

最佳化方法與應用二

MA5038-*

Chapter 12. Theory of Constrained Optimization

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Introduction

The second part of the textbook is about minimizing functions **subject to constraints** on the variables:

$$\min_{x \in \mathbb{R}^n} f(x) \quad \text{subject to} \quad \begin{cases} c_i(x) = 0, i \in \mathcal{E}, \\ c_i(x) \geq 0, i \in \mathcal{I}, \end{cases} \quad (1)$$

where f and the functions c_i are all smooth, real-valued functions on a subset of \mathbb{R}^n , and \mathcal{I} and \mathcal{E} are two finite sets of indices. As before, we call f the objective function, while $c_i, i \in \mathcal{E}$, are the equality constraints and $c_i, i \in \mathcal{I}$, are the inequality constraints. We define the feasible set Ω by

$$\Omega = \{x \mid (\forall i \in \mathcal{E})(c_i(x) = 0) \text{ and } (\forall i \in \mathcal{I})(c_i(x) \geq 0)\},$$

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In this chapter we derive mathematical characterizations of the solutions of (2). Two types of optimality conditions are discussed:

- ① Necessary conditions are conditions that must be satisfied by any solution point (under certain assumptions).
- ② Sufficient conditions are those that, if satisfied at a certain point x_* , guarantee that x_* is in fact a solution.

Optimality conditions for **unconstrained** optimization problems are:

- ① Necessary conditions: Local unconstrained minimizers x_* satisfies that $(\nabla f)(x_*) = 0$ and $(\nabla^2 f)(x_*)$ positive semi-definite.
- ② Sufficient conditions: Any point x_* at which $(\nabla f)(x_*) = 0$ and $(\nabla^2 f)(x_*)$ is positive definite is a strong local minimizer of f .

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Introduction

- **Local and global solutions**

We have seen already that global solutions are difficult to find even when there are no constraints. The situation may be improved when we add constraints, since the feasible set might exclude many of the local minima and it may be comparatively easy to pick the global minimum from those that remain. However, constraints can also make things more difficult. As an example, consider the problem

$$\min(x_2 + 100)^2 + 0.01x_1^2 \quad \text{subject to} \quad x_2 - \cos x_1 \geq 0,$$

illustrated in Figure 1. Without the constraint, the problem has the unique solution $(0, -100)^T$. With the constraint, there are local solutions near the points

$$x^{(k)} = (k\pi, -1)^T \quad \text{for } k = \pm 1, \pm 3, \pm 5, \dots$$

Introduction

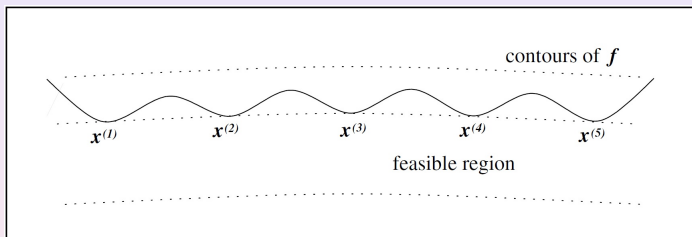


Figure 1: Constrained problem with many isolated local solutions.

Introduction

Definitions of the different types of local solutions are simple extensions of the corresponding definitions for the unconstrained case.

Definition

- 1 A vector x_* is a local solution of the problem (2) if $x_* \in \Omega$ and there is a neighborhood \mathcal{N} of x_* such that $f(x) \geq f(x_*)$ for $x \in \mathcal{N} \cap \Omega$.
- 2 A vector x_* is a strict local solution (also called a strong local solution) if $x_* \in \Omega$ and there is a neighborhood \mathcal{N} of x_* such that $f(x) > f(x_*)$ for all $x \in \mathcal{N} \cap \Omega$ with $x \neq x_*$.
- 3 A point x_* is an isolated local solution if $x_* \in \Omega$ and there is a neighborhood \mathcal{N} of x_* such that x_* is the only local solution in $\mathcal{N} \cap \Omega$.

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Introduction

- **Smoothness**

Smoothness of objective functions and constraints is an important issue in characterizing solutions, just as in the unconstrained case. It ensures that the objective function and the constraints all behave in a reasonably predictable way and therefore allows algorithms to make good choices for search directions.

We saw in Chapter 2 that graphs of non-smooth functions contain “kinks” or “jumps” where the smoothness breaks down. If we plot the feasible region for any given constrained optimization problem, we usually observe many kinks and sharp edges. Does this mean that the constraint functions that describe these regions are non-smooth? The answer is often no, because the non-smooth boundaries can often be described by a collection of smooth constraint functions.

Introduction

For example, Figure 2 shows a diamond-shaped feasible region in \mathbb{R}^2 that could be described by the single non-smooth constraint

$$\|x\|_1 \equiv |x_1| + |x_2| \leq 1.$$

It can also be described by the following set of smooth (in fact, linear) constraints:

$$x_1 + x_2 \leq 1, \quad x_1 - x_2 \leq 1, \quad -x_1 + x_2 \leq 1, \quad -x_1 - x_2 \leq 1. \quad (3)$$

Each of the four constraints represents one edge of the feasible polytope. In general, the constraint functions are chosen so that each one represents a smooth piece of the boundary of Ω .

Introduction

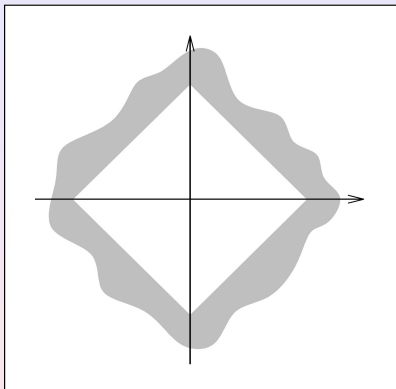


Figure 2: A feasible region with a non-smooth boundary can be described by smooth constraints.

Introduction

Non-smooth, unconstrained optimization problems can sometimes be reformulated as smooth constrained problems. An example is the unconstrained minimization of a function

$$f(x) = \max \{x^2, x\},$$

which has kinks at $x = 0$ and $x = 1$, and the solution at $x_* = 0$. We obtain a smooth, constrained formulation of this problem by adding an artificial variable t and writing

$$\min t \quad \text{s.t.} \quad t \geq x, t \geq x^2. \quad (4)$$

Reformulation techniques such as (3) and (4) are used often in cases where f is a maximum of a collection of functions or when f is a 1-norm or ∞ -norm of a vector function.

Introduction

In the examples above we expressed inequality constraints in a slightly different way from the form $c_i(x) \geq 0$ that appears in the definition (1). However, any collection of inequality constraints with \geq and \leq and nonzero right-hand sides can be expressed in the form $c_i(x) \geq 0$ by simple rearrangement of the inequality.

§12.1 Examples

To introduce the basic principles behind the characterization of solutions of constrained optimization problems, we work through three simple examples.

We begin with the definition of one important terminology.

Definition

The **active set** $\mathcal{A}(x)$ at any feasible x consists of the equality constraint indices from \mathcal{E} together with the indices of the inequality constraints i for which $c_i(x) = 0$; that is,

$$\mathcal{A}(x) = \mathcal{E} \cup \{i \in \mathcal{I} \mid c_i(x) = 0\}.$$

At a feasible point x , the inequality constraint $i \in \mathcal{I}$ is said to be active if $c_i(x) = 0$ and inactive if the strict inequality $c_i(x) > 0$ is satisfied.

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§12.1 Examples

• A Single equality constraint

Example

Our first example is a two-variable problem with a single equality constraint:

$$\min(x_1 + x_2) \quad \text{subject to} \quad x_1^2 + x_2^2 - 2 = 0 \quad (5)$$

(see Figure 12.3). In the language of (1), we have $f(x) = x_1 + x_2$, $\mathcal{I} = \emptyset$, $\mathcal{E} = \{1\}$, and $c_1(x) = x_1^2 + x_2^2 - 2$. We can see by inspection that the feasible set for this problem is the circle of radius $\sqrt{2}$ centered at the origin – just the boundary of this circle, not its interior. The solution x_* is obviously $(-1, -1)^T$. From any other point on the circle, it is easy to find a way to move that stays feasible (that is, remains on the circle) while decreasing f . For instance, from the point $x = (\sqrt{2}, 0)^T$ any move in the clockwise direction around the circle has the desired effect.

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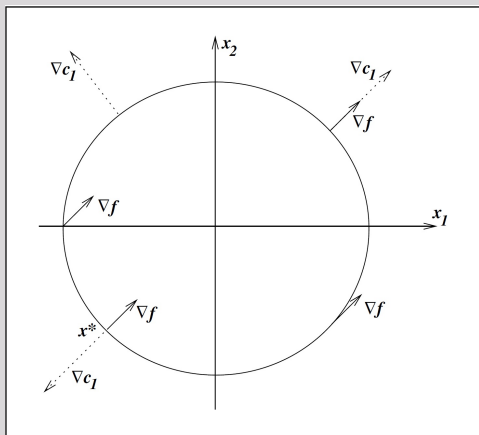


Figure 3: Problem (5), showing constraint and function gradients at various feasible points.

§12.1 Examples

Example (cont'd)

We also see from Figure 3 that at the solution x_* , the constraint normal $\nabla c_1(x_*)$ is parallel to $(\nabla f)(x_*)$. That is, there is a scalar λ_1^* (in this case $\lambda_1^* = -1/2$) such that

$$(\nabla f)(x_*) = \lambda_1^* \nabla c_1(x_*). \quad (6)$$

We can derive (6) by examining first-order Taylor series approximations to the objective and constraint functions. To retain feasibility with respect to the function $c_1(x) = 0$, we require any small (but nonzero) step s to satisfy that $c_1(x + s) = 0$; that is,

$$0 = c_1(x + s) \approx c_1(x) + \nabla c_1(x)^T s = \nabla c_1(x)^T s.$$

Hence, the step s retains feasibility with respect to c_1 , to first order, when it satisfies

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Similarly, if we want s to produce a decrease in f , we would have

$$0 > f(x+s) - f(x) \approx \nabla f(x)^T s,$$

or, to first order,

$$\nabla f(x)^T s < 0. \quad (8)$$

Existence of a small step s that satisfies both (7) and (8) strongly suggests existence of a direction d (where the size of d is not small; we could have $d \approx s/\|s\|$ to ensure that the norm of d is close to 1) with the same properties, namely

$$\nabla c_1(x)^T d = 0 \quad \text{and} \quad \nabla f(x)^T d < 0. \quad (9)$$

If, on the other hand, there is no direction d with the properties (9), then is it likely that we cannot find a small step s with the properties (7) and (8). In this case, x_* would appear to be a local minimizer.

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By drawing a picture, the reader can check that **the only way that a d satisfying (9) does not exist is if $\nabla f(x)$ and $\nabla c_1(x)$ are parallel**; that is, if the condition $\nabla f(x) = \lambda_1 \nabla c_1(x)$ holds at x , for some scalar λ_1 . If in fact $\nabla f(x)$ and $\nabla c_1(x)$ are not parallel, we can set

$$\bar{d} = -\left(\mathbf{I} - \frac{\nabla c_1(x) \nabla c_1(x)^T}{\|\nabla c_1(x)\|^2}\right) \nabla f(x); \quad d = \frac{\bar{d}}{\|\bar{d}\|}.$$

It is easy to verify that this d satisfies (9).

§12.1 Examples

Introduce the Lagrangian function

$$\mathcal{L}(x, \lambda_1) = f(x) - \lambda_1 c_1(x). \quad (10)$$

Since $\nabla_x \mathcal{L}(x, \lambda_1) = \nabla f(x) - \lambda_1 \nabla c_1(x)$, we can state the condition

$$(\nabla f)(x_*) = \lambda_1^* \nabla c_1(x_*) \quad (6)$$

equivalently as follows: At the solution x_* , there is a scalar λ_1^* such that

$$\nabla_x \mathcal{L}(x_*, \lambda_1^*) = 0. \quad (11)$$

This observation suggests that we can search for solutions of the equality-constrained problem (5) by seeking stationary points of the Lagrangian function. The scalar quantity λ_1 in (10) is called a **Lagrange multiplier** for the constraint $c_1(x) = 0$.

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- **A single inequality constraint**

Example

This is a slight modification of the first example, in which the equality constraint is replaced by an inequality. Consider

$$\min(x_1 + x_2) \quad \text{s.t.} \quad 2 - x_1^2 - x_2^2 \geq 0, \quad (12)$$

for which the feasible region consists of the circle of problem (5) and its interior (see Figure 4). Note that the constraint normal ∇c_1 points toward the interior of the feasible region at each point on the boundary of the circle. By inspection, we see that the solution is still $(-1, -1)^T$ and that the condition (6) holds for the value $\lambda_1^* = 1/2$. However, this inequality-constrained problem differs from the equality-constrained problem (5) of the first example in that the sign of the Lagrange multiplier plays a significant role.

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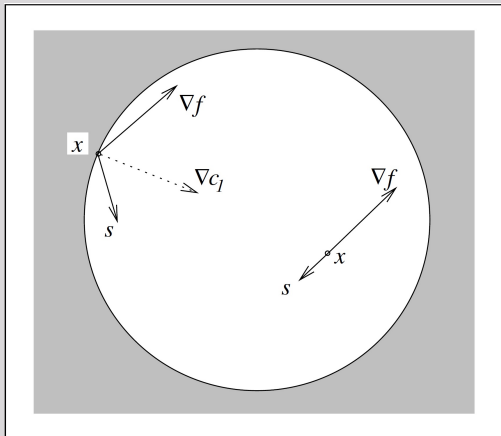


Figure 4: Improvement directions s from two feasible points x for the problem c at which the constraint is active and inactive, respectively.

§12.1 Examples

As before, we conjecture that a given feasible point x is not optimal if we can find a small step s that both retains feasibility and decreases the objective function f to first order. The main difference between problems (5) and (12) comes in the handling of the feasibility condition. As in (8), the step s improves the objective function, to first order, if $\nabla f(x)^T s < 0$. Meanwhile, s retains feasibility if

$$0 \leq c_1(x+s) \approx c_1(x) + \nabla c_1(x)^T s,$$

so, to first order, feasibility is retained if

$$c_1(x) + \nabla c_1(x)^T s \geq 0. \quad (13)$$

In determining whether a step s exists that satisfies both (8) and (13), we consider two cases, which are illustrated in Figure 4.

§12.1 Examples

Case I: Consider first the case in which x lies strictly inside the circle, so that the strict inequality $c_1(x) > 0$ holds. In this case, any step vector s satisfies the condition

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provided only that its length is sufficiently small. In fact, whenever $\nabla f(x) \neq 0$, we can obtain a step s that satisfies both

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Case I: Consider first the case in which x lies strictly inside the circle, so that the strict inequality $c_1(x) > 0$ holds. In this case, any step vector s satisfies the condition

$$c_1(x) + \nabla c_1(x)^T s \geq 0, \quad (13)$$

provided only that its length is sufficiently small. In fact, whenever $\nabla f(x) \neq 0$, we can obtain a step s that satisfies both

$$\nabla f(x)^T s < 0 \quad (8)$$

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Case II: Consider now the case in which x lies on the boundary of the circle, so that $c_1(x) = 0$. The conditions (8) and (13) therefore become

$$\nabla f(x)^T s < 0, \quad \nabla c_1(x)^T s \geq 0.$$

The first of these conditions defines an open half-space, while the second defines a closed half-space, as illustrated in Figure 5 in the next slide. It is clear from this figure that the intersection of these two regions is empty only when $\nabla f(x)$ and $\nabla c_1(x)$ point in the same direction; that is, when

$$\nabla f(x) = \lambda_1 \nabla c_1(x) \quad \text{for some } \lambda_1 \geq 0. \quad (15)$$

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§12.1 Examples

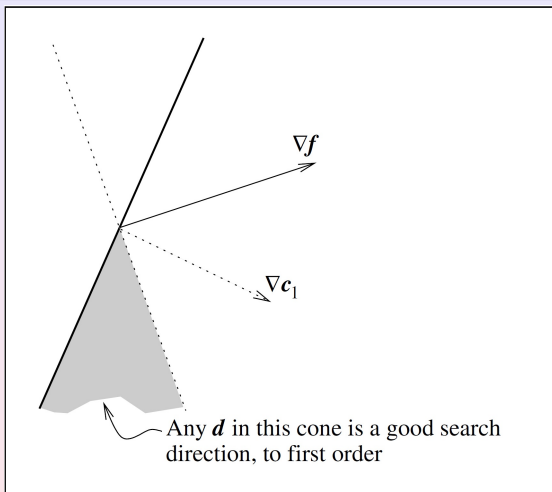


Figure 5: A direction d that satisfies both (8) and (13) lies in the intersection of a closed half-plane and an open half-plane.

§12.1 Examples

Note that the sign of the multiplier is significant here. If (6) were satisfied with a negative value of λ_1 , then $\nabla f(x)$ and $\nabla c_1(x)$ would point in opposite directions, and we see from Figure 5 that the set of directions that satisfy both (8) and (13) would make up an entire open half-plane.

