Proof: For $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^n$,

$$f'(\boldsymbol{y}) = f'(\boldsymbol{x}) + \int_0^1 f''(\boldsymbol{x} + \tau(\boldsymbol{y} - \boldsymbol{x}))(\boldsymbol{y} - \boldsymbol{x})d\tau$$

= $f'(\boldsymbol{x}) + \left(\int_0^1 f''(\boldsymbol{x} + \tau(\boldsymbol{y} - \boldsymbol{x}))d\tau\right)(\boldsymbol{y} - \boldsymbol{x}).$

Since $||f''(\boldsymbol{x})||_2 \leq L$,

$$\begin{split} \|f'(\boldsymbol{y}) - f'(\boldsymbol{x})\|_2 &\leq \left\| \int_0^1 f''(\boldsymbol{x} + \tau(\boldsymbol{y} - \boldsymbol{x})) d\tau \right\|_2 \|\boldsymbol{y} - \boldsymbol{x}\|_2 \\ &\leq \int_0^1 \|f''(\boldsymbol{x} + \tau(\boldsymbol{y} - \boldsymbol{x}))\|_2 d\tau \|\boldsymbol{y} - \boldsymbol{x}\|_2 \\ &\leq L \|\boldsymbol{y} - \boldsymbol{x}\|_2. \end{split}$$

On the other hand, for $\boldsymbol{s} \in \mathbb{R}^n$, and $\alpha \in \mathbb{R}$, $\alpha \neq 0$,

$$\|f'(x + \alpha s) - f'(x)\|_2 \le |\alpha|L\|s\|_2$$

Dividing both sides by $|\alpha|$ and taking the limit to zero,

$$\|f''(\boldsymbol{x})\boldsymbol{s}\|_2 \leq L\|\boldsymbol{s}\|_2, \quad \boldsymbol{s} \in \mathbb{R}^n.$$

Therefore, $||f''(\boldsymbol{x})||_2 \leq L$.

Example 3.3

1. The linear function $f(\boldsymbol{x}) = \alpha + \langle \boldsymbol{a}, \boldsymbol{x} \rangle \in \mathcal{C}^{2,1}_0(\mathbb{R}^n)$ since

$$f'(\boldsymbol{x}) = \boldsymbol{a}, \quad f''(\boldsymbol{x}) = \boldsymbol{O}.$$

2. The quadratic function $f(\mathbf{x}) = \alpha + \langle \mathbf{a}, \mathbf{x} \rangle + 1/2 \langle \mathbf{A}\mathbf{x}, \mathbf{x} \rangle$ with $\mathbf{A} = \mathbf{A}^T$ belongs to $\mathcal{C}_L^{2,1}(\mathbb{R}^n)$ where

$$f'(x) = a + Ax, \quad f''(x) = A, \quad L = ||A||_2.$$

3. The function $f(x) = \sqrt{1 + x^2} \in \mathcal{C}_1^{2,1}(\mathbb{R})$ since

$$f'(x) = \frac{x}{\sqrt{1+x^2}}, \quad f''(x) = \frac{1}{(1+x^2)^{3/2}} \le 1.$$

Lemma 3.4 Let $f \in \mathcal{C}_L^{1,1}(\mathbb{R}^n)$. Then for any $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^n$, we have

$$|f(\boldsymbol{y}) - f(\boldsymbol{x}) - \langle f'(\boldsymbol{x}), \boldsymbol{y} - \boldsymbol{x} \rangle| \leq rac{L}{2} \| \boldsymbol{y} - \boldsymbol{x} \|_2^2.$$

Proof:

For any $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^n$, we have

$$\begin{split} f(\boldsymbol{y}) &= f(\boldsymbol{x}) + \int_0^1 \langle f'(\boldsymbol{x} + \tau(\boldsymbol{y} - \boldsymbol{x})), \boldsymbol{y} - \boldsymbol{x} \rangle d\tau \\ &= f(\boldsymbol{x}) + \langle f'(\boldsymbol{x}), \boldsymbol{y} - \boldsymbol{x} \rangle + \int_0^1 \langle f'(\boldsymbol{x} + \tau(\boldsymbol{y} - \boldsymbol{x})) - f'(\boldsymbol{x}), \boldsymbol{y} - \boldsymbol{x} \rangle d\tau. \end{split}$$

