1 BASICS OF SET CONTSTRAINED AND UNCONSTRAINED OPTIMIZATION

1.1 INTRODUCTION

• We consider the **optimization problem**

minimize f(x) subject to $x \in \Omega$.

- The function $f: \mathbb{R}^n \to \mathbb{R}$ that we wish to minimize is a real-valued function called the **objective function**.
- The vector \mathbf{x} is an n-vector of **independent variables**: $\mathbf{x} = [x_1, ..., x_n]^{\mathsf{T}} \in \mathbb{R}^n$.
- The set Ω is a subset of \mathbb{R}^n called the **constraint set**, which takes the form $\Omega = \{x: h(x) = 0, g(x) \leq 0\}$, where h and g are given functions.
- The **minimizer** of f over Ω is a vector \mathbf{x} which results in the smallest value of the objective function.
- **Definition 1.1** Suppose that $f: \mathbb{R}^n \to \mathbb{R}$ is a real-valued function defined on some set $\Omega \subset \mathbb{R}^n$. A point $x^* \in \Omega$ is a **local minimizer** of f over Ω if there exists $\varepsilon > 0$ such that $f(x) \ge f^*(x)$ for all $x \in \Omega \setminus \{x^*\}$ and $||x x^*|| < \varepsilon$. A point $x^* \in \Omega$ is a **global minimizer** of f over Ω if $f(x) \ge f(x^*)$ for all $x \in \Omega \setminus \{x^*\}$.
- If x^* is a global minimizer of f over Ω , we write $f(x^*) = \min_{x \in \Omega} f(x)$ and $x^* = \underset{x \in \Omega}{\operatorname{argmin}} f(x)$.

Example 1.1.1. Suppose $f: \mathbb{R} \to \mathbb{R}$ is given by $f(x) = (x+1)^2 + 3$. Find $\arg\min_{x \in \Omega} f(x)$ where $\Omega = \{x: x \ge 0\}$.

$$x^* = \arg\min_{x \in \Omega} f(x) = 0.$$

Note: If $\Omega = \mathbb{R}$, then $x^* = \arg\min_{x \in \Omega} f(x) = -1$.

1.2 CONDITIONS FOR LOCAL MINIMIZERS

- Global minimizers are, in general, **difficult** to find. Therefore, in practice, we often have to be **satisfied** with finding local minimizers.
- The first-order derivative of $f: \mathbb{R}^n \to \mathbb{R}$, denoted Df(x), is

$$Df(\mathbf{x}) \triangleq \left[\frac{\partial f(\mathbf{x})}{\partial x_1}, \dots, \frac{\partial f(\mathbf{x})}{\partial x_n}\right].$$

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- The **gradient** $\nabla f(x)$ is the transpose of Df(x); that is, $\nabla f(x) = (Df(x))^{\mathsf{T}}$.
- The **second derivative** of $f: \mathbb{R}^n \to \mathbb{R}$ (also called the Hessian of f)) is

$$D^{2}f(\mathbf{x}) \triangleq \begin{bmatrix} \frac{\partial^{2}f}{\partial x_{1}^{2}}(\mathbf{x}) & \cdots & \frac{\partial^{2}f}{\partial x_{n}\partial x_{1}}(\mathbf{x}) \\ \vdots & \ddots & \vdots \\ \frac{\partial^{2}f}{\partial x_{1}\partial x_{n}}(\mathbf{x}) & \cdots & \frac{\partial^{2}f}{\partial x_{n}^{2}}(\mathbf{x}) \end{bmatrix}.$$

Example 1.2.1. Let $f(x_1, x_2) = 5x_1 + 8x_2 + x_1x_2 - x_1^2 - 2x_2^2$. Find Df(x) and $D^2f(x)$.