The optimality conditions for both cases I and II can again be summarized neatly using the Lagrangian function \mathcal{L} defined in

$$\mathcal{L}(x, \lambda_1) = f(x) - \lambda_1 c_1(x). \quad (10)$$

When no first-order feasible descent direction exists at some point x_* , we have that

$$\nabla_x \mathcal{L}(x_*, \lambda_1^*) = 0 \text{ for some } \lambda_1^* \geq 0, \quad (16)$$

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§12.1 Examples

Condition

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is known as a **complementarity condition** (互補條件); it implies that the Lagrange multiplier λ_1 can be strictly positive only when the corresponding constraint c_1 is active. Conditions of this type play a central role in constrained optimization, as we see in the sections that follow. In case I, we have that $c_1(x_*) > 0$, so (17) requires that $\lambda_1^* = 0$. Hence,

$$(\nabla f)(x_*) = \lambda_1^* \nabla c_1(x_*) \quad (6)$$

reduces to $(\nabla f)(x_*) = 0$, as required by (14). In case II, (17) allows λ_1^* to take on a non-negative value, so (16) becomes equivalent to

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§12.1 Examples

- **Two inequality constraints**

Example

Suppose we add an extra constraint to the problem (12) to obtain

$$\min(x_1 + x_2) \quad \text{s.t.} \quad 2 - x_1^2 - x_2^2 \geq 0, x_2 \geq 0, \quad (18)$$

for which the feasible region is the half-disk illustrated in Figure 6. It is easy to see that the solution lies at $(-\sqrt{2}, 0)^T$, a point at which both constraints are active. By repeating the arguments for the previous examples, we would expect a direction d of first-order feasible descent to satisfy

$$\nabla c_i(x)^T d \geq 0 \quad \text{for} \quad i \in \mathcal{I} = \{1, 2\} \quad (19a)$$

and

$$\nabla f(x)^T d < 0. \quad (19b)$$

§12.1 Examples

Example (cont'd)

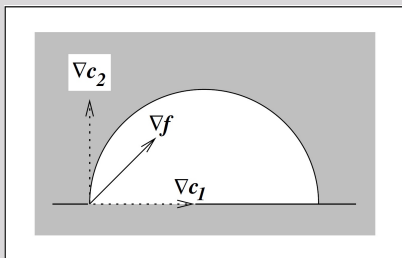


Figure 6: Problem (18), illustrating the gradients of the active constraints and objective at the solution.

However, it is clear from Figure 6 that no such direction can exist when $x = (-\sqrt{2}, 0)^T$. The conditions $\nabla c_i(x)^T d \geq 0$ are satisfied for $i = 1, 2$ only if $d = \alpha_1 \nabla c_1(x) + \alpha_2 \nabla c_2(x)$ for some $\alpha_1, \alpha_2 \geq 0$, but it is clear by inspection that all such vectors d satisfy $\nabla f(x)^T d \geq 0$.

§12.1 Examples

Example (cont'd)

Let us see how the Lagrangian and its derivatives behave for the problem (18) and the solution point $(-\sqrt{2}, 0)^T$. First, we include an additional term $\lambda_i c_i(x)$ in the Lagrangian for each additional constraint, so the definition of \mathcal{L} becomes

$$\mathcal{L}(x, \lambda) = f(x) - \lambda_1 c_1(x) - \lambda_2 c_2(x),$$

where $\lambda = (\lambda_1, \lambda_2)^T$ is the vector of Lagrange multipliers. The extension of condition (16) to this case is

$$\nabla_x \mathcal{L}(x_*, \lambda_*) = 0 \quad \text{for some } \lambda_* \geq 0, \quad (20)$$

where the inequality $\lambda_* \geq 0$ means that all components of λ_* are required to be non-negative. The non-negativity of the Lagrange multipliers is an important feature in the inequality constrained problem, and (20) will be shown in the next slide.

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§12.1 Examples

Example (cont'd)

By applying the complementarity condition (17) to both inequality constraints, we obtain

$$\lambda_1^* c_1(x_*) = 0, \quad \lambda_2^* c_2(x_*) = 0. \quad (21)$$

When $x_* = (-\sqrt{2}, 0)^T$, we have

$$(\nabla f)(x_*) = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad \nabla c_1(x_*) = \begin{bmatrix} 2\sqrt{2} \\ 0 \end{bmatrix}, \quad \nabla c_2(x_*) = \begin{bmatrix} 0 \\ 1 \end{bmatrix},$$

so that it is easy to verify that $\nabla_x \mathcal{L}(x_*, \lambda_*) = 0$ when we select λ_* as follows:

$$\lambda_* = \begin{bmatrix} 1/(2\sqrt{2}) \\ 1 \end{bmatrix}.$$

Note that both components of λ_* are positive, so that (20) is satisfied.

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Example (cont'd)

We consider now some other feasible points that are not solutions of (18), and examine the properties of the Lagrangian and its gradient at these points. For the point $x = (\sqrt{2}, 0)^T$, we again have that both constraints are active (see Figure 7 in the next slide). However, it is easy to identify vectors d that satisfies

$$\nabla c_i(x)^T d \geq 0 \quad \text{for } i \in \mathcal{I} = \{1, 2\}, \quad (19a)$$

$$\nabla f(x)^T d < 0. \quad (19b)$$

In fact, $d = (-1, 0)^T$ is one such vector (there are many others). For this value of x it is easy to verify that the condition $\nabla_x \mathcal{L}(x, \lambda) = 0$ is satisfied only when $\lambda = (-1/(2\sqrt{2}), 1)^T$. Note that the first component λ_1 is negative, so that the conditions (20) are not satisfied at this point.

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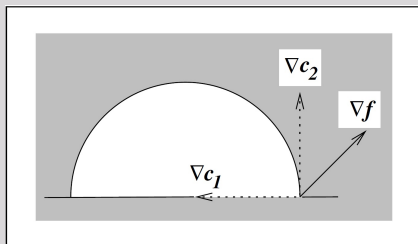


Figure 7: Problem (18), illustrating the gradients of the active constraints and objective at a non-optimal point.

§12.1 Examples

Example (cont'd)

Finally, we consider the point $x = (1, 0)^T$, at which only the second constraint c_2 is active. Since any small step s away from this point will continue to satisfy $c_1(x + s) > 0$, we need to consider only the behavior of c_2 and f in determining whether s is indeed a feasible descent step. Using the same reasoning as in the earlier examples, we find that the direction of feasible descent d must satisfy

$$\nabla c_2(x)^T d \geq 0, \quad \nabla f(x)^T d < 0. \quad (22)$$

By noting that

$$\nabla f(x) = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad \nabla c_2(x) = \begin{bmatrix} 0 \\ 1 \end{bmatrix},$$

it is easy to verify that the vector $d = (-1/2, 1/4)^T$ satisfies (22) and is therefore a descent direction.

§12.1 Examples

Example (cont'd)

To show that optimality conditions

$$\nabla_x \mathcal{L}(x_*, \lambda_*) = 0 \quad \text{for some } \lambda_* \geq 0 \quad (20)$$

and

$$\lambda_1^* c_1(x_*) = 0, \quad \lambda_2^* c_2(x_*) = 0, \quad (21)$$

fail, we note first from (21) that since $c_1(x) > 0$, we must have $\lambda_1 = 0$. Therefore, in trying to satisfy $\nabla_x \mathcal{L}(x, \lambda) = 0$, we are left to search for a value λ_2 such that $\nabla f(x) - \lambda_2 \nabla c_2(x) = 0$. No such λ_2 exists, and thus this point fails to satisfy the optimality conditions.

§12.2 Tangent Cone and Constraint Qualifications

在前一節中，我們通過檢查目標函數 f 和限制函數 c_i 的一階導數，來確定是否可以從給定的可行點 x 採取可行下降步驟。我們使用這些函數在 x 點展開的一階泰勒級數來形成一個目標函數和限制函數均為線性的近似問題。這種方法僅在線性近似在問題所涉及的點 x 附近捕捉到可行集的基本幾何特徵時才有意義。如果線性化近似與可行集根本不同，那麼我們不能期望線性近似提供有關原始問題的有用信息。因此，我們需要對在點 x 處 active constraint c_i 的性質作出假設，以確保線性近似在 x 附近與可行集相似。

在本節中，我們定義了在點 x 屬於閉集合 Ω 時，該點的 tangent cone $T_{\Omega}(x)$ 以及線性化可行方向集 $\mathcal{F}(x)$ 。我們還將討論 **constraint qualifications**，這些假設確保了可行集 Ω 及其在可行點 x 附近的線性化近似之間的相似性。

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§12.2 Tangent Cone and Constraint Qualifications

以下討論中的 Ω 均代表受限優化問題 (1) 的可行集。

Definition

- Given a feasible point x , we call $\{z_k\}$ a feasible sequence approaching x if $z_k \in \Omega$ (for all k sufficiently large) and $z_k \rightarrow x$.
- A tangent is a limiting direction of a feasible sequence. To be more precise, a vector d is said to be a tangent (or tangent vector) to Ω at a point x if there are a feasible sequence $\{z_k\}$ approaching x and a sequence of positive scalars $\{t_k\}$ with $t_k \rightarrow 0$ such that

$$\lim_{k \rightarrow \infty} \frac{z_k - x}{t_k} = d. \quad (23)$$

The collection of all tangents to Ω at x is called the **tangent cone** to the set Ω at x and is denoted by $T_{\Omega}(x)$.

§12.2 Tangent Cone and Constraint Qualifications

很容易看出 tangent cone $T_{\Omega}(x)$ 確實是一個 **cone** :

- ① $0 \in T_{\Omega}(x)$: 對所有 $k \in \mathbb{N}$ 令 $z_k \equiv x$ 。則 $\{z_k\}$ 是個可行數列。
- ② $d \in T_{\Omega}(x)$ and $\alpha > 0 \Rightarrow \alpha d \in T_{\Omega}(x)$: 若 $\{z_k\}$ 和 $\{t_k\}$ 滿足 (23) 式，將 t_k 替換成 $\alpha^{-1}t_k$ 可得 $\alpha d \in T_{\Omega}(x)$ 。

稍後，我們將受限優化問題

$$\min_{x \in \mathbb{R}^n} f(x) \quad \text{subject to} \quad \begin{cases} c_i(x) = 0, i \in \mathcal{E}, \\ c_i(x) \geq 0, i \in \mathcal{I}, \end{cases} \quad (1)$$

的局部解 x (等價地) 刻劃為「對所有收斂到 x 的可行數列 $\{z_k\}$ 都有對足夠大的 k 滿足 $f(z_k) \geq f(x)$ 這個性質」，並且推導出可確保這個性質成立的實用且可驗證的條件。我們通過在 x 點保持可行性的前進方向進行可行方向集的刻劃，在這一節中奠定相關基礎。

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§12.2 Tangent Cone and Constraint Qualifications

現在我們定義線性化可行方向集。回顧 active set 的定義：對於可行點 x ，active set $\mathcal{A}(x)$ 是所有使得限制條件 $c_i(x) = 0$ 的 index 集合，其符號表示為 $\mathcal{A}(x) = \mathcal{E} \cup \{i \in \mathcal{I} \mid c_i(x) = 0\}$ 。

Definition

Given a feasible point x and the active constraint set $\mathcal{A}(x)$, the set of linearized feasible directions $\mathcal{F}(x)$ is

$$\mathcal{F}(x) = \left\{ d \mid \begin{array}{l} d^T \nabla c_i(x) = 0 \text{ for all } i \in \mathcal{E}, \\ d^T \nabla c_i(x) \geq 0 \text{ for all } i \in \mathcal{A}(x) \cap \mathcal{I} \end{array} \right\}.$$

與 tangent cone 相同，非常容易驗證 $\mathcal{F}(x)$ 也是個 cone。

需要注意的是，tangent cone 的定義不依賴於集合 Ω 的代數表示，僅依賴於其幾何性質。然而，線性化可行方向集取決於屬於 active set 中的 i 限制函數 c_i 的定義。

§12.2 Tangent Cone and Constraint Qualifications

現在我們定義線性化可行方向集。回顧 active set 的定義：對於可行點 x ，active set $\mathcal{A}(x)$ 是所有使得限制條件 $c_i(x) = 0$ 的 index 集合，其符號表示為 $\mathcal{A}(x) = \mathcal{E} \cup \{i \in \mathcal{I} \mid c_i(x) = 0\}$ 。

Definition

Given a feasible point x and the active constraint set $\mathcal{A}(x)$, the set of linearized feasible directions $\mathcal{F}(x)$ is

$$\mathcal{F}(x) = \left\{ d \mid \begin{array}{l} d^T \nabla c_i(x) = 0 \text{ for all } i \in \mathcal{E}, \\ d^T \nabla c_i(x) \geq 0 \text{ for all } i \in \mathcal{A}(x) \cap \mathcal{I} \end{array} \right\}.$$

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§12.2 Tangent Cone and Constraint Qualifications

我們通過重新看 §12.1 中的兩個例子來說明 tangent cone 和線性化可行方向集。

Example (Revisit of the 1st example)

Recall the equality-constrained problem

$$\min(x_1 + x_2) \quad \text{s.t.} \quad x_1^2 + x_2^2 - 2 = 0. \quad (5)$$

Near the non-optimal point $x = (-\sqrt{2}, 0)^T$, Figure 8 shows a feasible sequence approaching x given by

$$z_k = \begin{bmatrix} -\sqrt{2 - 1/k^2} \\ -1/k \end{bmatrix}. \quad (24)$$

By choosing $t_k = \|z_k - x\|$, we find that $d = (0, -1)^T$ is a tangent. Note that the objective function $f(x) = x_1 + x_2$ increases strictly as we move along the sequence (24); that is, $f(z_{k+1}) > f(z_k)$ for all $k = 2, 3, \dots$. So x cannot be a solution of (5).

§12.2 Tangent Cone and Constraint Qualifications

Example (cont'd)

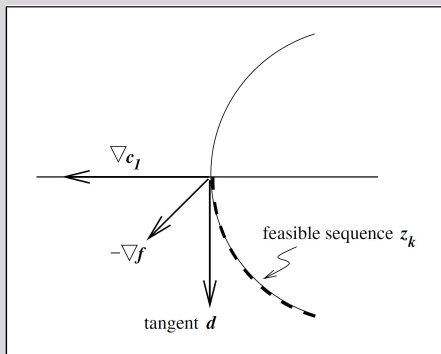


Figure 8: Constraint normal, objective gradient, and feasible sequence for problem (5).

§12.2 Tangent Cone and Constraint Qualifications

Example (cont'd)

Another feasible sequence is one that approaches $x = (-\sqrt{2}, 0)^T$ from the opposite direction given by

$$z_k = \begin{bmatrix} -\sqrt{2 - 1/k^2} \\ 1/k \end{bmatrix}.$$

It is easy to show that f decreases along this sequence and that the tangents corresponding to this sequence are $d = (0, \alpha)^T$. In summary, the tangent cone at $x = (-\sqrt{2}, 0)^T$ is $\{(0, d_2)^T \mid d_2 \in \mathbb{R}\}$.

By the definition of the linearized feasible direction, we have

$$d = (d_1, d_2)^T \in \mathcal{F}(x) \iff 0 = \nabla c_1(x)^T d = -2\sqrt{2}d_1.$$

Therefore, we obtain $\mathcal{F}(x) = \{(0, d_2)^T \mid d_2 \in \mathbb{R}\}$. In this case, we have $T_\Omega(x) = \mathcal{F}(x)$.

§12.2 Tangent Cone and Constraint Qualifications

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§12.2 Tangent Cone and Constraint Qualifications

Example (cont'd)

Suppose that the feasible set is defined instead by the formula $\Omega = \{x \mid c_1(x) = 0\}$, where

$$c_1(x) = (x_1^2 + x_2^2 - 2)^2 = 0. \quad (25)$$

Note that Ω is the same, but its algebraic specification has changed. The vector d belongs to the linearized feasible set if

$$\begin{aligned} 0 &= \nabla c_1(x)^T d = \begin{bmatrix} 4(x_1^2 + x_2^2 - 2)x_1 & 4(x_1^2 + x_2^2 - 2)x_2 \end{bmatrix} \begin{bmatrix} d_1 \\ d_2 \end{bmatrix} \\ &= \begin{bmatrix} 0 & 0 \end{bmatrix} \begin{bmatrix} d_1 \\ d_2 \end{bmatrix}, \end{aligned}$$

which is true for all $(d_1, d_2)^T$. Hence, we have $\mathcal{F}(x) = \mathbb{R}^2$, so for this algebraic specification of Ω , the tangent cone and linearized feasible sets differ.

§12.2 Tangent Cone and Constraint Qualifications

Example (Revisit of the 2nd example)

We now reconsider the problem

$$\min(x_1 + x_2) \quad \text{s.t.} \quad 2 - x_1^2 - x_2^2 \geq 0. \quad (12)$$

The solution $x = (-1, -1)^T$ is the same as the previous case, but there is a much more extensive collection of feasible sequences that converge to any given feasible point (see Figure 9).

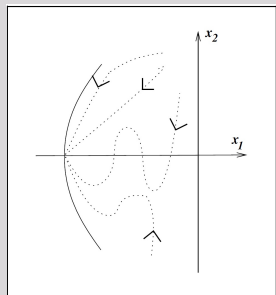


Figure 9: Feasible sequences converging to a particular feasible point for the region defined by $x_1^2 + x_2^2 \leq 2$.

§12.2 Tangent Cone and Constraint Qualifications

Example (cont'd)

From the point $x = (-\sqrt{2}, 0)^T$, the various feasible sequences defined above for the equality-constrained problem are still feasible for (12). There are also infinitely many feasible sequences that converge to $x = (-\sqrt{2}, 0)^T$ along a straight line from the interior of the circle.

These sequences have the form

$$z_k = (-\sqrt{2}, 0)^T + (1/k)w,$$

where w is any vector whose first component is positive ($w_1 > 0$).

The point z_k is feasible provided that $\|z_k\| \leq \sqrt{2}$; that is,

$$(-\sqrt{2} + w_1/k)^2 + (w_2/k)^2 \leq 2,$$

which is true when $k \geq (w_1^2 + w_2^2)/(2\sqrt{2}w_1)$.

§12.2 Tangent Cone and Constraint Qualifications

Example (cont'd)

From the point $x = (-\sqrt{2}, 0)^T$, the various feasible sequences defined above for the equality-constrained problem are still feasible for (12). There are also infinitely many feasible sequences that converge to $x = (-\sqrt{2}, 0)^T$ along a straight line from the interior of the circle. These sequences have the form

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§12.2 Tangent Cone and Constraint Qualifications

Example (cont'd)

In addition to these straight-line feasible sequences, we can also define an infinite variety of sequences that approach $(-\sqrt{2}, 0)^T$ along a curve from the interior of the circle. To summarize, the tangent cone to this set at $(-\sqrt{2}, 0)^T$ is $\{(w_1, w_2)^T \mid w_1 \geq 0\}$.

For the definition (12) of this feasible set, we have

$$d \in \mathcal{F}(x) \Leftrightarrow 0 \leq \nabla c_1(x)^T d = [-2x_1 \quad -2x_2] \begin{bmatrix} d_1 \\ d_2 \end{bmatrix} = 2\sqrt{2}d_1.$$

Hence, we obtain $\mathcal{F}(x) = T_{\Omega}(x)$ for this particular algebraic specification of the feasible set.

