic body with one cross-section.

We let $\tilde{\mathscr{L}}(\mu) = \mathscr{L}(\boldsymbol{u}(\mu), \mu)$ and set λ equal to the μ satisfying

$$\frac{\mathrm{d}\tilde{\mathscr{L}}}{\mathrm{d}\mu} = -\left(\frac{1}{k_1} + \frac{1}{k_2}\right)\mu + a = 0.$$

We also have

$$\frac{\mathrm{d}^2\tilde{\mathscr{L}}}{\mathrm{d}\mu^2} = -\left(\frac{1}{k_1} + \frac{1}{k_2}\right) < 0.$$

Hence,

$$\mathscr{L}(\boldsymbol{u}, \mu) \leq \mathscr{L}(\boldsymbol{u}, \lambda).$$

On the other hand, it is easy to see that $\mathscr{L}(\boldsymbol{u}, \lambda) \leq \mathscr{L}(\boldsymbol{v}, \lambda)$. □

Let us now visually confirm that the minimum in Exercise 2.9.3 is a saddle point of the Lagrange function. The variable in this problem was $(u_1, u_2, \lambda)^\top \in X = \mathbb{R}^3$. The current setting is difficult to illustrate. Hence we take $u_2 = 0$ (or, equivalently, $k_2 \to \infty$) and let $k_1 = 1$ and $a = 1$. Then

$$\mathscr{L}(u_1, \lambda) = \frac{1}{2}u_1^2 + \lambda(1 - u_1)$$

and the saddle point becomes $(u_1, \lambda) = (1, 1)$. Figure 2.23 shows the situation, from which we confirm the saddle point.

Here, we remark that λ refers to an internal force and that $-\mathscr{L}(\boldsymbol{u}, \boldsymbol{\lambda})$ is a complementary energy. Minimization of complementary energy is used in engineering when seeking internal forces from a given displacement.

Let us end this chapter with an application of the duality theorem with respect to an optimal design problems such as was treated in Chap. 1. As our

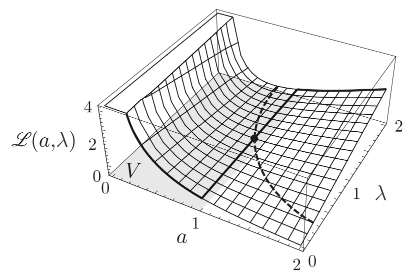


Fig. 2.25: Saddle point of Exercise 2.9.4.

observations in Section 1.1 and Sect. 2.2 showed, the optimal design problems considered in this book have been convex optimization problems. The duality theorem is thus applicable and the Lagrange function should form a saddle point with respect to the design variable and Lagrange multiplier at the minimizer of the optimal design problem. Let us take a look at this using a diagram.

In order to aid the illustration, we limit the number of variables to two. If one of the variables is a Lagrange multiplier, the number of design variables must be limited to one. Therefore, let us consider a one-dimensional linear elastic body with a single cross-sectional area, such as the one shown in Fig. 2.24.

Exercise 2.9.4 (Mean compliance minimization problem) Suppose that $e_{\mathrm{Y}} = 1$, $l = 1$, $c_1 = 1$ and $p = 1$. Find (a, u) satisfying

$$\min_{(a,u)\in\mathbb{R}^2} \left\{ f_0\left(u\right) = pu \;\middle|\; f_1\left(a\right) = la - c_1 \leq 0,\ \frac{e_{\mathrm{Y}}}{l} au = p \right\}.$$

Also graph the Lagrange function at this point on a diagram. □

Answer We have $\tilde{f}_0\left(a\right) = f_0\left(u\left(a\right)\right) = f_0\left(1/a\right) = 1/a$. The functions $\tilde{f}_0\left(a\right)$ and $f_1\left(a\right)$ are convex, and therefore

$$\min_{a\in\mathbb{R}} \left\{ \tilde{f}_0\left(a\right) \;\middle|\; f_1\left(a\right) \leq 0 \right\}$$

is a convex optimization problem. The Slater constraint qualification is clearly satisfied. The Lagrange function for this problem is given by

$$\mathscr{L}\left(a, \lambda\right) = \tilde{f}_0\left(a\right) + \lambda f_1\left(a\right) = \frac{1}{a} + \lambda\left(a - 1\right),$$

where $\lambda \in \mathbb{R}$ is a Lagrange multiplier with respect to $f_1\left(a\right) \leq 0$. We have

$$\mathscr{L}_a = -\frac{1}{a^2} + \lambda = 0, \quad \mathscr{L}_\lambda = a - 1 = 0,$$

and it follows that $(a, \lambda) = (1, 1)$ is a stationary point of $\mathscr{L}\left(a, \lambda\right)$. Figure 2.25 shows $\mathscr{L}$ in a neighborhood of this point, from which we can confirm the existence of the saddle point. □

2.10 Summary

Chapter 2 examined the theory of optimization problems in finite-dimensional vector spaces. The key points are as follows.

(1) Optimization problems are generally defined as finding an element at which a cost function attains its minimum value amongst a set of design variables. On the other hand, as we saw in Chap. 1, state and design variables are defined in optimal design problems, and cost functions are defined as functions of the design and state variables. In this case, state variables are uniquely determined via state equations. Here, in order to fit the optimal design problem into the framework of a general optimization problem, a state variable can be included in the design variable, and state equations should be viewed as equality constraints (Sect. 2.1).