$$Df(\mathbf{x}) = \left(\nabla f(\mathbf{x})\right)^{\mathsf{T}} = \left[\frac{\partial f}{\partial x_1}(\mathbf{x}), \frac{\partial f}{\partial x_2}(\mathbf{x})\right] = \left[5 + x_2 - 2x_1, 8 + x_1 - 4x_2\right]$$

and

$$D^{2}f(\mathbf{x}) = \begin{bmatrix} \frac{\partial^{2}f(\mathbf{x})}{\partial x_{1}^{2}} & \cdots & \frac{\partial^{2}f(\mathbf{x})}{\partial x_{n}\partial x_{1}} \\ \vdots & \ddots & \vdots \\ \frac{\partial^{2}f(\mathbf{x})}{\partial x_{1}\partial x_{n}} & \cdots & \frac{\partial^{2}f(\mathbf{x})}{\partial x_{n}^{2}} \end{bmatrix} = \begin{bmatrix} -2 & 1 \\ 1 & -4 \end{bmatrix}.$$

- Given an optimization problem with constraint set Ω , a minimizer may lie either in the **interior** or on the **boundary** of Ω . To study the case where it lies on the boundary, we need the notion of **feasible directions**.
- **Definition 1.2** A vector $\mathbf{d} \in \mathbb{R}^n$, $\mathbf{d} \neq \mathbf{0}$, is a **feasible direction** at $\mathbf{x} \in \Omega$ if there exists $\alpha_0 > 0$ such that $\mathbf{x} + \alpha \mathbf{d} \in \Omega$ for all $\alpha \in [0, \alpha_0]$.
- Let $f: \mathbb{R}^n \to \mathbb{R}$ be a real-valued function and let d be a feasible direction at $x \in \Omega$. The **directional derivative** of f in the direction d, denoted $\partial f/\partial d$, is the real-valued function defined by

$$\frac{\partial f(\mathbf{x})}{\partial \mathbf{d}} = \lim_{\alpha \to 0} \frac{f(\mathbf{x} + \alpha \mathbf{d}) - f(\mathbf{x})}{\alpha} = \langle \nabla f(\mathbf{x}), \mathbf{d} \rangle = \mathbf{d}^{\mathsf{T}} \nabla f(\mathbf{x}).$$

• If ||d|| = 1, then $\partial f/\partial d$ is the rate of increase of f at x in the direction d.

Example 1.2.2. Define $f: \mathbb{R}^3 \to \mathbb{R}$ by $f(x) = x_1 x_2 x_3$, and let $\mathbf{d} = \begin{bmatrix} 1/2, 1/2, 1/\sqrt{2} \end{bmatrix}^\mathsf{T}$. Find the directional derivative of f in the direction \mathbf{d} .

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$$\frac{\partial f(\mathbf{x})}{\partial \mathbf{d}} = \nabla f(\mathbf{x})^{\mathsf{T}} \mathbf{d} = [x_2 x_3, x_1 x_3, x_1 x_2] \begin{bmatrix} 1/2 \\ 1/2 \\ 1/\sqrt{2} \end{bmatrix} = \frac{x_2 x_3 + x_1 x_3 + \sqrt{2} x_1 x_2}{2}.$$

Note that $\|d\| = \sqrt{(1/2)^2 + (1/2)^2 + (1/\sqrt{2})^2} = 1$. The above is also the rate of increase of f at x in the direction d.

• Theorem 1.1 First-Order Necessary Condition (FONC). Let Ω be a subset of \mathbb{R}^n and $f \in C^1$ (i.e., the first derivative exists and is continuous) a real-valued function on Ω . If x^* is a local minimizer of f over Ω , then for any feasible direction d at x^* , we have

$$\mathbf{d}^{\mathsf{T}} \nabla f(\mathbf{x}^*) \geq 0.$$

• Corollary 1.1 Interior Case. Let Ω be a subset of \mathbb{R}^n and $f \in C^1$ a real-valued function on Ω . If x^* is a local minimizer of f over Ω and if x^* is an interior point of Ω , then

$$\nabla f(\mathbf{x}^*) = 0.$$

Example 1.2.2. Consider the problem

minimize
$$x_1^2 + 0.5x_2^2 + 3x_2 + 4.5$$
 subject to $x_1, x_2 \ge 0$.