§12.2 Tangent Cone and Constraint Qualifications

Example (cont'd)

In addition to these straight-line feasible sequences, we can also define an infinite variety of sequences that approach $(-\sqrt{2}, 0)^T$ along a curve from the interior of the circle. To summarize, the tangent cone to this set at $(-\sqrt{2}, 0)^T$ is $\{(w_1, w_2)^T \mid w_1 \geq 0\}$.

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§12.2 Tangent Cone and Constraint Qualifications

一般而言，我們有以下 Lemma。

Lemma

Let x be a feasible point. Then $T_{\Omega}(x) \subseteq \mathcal{F}(x)$.

Proof.

Let $d \in T_{\Omega}(x)$. Then there exist a feasible sequence $\{z_k\}$ and a sequence of positive scalars $\{t_k\}$ satisfying $\lim_{k \rightarrow \infty} t_k = 0$ and

$$\lim_{k \rightarrow \infty} \frac{z_k - x}{t_k} = d.$$

From the limit above, we have

$$z_k = x + t_k d + o(t_k);$$

thus Taylor's Theorem implies that

$$\begin{aligned} c_i(z_k) &= c_i(x) + \nabla c_i(x)^T (z_k - x) + o(\|z_k - x\|) \\ &= c_i(x) + t_k \nabla c_i(x)^T d + o(t_k). \end{aligned}$$

□

§12.2 Tangent Cone and Constraint Qualifications

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§12.2 Tangent Cone and Constraint Qualifications

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Therefore, for $i \in \mathcal{E}$, we have

$$0 = \frac{1}{t_k} c_i(z_k) = \nabla c_i(x)^T d + \frac{o(t_k)}{t_k},$$

while for $i \in \mathcal{A}(x) \cap \mathcal{I}$ we have

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Passing to the limit as $k \rightarrow \infty$, we obtain

- ① $\nabla c_i(x)^T d = 0$ if $i \in \mathcal{E}$.
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§12.2 Tangent Cone and Constraint Qualifications

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§12.2 Tangent Cone and Constraint Qualifications

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§12.2 Tangent Cone and Constraint Qualifications

Constraint qualifications 是保證線性化可行方向集 $\mathcal{F}(x)$ 與 tangent cone $T_{\Omega}(x)$ 相似的條件。事實上，大多數 constraint qualifications 都保證這兩個集合是相同的。正如之前提到的，這些條件確保了由在 x 點對集合 Ω 的代數描述進行線性化得到的 $\mathcal{F}(x)$ ，在 x 點附近捕捉了集合 Ω 的基本幾何特徵，就像 $T_{\Omega}(x)$ 所表示的那樣。

在第一個例子中， $T_{\Omega}(x)$ 和 $\mathcal{F}(x)$ 都由垂直軸組成，這在 x 的鄰域中與集合 Ω 在幾何上相似。作為更進一步的例子，考慮以下限制式：

$$c_1(x) = 1 - x_1^2 - (x_2 - 1)^2 \geq 0, \quad c_2(x) = -x_2 \geq 0, \quad (26)$$

對於這些限制，可行集是單點 $\Omega = \{(0, 0)^T\}$ （見圖 10）。

§12.2 Tangent Cone and Constraint Qualifications

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§12.2 Tangent Cone and Constraint Qualifications

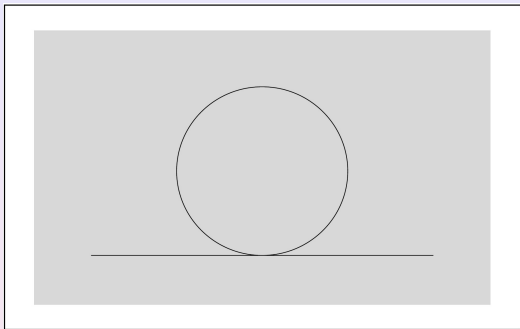


Figure 10: Problem (26), for which the feasible set is the single point of intersection between circle and line.

§12.2 Tangent Cone and Constraint Qualifications

對於點 $x = (0, 0)^T$ ，顯然 tangent cone 是 $T_{\Omega}(x) = \{(0, 0)^T\}$ ，因為所有收斂到 x 的可行數列必須對於所有足夠大的 k ，有 $z_k = x = (0, 0)^T$ 。此外，很容易顯示可行集的線性化近似是

$$\mathcal{F}(x) = \{(d_1, 0)^T \mid d_1 \in \mathbb{R}\},$$

即整個水平軸。在這種情況下，線性化可行方向集沒有捕捉到可行集的幾何特徵，因此不滿足 constraint qualifications。在演算法設計中最常使用的 constraint qualifications 是下一個定義的主題。

§12.2 Tangent Cone and Constraint Qualifications

Definition (LICQ)

For a given feasible point x (with corresponding active set $\mathcal{A}(x)$), we say that **the linear independence constraint qualification (LICQ) holds at x** if the set of active constraint gradients $\{\nabla c_i(x) \mid i \in \mathcal{A}(x)\}$ is linearly independent.

注意到 LICQ 條件在前述兩個例子（中的限制式與可行點）

$$c_1(x) = (x_1^2 + x_2^2 - 2)^2 = 0, \quad x = (-\sqrt{2}, 0)^T$$

和

$$c_1(x) = 1 - x_1^2 - (x_2 - 1)^2 \geq 0, \quad c_2(x) = -x_2 \geq 0, \quad x = (0, 0)^T$$

中並不滿足。一般來說，**如果滿足 LICQ，則任何一個 active constraint gradient 都不能為零**。我們將在 §12.6 中提及其他的 constraint qualifications。

§12.2 Tangent Cone and Constraint Qualifications

- **The relation between $T_{\Omega}(x)$ and $\mathcal{F}(x)$ given LICQ**

接下來的討論（包含後續章節），我們用 $A(x)$ 代表一個其列由在可行點 x 的 active constraint gradients 所組成的矩陣；亦即

$$A(x)^T = [\nabla c_i(x)]_{i \in \mathcal{A}(x)}. \quad (27)$$

我們首先建立以下 lemma。

Lemma

Let x be a feasible point at which the LICQ condition holds. Then for every $d \in \mathcal{F}(x)$ and sequence $\{t_k\}$ of positive scalars satisfying $\lim_{k \rightarrow \infty} t_k = 0$, there exists a feasible sequence $\{z_k\}$ such that

$$\lim_{k \rightarrow \infty} \frac{z_k - x}{t_k} = d \quad (23)$$

and

$$c_i(z_k) = t_k \nabla c_i(x)^T d \quad \forall i \in \mathcal{A}(x) \text{ and } k \gg 1. \quad (28)$$

§12.2 Tangent Cone and Constraint Qualifications

- The relation between $T_{\Omega}(x)$ and $\mathcal{F}(x)$ given LICQ

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§12.2 Tangent Cone and Constraint Qualifications

Proof.

W.L.O.G. we can assume that all the constraints c_i , $i = 1, 2, \dots, m$ are active at x . Let $d \in \mathcal{F}(x)$ be given, and suppose that $\{t_k\}_{k=0}^{\infty}$ is any sequence of positive scalars such $\lim_{k \rightarrow \infty} t_k = 0$. We first note that the $m \times n$ matrix $A(x)$ of active constraint gradients has full row rank m since the LICQ holds at x . By the fact that

the null space of $A(x) \oplus$ the range of $A(x)^T = \mathbb{R}^n$,

there exists an $n \times (n - m)$ matrix Z whose columns are a basis for the null space of $A(x)$; that is,

$$Z \in \mathbb{R}^{n \times (n-m)}, \quad Z \text{ has full column rank,} \quad A(x)Z = 0. \quad (29)$$

With $c \equiv [c_i]_{i \in \mathcal{A}(x)}$, define $R : \mathbb{R}^n \times \mathbb{R} \rightarrow \mathbb{R}^n$ by

$$R(z, t) = \begin{bmatrix} c(z) - tA(x)d \\ Z^T(z - x - td) \end{bmatrix}. \quad \square$$

§12.2 Tangent Cone and Constraint Qualifications

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§12.2 Tangent Cone and Constraint Qualifications

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$$Z \in \mathbb{R}^{n \times (n-m)}, \quad Z \text{ has full column rank,} \quad A(x)Z = 0. \quad (29)$$

With $c \equiv [c_i]_{i \in \mathcal{A}(x)}$, define $R : \mathbb{R}^n \times \mathbb{R} \rightarrow \mathbb{R}^n$ by

$$R(z, t) = \begin{bmatrix} c(z) - tA(x)d \\ Z^T(z - x - td) \end{bmatrix}. \quad \square$$

§12.2 Tangent Cone and Constraint Qualifications

Proof (cont'd).

Note that $R(x, 0) = 0$. Moreover, the Jacobian of $R(\cdot, \cdot)$ with respect to z at point $(z, t) = (x, 0)$ is

$$\nabla_z R(x, 0) = \begin{bmatrix} A(x) \\ Z^T \end{bmatrix},$$

which is non-singular by construction of Z . Therefore, the Implicit Function Theorem implies that the system

$$R(z, t) = \begin{bmatrix} c(z) - tA(x)d \\ Z^T(z - x - td) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad (30)$$

has a unique solution $z_k (\approx x)$ for all $t_k > 0$ sufficiently small. The Implicit Function Theorem also shows that $\lim_{k \rightarrow \infty} z_k = x$.

We claim that $\{z_k\}$ is a feasible sequence and satisfies desired properties (23) and (28). □

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§12.2 Tangent Cone and Constraint Qualifications

Proof (cont'd).

First we show that

$$\lim_{k \rightarrow \infty} \frac{z_k - x}{t_k} = d \quad (23)$$

holds for this choice of $\{z_k\}$. Using the facts that

- ① $R(z_k, t_k) = 0$ for sufficiently large k and
- ② $c(x) = [c_i(x)]_{i \in \mathcal{A}(x)} = 0$,

Taylor's Theorem implies that for k sufficiently large,

$$\begin{aligned} 0 &= R(z_k, t_k) = \begin{bmatrix} c(z_k) - t_k A(x)d \\ Z^T(z_k - x - t_k d) \end{bmatrix} \\ &= \begin{bmatrix} A(x)(z_k - x) + o(\|z_k - x\|) - t_k A(x)d \\ Z^T(z_k - x - t_k d) \end{bmatrix} \\ &= \begin{bmatrix} A(x) \\ Z^T \end{bmatrix} (z_k - x - t_k d) + o(\|z_k - x\|). \end{aligned}$$

□

§12.2 Tangent Cone and Constraint Qualifications

Proof (cont'd).

By dividing this expression by t_k and using non-singularity of the coefficient matrix in the first term, we obtain

$$\frac{z_k - x}{t_k} = d + o\left(\frac{\|z_k - x\|}{t_k}\right),$$

from which it follows that (23) is satisfied (details required). Moreover, since

$$R(z_k, t_k) = \begin{bmatrix} c(z_k) - t_k A(x)d \\ Z^T(z_k - x - t_k d) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

for sufficiently large k , we find that

$$c_i(z_k) = t_k \nabla c_i(x)^T d \quad \forall i \in \mathcal{A}(x) \text{ and } k \gg 1. \quad (28)$$

To conclude the lemma, we show that $\{z_k\}$ is a feasible sequence; that is, $c_i(z_k) = 0$ if $i \in \mathcal{E}$ and $c_i(z_k) \geq 0$ if $i \in \mathcal{I}$ for all sufficiently large k . □

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§12.2 Tangent Cone and Constraint Qualifications

Proof (cont'd).

Since $d \in \mathcal{F}(x)$, the definition of the set of linearized feasible directions implies that for sufficiently large k ,

$$\begin{aligned} i \in \mathcal{E} &\Rightarrow c_i(z_k) = t_k \nabla c_i(x)^T d = 0, \\ i \in \mathcal{A}(x) \cap \mathcal{I} &\Rightarrow c_i(z_k) = t_k \nabla c_i(x)^T d \geq 0. \end{aligned}$$

Moreover, if $i \in \mathcal{I} \cap \mathcal{A}(x)^c$, we must have $c_i(x) > 0$; thus by the fact that $\lim_{k \rightarrow \infty} z_k = x$ we have

$$c_i(z_k) > 0 \quad \forall k \gg 1.$$

Therefore, the continuity of c_i shows that for sufficiently large k ,

$$i \in \mathcal{I} \cap \mathcal{A}(x)^c \Rightarrow c_i(z_k) > 0.$$

Combining all the cases discussed above, we conclude that $\{z_k\}$ is indeed feasible. □

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§12.2 Tangent Cone and Constraint Qualifications

注意到對於一個可行點 x ，根據 tangent cone $T_{\Omega}(x)$ 的定義，前述 lemma 顯示只要在 x 點滿足 LICQ 條件，則有 $\mathcal{F}(x) \subseteq T_{\Omega}(x)$ 。結合關於 $T_{\Omega}(x) \subseteq \mathcal{F}(x)$ 的 lemma，我們得到以下結果：

Corollary

Let x be a feasible point at which the LICQ condition holds. Then $T_{\Omega}(x) = \mathcal{F}(x)$.

§12.3 First-Order Optimality Conditions

在本節中，我們首先陳述了 x_* 成為局部最小值的一階必要條件，並展示了這些條件在一個小例子中的滿足情況。該結果的證明將在後續章節中呈現。

作為陳述必要條件所需的預備工作，我們定義了問題 (1) 的 Lagrangian：

$$\mathcal{L}(x, \lambda) = f(x) - \sum_{i \in \mathcal{E} \cup \mathcal{I}} \lambda_i c_i(x). \quad (31)$$

以下定理中定義的必要條件稱為一階條件，因為它們關注意標函數和限制函數的梯度（一階導數向量）的性質。這些條件是本書其餘章節中描述的許多算法的基礎。

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§12.3 First-Order Optimality Conditions

Theorem (First-Order Necessary Conditions)

Suppose that x_* is a local solution of problem

$$\min_{x \in \mathbb{R}^n} f(x) \quad \text{subject to} \quad \begin{cases} c_i(x) = 0, i \in \mathcal{E}, \\ c_i(x) \geq 0, i \in \mathcal{I}, \end{cases} \quad (1)$$

that the functions f and c_i in (1) are continuously differentiable, and that the LICQ holds at x_* . Then there is a Lagrange multiplier vector λ_* , with components λ_i^* , $i \in \mathcal{E} \cup \mathcal{I}$, such that the following conditions are satisfied.

$$\nabla_x \mathcal{L}(x_*, \lambda_*) = 0, \quad (32a)$$

$$c_i(x_*) = 0 \quad \text{for all } i \in \mathcal{E}, \quad (32b)$$

$$c_i(x_*) \geq 0 \quad \text{for all } i \in \mathcal{I}, \quad (32c)$$

$$\lambda_i^* \geq 0 \quad \text{for all } i \in \mathcal{I}, \quad (32d)$$

$$\lambda_i^* c_i(x_*) = 0 \quad \text{for all } i \in \mathcal{E} \cup \mathcal{I}. \quad (32e)$$

§12.3 First-Order Optimality Conditions

- 1 條件 (32) 通常被稱為 Karush-Kuhn-Tucker 條件，簡稱 KKT 條件。
- 2 一個可行點 x_* 被稱為是一個 KKT point 如果存在 λ_* 使得 KKT 條件滿足。如此的 (x_*, λ_*) 也被稱為一個 KKT pair。
- 3 最後一個條件

$$\lambda_i^* c_i(x_*) = 0 \quad \text{for all } i \in \mathcal{E} \cup \mathcal{I} \quad (32e)$$

是互補條件：其意味著要麼限制 i 是 active，要麼 $\lambda_i^* = 0$ ，或者可能兩者都是。特別地，對於 inactive 的不等式限制對應的 Lagrange 乘子則為零，我們可以從 (32a) 中刪除不屬於 $\mathcal{A}(x_*)$ 的指標 i 所對應的項，並將此條件重寫為：

$$0 = \nabla_x \mathcal{L}(x_*, \lambda_*) = \nabla f(x_*) - \sum_{i \in \mathcal{A}(x_*)} \lambda_i^* \nabla c_i(x_*).$$

一階必要條件的證明相當複雜，但對於我們理解受限優化很重要，因此我們將在下一節中進行介紹。

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§12.3 First-Order Optimality Conditions

互補性的一個特殊情況很重要，值得給予自己的定義。

Definition (Strict Complementarity)

Given a local solution x_* of problem (1) and a vector λ_* satisfying (32), we say that the **strict complementarity condition holds** if exactly one of λ_i^* and $c_i(x_*)$ is zero for each index $i \in \mathcal{I}$; that is, $\lambda_i^* > 0$ for each $i \in \mathcal{I} \cap \mathcal{A}(x_*)$.

嚴格互補性的滿足通常使演算法更容易確定 active set $\mathcal{A}(x_*)$ 並迅速收斂到解 x_* 。對於給定問題 (1) 和解 x_* ，可能存在許多滿足條件 (32) 的向量 λ_* 。然而，當在 x_* 處滿足 LICQ 時，最優的 λ_* 是唯一的。

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§12.3 First-Order Optimality Conditions

在結束本節之前，我們通過另一個例子來說明 KKT 條件。

Example

Consider the minimization problem

$$\min_x \left(x_1 - \frac{3}{2} \right)^2 + \left(x_2 - \frac{1}{2} \right)^4 \quad \text{s.t.} \quad \begin{bmatrix} 1 - x_1 - x_2 \\ 1 - x_1 + x_2 \\ 1 + x_1 - x_2 \\ 1 + x_1 + x_2 \end{bmatrix} \geq 0. \quad (33)$$

From Figure 11 we see that the solution is $x_* = (1, 0)^T$ at which the first and second constraints in (33) are active. Denoting them by c_1 and c_2 (and the inactive constraints by c_3 and c_4) so that $\mathcal{A}(x_*) = \{1, 2\}$, we have that

$$\nabla f(x_*) = \begin{bmatrix} -1 \\ -\frac{1}{2} \end{bmatrix}, \quad \nabla c_1(x_*) = \begin{bmatrix} -1 \\ -1 \end{bmatrix}, \quad \nabla c_2(x_*) = \begin{bmatrix} -1 \\ 1 \end{bmatrix}.$$

§12.3 First-Order Optimality Conditions

Example (cont'd)

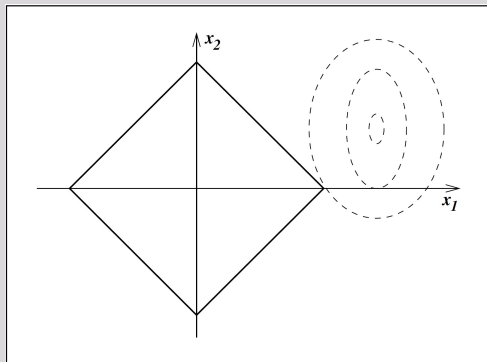


Figure 11: Inequality-constrained problem (33) with solution at $(1, 0)^T$.