Therefore,

$$\begin{split} |f(\boldsymbol{y}) - f(\boldsymbol{x}) - \langle f'(\boldsymbol{x}), \boldsymbol{y} - \boldsymbol{x} \rangle| &= \left| \int_0^1 \langle f'(\boldsymbol{x} + \tau(\boldsymbol{y} - \boldsymbol{x})) - f'(\boldsymbol{x}), \boldsymbol{y} - \boldsymbol{x} \rangle d\tau \right| \\ &\leq \int_0^1 |\langle f'(\boldsymbol{x} + \tau(\boldsymbol{y} - \boldsymbol{x})) - f'(\boldsymbol{x}), \boldsymbol{y} - \boldsymbol{x} \rangle| d\tau \\ &\leq \int_0^1 \|f'(\boldsymbol{x} + \tau(\boldsymbol{y} - \boldsymbol{x})) - f'(\boldsymbol{x})\|_2 \|\boldsymbol{y} - \boldsymbol{x}\|_2 d\tau \\ &\leq \int_0^1 \tau L \|\boldsymbol{y} - \boldsymbol{x}\|_2^2 d\tau = \frac{L}{2} \|\boldsymbol{y} - \boldsymbol{x}\|_2^2. \end{split}$$

Consider a function $f \in \mathcal{C}_L^{1,1}(\mathbb{R}^n)$. Let us fix $\boldsymbol{x}_0 \in \mathbb{R}^n$, and define two quadratic functions:

$$\phi_1(\boldsymbol{x}) = f(\boldsymbol{x}_0) + \langle f'(\boldsymbol{x}_0), \boldsymbol{x} - \boldsymbol{x}_0 \rangle - \frac{L}{2} \| \boldsymbol{x} - \boldsymbol{x}_0 \|_2^2,$$

$$\phi_2(\boldsymbol{x}) = f(\boldsymbol{x}_0) + \langle f'(\boldsymbol{x}_0), \boldsymbol{x} - \boldsymbol{x}_0 \rangle + \frac{L}{2} \| \boldsymbol{x} - \boldsymbol{x}_0 \|_2^2.$$

Then the graph of the function f is located between the graphs of ϕ_1 and ϕ_2 :

$$\phi_1(\boldsymbol{x}) \leq f(\boldsymbol{x}) \leq \phi_2(\boldsymbol{x}), \quad \boldsymbol{x} \in \mathbb{R}^n.$$

Lemma 3.5 Let $f \in \mathcal{C}^{2,2}_M(\mathbb{R}^n)$. Then for all $x, y \in \mathbb{R}^n$, we have

$$\|f'(\boldsymbol{y}) - f'(\boldsymbol{x}) - f''(\boldsymbol{x})(\boldsymbol{y} - \boldsymbol{x})\|_2 \le \frac{M}{2} \|\boldsymbol{y} - \boldsymbol{x}\|_2^2,$$
$$|f(\boldsymbol{y}) - f(\boldsymbol{x}) - \langle f'(\boldsymbol{x}), \boldsymbol{y} - \boldsymbol{x} \rangle - \frac{1}{2} \langle f''(\boldsymbol{x})(\boldsymbol{y} - \boldsymbol{x}), \boldsymbol{y} - \boldsymbol{x} \rangle| \le \frac{M}{6} \|\boldsymbol{y} - \boldsymbol{x}\|_2^3$$

Lemma 3.6 Let $f \in \mathcal{C}_M^{2,2}(\mathbb{R}^n)$, with $\|f''(\boldsymbol{x}) - f''(\boldsymbol{y})\|_2 \leq M \|\boldsymbol{x} - \boldsymbol{y}\|_2$. Then

$$f''(\boldsymbol{x}) - M \|\boldsymbol{y} - \boldsymbol{x}\|_2 \boldsymbol{I} \leq f''(\boldsymbol{y}) \leq f''(\boldsymbol{x}) + M \|\boldsymbol{y} - \boldsymbol{x}\|_2 \boldsymbol{I}$$