- (a) Is the first-order necessary condition (FONC) for a local minimizer satisfied at $x = [1,3]^T$?
- (b) Is the FONC for a local minimizer satisfied at $x = [0, 3]^{T}$?
- (c) Is the FONC for a local minimizer satisfied at $x = [1, 0]^{\mathsf{T}}$?
- (d) Is the FONC for a local minimizer satisfied at $x = [1, 0]^{\mathsf{T}}$?
- (a) At $\boldsymbol{x} = [1,3]^{\mathsf{T}}$, we have $\nabla f(\boldsymbol{x}) = [2x_1,x_2+3]^{\mathsf{T}} = [2,6]^{\mathsf{T}}$. The point $\boldsymbol{x} = [1,3]^{\mathsf{T}}$ is an interior point of $\Omega = \{\boldsymbol{x}: x_1 \geq 0, x_2 \geq 0\}$. Hence, the FONC requires that $\nabla f(\boldsymbol{x}) = 0$.

The point $x = [1, 3]^T$ does not satisfy the FONC for a local minimizer.

(b) At $\mathbf{x} = [0,3]^{\mathsf{T}}$, we have $\nabla f(\mathbf{x}) = [2x_1, x_2 + 3]^{\mathsf{T}} = [0,6]^{\mathsf{T}}$, and hence $\mathbf{d}^{\mathsf{T}} \nabla f(\mathbf{x}) = 6d_2$, where $\mathbf{d} = [d_1, d_2]^{\mathsf{T}}$. For \mathbf{d} to be feasible at \mathbf{x} , we need $d_1 \geq 0$ and d_2 can take an arbitrary value in \mathbb{R} .

The point $\mathbf{x} = [1,3]^{\mathsf{T}}$ does not satisfy the FONC for a minimizer because d_2 is allowed to be less than zero. For example, $\mathbf{d} = [1,-1]^{\mathsf{T}}$ is a feasible direction, but $\mathbf{d}^{\mathsf{T}} \nabla f(\mathbf{x}) = -6 < 0$.

(c) At $\mathbf{x} = [1,0]^{\mathsf{T}}$, we have $\nabla f(\mathbf{x}) = [2x_1, x_2 + 3]^{\mathsf{T}} = [2,3]^{\mathsf{T}}$, and hence $\mathbf{d}^{\mathsf{T}} \nabla f(\mathbf{x}) = 2d_1 + 3d_2$, where $\mathbf{d} = [d_1, d_2]^{\mathsf{T}}$. For \mathbf{d} to be feasible at \mathbf{x} , we need $d_2 \geq 0$ and d_1 can take an arbitrary value in \mathbb{R} .

The point $\mathbf{x} = [1, 0]^{\mathsf{T}}$ does not satisfy the FONC for a minimizer because d_1 is allowed to be less than zero. For example, $\mathbf{d} = [-5, 1]^{\mathsf{T}}$ is a feasible direction, but $\mathbf{d}^{\mathsf{T}} \nabla f(\mathbf{x}) = -7 < 0$

(d) At $\mathbf{x} = [0,0]^{\mathsf{T}}$, we have $\nabla f(\mathbf{x}) = [2x_1, x_2 + 3]^{\mathsf{T}} = [0,3]^{\mathsf{T}}$, and hence $\mathbf{d}^{\mathsf{T}} \nabla f(\mathbf{x}) = 3d_2$, where $\mathbf{d} = [d_1, d_2]^{\mathsf{T}}$. For \mathbf{d} to be feasible at \mathbf{x} , we need $d_1 \geq 0$ and $d_2 \geq 0$. The point $\mathbf{x} = [1,0]^{\mathsf{T}}$ satisfies the FONC because $\mathbf{d}^{\mathsf{T}} \nabla f(\mathbf{x}) = 3d_2 \geq 0$.

