OR4030 OPTIMIZATION Chapter 2
Mathematical Background for Nonlinear Optimization
2.1 Sets

Neighborhood

The *ε-neighborhood* of a point $x = (x_1, x_2, \ldots, x_n)^T \in \Re^n$ is the set of points inside the ball with center x and radius $\varepsilon > 0$:

$$N_\varepsilon(x) = \{y \in \Re^n : \|y - x\| < \varepsilon\},$$

where $\|y - x\| = \sqrt{\sum_{j=1}^n (y_j - x_j)^2}$ for $y = (y_1, y_2, \ldots, y_n)^T$.

Open Sets

A set S is called *open* if around every point in S there is a neighborhood that is contained in S. For example, $\Re^n$, $\emptyset$ and the open interval (a, b) in $\Re^1$ (or simply written as $\Re$) are open sets.

Closed Sets

A set S in $\Re^n$ is called *closed* if its complement S' (i.e., the set $\Re^n \setminus S$) is an open set. For example, $\Re^n$, $\emptyset$ and the closed interval $[a, b]$ in $\Re$ are closed sets.

Bounded Sets

A set is *bounded* if it can be contained in a ball of a sufficiently large radius. For example, the open interval (a, b) and the closed interval $[a, b]$ in $\Re$ are both bounded sets (here a and b are two finite numbers).

Compact Sets

A set is *compact* if it is both closed and bounded. For example, the closed interval $[a, b]$ is a compact set.

2.2 Convex Sets

A set S in $\Re^n$ is *convex* if for any elements $\bar{x}$ and $\hat{x}$ of S,

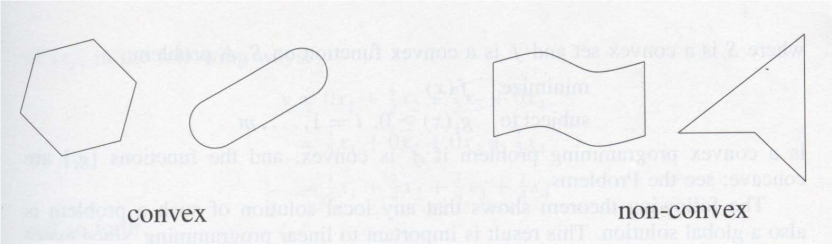
$$\lambda\bar{x} + (1-\lambda)\hat{x} \in S$$

for all values of λ such that $0 \leq \lambda \leq 1$.

The set

$$\begin{aligned} & \{\lambda\bar{x} + (1-\lambda)\hat{x} \mid 0 \leq \lambda \leq 1\} \\ = \; & \{\hat{x} + \lambda(\bar{x} - \hat{x}) \mid 0 \leq \lambda \leq 1\} \end{aligned}$$

is the line segment joining $\bar{x}$ and $\hat{x}$. So, S is a convex set if and only if for every pair of $\bar{x}$ and $\hat{x}$ in S, the line segment joining $\bar{x}$ and $\hat{x}$ also lies in S.



Convex and Non-convex Sets

It is easy to check by the definition that the following sets are all convex sets.

- Any line:
$$L = \{x + \lambda v \mid \lambda \in \Re\}$$
for a given point (or say a vector) x and a given vector v in $\Re^n$.
- Any half line or ray:
$$L = \{x + \lambda v \mid \lambda \geq 0\}$$
for a given point x and a given vector v in $\Re^n$.

- Any closed half-space

$$F^+ = \{y \in \Re^n \mid \bar{x}^T y \geq \alpha\}$$

for a given vector $\bar{x}$ in $\Re^n$ and a given real number α.

- Any open half-space

$$F = \{y \in \Re^n \mid \bar{x}^T y > \alpha\}$$

for a given vector $\bar{x}$ in $\Re^n$ and a given real number α.

- Any closed ball

$$B^+(\bar{x}, r) = \{y \in \Re^n \mid \|y - \bar{x}\| \leq r\}$$

or open ball

$$B(\bar{x}, r) = \{y \in \Re^n \mid \|y - \bar{x}\| < r\},$$

where $\bar{x}$ is a given point in $\Re^n$, and r is a positive number.

- The intersection of a number of convex sets C_i in $\Re^n$, $i = 1, 2, \ldots, k$:

$$C = \{\bigcap_{i=1}^{k} C_i \mid C_i, i = 1, \ldots, k, \text{ are convex sets}\}.$$

- The solution set to the linear equations

$$S = \{x \in \Re^n \mid Ax = b\},$$

where $A \in \Re^{m \times n}$ (i.e., a $m \times n$ real matrix), and $b \in \Re^m$.
- For p given points $x^1, x^2, \ldots, x^p$ in $\Re^n$, any vector

$$\sum_{i=1}^{p} \lambda_i x^i = \lambda_1 x^1 + \lambda_2 x^2 + \cdots + \lambda_p x^p$$

is called a *convex combination of $x^1, \ldots, x^p$*, if all numbers λ_i satisfy that

$$\lambda_i \geq 0, \; i = 1, \ldots, p; \quad \text{and} \; \sum_{i=1}^{p} \lambda_i = 1.$$

For p given points $x^1, x^2, \ldots, x^p$ in $\Re^n$, all their convex combinations:

$$C = \{\sum_{i=1}^{p} \lambda_i x^i \mid \lambda_i \geq 0,\ \sum_{i=1}^{p} \lambda_i = 1\}$$

form a convex set. This set is called the convex hull of points $x^1, x^2, \ldots, x^p$.