Proof:

Since $f \in \mathcal{C}_M^{2,2}(\mathbb{R}^n)$, $\|f''(\boldsymbol{y}) - f''(\boldsymbol{x})\|_2 \leq M \|\boldsymbol{y} - \boldsymbol{x}\|_2$. This means that the eigenvalues of the symmetric matrix $f''(\boldsymbol{y}) - f''(\boldsymbol{x})$ satisfy:

$$|\lambda_i(f''(\boldsymbol{y}) - f''(\boldsymbol{x}))| \le M \|\boldsymbol{y} - \boldsymbol{x}\|_2, \quad i = 1, 2, \dots, n.$$

Therefore,

$$-M\|oldsymbol{y}-oldsymbol{x}\|_2oldsymbol{I} \preceq f''(oldsymbol{y}) - f''(oldsymbol{x}) \preceq M\|oldsymbol{y}-oldsymbol{x}\|_2oldsymbol{I}.$$

3.1Exercises

1. Prove Lemma 3.5.

4 Optimality Conditions for Differentiable Functions in \mathbb{R}^n

Let $f(\boldsymbol{x})$ be differentiable at $\bar{\boldsymbol{x}}$. Then for $\boldsymbol{y} \in \mathbb{R}^n$, we have

$$f(\boldsymbol{y}) = f(\bar{\boldsymbol{x}}) + \langle f'(\bar{\boldsymbol{x}}), \boldsymbol{y} - \bar{\boldsymbol{x}} \rangle + o(\|\boldsymbol{y} - \bar{\boldsymbol{x}}\|_2),$$

where o(r) is some function of r > 0 such that

$$\lim_{r \to 0} \frac{1}{r} o(r) = 0, \ o(0) = 0.$$

Let s be a direction in \mathbb{R}^n such that $||s||_2 = 1$. Consider the local decrease (or increase) of f(x) along s:

$$\Delta(\boldsymbol{s}) = \lim_{\alpha \to 0} \frac{1}{\alpha} \left[f(\bar{\boldsymbol{x}} + \alpha \boldsymbol{s}) - f(\bar{\boldsymbol{x}}) \right]$$

Since $f(\bar{\boldsymbol{x}} + \alpha \boldsymbol{s}) - f(\bar{\boldsymbol{x}}) = \alpha \langle f'(\bar{\boldsymbol{x}}), \boldsymbol{s} \rangle + o(\|\alpha \boldsymbol{s}\|_2)$, we have $\Delta(\boldsymbol{s}) = \langle f'(\bar{\boldsymbol{x}}), \boldsymbol{s} \rangle$. Using the Cauchy-Schwartz inequality $-\|\boldsymbol{x}\|_2 \|\boldsymbol{y}\|_2 \leq \langle \boldsymbol{x}, \boldsymbol{y} \rangle \leq \|\boldsymbol{x}\|_2 \|\boldsymbol{y}\|_2$,

$$\Delta(\boldsymbol{s}) = \langle f'(\bar{\boldsymbol{x}}), \boldsymbol{s} \rangle \ge - \|f'(\bar{\boldsymbol{x}})\|_2.$$

Choosing the direction $\bar{\boldsymbol{s}} = -f'(\bar{\boldsymbol{x}})/\|f'(\bar{\boldsymbol{x}})\|_2$,

$$\Delta(\bar{\boldsymbol{s}}) = -\left\langle f'(\bar{\boldsymbol{x}}), \frac{f'(\bar{\boldsymbol{x}})}{\|f'(\bar{\boldsymbol{x}})\|_2} \right\rangle = -\|f'(\bar{\boldsymbol{x}})\|_2$$

Thus, the direction $-f'(\bar{x})$ is the direction of the fastest local decrease of f(x) at point \bar{x} .