Example 1.2.2. Consider the set-constrained problem

minimize
$$f(x)$$
 subject to $x \in \Omega = \{[x_1, x_2]^T : x_1^2 + x_2^2 = 1\}.$

- (a) Consider a point $x^* \in \Omega$. Specify all feasible directions at x^* .
- (b) Which points in Ω satisfy the FONC for this set-constrained problem?
- (c) Based on part (b), is the FONC for this set-constrained problem useful for eliminating local-minimizer candidates?
- (d) Suppose that we use polar coordinates to parameterize points $x \in \Omega$ in terms of a single parameter θ :

$$x_1 = \cos \theta$$
 $x_2 = \sin \theta$.

Now use the FONC for unconstrained problems (with respect to θ) to derive a necessary condition of this sort: if $\mathbf{x}^* \in \Omega$ is a local minimizer, then $\mathbf{d}^\mathsf{T} \nabla f(\mathbf{x}^*) = 0$ for all \mathbf{d} satisfying a "certain condition." Specify what this certain condition is.

- (a) There are no feasible directions at any x^* .
- (b) Because of part a, all points in Ω satisfy the FONC for this set-constrained problem.
- (c) No, the FONC for this set-constrained problem is not useful for eliminating local-minimizer candidates.
- (d) Write $h(\theta) = f(g(\theta))$, where $g: \mathbb{R} \to \mathbb{R}^2$ is given by the equations relating θ to $\mathbf{x} = [x_1, x_2]^\mathsf{T}$. Note that $Dg(\theta) = [-\sin\theta, \cos\theta]^\mathsf{T}$. Hence, by the chain rule,

$$h'(\theta) = Df(g(\theta))Dg(\theta) = Dg(\theta)^{\mathsf{T}}\nabla f(g(\theta)).$$

Notice that $Dg(\theta)$ is **tangent** to Ω at $\mathbf{x} = g(\theta)$. Alternatively, we could say that $Dg(\theta)$ is orthogonal to $\mathbf{x} = g(\theta)$. Suppose that $\mathbf{x}^* \in \Omega$ is a local minimizer. Write $\mathbf{x}^* = g(\theta^*)$. Then θ^* is an unconstrained minimizer of h. By the FONC for unconstrained problems, $h'(\theta^*) = 0$, which implies that $\mathbf{d}^\mathsf{T} \nabla f(\mathbf{x}^*) = 0$ for all \mathbf{d} tangent to Ω at \mathbf{x}^* (or, alternatively, for all \mathbf{d} orthogonal to \mathbf{x}^*).

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• Theorem 1.2 Second-Order Necessary Condition (SONC). Let $\Omega \subset \mathbb{R}^n$, $f \in C^2$ a function on Ω , x^* a local minimizer of f over Ω , and d a feasible direction at x^* . If $d^{\mathsf{T}}\nabla f(x^*) = 0$, then

$$\mathbf{d}^{\mathsf{T}}\mathbf{F}(\mathbf{x}^*)\mathbf{d} \geq 0$$
,

where F is the Hessian of f.

• Corollary 1.2 Interior Case. Let x^* be an interior point of $\Omega \subset \mathbb{R}^n$. If x^* is a local minimizer of $f: \Omega \to \mathbb{R}$, $f \in C^2$, then

$$\nabla f(\mathbf{x}^*) = \mathbf{0},$$

and $F(x^*)$ is positive semidefinite $(F(x^*) \ge 0)$; that is, for all $d \in \mathbb{R}^n$,

$$d^{\mathsf{T}}F(x^*)d \geq 0.$$

Example 1.6 Consider a function of one variable $f(x) = x^3$, $f: \mathbb{R} \to \mathbb{R}$. Does the point x = 0 satisfy both the FONC and SONC?

x = 0 is an interior point. Then, $\nabla f(x^*) = 3x^2$ and $F(x^*) = 6x$. Hence, both the FONC and SONC are satisfied: $\nabla f(0) = 0$ and F(0) = 0.

Example 1.7 Consider a function $f: \mathbb{R}^2 \to \mathbb{R}$, where $f(x) = x_1^2 - x_2^2$. Does the point $x = [0,0]^T$ satisfy both the FONC and SONC?

The FONC requires that $\nabla f(\mathbf{x}) = [2x_1, -2x_2]^{\mathsf{T}} = 0$. Thus, $\mathbf{x} = [0, 0]^{\mathsf{T}}$ satisfies the FONC.