Therefore, the KKT conditions (32a)-(32e) are satisfied when we set $\lambda_* = (3/4, 1/4, 0, 0)^T$.

§12.4 First-Order Optimality Conditions: Proof

- **A fundamental necessary condition**

如前所述，點 x 被稱為是受限優化問題

$$\min_{x \in \mathbb{R}^n} f(x) \quad \text{subject to} \quad \begin{cases} c_i(x) = 0, i \in \mathcal{E}, \\ c_i(x) \geq 0, i \in \mathcal{I}, \end{cases} \quad (1)$$

的一個局部解如果所有收斂到 x 的可行數列 $\{z_k\}$ 對足夠大的 k 都滿足 $f(z_k) \geq f(x)$ 。以下結果顯示，如果存在這樣的一個數列，則其極限方向必須與目標函數梯度有非負內積。

Theorem

If x_* is a local solution of (1), then we have

$$(\nabla f)(x_*)^T d \geq 0 \quad \text{for all } d \in T_{\Omega}(x_*).$$

§12.4 First-Order Optimality Conditions: Proof

Proof.

Suppose the contrary that there exists $d \in T_{\Omega}(x_*)$ for which $(\nabla f)(x_*)^T d < 0$. Let $\{z_k\} \subseteq \Omega$ and $\{t_k\} \subseteq \mathbb{R}^+$ be sequences satisfying

$$\lim_{k \rightarrow \infty} t_k = 0 \quad \text{and} \quad \lim_{k \rightarrow \infty} \frac{z_k - x_*}{t_k} = d.$$

By Taylor's Theorem,

$$\begin{aligned} f(z_k) &= f(x_*) + (z_k - x_*)^T (\nabla f)(x_*) + o(\|z_k - x_*\|) \\ &= f(x_*) + t_k d^T (\nabla f)(x_*) + o(t_k). \end{aligned}$$

Since $d^T (\nabla f)(x_*) < 0$, the remainder term is eventually dominated by the first-order term; thus

$$f(z_k) < f(x_*) + \frac{1}{2} t_k d^T (\nabla f)(x_*) \quad \forall k \gg 1.$$

Since $d^T (\nabla f)(x_*) < 0$, x_* cannot be a local solution. □

§12.4 First-Order Optimality Conditions: Proof

這個結果的逆命題不一定成立。也就是說，即使對於所有的 $T_{\Omega}(x_*)$ 中的 d 都有 $(\nabla f)(x_*)^T d \geq 0$ ， x_* 仍然不一定是一個局部最小值。下面是一個有兩個變數的受限優化問題的例子，如圖 12 所示。

$$\min x_2 \quad \text{subject to} \quad x_2 \geq -x_1^2. \quad (34)$$

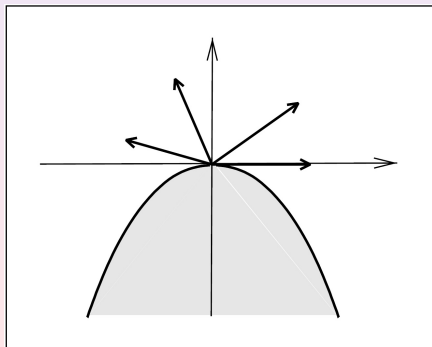


Figure 12: Problem (34), showing various limiting directions of feasible sequences at the point $(0,0)^T$.

§12.4 First-Order Optimality Conditions: Proof

這個問題實際上是無界的，但讓我們來檢視它在 $x_* = (0, 0)^T$ 的行為。不難證明所有可行數列的極限方向 $d = (d_1, d_2)^T$ 必須滿足 $d_2 \geq 0$ ，因此由 $(\nabla f)(x_*) = (0, 1)^T$ 我們得到

$$(\nabla f)(x_*)^T d = d_2 \geq 0.$$

然而， x_* 顯然不是一個局部最小值：對於 $\alpha > 0$ 的點 $(\alpha, -\alpha^2)^T$ 之函數值小於在 x_* 的函數值，並且可以通過將 α 設置足夠小來使其趨近於 x_* 。

§12.4 First-Order Optimality Conditions: Proof

• Farkas' lemma

證明一階必要條件中最重要的一步是一個被稱為 Farkas' Lemma 的古典 alternative 定理。該 lemma 考慮一個定義如下的 cone K :

$$K = \{By + Cw \mid y \geq 0\}, \quad (35)$$

其中 B 和 C 分別為給定的 $n \times m$ 和 $n \times p$ 的矩陣，而 y 和 w 是適當維度的任意向量。根據 Farkas' Lemma，對於給定的 \mathbb{R}^n 向量 g ，有兩種情況之一（且僅有一種）為真：要麼 g 屬於 K ，要麼存在一個 \mathbb{R}^n 向量 d 使得

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§12.4 First-Order Optimality Conditions: Proof

這兩種情況在圖 13 中以 B 有三行、 C 為空、以及 $n = 2$ 的情況做了展示。需要注意的是，在第二種情況中，向量 d 定義了一個分割超平面 (separating hyperplane)，這是在 \mathbb{R}^n 中的一個平面，它將向量 g 與 cone K 分開。

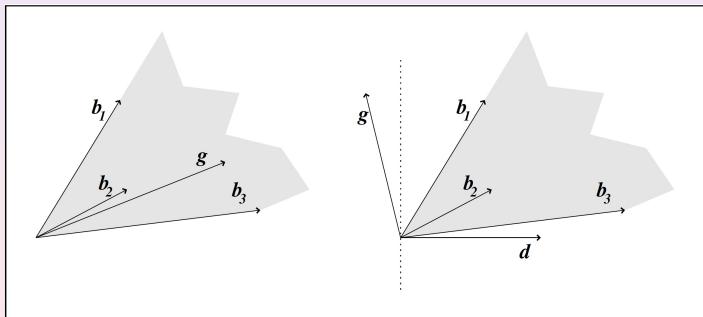


Figure 13: Farkas' Lemma: either $g \in K$ (left) or there is a separating hyperplane (right).

§12.4 First-Order Optimality Conditions: Proof

Lemma (Farkas)

Let $B \in \mathbb{R}^{n \times m}$, $C \in \mathbb{R}^{n \times p}$ be given, and K be a set defined by

$$K = \{By + Cw \mid y \geq 0, w \in \mathbb{R}^p\}. \quad (35)$$

For a given vector $g \in \mathbb{R}^n$, we have either that $g \in K$ or that there exists $d \in \mathbb{R}^n$ satisfying

$$g^T d < 0, \quad B^T d \geq 0, \quad C^T d = 0, \quad (36)$$

but **not both**.

Proof.

We show first that the two alternatives cannot hold simultaneously. If $g \in K$, there exist vectors $y \geq 0$ and w such that $g = By + Cw$. If there also exists a d with the property (36), we have

$$0 > d^T g = d^T By + d^T Cw = (B^T d)^T y + (C^T d)^T w \geq 0.$$

Hence, we cannot have both alternatives holding at once. □

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Proof (cont'd).

We now show that one of the alternatives holds. To be precise, we show how to construct d with the properties (36) in the case that $g \notin K$. For this part of the proof, we need to use the property that K is a closed set – a fact that is intuitively obvious but not trivial to prove (see Lemma 12.15 in the textbook). Let $\{s_k\} \subseteq K$ be a minimizing sequence satisfying

$$\inf_{s \in K} \|s - g\| \leq \|s_k - g\| < \inf_{s \in K} \|s - g\| + \frac{1}{k}.$$

Then the fact that $\{s_k\} \subseteq K \cap B[g, \inf_{s \in K} \|s - g\| + 1]$ implies that there exists a convergent subsequence $\{s_{k_j}\}$ with limit $\hat{s} \in K$. Such \hat{s} is the vector in K that is closet to g in the sense of the Euclidean norm. Since $\hat{s} \in K$, we have from the fact that K is a cone that $\alpha \hat{s} \in K$ for all scalars $\alpha \geq 0$. □

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Since $\|\alpha\hat{s} - g\|^2$ is minimized by $\alpha = 1$, we have

$$\left. \frac{d}{d\alpha} \right|_{\alpha=1} \|\alpha\hat{s} - g\|^2 = 0 \quad \Rightarrow \quad \hat{s}^T(\hat{s} - g) = 0. \quad (37)$$

Now, let s be any other vector in K . Since K is convex, we have by the minimizing property of \hat{s} that

$$\|\hat{s} + \theta(s - \hat{s}) - g\|^2 \geq \|\hat{s} - g\|^2 \quad \text{for all } \theta \in [0, 1],$$

and hence

$$2\theta(s - \hat{s})^T(\hat{s} - g) + \theta^2\|s - \hat{s}\|^2 \geq 0 \quad \text{for all } \theta \in [0, 1].$$

By dividing this expression by θ and taking the limit as $\theta \searrow 0$, we have $(s - \hat{s})^T(\hat{s} - g) \geq 0$. Therefore, because of (37),

$$s^T(\hat{s} - g) \geq 0 \quad \text{for all } s \in K. \quad (38)$$

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$$d^T g = d^T (\hat{s} - d) = (\hat{s} - g)^T \hat{s} - d^T d = -\|d\|^2 < 0,$$

so that d satisfies the first property in (36).

From (38), we have that $d^T s \geq 0$ for all $s \in K$, so that

$$d^T (By + Cw) \geq 0 \quad \text{for all } y \geq 0 \text{ and all } w.$$

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$$N = \left\{ \sum_{i \in \mathcal{A}(x_*)} \lambda_i \nabla c_i(x_*) \mid \{\lambda_i\}_{i \in \mathcal{A}(x_*)} \subseteq \mathbb{R}, \lambda_i \geq 0 \text{ if } i \in \mathcal{A}(x_*) \cap \mathcal{I} \right\},$$

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因此，如果對於所有屬於 $\mathcal{F}(x_*)$ 的向量 d 都有 $\nabla f(x_*)^T d \geq 0$ 的話，則 $(\nabla f)(x_*)$ 屬於 cone N 。

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§12.4 First-Order Optimality Conditions: Proof

Theorem (First-Order Necessary Conditions)

Suppose that x_* is a local solution of problem

$$\min_{x \in \mathbb{R}^n} f(x) \quad \text{subject to} \quad \begin{cases} c_i(x) = 0, i \in \mathcal{E}, \\ c_i(x) \geq 0, i \in \mathcal{I}, \end{cases} \quad (1)$$

that the functions f and c_i in (1) are continuously differentiable, and that the LICQ holds at x_* . Then there is a Lagrange multiplier vector λ_* , with components λ_i^* , $i \in \mathcal{E} \cup \mathcal{I}$, such that the following conditions are satisfied.

$$\nabla_x \mathcal{L}(x_*, \lambda_*) = 0, \quad (32a)$$

$$c_i(x_*) = 0 \quad \text{for all } i \in \mathcal{E}, \quad (32b)$$

$$c_i(x_*) \geq 0 \quad \text{for all } i \in \mathcal{I}, \quad (32c)$$

$$\lambda_i^* \geq 0 \quad \text{for all } i \in \mathcal{I}, \quad (32d)$$

$$\lambda_i^* c_i(x_*) = 0 \quad \text{for all } i \in \mathcal{E} \cup \mathcal{I}. \quad (32e)$$

§12.4 First-Order Optimality Conditions: Proof

Proof.

Suppose that $x_* \in \mathbb{R}^n$ is a local solution of (1) at which the LICQ holds. Then the established lemmas and theorem show that

$$T_{\Omega}(x_*) = \mathcal{F}(x_*) \quad \text{and} \quad d^T(\nabla f)(x_*) \geq 0 \quad \forall d \in T_{\Omega}(x_*).$$

Therefore, $d^T(\nabla f)(x_*) \geq 0$ for all $d \in \mathcal{F}(x_*)$; thus Farkas' Lemma implies that there are multipliers $\{\lambda_i\}_{i \in \mathcal{A}(x_*)} \subseteq \mathbb{R}$ such that

$$(\nabla f)(x_*) = \sum_{i \in \mathcal{A}(x_*)} \lambda_i \nabla c_i(x_*), \quad \lambda_i \geq 0 \text{ if } i \in \mathcal{A}(x_*) \cap \mathcal{I}. \quad (39)$$

Define the vector λ_* by

$$\lambda_i^* = \begin{cases} \lambda_i & \text{if } i \in \mathcal{A}(x_*), \\ 0 & \text{if } i \in \mathcal{I} \setminus \mathcal{A}(x_*), \end{cases} \quad (40)$$

We claim that this choice of λ_* , together with our local solution x_* , satisfies the conditions (32). □

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§12.4 First-Order Optimality Conditions: Proof

Proof (cont'd).

We check these conditions in turn.

- ① The condition (32a) follows immediately from (39) and the definitions (31) of the Lagrangian function and (40) of λ_* .
- ② Since x_* is feasible, the conditions (32b) and (32c) are satisfied.
- ③ We have from (39) that $\lambda_i^* \geq 0$ for $i \in \mathcal{A}(x_*) \cap \mathcal{I}$, while from (40), $\lambda_i^* = 0$ for $i \in \mathcal{I} \setminus \mathcal{A}(x_*)$. Hence, $\lambda_i^* \geq 0$ for $i \in \mathcal{I}$, so that (32d) holds.
- ④ We have for $i \in \mathcal{A}(x_*) \cap \mathcal{I}$ that $c_i(x_*) = 0$, while for $i \in \mathcal{I} \setminus \mathcal{A}(x_*)$, we have $\lambda_i^* = 0$. Hence $\lambda_i^* c_i(x_*) = 0$ for $i \in \mathcal{I}$, so that (32e) is satisfied as well.

The proof is complete. □

§12.4 First-Order Optimality Conditions: Proof

在定理的證明中，在局部解 x_* 的 LICQ 要求是為了證明條件

$$T_{\Omega}(x_*) = \mathcal{F}(x_*). \quad (41)$$

因此，對定理證明做些許修改我們得到以下定理。

Theorem (First-Order Necessary Conditions)

Suppose that x_ is a local solution of the constrained optimization problem (1) in which the functions f and c_i are continuously differentiable. If (41) holds, then there is a Lagrange multiplier vector λ_* with components λ_i^* such that*

$$\nabla_x \mathcal{L}(x_*, \lambda_*) = 0, \quad (32a)$$

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§12.5 Second-Order Conditions

到目前為止我們描述了在局部解 x_* 處目標函數 f 的一階導數和 active 限制 c_i 如何相互關聯的一階必要條件 - 即 KKT 條件。當這些條件滿足時，在該點沿任何 $\mathcal{F}(x_*)$ 中的向量 w 方向的些微移動，目標函數的一階近似的函數值要麼增加了（即 $w^T(\nabla f)(x_*) > 0$ ），要麼保持不變（即 $w^T(\nabla f)(x_*) = 0$ ）。

假設 $w \in \mathcal{F}(x_*)$ 且 $w^T(\nabla f)(x_*) = 0$ 。那麼單從一階導數的訊息中，並無法判斷在解 x_* 處沿 w 方向做些微移動時，目標函數 f 的函數值是否會增加或減少。在本節中，我們使用二階條件檢查目標函數 f 和限制函數 c_i 的泰勒級數展開中的二階導數項，以這些額外資訊幫助我們判斷 f 函數值是增加還是減少。基本上，二階條件關注於 Lagrangian 在“未定方向” - 即在解 x_* 使得 $w^T(\nabla f)(x_*) = 0$ 成立的 $\mathcal{F}(x_*)$ 中的的方向 - 上的曲率。

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§12.5 Second-Order Conditions

給定 $\mathcal{F}(x_*)$ 和滿足 KKT 條件 (32) 的一些 Lagrange 乘子向量 λ_* ，我們定義 critical cone $\mathcal{C}(x_*, \lambda_*)$ 如下：

$$\mathcal{C}(x_*, \lambda_*) = \left\{ w \in \mathcal{F}(x_*) \mid \nabla c_i(x_*)^T w = 0 \text{ if } i \in \mathcal{A}(x_*) \cap \mathcal{I} \ \& \ \lambda_i^* > 0 \right\}$$

或是進一步由 $\mathcal{F}(x_*)$ 的定義有以下等價條件

$$w \in \mathcal{C}(x_*, \lambda_*) \Leftrightarrow \begin{cases} \nabla c_i(x_*)^T w = 0 & \text{if } i \in \mathcal{E}, \\ \nabla c_i(x_*)^T w = 0 & \text{if } i \in \mathcal{A}(x_*) \cap \mathcal{I} \text{ and } \lambda_i^* > 0, \\ \nabla c_i(x_*)^T w \geq 0 & \text{if } i \in \mathcal{A}(x_*) \cap \mathcal{I} \text{ and } \lambda_i^* = 0. \end{cases} \quad (42)$$

Critical cone 包含那些即使在我們對目標函數進行微小更改時也會趨向於“附著”於所對應的 Lagrange 乘子分量為正的 active 不等式限制以及等式限制的方向。

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§12.5 Second-Order Conditions

根據 critical cone 的定義 (42) 和對於所有 $\mathcal{I} \setminus \mathcal{A}(x_*)$ 中的 inactive index i 有 $\lambda_i^* = 0$ 的事實，我們立即得到：

$$w \in \mathcal{C}(x_*, \lambda_*) \Rightarrow \lambda_i^* \nabla c_i(x_*)^T w = 0 \text{ if } i \in \mathcal{E} \cup \mathcal{I}. \quad (43)$$