(2) The gradient of a cost function is 0 at local minimizers of unconstrained optimization problems (Theorem 2.5.2). Moreover, if the Hesse matrix is positive definite at the stationary point (gradient 0) of the cost function, then it is a local minimizer (Theorem 2.5.5). Furthermore, if the cost function is convex, the local minimizer yields the global minimum (Theorem 2.5.6 or Corollary 2.7.3).

(3) At a local minimum of an optimization problem under equality constraints, the Lagrange function is stationary (Theorem 2.6.4). Also, when the Hesse matrix of the Lagrange function is positive definite with respect to variation of a variable satisfying an equality constraint at a stationary point of the Lagrange function, it follows that the stationary point is a local minimizer (Theorem 2.6.7). Furthermore, if the optimization problem is convex, the stationary point of the Lagrange function is a global minimizer (Corollary 2.7.10).

(4) The KKT conditions hold at local minimizers of optimization problems under inequality constraints (Theorem 2.7.5). If the Hesse matrix of the Lagrange function with respect to arbitrary variation of a variable satisfying an inequality constraint is positive definite at the point where the KKT condition is satisfied, then that point is a local minimizer (Theorem 2.7.8). Furthermore, if the optimization problem is convex, a point satisfying the KKT condition yields the global minimum (Theorem 2.7.9).

(5) At local minimizers of optimization problems under equality and inequality constraints, KKT conditions are established from the derivative of the cost function with respect to the independent variation of an unconstrained variable while an equality constraint is satisfied (Eqs. (2.8.5)–(2.8.8)).

(6) Minimizers of convex optimization problems which include inequality constraints form saddle points of their Lagrange functions (Theorem 2.9.2).

The literature of optimization theory is vast. In addition to the references cited in this chapter we also refer to [2,3,7,8,11,12].

2.11 Practice Problems

2.1 In Definition 2.4.5, if $\boldsymbol{A}$ is positive definite, show that α equals the minimum value of the eigenvalues of $\boldsymbol{A}$. Also show that if $\boldsymbol{A}$ is negative definite, that $-\alpha$ equals the maximum value of the eigenvalues of $\boldsymbol{A}$. (Hint: Refer to Theorem A.2.1.)

2.2 Let $f : \mathbb{R}^2 \mapsto \mathbb{R}$ be the function

$$f(x_1, x_2) = \frac{1}{2}\left(ax_1^2 + 2bx_1x_2 + cx_2^2\right) + dx_1 + ex_2,$$

where $a, b, c, d \in \mathbb{R}$ are constants. Derive necessary conditions for f to attain a minimum value. Also show that a sufficient condition is $a > 0$ and $ac - b^2 > 0$. The Sylvester criterion (Theorem A.2.2) may of course be used.

2.3 Amongst the set of rectangles whose perimeter is less than a given value, show that the one with the largest area is a square.

- Let the length of the sides of the rectangle be expressed by $\boldsymbol{x} = (x_1, x_2)^\top \in \mathbb{R}^2$. Construct the problem by defining a positive real constant constraining the perimeter length to be c_1.
- Define the Lagrange function and find the KKT conditions.
- Show that if a solution satisfies the KKT conditions, then it is a global minimizer. (Hint: Consider whether or not this is a convex optimization problem. If it is not, show that the problem in which the cost function is recreated using functions (denoted by $\tilde{f}_0$ here) with respect to the set of constrained variables is a convex optimization problem.)

References

[1] Bartle, R. G. *The Elements of Real Analysis, 2nd Ed.* Wiley, New York, 1976.

[2] Bazaraa, M. S. and Shetty, C. M. *Nonlinear Programming: Theory and Algorithms.* Wiley, New York, 1979.

[3] Chong, E. K. P. and Żak, S. H. *An Introduction to Optimization.* Wiley, New York, 2008.

[4] Fujita, H., Konno, H., and Tanabe, K. *Optimization Method (in Japanese).* Iwanami Shoten, Tokyo, 1994.

[5] Fukushima, M. *Basics of Nonlinear Optimization (in Japanese).* Asakura Publishing, Tokyo, 2001.

[6] Güler, O. *Foundations of Optimization.* Springer, New York, 2010.

[7] Jeter, M. W. *Mathematical Programming: An Introduction to Optimization.* M. Dekker, Inc., New York, 1986.

[8] Kushimoto, S. *Basics of Optimization Problems (in Japanese).* Morikita Publishing, Tokyo, 1979.

[9] Rudin, W. *Principles of Mathematical Analysis.* McGraw-Hill, New York, 1976.

[10] Takagi, T. *Analysis Overview, 3rd Rev. (in Japanese).* Iwanami Shoten, Tokyo, 1961.

[11] Tamura, A. and Matsumura, M. *Optimization Method (in Japanese).* Kyoritsu Shuppan, Tokyo, 2002.

[12] Yabe, H. *Engineering Basics: Optimization and Its Applications (in Japanese).* Suurikougaku-sha, Tokyo, 2006.