Theorem 4.1 (First-order necessary optimality condition) Let x^* be a local minimum of the differentiable function f(x). Then

$$f'(\boldsymbol{x}^*) = \boldsymbol{0}.$$

Proof:

Let \boldsymbol{x}^* be the local minimum of $f(\boldsymbol{x})$. Then, there is r > 0 such that for all \boldsymbol{y} with $\|\boldsymbol{y} - \boldsymbol{x}^*\|_2 \le r$, $f(\boldsymbol{y}) \ge f(\boldsymbol{x}^*)$.

Since f is differentiable,

$$f(\boldsymbol{y}) = f(\boldsymbol{x}^*) + \langle f'(\boldsymbol{x}^*), \boldsymbol{y} - \boldsymbol{x}^* \rangle + o(\|\boldsymbol{y} - \boldsymbol{x}^*\|_2) \ge f(\boldsymbol{x}^*).$$

Dividing by $\|\boldsymbol{y} - \boldsymbol{x}^*\|_2$, and taking the limit $\boldsymbol{y} \to \boldsymbol{x}^*$,

$$\langle f'(\boldsymbol{x}^*), \boldsymbol{s} \rangle \ge 0, \quad \forall \boldsymbol{s} \in \mathbb{R}^n, \quad \|\boldsymbol{s}\|_2 = 1.$$

Consider the opposite direction -s, and then we conclude that

$$\langle f'(\boldsymbol{x}^*), \boldsymbol{s} \rangle = 0, \quad \forall \boldsymbol{s} \in \mathbb{R}^n, \quad \|\boldsymbol{s}\|_2 = 1.$$

Choosing $\boldsymbol{s} = \boldsymbol{e}_i$ (i = 1, 2, ..., n), we conclude that $f'(\boldsymbol{x}^*) = 0$.

Remark 4.2 For the first-order sufficient optimality condition, we need convexity for the function f(x).

Corollary 4.3 Let x^* be a local minimum of a differentiable function f(x) subject to linear equality constraints

$$\boldsymbol{x} \in \mathcal{L} := \{ \boldsymbol{x} \in \mathbb{R}^n \mid \boldsymbol{A} \boldsymbol{x} = \boldsymbol{b} \} \neq \emptyset,$$

where $\boldsymbol{A} \in \mathbb{R}^{m \times n}$, $\boldsymbol{b} \in \mathbb{R}^m$, m < n.

Then, there exists a vector of multipliers $\boldsymbol{\lambda}^*$ such that

$$f'(\boldsymbol{x}^*) = \boldsymbol{A}^T \boldsymbol{\lambda}^*$$

Proof:

Consider the vectors u_i (i = 1, 2, ..., k) with $k \ge n - m$ which form an orthonormal basis of the null space of A. Then, $x \in \mathcal{L}$ can be represented as

$$oldsymbol{x} = oldsymbol{x}(oldsymbol{t}) := oldsymbol{x}^* + \sum_{i=1}^k t_i oldsymbol{u}_i, \quad oldsymbol{t} \in \mathbb{R}^k.$$

Moreover, the point t = 0 is the local minimal solution of the function $\phi(t) = f(x(t))$.

From Theorem 4.1, $\phi'(\mathbf{0}) = \mathbf{0}$. That is,

$$\frac{d\phi}{dt_i}(\mathbf{0}) = \langle f'(\boldsymbol{x}^*), \boldsymbol{u}_i \rangle = 0, \quad i = 1, 2, \dots, k$$

Now there is t^* and λ^* such that

$$f'(\boldsymbol{x}^*) = \sum_{i=1}^k t_i^* \boldsymbol{u}_i + \boldsymbol{A}^T \boldsymbol{\lambda}^*.$$

For each i = 1, 2, ..., k,

$$\langle f'(\boldsymbol{x}^*), \boldsymbol{u}_i \rangle = t_i^* = 0.$$

Therefore, we have the result.

The following type of result is called *theorems of the alternative*, and are closed related to duality theory in optimization.