The Hessian matrix of f is

$$F(x) = \begin{bmatrix} 2 & 0 \\ 0 & -2 \end{bmatrix}$$

The Hessian matrix is indefinite; that is, for some $\mathbf{d}_1 \in \mathbb{R}^2$ we have $\mathbf{d}_1^\mathsf{T} \mathbf{F} \mathbf{d}_1 > 0$ (e.g., $\mathbf{d}_1 = [1,0]^\mathsf{T}$); and, for some \mathbf{d}_2 , we have $\mathbf{d}_2^\mathsf{T} \mathbf{F} \mathbf{d}_2 < 0$ (e.g., $\mathbf{d}_2 = [0,1]^\mathsf{T}$). Thus, $\mathbf{x} = [0,0]^\mathsf{T}$ does not satisfy the SONC, and hence it is not a minimizer.

- Theorem 1.3 Second-Order Sufficient Condition (SOSC), Interior Case. Let $f \in C^2$ be defined on a region in which x^* is an interior point. Suppose that
 - 1. $\nabla f(\mathbf{x}^*) = 0$.
 - 2. $F(x^*) > 0$.

Then, x^* is a strict local minimizer of f.

Example 1.8 Let $f(x) = x_1^2 + x_2^2$. We have Consider a function $f: \mathbb{R}^2 \to \mathbb{R}$, where $f(x) = x_1^2 - x_2^2$. Does the point $x = [0, 0]^T$ satisfy the FONC, SONC, and SOSC?

We have $\nabla f(x) = [2x_1, 2x_2]^{\mathsf{T}} = 0$ if and only if $x = [0, 0]^{\mathsf{T}}$. For all $x \in \mathbb{R}^2$, we have

$$F(x) = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix} > 0.$$

satisfies the FONC, SONC, and SOSC.

APPENDEX

• Theorem 1.1 First-Order Necessary Condition (FONC). Let Ω be a subset of \mathbb{R}^n and $f \in C^1$ (i.e., the first derivative exists and is continuous) a real-valued function on Ω . If x^* is a local minimizer of f over Ω , then for any feasible direction d at x^* , we have

$$\boldsymbol{d}^{\mathsf{T}} \nabla f(\boldsymbol{x}^*) \geq 0.$$

Proof. Define

$$x(\alpha) = x^* + \alpha d \in \Omega.$$

Note that $x(0) = x^*$. Define the composite function

$$\phi(\alpha) = f(\mathbf{x}(\alpha)).$$

Then, by Taylor's theorem,

$$f(\mathbf{x}^* + \alpha \mathbf{d}) - f(\mathbf{x}^*) = \phi(\alpha) - \phi(0) = \phi'(0)\alpha + o(\alpha) = \alpha \mathbf{d}^{\mathsf{T}} \nabla f(\mathbf{x}(0)) + o(\alpha),$$

where $\alpha \ge 0$. Thus, if $\phi(\alpha) \ge \phi(0)$, that is, $f(x^* + \alpha d) \ge f(x^*)$ for sufficiently small values of $\alpha > 0$, then we have to have $d^{\mathsf{T}} \nabla f(x(0)) \ge 0$.

• Corollary 1.1 Interior Case. Let Ω be a subset of \mathbb{R}^n and $f \in C^1$ a real-valued function on Ω . If x^* is a local minimizer of f over Ω and if x^* is an interior point of Ω , then

$$\nabla f(\mathbf{x}^*) = 0.$$

Proof. Suppose that f has a local minimizer x^* that is an interior point of Ω . Because x^* is an interior point of Ω , the set of feasible directions at x^* is the whole of \mathbb{R}^n . Thus, for any $d \in \mathbb{R}^n$, $d^{\mathsf{T}} \nabla f(x^*) \geq 0$ and $-d^{\mathsf{T}} \nabla f(x^*) \geq 0$. Hence, $d^{\mathsf{T}} \nabla f(x^*) = 0$ for all $d \in \mathbb{R}^n$, which implies that $\nabla f(x^*) = 0$.