因此，根據第一個 KKT 條件 (32a) 和 Lagrangian 的定義 (31)，我們有：

$$w \in \mathcal{C}(x_*, \lambda_*) \Rightarrow w^T (\nabla f)(x_*) = \sum_{i \in \mathcal{E} \cup \mathcal{I}} \lambda_i^* w^T \nabla c_i(x_*) = 0.$$

因此，critical cone $\mathcal{C}(x_*, \lambda_*)$ 包含了從一階導數信息無法確定 f 是否增加或減少來自於 $\mathcal{F}(x_*)$ 的方向。

Remark: 一個簡單記 $\mathcal{C}(x_*, \lambda_*)$ 的方式為 $\mathcal{F}(x_*)$ 中將所對應之 Lagrange 乘子非零的不等式限制全部視為等式限制後而得的新 $\mathcal{F}(x_*)$ 。

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§12.5 Second-Order Conditions

Example

Consider the problem

$$\min x_1 \quad \text{subject to} \quad x_2 \geq 0, 1 - (x_1 - 1)^2 - x_2^2 \geq 0, \quad (44)$$

illustrated in Figure 14. It is not difficult to see that the solution is $x_* = (0, 0)^T$, with active set $\mathcal{A}(x_*) = \{1, 2\}$ and a unique optimal Lagrange multiplier $\lambda_* = (0, 0.5)^T$. Since the gradients of the active constraints at x_* are $(0, 1)^T$ and $(2, 0)^T$, respectively, the LICQ holds, so the optimal multiplier is unique. The linearized feasible set is then

$$\mathcal{F}(x_*) = \left\{ d \mid d^T \begin{bmatrix} 0 \\ 1 \end{bmatrix} \geq 0, d^T \begin{bmatrix} 2 \\ 0 \end{bmatrix} \geq 0 \right\} = \{d \mid d \geq 0\},$$

while the critical cone is

$$\mathcal{C}(x_*, \lambda_*) = \left\{ w \in \mathcal{F}(x_*) \mid w^T \begin{bmatrix} 2 \\ 0 \end{bmatrix} = 0 \right\} = \{(0, w_2)^T \mid w_2 \geq 0\}.$$

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§12.5 Second-Order Conditions

Example (cont'd)

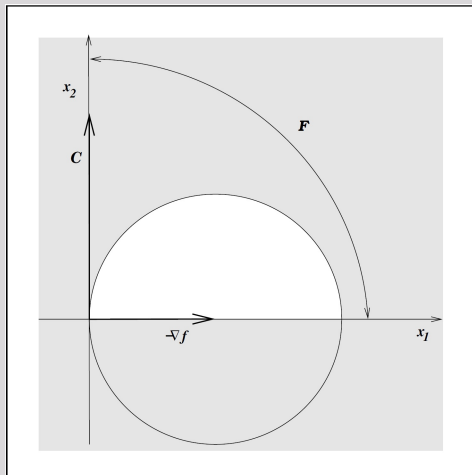


Figure 14: Problem (44), showing $\mathcal{F}(x_*)$ and $\mathcal{C}(x_*, \lambda_*)$.

§12.5 Second-Order Conditions

以下定理涉及二階導數的必要條件。

Theorem (Second-Order Necessary Conditions)

Suppose that x_* is a local solution of

$$\min_{x \in \mathbb{R}^n} f(x) \quad \text{subject to} \quad \begin{cases} c_i(x) = 0, i \in \mathcal{E}, \\ c_i(x) \geq 0, i \in \mathcal{I}, \end{cases} \quad (1)$$

and that the LICQ condition is satisfied at x_* . Let λ_* be the Lagrange multiplier vector for which the KKT conditions

$$\nabla_x \mathcal{L}(x_*, \lambda_*) = 0, \quad (32a)$$

$$c_i(x_*) = 0 \quad \text{for all } i \in \mathcal{E}, \quad (32b)$$

$$c_i(x_*) \geq 0 \quad \text{for all } i \in \mathcal{I}, \quad (32c)$$

$$\lambda_i^* \geq 0 \quad \text{for all } i \in \mathcal{I}, \quad (32d)$$

$$\lambda_i^* c_i(x_*) = 0 \quad \text{for all } i \in \mathcal{E} \cup \mathcal{I}. \quad (32e)$$

are satisfied. Then

$$w^T \nabla_{xx}^2 \mathcal{L}(x_*, \lambda_*) w \geq 0 \quad \text{for all } w \in \mathcal{C}(x_*, \lambda_*). \quad (45)$$

§12.5 Second-Order Conditions

Proof.

Let $w \in \mathcal{C}(x_*, \lambda_*)$ be given. Since the LICQ condition holds at x_* and $\mathcal{C}(x_*, \lambda_*) \subseteq \mathcal{F}(x_*)$, there exist a feasible sequence $\{z_k\}$ approaching x_* and a sequence $\{t_k\}$ of positive scalars approaching 0 such that

$$\lim_{k \rightarrow \infty} \frac{z_k - x_*}{t_k} = w \quad (23)$$

and

$$c_i(z_k) = t_k \nabla c_i(x_*)^T w \quad \forall i \in \mathcal{A}(x_*) \text{ and } k \gg 1. \quad (28)$$

The fact that the multiplier corresponding to inactive constraint is zero implies that for k sufficiently large,

$$\begin{aligned} \mathcal{L}(z_k, \lambda_*) &= f(z_k) - \sum_{i \in \mathcal{E} \cup \mathcal{I}} \lambda_i^* c_i(z_k) = f(z_k) - \sum_{i \in \mathcal{A}(x_*)} \lambda_i^* c_i(z_k) \\ &= f(z_k) - t_k \sum_{i \in \mathcal{A}(x_*)} \lambda_i^* \nabla c_i(x_*)^T w. \quad \square \end{aligned}$$

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§12.5 Second-Order Conditions

Proof (cont'd).

Since $w \in \mathcal{C}(x_*, \lambda_*)$, using (43) (which shows that $\lambda_i^* \nabla c_i(x_*)^T w = 0$ for all $i \in \mathcal{E} \cup \mathcal{I}$) we obtain that

$$\mathcal{L}(z_k, \lambda_*) = f(z_k).$$

On the other hand, using Taylor's Theorem expression and continuity of the Hessians $\nabla^2 f$ and $\nabla^2 c_i$, $i \in \mathcal{E} \cup \mathcal{I}$, we obtain

$$\begin{aligned} \mathcal{L}(z_k, \lambda_*) &= \mathcal{L}(x_*, \lambda_*) + (z_k - x_*)^T \nabla_x \mathcal{L}(x_*, \lambda_*) & (46) \\ &\quad + \frac{1}{2} (z_k - x_*)^T \nabla_{xx}^2 \mathcal{L}(x_*, \lambda_*) (z_k - x_*) + o(\|z_k - x_*\|^2). \end{aligned}$$

By the complementarity conditions (32e), $\mathcal{L}(x_*, \lambda_*) = f(x_*)$. From (32a), $\nabla_x \mathcal{L}(x_*, \lambda_*) = 0$ so the second term on the right-hand side is zero. Also note that the limit (23) can be rewritten as

$$z_k - x_* = t_k w + o(t_k).$$

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§12.5 Second-Order Conditions

Proof (cont'd).

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§12.5 Second-Order Conditions

Proof (cont'd).

Therefore,

$$f(z_k) = f(x_*) + \frac{1}{2}t_k^2 w^T \nabla_{xx}^2 \mathcal{L}(x_*, \lambda_*) w + o(t_k^2).$$

If $w^T \nabla_{xx}^2 \mathcal{L}(x_*, \lambda_*) w < 0$, then $f(z_k) < f(x_*)$ for $k \gg 1$, contradicting the fact that x_* is a local solution. Hence, the condition

$$w^T \nabla_{xx}^2 \mathcal{L}(x_*, \lambda_*) w \geq 0 \quad \text{for all } w \in \mathcal{C}(x_*, \lambda_*) \quad (45)$$

must hold, as claimed. \square

下一個定理中所述的二階充分條件看起來非常像剛才討論的必要條件，但不同之處在於：

- ① 不需要要求 **the constraint qualification**，以及
- ② 不等式 (45) 被更嚴格的不等式

$$w^T \nabla_{xx}^2 \mathcal{L}(x_*, \lambda_*) w > 0 \quad \text{for all } w \in \mathcal{C}(x_*, \lambda_*) \setminus \{0\} \quad (48)$$

所取代。

§12.5 Second-Order Conditions

Proof (cont'd).

Therefore,

$$f(z_k) = f(x_*) + \frac{1}{2}t_k^2 w^T \nabla_{xx}^2 \mathcal{L}(x_*, \lambda_*) w + o(t_k^2).$$

If $w^T \nabla_{xx}^2 \mathcal{L}(x_*, \lambda_*) w < 0$, then $f(z_k) < f(x_*)$ for $k \gg 1$, contradicting the fact that x_* is a local solution. Hence, the condition

$$w^T \nabla_{xx}^2 \mathcal{L}(x_*, \lambda_*) w \geq 0 \quad \text{for all } w \in \mathcal{C}(x_*, \lambda_*) \quad (45)$$

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§12.5 Second-Order Conditions

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所取代。

§12.5 Second-Order Conditions

Theorem (Second-Order Sufficient Conditions)

Suppose that for some feasible point $x_* \in \mathbb{R}^n$ there is a Lagrange multiplier vector λ_* such that the KKT conditions

$$\nabla_x \mathcal{L}(x_*, \lambda_*) = 0, \quad (32a)$$

$$c_i(x_*) = 0 \quad \text{for all } i \in \mathcal{E}, \quad (32b)$$

$$c_i(x_*) \geq 0 \quad \text{for all } i \in \mathcal{I}, \quad (32c)$$

$$\lambda_i^* \geq 0 \quad \text{for all } i \in \mathcal{I}, \quad (32d)$$

$$\lambda_i^* c_i(x_*) = 0 \quad \text{for all } i \in \mathcal{E} \cup \mathcal{I}. \quad (32e)$$

are satisfied. Suppose also that

$$w^T \nabla_{xx}^2 \mathcal{L}(x_*, \lambda_*) w > 0 \quad \text{for all } w \in \mathcal{C}(x_*, \lambda_*) \setminus \{0\}. \quad (48)$$

Then x_* is a strict local solution for

$$\min_{x \in \mathbb{R}^n} f(x) \quad \text{subject to} \quad \begin{cases} c_i(x) = 0, i \in \mathcal{E}, \\ c_i(x) \geq 0, i \in \mathcal{I}. \end{cases} \quad (1)$$

§12.5 Second-Order Conditions

Proof.

Before proceeding, note that the set $\bar{\mathcal{C}} = \{d \in \mathcal{C}(x_*, \lambda_*) \mid \|d\| = 1\}$ is a compact subset of $\mathcal{C}(x_*, \lambda_*)$, so by (48),

$$\min_{d \in \bar{\mathcal{C}}} d^T \nabla_{xx}^2 \mathcal{L}(x_*, \lambda_*) d \equiv \sigma > 0.$$

Since $\mathcal{C}(x_*, \lambda_*)$ is a cone, we have that $w/\|w\| \in \bar{\mathcal{C}}$ if and only if $w \in \mathcal{C}(x_*, \lambda_*) \setminus \{0\}$. Therefore, condition (48) implies that

$$w^T \nabla_{xx}^2 \mathcal{L}(x_*, \lambda_*) w \geq \sigma \|w\|^2 \quad \text{for all } w \in \mathcal{C}(x_*, \lambda_*), \quad (49)$$

where $\sigma > 0$ is defined above. Moreover, by Taylor's Theorem the KKT condition (32a,e) shows that

$$\begin{aligned} \mathcal{L}(x, \lambda_*) &= f(x_*) + \frac{1}{2}(x - x_*)^T \nabla_{xx}^2 \mathcal{L}(x_*, \lambda_*) (x - x_*) \\ &\quad + o(\|x - x_*\|^2). \end{aligned} \quad (50)$$

□

§12.5 Second-Order Conditions

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§12.5 Second-Order Conditions

Proof (cont'd).

Now we prove the result by showing that every feasible sequence $\{z_k\}$ approaching x_* satisfies

$$f(z_k) \geq f(x_*) + \frac{\sigma}{4} \|z_k - x_*\|^2 \quad \forall k \gg 1.$$

Suppose the contrary that there is a feasible sequence $\{z_k\}$ approaching x_* with

$$f(z_k) < f(x_*) + \frac{\sigma}{4} \|z_k - x_*\|^2 \quad \forall k \gg 1. \quad (51)$$

By taking a subsequence if necessary, we can identify a limiting direction d such that

$$\lim_{k \rightarrow \infty} \frac{z_k - x_*}{\|z_k - x_*\|} = d.$$

We then have $d \in T_\Omega(x_*)$, and the fact that $T_\Omega(x_*) \subseteq \mathcal{F}(x_*)$ shows that $d \in \mathcal{F}(x_*)$. Next we show that $d \in \mathcal{C}(x_*, \lambda_*)$. □

§12.5 Second-Order Conditions

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§12.5 Second-Order Conditions

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$$z_k - x_* = t_k d + o(t_k), \quad t_k = \|z_k - x_*\|.$$

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§12.5 Second-Order Conditions

Proof (cont'd).

If d were not in $\mathcal{C}(x_*, \lambda_*)$, we could identify some index $j \in \mathcal{A}(x_*) \cap \mathcal{I}$ such that the strict positivity condition

$$\lambda_j^* \nabla c_j(x_*)^T d > 0 \quad (52)$$

is satisfied, while for the remaining indices $i \in \mathcal{A}(x_*)$, we have

$$\lambda_i^* \nabla c_i(x_*)^T d \geq 0.$$

From Taylor's Theorem, for this particular value of j we have that

$$\begin{aligned} \lambda_j^* c_j(z_k) &= \lambda_j^* c_j(x_*) + \lambda_j^* \nabla c_j(x_*)^T (z_k - x_*) + o(\|z_k - x_*\|) \\ &= t_k \lambda_j^* \nabla c_j(x_*)^T d + o(t_k). \end{aligned}$$

Recall the Lagrange function

$$\mathcal{L}(x, \lambda) = f(x) - \sum_{i \in \mathcal{E} \cup \mathcal{I}} \lambda_i c_i(x). \quad \square$$

§12.5 Second-Order Conditions

Proof (cont'd).

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§12.5 Second-Order Conditions

Proof (cont'd).

Since $\{z_k\}$ is feasible, the KKT condition (32d) implies that

$$\begin{aligned} \mathcal{L}(z_k, \lambda_*) &= f(z_k) - \sum_{i \in \mathcal{E} \cup \mathcal{I}} \lambda_i^* c_i(z_k) \leq f(z_k) - \lambda_j^* c_j(z_k) \\ &\leq f(z_k) - t_k \lambda_j^* \nabla c_j(x_*)^T d + o(t_k). \end{aligned} \quad (53)$$

On the other hand, (50) shows that

$$\mathcal{L}(z_k, \lambda_*) = f(x_*) + \frac{1}{2} t_k^2 d^T \nabla_{xx}^2 \mathcal{L}(x_*, \lambda_*) d + o(t_k^2);$$

thus, combining the equality above and (53), we conclude that

$$f(z_k) \geq f(x_*) + t_k \lambda_j^* \nabla c_j(x_*)^T d + o(t_k),$$

which, because of (52), is a contradiction to

$$f(z_k) < f(x_*) + \frac{\sigma}{4} \|z_k - x_*\|^2 \quad \forall k \gg 1. \quad (51)$$

§12.5 Second-Order Conditions

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§12.5 Second-Order Conditions

Proof (cont'd).

Therefore, $d \in \mathcal{C}(x_*, \lambda_*)$, and hence (49) shows that

$$d^T \nabla_{xx}^2 \mathcal{L}(x_*, \lambda_*) d \geq \sigma \|d\|^2.$$

By the Taylor series estimate (50), we obtain that

$$\begin{aligned} f(z_k) &\geq f(z_k) - \sum_{i \in \mathcal{E} \cup \mathcal{I}} \lambda_i^* c_i(z_k) = \mathcal{L}(z_k, \lambda_*) \\ &= f(x_*) + \frac{1}{2} t_k^2 d^T \nabla_{xx}^2 \mathcal{L}(x_*, \lambda_*) d + o(t_k^2) \\ &\geq f(x_*) + \frac{\sigma}{2} \|z_k - x_*\|^2 + o(\|z_k - x_*\|^2). \end{aligned}$$

This inequality again yields the contradiction to (51). Therefore, every feasible sequence $\{z_k\}$ approaching x_* must satisfy

$$f(z_k) \geq f(x_*) + \frac{\sigma}{4} \|z_k - x_*\|^2 \quad \forall k \gg 1,$$

so x_* is a strict local solution. □

§12.5 Second-Order Conditions

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§12.5 Second-Order Conditions

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$$f(z_k) \geq f(x_*) + \frac{\sigma}{4} \|z_k - x_*\|^2 \quad \forall k \gg 1,$$

so x_* is a strict local solution. □

§12.5 Second-Order Conditions

Example

We now return to the 2nd example in Section 12.1 to check the second-order conditions for problem

$$\min(x_1 + x_2) \quad \text{s.t.} \quad 2 - x_1^2 - x_2^2 \geq 0. \quad (12)$$

In this problem we have the Lagrange function

$$\mathcal{L}(x, \lambda) = (x_1 + x_2) - \lambda_1(2 - x_1^2 - x_2^2),$$

and $\mathcal{E} = \emptyset$, $\mathcal{I} = \{1\}$. The KKT conditions (32) are satisfied by $x_* = (-1, -1)^T$, with $\lambda_1^* = 1/2$. The Lagrangian Hessian at x_* is

$$\nabla_{xx}^2 \mathcal{L}(x_*, \lambda_*) = \begin{bmatrix} 2\lambda_1^* & 0 \\ 0 & 2\lambda_1^* \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

which is positive definite, so it certainly satisfies the conditions of the theorem above. We conclude that $x_* = (-1, -1)^T$ is a strict local solution for (12).