Corollary 4.4 Given $A \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^m$, $c \in \mathbb{R}^n$, $\eta \in \mathbb{R}$, either

$$\begin{cases} \langle \boldsymbol{c}, \boldsymbol{x} \rangle < \eta \\ \boldsymbol{A} \boldsymbol{x} = \boldsymbol{b} \end{cases} \text{ has a solution } \boldsymbol{x} \in \mathbb{R}^n, \tag{1}$$

or

$$\begin{pmatrix}
\begin{cases}
\langle \boldsymbol{b}, \boldsymbol{\lambda} \rangle > 0 \\
\boldsymbol{A}^T \boldsymbol{\lambda} = \boldsymbol{0} \\
\text{or} \\
\begin{cases}
\langle \boldsymbol{b}, \boldsymbol{\lambda} \rangle \ge \eta \\
\boldsymbol{A}^T \boldsymbol{\lambda} = \boldsymbol{c}
\end{pmatrix}$$
has a solution $\boldsymbol{\lambda} \in \mathbb{R}^m$, (2)

but never both

Proof:

Let us first show that if $\exists x \in \mathbb{R}^n$ satisfying (1), $\exists \lambda \in \mathbb{R}^m$ satisfying (2). Let us assume by contradiction that $\exists \lambda$. Then $\langle \lambda, Ax \rangle = \langle \lambda, b \rangle$ and in the homogeneous case it gives $0 = \langle \lambda, b \rangle > 0$ and in the non-homogeneous case it gives $\eta > \langle c, x \rangle = \langle \lambda, b \rangle \ge \eta$. Both of cases are impossible.

Now, let us assume that $\exists x \in \mathbb{R}^n$ satisfying (1). If additionally $\exists x \in \mathbb{R}^n$ such that Ax = b, it means that the columns of the matrix A do not spam the vector b. Therefore, there is $0 \neq \lambda \in \mathbb{R}^m$ which is orthogonal to all of these columns and $\langle b, \lambda \rangle \neq 0$. Selecting the correct sign, we constructed a λ which satisfies the homogeneous system of (2). Now, if for all x such that Ax = b we have $\langle c, x \rangle \geq \eta$, it means that the minimization of the function $f(x) = \langle c, x \rangle$ subject to Ax = b has an optimal solution x^* with $f(x^*) \geq \eta$ (since $\exists x \in \mathbb{R}^n$ such that Ax = b, we can always assume that $m \leq n$ eliminating redundant linear constraints from the system. If n = m and A is nonsingular, take $\lambda = A^{-T}c$. Otherwise, we can eliminate again redundant linear constraint to have n > m). From Corollary 4.3, $\exists \lambda \in \mathbb{R}^m$ such that $A^T\lambda = c$, and $\langle b, \lambda \rangle = \langle x^*, A^T\lambda \rangle = \langle x^*, c \rangle \geq \eta$.

If $f(\boldsymbol{x})$ is twice differentiable at $\bar{\boldsymbol{x}} \in \mathbb{R}^n$, then for $\boldsymbol{y} \in \mathbb{R}^n$, we have

$$f'(y) = f'(\bar{x}) + f''(\bar{x})(y - \bar{x}) + o(||y - \bar{x}||_2),$$

where $\boldsymbol{o}(r)$ is such that $\lim_{r\to 0} \|\boldsymbol{o}(r)\|_2/r = 0$ and $\boldsymbol{o}(0) = 0$.

Theorem 4.5 (Second-order necessary optimality condition) Let x^* be a local minimum of a twice continuously differentiable function f(x). Then

$$f'(\boldsymbol{x}^*) = 0, \qquad f''(\boldsymbol{x}^*) \succeq \boldsymbol{O}.$$

Proof:

Since \boldsymbol{x}^* is a local minimum of $f(\boldsymbol{x})$, $\exists r > 0$ such that for all $\boldsymbol{y} \in \mathbb{R}^n$ which satisfy $\|\boldsymbol{y} - \boldsymbol{x}^*\|_2 \leq r$, $f(\boldsymbol{y}) \geq f(\boldsymbol{x}^*)$.