• Theorem 1.2 Second-Order Necessary Condition (SONC). Let $\Omega \subset \mathbb{R}^n$, $f \in C^2$ a function on Ω , x^* a local minimizer of f over Ω , and d a feasible direction at x^* . If $d^T \nabla f(x^*) = 0$, then

$$\mathbf{d}^{\mathsf{T}}\mathbf{F}(\mathbf{x}^*)\mathbf{d}\geq 0$$
,

where \mathbf{F} is the Hessian of f.

Proof. We prove the result by contradiction. Suppose there is a feasible direction \boldsymbol{d} at \boldsymbol{x}^* such that $\boldsymbol{d}^\top \nabla f(\boldsymbol{x}^*) = 0$ and $\boldsymbol{d}^\top F(\boldsymbol{x}^*) \boldsymbol{d} < 0$. Let $\boldsymbol{x}(\alpha) = \boldsymbol{x}^* + \alpha \boldsymbol{d}$ and define the composite function $\phi(\alpha) = f(\boldsymbol{x}^* + \alpha \boldsymbol{d}) = f(\boldsymbol{x}(\alpha))$. Then, by Taylor's theorem,

$$\phi(\alpha) = \phi(0) + \phi''(0) \frac{\alpha^2}{2} + o(\alpha^2),$$

where by assumption, $\phi'(0) = \mathbf{d}^{\mathsf{T}} \nabla F(\mathbf{x}^*) = 0$ and $\phi''(0) = \mathbf{d}^{\mathsf{T}} \mathbf{F}(\mathbf{x}^*) \mathbf{d} < 0$.

For sufficiently small α ,

$$\phi(\alpha) - \phi(0) = \phi''(0) \frac{\alpha^2}{2} + o(\alpha^2) < 0,$$

that is,

$$f(\mathbf{x}^* + \alpha \mathbf{d}) < f(\mathbf{x}^*).$$

which contradicts the assumption that x^* is a local minimizer. Thus,

$$\phi''(0) = d^{\mathsf{T}} F(x^*) d \ge 0.$$

• Corollary 1.2 Interior Case. Let x^* be an interior point of $\Omega \subset \mathbb{R}^n$. If x^* is a local minimizer of $f: \Omega \to \mathbb{R}$, $f \in C^2$, then

$$\nabla f(\mathbf{x}^*) = \mathbf{0}$$

and $F(x^*)$ is positive semidefinite ($F(x^*) \ge 0$); that is, for all $d \in \mathbb{R}^n$,

$$d^{\mathsf{T}}F(x^*)d \geq 0.$$

Proof. If x^* is an interior point, then all directions are feasible. The result then follows from Corollary 1.1 and Theorem 1.2.

- Theorem 1.3 Second-Order Sufficient Condition (SOSC), Interior Case. Let $f \in C^2$ be defined on a region in which x^* is an interior point. Suppose that
 - 1. $\nabla f(\mathbf{x}^*) = 0$.
 - 2. $F(x^*) > 0$.

Then, x^* is a strict local minimizer of f.

Proof. Because $f \in C^2$, we have $F(x^*) = F^{\mathsf{T}}(x^*)$. Using assumption 2 and Rayleigh's inequality it follows that if $d \neq 0$, then $0 < \lambda_{\min}(F(x^*)) ||d||^2 \le d^{\mathsf{T}} F(x^*) d$.

By Taylor's theorem and assumption 1,

$$f(\mathbf{x}^* + \mathbf{d}) - f(\mathbf{x}^*) = \frac{1}{2}\mathbf{d}^{\mathsf{T}}\mathbf{F}(\mathbf{x}^*)\mathbf{d} + o(\|\mathbf{d}\|^2) \ge \frac{\lambda_{\min}(\mathbf{F}(\mathbf{x}^*))}{2}\|\mathbf{d}\|^2 + o(\|\mathbf{d}\|^2).$$

Hence, for all d such that ||d|| is sufficiently small,

$$f(\mathbf{x}^* + \mathbf{d}) > f(\mathbf{x}^*),$$

which completes the proof.