§12.5 Second-Order Conditions

Example

For a more complex example, consider the problem

$$\min -0.1(x_1 - 4)^2 + x_2^2 \quad \text{s.t.} \quad x_1^2 + x_2^2 - 1 \geq 0, \quad (54)$$

in which we seek to minimize a non-convex function over the **exterior** of the unit circle. Obviously, the objective function is not bounded below on the feasible region, since we can take the feasible sequence

$$\begin{bmatrix} 10 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 20 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 30 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 40 \\ 0 \end{bmatrix}, \quad \dots$$

and note that $f(x)$ approaches $-\infty$ along this sequence. Therefore, no global solution exists, but it may still be possible to identify a strict local solution on the boundary of the constraint. We search for such a solution by using the KKT conditions (32) and the second-order conditions of in the previous theorem.

§12.5 Second-Order Conditions

Example (cont'd)

By defining the Lagrangian for (54) in the usual way, it is easy to verify that

$$\nabla_x \mathcal{L}(x, \lambda) = \begin{bmatrix} -0.2(x_1 - 4) - 2\lambda_1 x_1 \\ 2x_2 - 2\lambda_1 x_2 \end{bmatrix}, \quad (55a)$$

$$\nabla_{xx}^2 \mathcal{L}(x, \lambda) = \begin{bmatrix} -0.2 - 2\lambda_1 & 0 \\ 0 & 2 - 2\lambda_1 \end{bmatrix}. \quad (55b)$$

The point $x_* = (1, 0)^T$ satisfies the KKT conditions with $\lambda_1^* = 0.3$ and the active set $\mathcal{A}(x_*) = \{1\}$. To check that the second-order sufficient conditions are satisfied at this point, we note that

$$\nabla c_1(x_*) = \begin{bmatrix} 2 \\ 0 \end{bmatrix}$$

so that the critical cone is simply

$$\mathcal{C}(x_*, \lambda_*) = \{(0, w_2)^T \mid w_2 \in \mathbb{R}\}.$$

§12.5 Second-Order Conditions

Example (cont'd)

Now, by substituting x_* and λ_* into (55b), we have for any $w \in \mathcal{C}(x_*, \lambda_*)$ with $w \neq 0$ that $w_2 \neq 0$ and thus

$$\begin{aligned} w^T \nabla_{xx}^2 \mathcal{L}(x_*, \lambda_*) w &= \begin{bmatrix} 0 & w_2 \end{bmatrix} \begin{bmatrix} -0.4 & 0 \\ 0 & 1.4 \end{bmatrix} \begin{bmatrix} 0 \\ w_2 \end{bmatrix} \\ &= 1.4w_2^2 > 0. \end{aligned}$$

Hence, the second-order sufficient conditions are satisfied, and we conclude from the previous theorem that $(1, 0)^T$ is a strict local solution for (54).

§12.5 Second-Order Conditions

• Second-order conditions and projected Hessians

二階條件在某些情況下會以一種比

$$w^T \nabla_{xx}^2 \mathcal{L}(x_*, \lambda_*) w \geq 0 \quad \text{for all } w \in \mathcal{C}(x_*, \lambda_*) \quad (45)$$

與

$$w^T \nabla_{xx}^2 \mathcal{L}(x_*, \lambda_*) w > 0 \quad \text{for all } w \in \mathcal{C}(x_*, \lambda_*) \setminus \{0\} \quad (48)$$

稍微弱但更容易驗證的形式陳述。以下我們討論在滿足 KKT 條件 (32) 的乘子 λ_* 滿足嚴格互補性（且是唯一的）時的情況。在這種情況下，二階條件的形式可使用 Lagrangian 的 Hessian 矩陣 $\nabla_{xx}^2 \mathcal{L}(x_*, \lambda_*)$ 對與 $\mathcal{C}(x_*, \lambda_*)$ 相關的子空間的前後投影 (two-sided projection) 來進行展示。

§12.5 Second-Order Conditions

注意到當滿足 KKT 條件 (32) 的乘子 λ_* 滿足嚴格互補性 (即對於每個在 $\mathcal{I} \cap \mathcal{A}(x_*)$ 中的 index i 都有 $\lambda_i^* > 0$) 時, 我們有 $w \in \mathcal{C}(x_*, \lambda_*)$ 若且唯若

$$\begin{cases} \nabla c_i(x_*)^T w = 0 & \text{if } i \in \mathcal{E}, \\ \nabla c_i(x_*)^T w = 0 & \text{if } i \in \mathcal{A}(x_*) \cap \mathcal{I} \text{ and } \lambda_i^* > 0, \\ \nabla c_i(x_*)^T w \geq 0 & \text{if } i \in \mathcal{A}(x_*) \cap \mathcal{I} \text{ and } \lambda_i^* = 0. \end{cases}$$

因此, 當滿足 KKT 條件 (32) 的乘子 λ_* 滿足嚴格互補性時

$$\mathcal{C}(x_*, \lambda_*) = \text{Null}([\nabla c_i(x_*)^T]_{i \in \mathcal{A}(x_*)}) = \text{Null}(A(x_*)),$$

其中 $A(x_*) \equiv [\nabla c_i(x_*)^T]_{i \in \mathcal{A}(x_*)}$ 如 (27) 式中所定義。換句話說, 在這種情況下, $\mathcal{C}(x_*, \lambda_*)$ 是在 x_* 處的 active constraint gradient 形成的矩陣的 null space。

§12.5 Second-Order Conditions

注意到當滿足 KKT 條件 (32) 的乘子 λ_* 滿足嚴格互補性 (即對於每個在 $\mathcal{I} \cap \mathcal{A}(x_*)$ 中的 index i 都有 $\lambda_i^* > 0$) 時，我們有 $w \in \mathcal{C}(x_*, \lambda_*)$ 若且唯若

$$\begin{cases} \nabla c_i(x_*)^T w = 0 & \text{if } i \in \mathcal{E}, \\ \nabla c_i(x_*)^T w = 0 & \text{if } i \in \mathcal{A}(x_*) \cap \mathcal{I} \text{ and } \lambda_i^* > 0, \\ \nabla c_i(x_*)^T w \geq 0 & \text{if } i \in \mathcal{A}(x_*) \cap \mathcal{I} \text{ and } \lambda_i^* = 0. \end{cases}$$

因此，當滿足 KKT 條件 (32) 的乘子 λ_* 滿足嚴格互補性時

$$\mathcal{C}(x_*, \lambda_*) = \text{Null}([\nabla c_i(x_*)^T]_{i \in \mathcal{A}(x_*)}) = \text{Null}(A(x_*)),$$

其中 $A(x_*) \equiv [\nabla c_i(x_*)^T]_{i \in \mathcal{A}(x_*)}$ 如 (27) 式中所定義。換句話說，在這種情況下， $\mathcal{C}(x_*, \lambda_*)$ 是在 x_* 處的 active constraint gradient 形成的矩陣的 null space。

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§12.5 Second-Order Conditions

與 (29) 類似，由於

the null space of $A(x_*) \oplus$ the range of $A(x_*)^T = \mathbb{R}^n$,

我們可以定義一個具有滿秩的 $n \times (n - \text{rank}(A(x_*)))$ 矩陣 Z ，其行向量 span 空間 $\mathcal{C}(x_*, \lambda_*)$ ；即

$$\mathcal{C}(x_*, \lambda_*) = \left\{ Zu \mid u \in \mathbb{R}^{n - \text{rank}(A(x_*))} \right\}.$$

因此，如果除了滿足 KKT 條件 (32) 的乘子 λ_* 滿足嚴格互補性外更進一步假設乘子的唯一性（例如說在 x_* 處滿足 LICQ 條件時），則 $A(x_*)$ 有滿秩且

$$\mathcal{C}(x_*, \lambda_*) = \left\{ Zu \mid u \in \mathbb{R}^{n - |\mathcal{A}(x_*)|} \right\},$$

因為在此情況下在 x_* active constraint 的個數 $|\mathcal{A}(x_*)|$ 恰為 $A(x_*)^T$ 的 range 的維度。

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因此，當滿足 KKT 條件 (32) 的乘子 λ_* 滿足嚴格互補性（且又是唯一）時，二階必要條件

$$w^T \nabla_{xx}^2 \mathcal{L}(x_*, \lambda_*) w \geq 0 \quad \text{for all } w \in \mathcal{C}(x_*, \lambda_*) \quad (45)$$

可以重新陳述為

$$u^T Z^T \nabla_{xx}^2 \mathcal{L}(x_*, \lambda_*) Z u \geq 0 \quad \forall u \in \mathbb{R}^{n-\text{rank}(A(x_*))},$$

或者更簡潔地說，「 $Z^T \nabla_{xx}^2 \mathcal{L}(x_*, \lambda_*) Z$ 為半正定矩陣」。同樣地，二階充分條件

$$w^T \nabla_{xx}^2 \mathcal{L}(x_*, \lambda_*) w > 0 \quad \text{for all } w \in \mathcal{C}(x_*, \lambda_*) \setminus \{0\} \quad (48)$$

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接下來我們將展示， Z 可以通過數值計算獲得，因此正定性（及半正定性）條件實際上可以被檢驗。

計算矩陣 Z 的一種方法是將 active constraint gradient 矩陣應用 QR 分解。在上述的一種最簡單的情況中（即乘子 λ_* 滿足嚴格互補性且為唯一的），我們將 $A(x_*)$ 定義為 (27) 式中的形式，並將其轉置的 QR 分解表示為

$$A(x_*)^T = Q \begin{bmatrix} R \\ 0 \end{bmatrix} = [Q_1 \quad Q_2] \begin{bmatrix} R \\ 0 \end{bmatrix} = Q_1 R,$$

其中 R 是一個上三角方陣， Q 是 $n \times n$ 的正交矩陣。如果 R 是可逆的，我們可以設置 $Z = Q_2$ 。如果 R 是 singular 的（表示 active constraint gradient 線性相依），則在 QR 過程中使用 column pivoting 的些微增強程序可以用來決定 Z 。

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§12.6 Other Constraint Qualifications

在本節中我們重新考慮 constraint qualifications，即在 §12.2 和 §12.4 討論的條件，確保對可行集 Ω 的線性化近似捕捉了和解 x_* 附近 Ω 的基本形狀。

當所有 active constraint 是線性的情況下，亦即存在 $a_i \in \mathbb{R}^n$ 以及 $b_i \in \mathbb{R}$ 使得

$$c_i(x) = a_i^T x + b_i \quad (56)$$

的情況下，線性化可行方向集 $\mathcal{F}(x_*)$ 顯然是對實際可行集的適當表示。對於這種情況，不難證明以下的 Lemma。

Lemma

Suppose that at some $x_ \in \Omega$, all active constraints $c_i(\cdot)$, $i \in \mathcal{A}(x_*)$, are linear functions. Then $\mathcal{F}(x_*) = T_\Omega(x_*)$.*

注意到 $\mathcal{F}(x_*) = T_\Omega(x_*)$ 是 KKT 條件成立的條件（之一）。

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Proof of Lemma (in the previous slide).

It suffices to show that $\mathcal{F}(x_*) \subseteq T_\Omega(x_*)$. Let $w \in \mathcal{F}(x_*)$. By the definition of feasible direction set and the form (56) of the constraints,

$$\mathcal{F}(x_*) = \left\{ d \mid \begin{array}{l} a_i^T d = 0 \text{ for all } i \in \mathcal{E}, \\ a_i^T d \geq 0 \text{ for all } i \in \mathcal{A}(x_*) \cap \mathcal{I} \end{array} \right\}.$$

First, note that there is a positive scalar \bar{t} such that the inactive constraints remain inactive at $x_* + tw$, for all $t \in [0, \bar{t}]$; that is,

$$c_i(x_* + tw) > 0 \quad \text{for all } i \in \mathcal{I} \setminus \mathcal{A}(x_*) \text{ and all } t \in [0, \bar{t}].$$

Now define the sequence z_k by

$$z_k = x_* + (\bar{t}/k)w, \quad k = 1, 2, \dots$$

By the choice of \bar{t} , we find that z_k is feasible with respect to the inactive inequality constraints $i \in \mathcal{I} \setminus \mathcal{A}(x_*)$. □

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Proof (cont'd).

Moreover, since $a_i^T w \geq 0$ for all $i \in \mathcal{I} \cap \mathcal{A}(x_*)$, we find that for all $i \in \mathcal{I} \cap \mathcal{A}(x_*)$,

$$c_i(z_k) = c_i(z_k) - c_i(x_*) = a_i^T(z_k - x_*) = (\bar{t}/k)a_i^T w \geq 0,$$

so that z_k is also feasible with respect to the active inequality constraints c_i , $i \in \mathcal{I} \cap \mathcal{A}(x_*)$. Finally, for $i \in \mathcal{E}$, by the fact that x_* is feasible and $w \in \mathcal{F}(x_*)$, we have $a_i^T w = 0$ so that

$$a_i^T z_k + b_i = a_i^T(x_* + (\bar{t}/k)w) + b_i = a_i^T x_* + b_i = 0;$$

thus z_k is feasible with respect to the equality constraints c_i , $i \in \mathcal{E}$. Hence, z_k is feasible for each $k = 1, 2, \dots$. In addition, we have that

$$\frac{z_k - x_*}{\bar{t}/k} = \frac{(\bar{t}/k)w}{\bar{t}/k} = w,$$

so that w is the limiting direction of $\{z_k\}$. Hence, $w \in T_\Omega(x_*)$. \square

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§12.6 Other Constraint Qualifications

雖然「所有 active constraint 都是線性的」這一條件是另一個 constraint qualification，但它既不比 LICQ 條件更弱也不更強；亦即有些情況下一個條件被滿足而另一個條件不被滿足。

Example

Let $c_1(x_1, x_2) = x_1 + x_2 - 1$ and $c_2(x_1, x_2) = 2x_1 + 2x_2 - 2$. Then at $x = (1, 0)^T$, $\mathcal{A}(x) = \{1, 2\}$ but clearly

$$[\nabla c_i(x)]_{i \in \mathcal{A}(x)} \equiv [\nabla c_1(x) : \nabla c_2(x)]$$

does not has full rank; thus LICQ does not hold at x .

§12.6 Other Constraint Qualifications

另一個有用的 LICQ 的推廣是 Mangasarian-Fromovitz constraint qualification (MFCQ)。

Definition (MFCQ)

We say that the Mangasarian-Fromovitz constraint qualification (MFCQ) holds at x_* if there exists a vector $w \in \mathbb{R}^n$ such that

$$\begin{aligned}\nabla c_i(x_*)^T w &> 0 \quad \text{for all } i \in \mathcal{A}(x_*) \cap \mathcal{I}, \\ \nabla c_i(x_*)^T w &= 0 \quad \text{for all } i \in \mathcal{E},\end{aligned}$$

and the set of **equality** constraint gradients $\{\nabla c_i(x_*) \mid i \in \mathcal{E}\}$ is linearly independent.

需要注意涉及 active inequality constraint 的“嚴格”不等式。

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§12.6 Other Constraint Qualifications

Remark: (應用 §12.9 的對偶理論) 可以證明

存在 $w \in \mathbb{R}^n$ 滿足

$$\nabla c_i(x_*)^T w > 0 \text{ for all } i \in \mathcal{A}(x_*) \cap \mathcal{I},$$

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等價於

受限優化問題

$$\max_{\lambda \in \mathbb{R}^{|\mathcal{A}(x_*)|}} \sum_{i \in \mathcal{A}(x_*) \cap \mathcal{I}} \lambda_i \text{ subject to } \begin{cases} \sum_{i \in \mathcal{A}(x_*)} \lambda_i \nabla c_i(x_*) = 0, \\ \lambda_i \geq 0, \quad i \in \mathcal{A}(x_*) \cap \mathcal{I}, \end{cases}$$

的極值為零。

注意到上述受限優化問題的極植為零意謂著

$$\left\{ [\nabla c_i(x_*)]_{i \in \mathcal{A}(x_*) \cap \mathcal{I}} y \mid y \geq 0 \right\} \cap \left\{ [\nabla c_i(x_*)]_{i \in \mathcal{E}} w \mid w \in \mathbb{R}^{|\mathcal{E}|} \right\} = \{0\}.$$

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§12.6 Other Constraint Qualifications

在加入 $\{\nabla c_i(x_*) \mid i \in \mathcal{E}\}$ 是線性獨立集的條件後，我們得到

Theorem

Let $x \in \Omega$. Then MFCQ holds at x if and only if the system (for λ)

$$\begin{aligned} \sum_{i \in \mathcal{E} \cup \mathcal{I}} \lambda_i \nabla c_i(x) &= 0, \\ \lambda_i c_i(x) &= 0, \quad i \in \mathcal{I}, \\ \lambda_i &\geq 0, \quad i \in \mathcal{I}, \end{aligned}$$

only has zero solution.

因此，MFCQ 條件與 LICQ 條件不同之處在於驗證向量間的“線性獨立性”時，在 active constraint gradients 的“線性組合”中不等式限制所對應的係數必須非負。然後該注意到的是我們無法由上述定理下結論說若 MFCQ 在 local solution x_* 滿足，則其對應滿足 KKT 條件的 λ_* （若存在的話）的唯一性。

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因此，MFCQ 條件與 LICQ 條件不同之處在於驗證向量間的“線性獨立性”時，在 active constraint gradients 的“線性組合”中不等式限制所對應的係數必須非負。然後該注意到的是我們無法由上述定理下結論說若 MFCQ 在 local solution x_* 滿足，則其對應滿足 KKT 條件的 λ_* （若存在的話）的唯一性。

§12.6 Other Constraint Qualifications

MFCQ 是比 LICQ 更弱的條件。 如果 LICQ 被滿足，則 active constraint gradient 有滿秩，因此以下系統所定義的等式系統

$$\begin{aligned}\nabla c_i(x_*)^T w &= 1 \quad \text{for all } i \in \mathcal{A}(x_*) \cap \mathcal{I}, \\ \nabla c_i(x_*)^T w &= 0 \quad \text{for all } i \in \mathcal{E},\end{aligned}$$

有解 w 。因此，我們可以選擇此 w 恰好是 MFCQ 定義中的向量。另一方面，可以輕易構造出滿足 MFCQ 但不滿足 LICQ 的例子。

Example

Let

$$\begin{aligned}c_1(x_1, x_2) &= 2 - (x_1 - 1)^2 - (x_2 - 1)^2, \\ c_2(x_1, x_2) &= 2 - (x_1 - 1)^2 - (x_2 + 1)^2, \\ c_3(x_1, x_2) &= x_1\end{aligned}$$

be the constraint functions for inequality constraints. Then MFCQ holds at $x = (0, 0)^T$ but LICQ does not hold at x .