From Theorem 4.1, $f'(\boldsymbol{x}^*) = 0$. Then

$$f(\boldsymbol{y}) = f(\boldsymbol{x}^*) + \frac{1}{2} \langle f''(\boldsymbol{x}^*)(\boldsymbol{y} - \boldsymbol{x}^*), \boldsymbol{y} - \boldsymbol{x}^* \rangle + o(\|\boldsymbol{y} - \boldsymbol{x}^*\|_2^2) \ge f(\boldsymbol{x}^*).$$

And $\langle f''(\boldsymbol{x}^*)\boldsymbol{s}, \boldsymbol{s} \rangle \geq 0, \ \forall \boldsymbol{s} \in \mathbb{R}^n \text{ with } \|\boldsymbol{s}\|_2 = 1.$

Theorem 4.6 (Second-order sufficient optimality condition) Let the function f(x) be twice continuously differentiable on \mathbb{R}^n , and let x^* satisfy the following conditions:

$$f'(\boldsymbol{x}^*) = 0, \quad f''(\boldsymbol{x}^*) \succ \boldsymbol{O}.$$

Then, \boldsymbol{x}^* is a strict local minimum of $f(\boldsymbol{x})$.

Proof:

In a small neighborhood of \boldsymbol{x}^* , function $f(\boldsymbol{x}^*)$ can be represented as:

$$f(y) = f(x^*) + \frac{1}{2} \langle f''(x^*)(y - x^*), y - x^* \rangle + o(||y - x^*||_2^2).$$

Since $o(r)/r \to 0$, there is a $\bar{r} > 0$ such that for all $r \in [0, \bar{r}]$,

$$|o(r)| \leq \frac{r}{4}\lambda_1(f''(\boldsymbol{x}^*)),$$

where $\lambda_1(f''(\boldsymbol{x}^*))$ is the smallest eigenvalue of the symmetric matrix $f''(\boldsymbol{x}^*)$ which is positive. Then

$$f(\boldsymbol{y}) \ge f(\boldsymbol{x}^*) + rac{1}{2}\lambda_1(f''(\boldsymbol{x}^*))\|\boldsymbol{y} - \boldsymbol{x}^*\|_2^2 + o(\|\boldsymbol{y} - \boldsymbol{x}^*\|_2^2).$$

Considering that $\bar{r} < 1$, $|o(r^2)| \le r^2/4\lambda_1(f''(\boldsymbol{x}^*))$ for $r \in [0, \bar{r}]$, finally

$$f(\boldsymbol{y}) \ge f(\boldsymbol{x}^*) + \frac{1}{4}\lambda_1(f''(\boldsymbol{x}^*)) \|\boldsymbol{y} - \boldsymbol{x}^*\|_2^2 > f(\boldsymbol{x}^*).$$

1. Let $f : \mathbb{R}^n \to \mathbb{R}, g : \mathbb{R}^n \to \mathbb{R}^m$ continuously differentiable functions and $h \in \mathbb{R}^m$. Define the following optimization problem.

$$\left\{egin{array}{ll} ext{minimize} & f(m{x}) \ ext{subject to} & g(m{x}) = m{h} \ & m{x} \in \mathbb{R}^n \end{array}
ight.$$

Write the Karush-Kuhn-Tucker (KKT) conditions corresponding to the above problem.

- 2. In view of Theorem 4.6, find a twice continuously differentiable function on \mathbb{R}^n which satisfies $f'(\boldsymbol{x}^*) = 0$, $f''(\boldsymbol{x}^*) \succeq \boldsymbol{O}$, but \boldsymbol{x}^* is not a local minimum of $f(\boldsymbol{x})$.
- 3. Let $f : \mathbb{R}^n \to \mathbb{R}$ be a continuous differentiable and convex function. If $x^* \in \mathbb{R}^n$ is such that $f'(x^*) = 0$, then show that x^* is a global minimum for f(x).