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可以證明在 MFCQ 替換了 LICQ 後的一階必要條件（即 KKT 條件）結果（本書未證）。MFCQ 產生了一個很好的性質，即它等價於滿足 KKT 條件 (32) 的 Lagrange 乘子向量 λ_* 的集合的緊緻性（在 LICQ 的情況下，這個集合由一個唯一的向量 λ_* 組成，因此在自動有界）。

需要注意的是，constraint qualifications 是使得線性逼近足夠的充分條件而非必要條件。例如，考慮由 $x_2 \geq -x_1^2$ 和 $x_2 \leq x_1^2$ 定義的集合以及可行點 $x_* = (0, 0)^T$ 。我們討論過的任何 constraint qualifications 都不滿足，但線性逼近

$$\mathcal{F}(x_*) = \{(w_1, 0)^T \mid w_1 \in \mathbb{R}\}$$

仍準確地反映了在 x_* 附近的可行集的幾何形狀。

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§12.7 A Geometric Viewpoint

最後，我們提到一個替代的一階最優性條件，它僅僅取決於可行集 Ω 的幾何形狀，而不取決於在限制函數的代數描述。從幾何角度來看，我們的問題 (1) 可以陳述為

$$\min f(x) \quad \text{subject to} \quad x \in \Omega, \quad (57)$$

其中 Ω 是可行集。

首先，我們定義在可行點 x 處的集合 Ω 的 normal cone。

Definition

The normal cone to the set Ω at a point $x \in \Omega$ is defined as

$$N_{\Omega}(x) = \left\{ v \mid v^T w \leq 0 \text{ for all } w \in T_{\Omega}(x) \right\},$$

where $T_{\Omega}(x)$ is the tangent cone to the set Ω at x . Each vector $v \in N_{\Omega}(x)$ is said to be a normal vector.

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對於問題 (57) 的一階必要條件非常簡單而清晰。

Theorem

Suppose that x_* is a local minimizer of f in Ω . Then

$$-\nabla f(x_*) \in N_{\Omega}(x_*).$$

Proof.

Let $d \in T_{\Omega}(x_*)$ be given, there exist a feasible sequence $\{z_k\}$ and a sequence of positive scalars $\{t_k\}$ such that

$$z_k = x_* + t_k d + o(t_k) \quad \forall k \in \mathbb{N}.$$

Since x_* is a local solution and f is continuously differentiable, by Taylor's Theorem we have

$$0 \leq f(z_k) - f(x_*) = t_k \nabla f(x_*)^T d + o(t_k).$$

By dividing by t_k and passing to the limit as $k \rightarrow \infty$, we find that $\nabla f(x_*)^T d \geq 0$. □

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Proof (cont'd).

Therefore,

$$-\nabla f(x_*)^T d \leq 0 \quad \forall d \in T_\Omega(x_*).$$

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由問題 (1) 局部解所滿足的一階必要條件 (KKT 條件)，我們發現上述定理暗含了 $N_\Omega(x_*)$ 與 active constraint gradients 的 conic combination

$$N = \left\{ \sum_{i \in \mathcal{A}(x_*)} \lambda_i \nabla c_i(x_*) \mid \{\lambda_i\}_{i \in \mathcal{A}(x_*)} \subseteq \mathbb{R}, \lambda_i \geq 0 \text{ if } i \in \mathcal{A}(x_*) \cap \mathcal{I} \right\}$$

之間存在密切關係。當 LICQ 條件成立時，兩者相同 (除了正負號的改變)。

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Lemma

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By Farkas' Lemma, we have that

$$g \in N \iff g^T d \geq 0 \text{ for all } d \in \mathcal{F}(x_*).$$

Since LICQ holds at x_* , $\mathcal{F}(x_*) = T_\Omega(x_*)$; thus it follows by switching the sign of this expression that

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§12.8 Lagrange Multipliers and Sensitivity

在最優性理論中，Lagrange 乘子具有直觀的意義。在這一節中，我們將“證明”每個 Lagrange 乘子 λ_i^* 向我們傳達了一些關於最優目標值 $f(x_*)$ 對於限制 c_i 的存在的敏感性訊息。換句話說， λ_i^* 指示了 f 如何在特定限制 c_i 下「推動」或「拉扯」解 x_* 。

當我們選擇一個 inactive 的限制 $i \notin \mathcal{A}(x_*)$ 時， $c_i(x_*) > 0$ ，解 x_* 和函數值 $f(x_*)$ 對於此限制的存在與否是不在意的。如果我們對此 c_i 進行微小的擾動，它仍然會是 inactive 的， x_* 仍然是優化問題的局部解。由於從 KKT 條件 (32e) 中得出 $\lambda_i^* = 0$ ，Lagrange 乘子準確地表明限制 i 不重要。

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接下來假設限制 i 是 active 的，現在讓我們對此限制的右手邊進行微小擾動，要求，比如說，讓 $c_i(x) \geq -\varepsilon \|\nabla c_i(x_*)\|$ 而不是 $c_i(x) \geq 0$ 。假設 ε 足夠小，以至於擾動後的解 $x_*(\varepsilon)$ 仍然具有相同的 active constraint set（意即原先是 active 的在擾動後依然是 active 的），並且 Lagrange 乘子受到的擾動不大（這些條件可以通過嚴格互補性和二階條件的幫助而被更嚴格地定義）。於是我們發現

$$-\varepsilon \|\nabla c_i(x_*)\| = c_i(x_*(\varepsilon)) - c_i(x_*) \approx (x_*(\varepsilon) - x_*)^T \nabla c_i(x_*),$$

且對所有不等於 i 的 $j \in \mathcal{A}(x_*)$ 我們有

$$0 = c_j(x_*(\varepsilon)) - c_j(x_*) \approx (x_*(\varepsilon) - x_*)^T \nabla c_j(x_*).$$

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同時，可以借助 KKT 條件

$$\nabla_x \mathcal{L}(x_*, \lambda_*) = 0. \quad (32a)$$

來估計 $f(x_*(\varepsilon))$ 的值。由 Taylor 定理與上述條件我們有

$$\begin{aligned} f(x_*(\varepsilon)) - f(x_*) &\approx (x_*(\varepsilon) - x_*)^T \nabla f(x_*) \\ &= \sum_{j \in \mathcal{A}(x_*)} \lambda_j^* (x_*(\varepsilon) - x_*)^T \nabla c_j(x_*) \\ &\approx -\varepsilon \|\nabla c_i(x_*)\| \lambda_i^*. \end{aligned}$$

左右同除 ε 後取 ε 趨近到 0 的極限，我們發現解集合 $x_*(\varepsilon)$ 滿足

$$\left. \frac{d}{d\varepsilon} \right|_{\varepsilon=0} f(x_*(\varepsilon)) = -\lambda_i^* \|\nabla c_i(x_*)\|. \quad (58)$$

§12.8 Lagrange Multipliers and Sensitivity

敏感度分析會得出以下結論：如果 $\lambda_i^* \|\nabla c_i(x_*)\|$ 很大，那麼最優值對於第 i 個限制的存在是敏感的，而如果這個量很小，則依賴性不會太強。如果對於某些 active constraint λ_i^* 恰好等於零，那麼在某些方向上對 c_i 的微小擾動幾乎不會對最優目標值產生影響；在一階近似下，這種變化是零。這個討論促使我們給出以下定義。

Definition

Let x_* be a solution of the problem (1), and suppose that the KKT conditions (32) are satisfied. We say that an inequality constraint c_i is **strongly active** or **binding** if $i \in \mathcal{A}(x_*)$ and $\lambda_i^* > 0$ for some Lagrange multiplier λ_* satisfying (32). We say that c_i is weakly active if $i \in \mathcal{A}(x_*)$ and $\lambda_i^* = 0$ for all λ_* satisfying (32).

§12.8 Lagrange Multipliers and Sensitivity

需要注意的是，上述的敏感度分析獨立於各個限制的尺度。例如，我們可以通過將某些 active constraint c_i 替換為 $10c_i$ 來改變問題的表述。新問題實際上是等價的（即，它具有相同的可行集和相同的解），但與 c_i 對應的最優乘子 λ_i^* 將被 $\lambda_i^*/10$ 所取代。然而，由於 $\|\nabla c_i(x_*)\|$ 被 $10\|\nabla c_i(x_*)\|$ 所取代，乘積 $\lambda_i^*\|\nabla c_i(x_*)\|$ 並不會改變。另一方面，如果我們將目標函數 f 替換為 $10f$ ，那麼 KKT 條件 (32) 中的乘子 $10\lambda_i^*$ 都需要被 $10\lambda_i^*$ 所取代。因此，在 (58) 中，我們看到對於擾動的 f 的敏感性增加了 10 倍，這正是我們所期望的。

§12.9 Duality

在本節中，我們介紹非線性規劃的對偶理論 (duality theory) 中的一些要素。對偶理論被用來啟發和發展一些重要的演算法，包括第 17 章要提到的 Augmented Lagrangian Method。對偶理論的完整論述超越了非線性規劃，為 convex non-smooth optimization 甚至離散最佳化領域提供了重要的洞見。其對線性規劃的特殊應用對該領域的發展至關重要；這個部份請參考第 13 章。

對偶理論告訴我們如何從原本最佳化問題的函數和數據去構建一個替代問題。這個替代原問題的「對偶」問題 (dual problem) 與原本的最佳化問題（為了對比起見，在這種情況下有時被稱為 primal 問題）有著迷人的相關性。在某些情況下，對偶問題在計算上比原本的問題更容易解決。在其他情況下，對偶問題可以用來輕鬆地取得原問題中目標函數的下界。

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如上所述，對偶問題也已被用來設計解決 primal 問題的算法。本節中的結果大多局限於受限優化問題 (1) 的特殊情況，其中：

- ① 沒有等式限制（或是只有線性等式限制 – 這個 case 可以將等式限制轉換成 ② 中提到的不等式限制），即 $\mathcal{E} = \emptyset$ ，且
- ② 目標函數 f 和「負的」不等式限制之限制函數 $-c_i$ 是凸函數，即討論的是 convex optimization。

為了簡化，我們假設有 m 個不等式限制。定義一個向量值函數 $c(x) \equiv (c_1(x), c_2(x), \dots, c_m(x))^T$ ，我們可以將問題重寫為：

$$\min_{x \in \mathbb{R}^n} f(x) \quad \text{subject to} \quad c(x) \geq 0 \quad (59)$$

上述受限優化問題所對應之 Lagrangian (10) 簡單表示為

$$\mathcal{L}(x, \lambda) = f(x) - \lambda^T c(x),$$

其中 $\lambda \in \mathbb{R}^m$ 是 Lagrange 乘子向量。

§12.9 Duality

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Convexity

在繼續進行討論之前，我們必須先探討一個凸函數的等價性質。
首先我們先回顧凸集合與凸函數的定義。

Definition

A subset C of a vector space is said to be convex if

$$(1-t)x + ty \in C \quad \forall x, y \in C, t \in [0, 1].$$

Definition

Let C be a convex set, and $f: C \rightarrow \mathbb{R}$ be a function.

- ① f is said to be convex if for all $x, y \in C$ and $t \in [0, 1]$,

$$f((1-t)x + ty) \leq (1-t)f(x) + tf(y).$$

- ② f is said to be strictly convex if for all distinct $x, y \in C$ and $t \in (0, 1)$,

$$f((1-t)x + ty) < (1-t)f(x) + tf(y).$$

接下來的定理刻劃了可微的凸函數的等價條件。

Convexity

Theorem

Let C be a convex set, and $f: C \rightarrow \mathbb{R}$ be a differentiable function.

- ① f is convex if and only if

$$f(y) \geq f(x) + \nabla f(x)^T(y - x) \quad \forall x, y \in C.$$

- ② f is strictly convex if and only if

$$f(y) > f(x) + \nabla f(x)^T(y - x) \quad \forall x, y \in C, x \neq y.$$

Proof.

- ① (\Rightarrow) Let $x, y \in C$. For all $t \in [0, 1]$,

$$f((1-t)x + ty) \leq (1-t)f(x) + tf(y);$$

thus for $t \in (0, 1]$,

$$\nabla f(x)^T(y - x) = \lim_{t \rightarrow 0^+} \frac{f((1-t)x + ty) - f(x)}{t} \leq f(y) - f(x).$$

Note that the limit is the directional derivative of f at x along direction $y - x$; thus □

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Proof (cont'd).

- ① (\Leftarrow) Let $x, y \in C$, $t \in [0, 1]$, and suppose that

$$f(w) \geq f(z) + \nabla f(z)^T(w - z) \quad \forall w, z \in C.$$

Let $z = (1-t)x + ty$ and $w = x$ or $w = y$ in the inequality above, we obtain

$$f(x) \geq f((1-t)x + ty) + \nabla f((1-t)x + ty)^T(t(y - x))$$

and

$$f(y) \geq f((1-t)x + ty) + \nabla f((1-t)x + ty)^T((1-t)(x - y)).$$

Therefore,

$$\begin{aligned} (1-t)f(x) + tf(y) &\geq (1-t)f((1-t)x + ty) + tf((1-t)x + ty) \\ &= f((1-t)x + ty); \end{aligned}$$

thus f is convex. □

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$$f(x) \geq f((1-t)x + ty) + t \nabla f((1-t)x + ty)^T(y - x)$$

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$$f(x) > f((1-t)x + ty) + t \nabla f((1-t)x + ty)^T(y - x)$$

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thus f is **strictly** convex. □

Convexity

Proof (cont'd).

② (\Rightarrow) From ① we have

$$f(y) \geq f(x) + \nabla f(x)^T(y - x) \quad \forall x, y \in C, x \neq y.$$

so it suffices to show that

$$f(y) \neq f(x) + \nabla f(x)^T(y - x) \quad \forall x, y \in C, x \neq y.$$

Suppose the contrary that there exist $x, y \in C, x \neq y$ such that

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$$\begin{aligned} f(z) &< (1-t)f(x) + tf(y) = f(x) + t[f(y) - f(x)] \\ &= f(x) + t\nabla f(x)^T(y - x) \\ &= f(x) + \nabla f(x)^T(z - x) \leq f(z), \end{aligned}$$

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§12.9 Duality

對偶目標函數 $q: \mathbb{R}^n \rightarrow \mathbb{R}$ 被定義為

$$q(\lambda) \equiv \inf_x \mathcal{L}(x, \lambda), \quad (60)$$

其中 q 的定義域是使 q 值有限的 λ 的集合；也就是說，

$$\mathcal{D} \equiv \text{Dom}(q) = \{\lambda \mid q(\lambda) > -\infty\}.$$

需要注意的是，在 (60) 中計算 infimum 時，需要找到給定 λ 後函數 $\mathcal{L}(\cdot, \lambda)$ 的全域 minimizer，然而正如我們在第 2 章中所指出的，這在實踐中可能非常困難。不過，當 f 和 $-c_i$ 都是凸函數且 $\lambda \geq 0$ （這是我們最感興趣的情況），函數 $\mathcal{L}(\cdot, \lambda)$ 也是凸函數。在這種情況下，所有局部最小值都是全域最小值，因此計算 $q(\lambda)$ 變得更加實際。

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受限優化問題

$$\min_{x \in \mathbb{R}^n} f(x) \quad \text{subject to} \quad c(x) \geq 0 \quad (59)$$

的對偶問題是以下的受限優化（最大化）問題

$$\max_{\lambda \in \mathbb{R}^n} q(\lambda) \quad \text{subject to} \quad \lambda \geq 0. \quad (61)$$

Example

Consider the problem

$$\min_{(x_1, x_2)} 0.5(x_1^2 + x_2^2) \quad \text{subject to} \quad x_1 - 1 \geq 0. \quad (62)$$

The Lagrangian is

$$\mathcal{L}(x_1, x_2, \lambda) = 0.5(x_1^2 + x_2^2) - \lambda(x_1 - 1).$$

If we hold λ fixed, \mathcal{L} a convex function of $(x_1, x_2)^T$; thus the infimum of \mathcal{L} is achieved when the partial derivatives with respect to x_1 and x_2 are zero; that is, $x_1 - \lambda = 0$, $x_2 = 0$.

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§12.9 Duality

Example (cont'd)

By substituting these infimal values into $\mathcal{L}(x_1, x_2, \lambda)$, we obtain the dual objective (60):

$$q(\lambda) = 0.5(\lambda^2 + 0) - \lambda(\lambda - 1) = -0.5\lambda^2 + \lambda.$$

Hence, the dual problem of (61) is

$$\max_{\lambda \geq 0} -0.5\lambda^2 + \lambda \quad (63)$$

which clearly has the solution $\lambda = 1$.

在本節的剩餘部分，我們將展示對偶問題如何與受限優化問題

$$\min_{x \in \mathbb{R}^n} f(x) \quad \text{subject to} \quad c(x) \geq 0 \quad (59)$$

相關聯。我們的第一個結果涉及到對偶目標函數 q 的凹性 (concavity) 和其定義域 \mathcal{D} 的凸性 (convexity)。

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Theorem

The function q defined by (60) is concave and its domain \mathcal{D} is convex.

Proof.

For any λ_0 and λ_1 in \mathbb{R}^m , any $x \in \mathbb{R}^n$, and any $\alpha \in [0, 1]$, we have

$$\mathcal{L}(x, (1 - \alpha)\lambda_0 + \alpha\lambda_1) = (1 - \alpha)\mathcal{L}(x, \lambda_0) + \alpha\mathcal{L}(x, \lambda_1).$$

By the fact that **the infimum of a sum is greater than or equal to the sum of infimums**, taking the infimum of both sides in the expression above we obtain

$$q((1 - \alpha)\lambda_0 + \alpha\lambda_1) \geq (1 - \alpha)q(\lambda_0) + \alpha q(\lambda_1),$$

confirming concavity of q . If both λ_0 and λ_1 belong to \mathcal{D} , this inequality implies that $q((1 - \alpha)\lambda_0 + \alpha\lambda_1) > -\infty$ also, and therefore $(1 - \alpha)\lambda_0 + \alpha\lambda_1 \in \mathcal{D}$, verifying convexity of \mathcal{D} . \square

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§12.9 Duality

接下來我們將證明對偶問題

$$\max_{\lambda \in \mathbb{R}^n} q(\lambda) \quad \text{subject to} \quad \lambda \geq 0 \quad (61)$$

的最大值給出了 primal 問題

$$\min_{x \in \mathbb{R}^n} f(x) \quad \text{subject to} \quad c(x) \geq 0. \quad (59)$$

最小值的一個下界。這個結果是根據以下的定理。

Theorem (Weak Duality)

For any \bar{x} feasible for (59) and any $\bar{\lambda} \geq 0$, we have $q(\bar{\lambda}) \leq f(\bar{x})$.

Proof.

By the definition of q ,

$$q(\bar{\lambda}) = \inf_x [f(x) - \bar{\lambda}^T c(x)] \leq f(\bar{x}) - \bar{\lambda}^T c(\bar{x}) \leq f(\bar{x}),$$

where the final inequality follows from $\bar{\lambda} \geq 0$ and $c(\bar{x}) \geq 0$. \square

§12.9 Duality

接下來我們將證明對偶問題

$$\max_{\lambda \in \mathbb{R}^n} q(\lambda) \quad \text{subject to} \quad \lambda \geq 0 \quad (61)$$

的最大值給出了 primal 問題

$$\min_{x \in \mathbb{R}^n} f(x) \quad \text{subject to} \quad c(x) \geq 0. \quad (59)$$

最小值的一個下界。這個結果是根據以下的定理。

Theorem (Weak Duality)

For any \bar{x} feasible for (59) and any $\bar{\lambda} \geq 0$, we have $q(\bar{\lambda}) \leq f(\bar{x})$.

Proof.

By the definition of q ,

$$q(\bar{\lambda}) = \inf_x [f(x) - \bar{\lambda}^T c(x)] \leq f(\bar{x}) - \bar{\lambda}^T c(\bar{x}) \leq f(\bar{x}),$$

where the final inequality follows from $\bar{\lambda} \geq 0$ and $c(\bar{x}) \geq 0$. \square

§12.9 Duality

對於本節最後的幾個結果，我們注意到適用於

$$\min_{x \in \mathbb{R}^n} f(x) \quad \text{subject to} \quad c(x) \geq 0 \quad (59)$$

的 KKT 條件 (32) 如下所示：

$$\nabla f(\bar{x}) - \nabla c(\bar{x})\bar{\lambda} = 0, \quad (64a)$$

$$c(\bar{x}) \geq 0, \quad (64b)$$

$$\bar{\lambda} \geq 0, \quad (64c)$$

$$\bar{\lambda}_i c_i(\bar{x}) = 0, \quad i = 1, 2, \dots, m, \quad (64d)$$

其中 $\nabla c(x)$ 是由以下的 $n \times m$ 矩陣所以定義：

$$\nabla c(x) = [\nabla c_1(x) : \nabla c_2(x) : \dots : \nabla c_m(x)].$$

下一個結果顯示了對於 (59) 的最優 Lagrange 乘子在一定條件下是對偶問題 (61) 的解。

§12.9 Duality

Theorem

Suppose that f and $-c_i$, $i = 1, 2, \dots, m$ are convex functions on \mathbb{R}^n that are differentiable at a KKT point \bar{x} to

$$\min_{x \in \mathbb{R}^n} f(x) \quad \text{subject to} \quad c(x) \geq 0, \quad (59)$$

where $c(x) \equiv (c_1(x), c_2(x), \dots, c_m(x))^T$. Then \bar{x} is a solution to (59). Moreover, any $\bar{\lambda}$ for which $(\bar{x}, \bar{\lambda})$ satisfies the KKT conditions

$$\nabla f(\bar{x}) - \nabla c(\bar{x})\bar{\lambda} = 0, \quad (64a)$$

$$c(\bar{x}) \geq 0, \quad (64b)$$

$$\bar{\lambda} \geq 0, \quad (64c)$$

$$\bar{\lambda}_i c_i(\bar{x}) = 0, \quad i = 1, 2, \dots, m, \quad (64d)$$

is a local solution of the dual problem

$$\max_{\lambda \in \mathbb{R}^n} q(\lambda) \quad \text{subject to} \quad \lambda \geq 0. \quad (61)$$

§12.9 Duality

Proof.

Suppose that $(\bar{x}, \bar{\lambda})$ satisfies the KKT condition (64). We have from $\bar{\lambda} \geq 0$ that $\mathcal{L}(\cdot, \bar{\lambda})$ is a convex and differentiable function. Hence, for any x , we have

$$\mathcal{L}(x, \bar{\lambda}) \geq \mathcal{L}(\bar{x}, \bar{\lambda}) + \nabla_x \mathcal{L}(\bar{x}, \bar{\lambda})^T (x - \bar{x}) = \mathcal{L}(\bar{x}, \bar{\lambda}),$$

where the last equality follows from (64a). Therefore, we have

$$q(\bar{\lambda}) = \inf_x \mathcal{L}(x, \bar{\lambda}) = \mathcal{L}(\bar{x}, \bar{\lambda}) = f(\bar{x}) - \bar{\lambda}^T c(\bar{x}) = f(\bar{x}),$$

where the last equality follows from (64d).

On the other hand, the weak duality implies that

$$q(\lambda) \leq f(\bar{x}) \quad \forall \lambda \geq 0;$$

thus it follows from $q(\bar{\lambda}) = f(\bar{x})$ that \bar{x} is a solution to (59) and $\bar{\lambda}$ is a solution of (61). □

§12.9 Duality

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Suppose that $(\bar{x}, \bar{\lambda})$ satisfies the KKT condition (64). We have from $\bar{\lambda} \geq 0$ that $\mathcal{L}(\cdot, \bar{\lambda})$ is a convex and differentiable function. Hence, for any x , we have

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§12.9 Duality

注意到如果函數是連續可微的，並且像 LICQ 這樣的 constraint qualification 在 (59) 的局部解 \bar{x} 處成立（或是 $T_{\Omega}(\bar{x}) = \mathcal{F}(\bar{x})$ ），那麼滿足 KKT 條件的最優 Lagrange 乘子是存在的。這個觀察證明了如下 Corollary。

Corollary

Suppose that f and $-c_i$, $i = 1, 2, \dots, m$ be convex functions on \mathbb{R}^n that are differentiable at a solution \bar{x} to

$$\min_{x \in \mathbb{R}^n} f(x) \quad \text{subject to} \quad c(x) \geq 0, \quad (59)$$

If LICQ holds at \bar{x} ; that is, $\{\nabla c_i(\bar{x}) \mid i \in \mathcal{A}(\bar{x})\}$ is linearly independent or equivalently, the matrix $[\nabla c_i(\bar{x})]_{i \in \mathcal{A}(\bar{x})}$ has full rank, then there is a solution of the dual problem

$$\max_{\lambda \in \mathbb{R}^m} q(\lambda) \quad \text{subject to} \quad \lambda \geq 0. \quad (61)$$

§12.9 Duality

Example

In previous example of solving

$$\min_{(x_1, x_2)} 0.5(x_1^2 + x_2^2) \quad \text{subject to} \quad x_1 - 1 \geq 0, \quad (62)$$

we see that $\lambda = 1$ is both an optimal Lagrange multiplier for problem (62) and a solution of its dual problem

$$\max_{\lambda \geq 0} -0.5\lambda^2 + \lambda. \quad (63)$$

Note too that the optimal objective for both problems is 0.5.

接下來我們證明了前一個定理的部分逆命題，它顯示對偶問題 (61) 的解有時可以用來推導原始問題 (59) 的解。此逆命題的關鍵條件是函數 $\mathcal{L}(\cdot, \hat{\lambda})$ 在某個特別 $\hat{\lambda}$ 值的嚴格凸性。我們注意到，如果 f 是嚴格凸的，或者如果對於某個 $i = 1, 2, \dots, m$ ， $-c_i$ 是嚴格凸的且 $\hat{\lambda}_i > 0$ ，則這個條件成立。

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§12.9 Duality

Theorem

Suppose that f and $-c_i$, $i = 1, 2, \dots, m$ are convex and continuously differentiable on \mathbb{R}^n . Suppose that

- 1 \bar{x} is a solution of

$$\min_{x \in \mathbb{R}^n} f(x) \quad \text{subject to} \quad c(x) \geq 0, \quad (59)$$

and LICQ holds at \bar{x} (or $T_{\Omega}(\bar{x}) = \mathcal{F}(\bar{x})$);

- 2 $\hat{\lambda}$ solves the dual problem

$$\max_{\lambda \in \mathbb{R}^m} q(\lambda) \quad \text{subject to} \quad \lambda \geq 0, \quad (61)$$

and the infimum $\inf_x \mathcal{L}(x, \hat{\lambda})$ is attained at \hat{x} .

Assume further that $\mathcal{L}(\cdot, \hat{\lambda})$ is a strictly convex function. Then $\bar{x} = \hat{x}$ (that is, \hat{x} is the unique solution of (59)), and $\hat{\lambda}$ is a Lagrange multiplier for \bar{x} (that is, $(\bar{x}, \hat{\lambda})$ satisfies the KKT condition).

§12.9 Duality

Proof.

Suppose the contrary that $\bar{x} \neq \hat{x}$. Since $\hat{x} = \arg \min_x \mathcal{L}(x, \hat{\lambda})$, we have $\nabla_x \mathcal{L}(\hat{x}, \hat{\lambda}) = 0$; thus the strict convexity of $\mathcal{L}(\cdot, \hat{\lambda})$ implies that

$$\mathcal{L}(\bar{x}, \hat{\lambda}) - \mathcal{L}(\hat{x}, \hat{\lambda}) > \nabla_x \mathcal{L}(\hat{x}, \hat{\lambda})^T (\bar{x} - \hat{x}) = 0.$$

Since LICQ holds at \bar{x} , there is $\bar{\lambda}$ satisfying the KKT conditions (64).

By the previous theorem $\bar{\lambda}$ solves the dual problem (61) so that

$$\mathcal{L}(\bar{x}, \bar{\lambda}) = q(\bar{\lambda}) = q(\hat{\lambda}) = \mathcal{L}(\hat{x}, \hat{\lambda}).$$

Therefore,

$$\mathcal{L}(\bar{x}, \hat{\lambda}) > \mathcal{L}(\hat{x}, \hat{\lambda}) = \mathcal{L}(\bar{x}, \bar{\lambda}).$$

In particular,

$$-\hat{\lambda}^T c(\bar{x}) > -\bar{\lambda}^T c(\bar{x}) = 0,$$

where the final equality follows from the KKT condition (64d). Since $\hat{\lambda} \geq 0$ and $c(\bar{x}) \geq 0$, we have $-\hat{\lambda}^T c(\bar{x}) \leq 0$, a contradiction. \square

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§12.9 Duality

Proof (cont'd).

Therefore, $\bar{x} = \hat{x}$. Moreover, the identities (from the previous slide)

$$\mathcal{L}(\bar{x}, \bar{\lambda}) = \mathcal{L}(\hat{x}, \hat{\lambda}) \quad \text{and} \quad f(\bar{x}) = \mathcal{L}(\bar{x}, \bar{\lambda})$$

imply that $f(\bar{x}) = \mathcal{L}(\bar{x}, \hat{\lambda})$. This identity shows that $\hat{\lambda}^T c(\bar{x}) = 0$. Since $\hat{\lambda} \geq 0$ and $c(\bar{x}) \geq 0$, we must have $\hat{\lambda}_i c_i(\bar{x}) = 0$ for all $1 \leq i \leq m$; thus the KKT condition holds at $(\bar{x}, \hat{\lambda})$. \square

Example

In previous example of solving

$$\min_{(x_1, x_2)} 0.5(x_1^2 + x_2^2) \quad \text{subject to} \quad x_1 - 1 \geq 0, \quad (62)$$

at the dual solution $\lambda = 1$, the infimum of $\mathcal{L}(x_1, x_2, \lambda)$ is achieved at $(x_1, x_2) = (1, 0)^T$, which is the solution of the original problem (62).

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§12.9 Duality

一個與先前討論的對偶問題稍微不同但對於計算很方便的對偶形式是 Wolfe 對偶，其表述如下：

$$\max_{x, \lambda} \mathcal{L}(x, \lambda) \quad \text{subject to} \quad \nabla_x \mathcal{L}(x, \lambda) = 0, \quad \lambda \geq 0. \quad (65)$$

以下的結果解釋了 Wolfe 對偶與受限優化問題

$$\min_{x \in \mathbb{R}^n} f(x) \quad \text{subject to} \quad c(x) \geq 0 \quad (59)$$

的關係。

Theorem

Suppose that f and $-c_i$, $i = 1, 2, \dots, m$ are convex and continuously differentiable on \mathbb{R}^n . Suppose that $(\bar{x}, \bar{\lambda})$ is a solution pair of (59) at which LICQ holds; that is, \bar{x} is a solution of (59) and $\bar{\lambda}$ is a corresponding Lagrange multiplier vector (whose existence is guaranteed by one of previous theorem). Then $(\bar{x}, \bar{\lambda})$ solves the problem (65).

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§12.9 Duality

Proof.

Since $(\bar{x}, \bar{\lambda})$ is a solution pair of (59), it holds the KKT conditions (64) so that $(\bar{x}, \bar{\lambda})$ satisfies the constraint

$$\nabla_x \mathcal{L}(x, \lambda) = 0, \quad \lambda \geq 0 \quad (66)$$

and that $\mathcal{L}(\bar{x}, \bar{\lambda}) = f(\bar{x})$. Therefore, for any pair (x, λ) that satisfies (66) we have that

$$\begin{aligned} \mathcal{L}(\bar{x}, \bar{\lambda}) = f(\bar{x}) &\geq f(\bar{x}) - \lambda^T c(\bar{x}) = \mathcal{L}(\bar{x}, \lambda) \\ &\geq \mathcal{L}(x, \lambda) + \nabla_x \mathcal{L}(x, \lambda)^T (\bar{x} - x) = \mathcal{L}(x, \lambda), \end{aligned}$$

where the second inequality follows from the convexity of $\mathcal{L}(\cdot, \lambda)$. We have therefore shown that $(\bar{x}, \bar{\lambda})$ maximizes \mathcal{L} over the constraints (66), and hence solves

$$\max_{x, \lambda} \mathcal{L}(x, \lambda) \quad \text{subject to} \quad \nabla_x \mathcal{L}(x, \lambda) = 0, \quad \lambda \geq 0. \quad (65)$$

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§12.9 Duality

Example (Linear Programming)

An important special case of (59) is the linear programming problem

$$\min c^T x \quad \text{subject to} \quad Ax - b \geq 0, \quad (67)$$

for which the dual objective is

$$q(\lambda) = \inf_x c^T x - \lambda^T (Ax - b) = \inf_x (c - A^T \lambda)^T x + b^T \lambda.$$

If $c - A^T \lambda \neq 0$, the infimum is clearly $-\infty$ (we can set x to be a large negative multiple of $-(c - A^T \lambda)$ to make q arbitrarily large and negative). When $c - A^T \lambda = 0$, on the other hand, the dual objective is simply $b^T \lambda$. In maximizing q , we can exclude λ for which $c - A^T \lambda \neq 0$ from consideration. Hence, we can write the dual problem (61) as follows:

$$\max_{\lambda} b^T \lambda \quad \text{subject to} \quad A^T \lambda = c, \lambda \geq 0. \quad (68)$$

§12.9 Duality

Example (Linear Programming (cont'd))

The Wolfe dual of (67) can be written as

$$\max_{x, \lambda} c^T x - \lambda^T (Ax - b) \quad \text{subject to} \quad A^T \lambda = c, \lambda \geq 0,$$

and by substituting the constraint $A^T \lambda - c = 0$ into the objective we obtain (68) again. For some matrices A , the dual problem (68) may be computationally easier to solve than the original problem (67).

Example (Convex Quadratic Programming)

Consider

$$\min_x \frac{1}{2} x^T G x + c^T x \quad \text{subject to} \quad Ax - b \geq 0,$$

where G is a symmetric positive definite matrix. The dual objective for this problem is

$$q(\lambda) = \inf_x \mathcal{L}(x, \lambda) = \inf_x \frac{1}{2} x^T G x + c^T x - \lambda^T (Ax - b).$$

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Example (Linear Programming (cont'd))

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§12.9 Duality

Example (Convex Quadratic Programming (cont'd))

Since G is positive definite, $\mathcal{L}(\cdot, \lambda)$ is a strictly convex quadratic function; thus the infimum is achieved when $\nabla_x \mathcal{L}(x, \lambda) = 0$; that is,

$$Gx + c - A^T \lambda = 0. \quad (69)$$

Hence, we can substitute for x in the infimum expression and write the dual objective explicitly as follows:

$$q(\lambda) = -\frac{1}{2}(A^T \lambda - c)^T G^{-1}(A^T \lambda - c) + b^T \lambda.$$

Alternatively, we can write the Wolfe dual form (65) by retaining x as a variable and including the constraint (69) explicitly in the dual problem, to obtain

$$\max_{(x, \lambda)} \frac{1}{2} x^T G x + c^T x - \lambda^T (A x - b) \quad \text{subject to} \quad G x + c - A^T \lambda = 0, \lambda \geq 0.$$

§12.9 Duality

Example (Convex Quadratic Programming (cont'd))

To make it clearer that the objective is concave, we can use the constraint to substitute $(c - A^T \lambda)^T x = -x^T G x$ in the objective, and rewrite the dual formulation as follows:

$$\max_{(x, \lambda)} -\frac{1}{2} x^T G x + \lambda^T b \quad \text{subject to} \quad Gx + c - A^T \lambda = 0, \lambda \geq 0.$$

注意到 Wolfe 對偶形式只需要 G 是正半定的。