Note that for three points x^1, x^2 and x^3 in $\Re^2$, all their convex combinations form the triangular region with x^1, x^2 and x^3 as its vertexes.

Limits

The equation

$$\lim_{x \longrightarrow c} f(x) = d$$

means that as the single variable x gets very close to the number c (but is not necessary equal to c), the value of $f(x)$ gets arbitrarily close to the value d.

It is also possible that

$$\lim_{x \longrightarrow c} f(x)$$

may not exist.

Continuity

A function $f(x)$ is *continuous* at a point (or say a value) c if

$$\lim_{x \to c} f(x) = f(c).$$

If $f(x)$ is not continuous at c, we say that $f(x)$ is *discontinuous* (or has a discontinuity) at c.

Differentiation

The *derivative* of $f(x)$ at a point c is defined by

$$f'(c) = \frac{df(c)}{dx} = \left.\frac{df}{dx}\right|_{x=c} = \lim_{\Delta x \to 0} \frac{f(c + \Delta x) - f(c)}{\Delta x}$$

provided that the limit exists. When the limit exists, we say that $f(x)$ is *differentiable* at c. Note also that if $f(x)$ is differentiable at c, then $f(x)$ is continuous at c.

Higher Derivatives

Furthermore, we can define

$$f^{(2)}(c) = f''(c) = \frac{d^2 f(c)}{dx^2} = \left.\frac{d^2 f}{dx^2}\right|_{x=c}$$

to be the derivative of function $f'(x)$ at point $x = c$.

Similarly, we define (if it exists) $f^{(k)}(c)$ to be the derivative of $f^{(k-1)}(x)$ at $x = c$ for $k \geq 3$.

Continuously Differentiable Functions

- $f \in C^0(S)$
  - $\sim$ f is a real-valued continuous function in its domain S.

- $f \in C^1(S)$
  - $\sim$ f is a real-valued continuously differentiable function in S
  - $\sim$ i.e., f' exists and is continuous everywhere in S.

- $f \in C^k(S)$, where $k = 1, 2, 3, \ldots$
  - $\sim$ f is a real-valued kth-order continuously differentiable function in S
  - $\sim$ i.e., $f^{(k)}$ exists and is continuous everywhere in its domain

Taylor's Theorem

Suppose $f^{(k+1)}$ exists for every point on the interval $[a, b]$. Let $c \in [a, b]$. Then for every $x \in [a, b]$, there exists h between c and x with

$$f(x) = P_k(x) + R_k(x),$$

where

$$\begin{aligned} P_k(x) &= f(c) + f'(c)(x-c) + \frac{f''(c)}{2!}(x-c)^2 + \cdots \\ &\quad + \frac{f^{(k)}(c)}{k!}(x-c)^k, \\ R_k(x) &= \frac{f^{(k+1)}(h)}{(k+1)!}(x-c)^{k+1}. \end{aligned}$$

Here

$P_k(x)$ is called the *kth-order Taylor series expansion* of f about c, and

$R_k(x)$ is called the *remainder term* (or *truncation error*) associated with $P_k(x)$.

The infinite series obtained by taking the limit of $P_k(x)$ as $k \longrightarrow \infty$ is called the *Taylor series* of f about c.

We can use $P_k(x)$ to approximate $f(x)$: $f(x) \approx P_k(x)$ with an error of $R_k(x)$.

Partial Derivatives and the Gradient Vector

The *partial derivative* of f with respect to the variable x_j is

$$\frac{\partial f}{\partial x_j} = \lim_{\Delta x_j \to 0} \frac{f(x_1, \ldots, x_j + \Delta x_j, \ldots, x_n) - f(x_1, \ldots, x_j, \ldots, x_n)}{\Delta x_j}.$$

The *gradient* of f is defined by:

$$\nabla f = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{bmatrix}.$$

Second-Order Partial Derivatives and the Hessian Matrix

We use the notation

$$\frac{\partial^2 f}{\partial x_i \, \partial x_j}$$

to denote a *second-order partial derivative* of f.

To find $\frac{\partial^2 f}{\partial x_i \, \partial x_j}$, we first find $\frac{\partial f}{\partial x_j}$ and then take its partial derivative with respect to x_i, i.e.,

$$\frac{\partial^2 f}{\partial x_i \, \partial x_j} = \frac{\partial}{\partial x_i}\left[\frac{\partial f}{\partial x_j}\right].$$

If the second-order partial derivatives exist and are everywhere continuous, then

$$\frac{\partial^2 f}{\partial x_i \, \partial x_j} = \frac{\partial^2 f}{\partial x_j \, \partial x_i}.$$

Suppose $f \in C^2(\Re^n)$. The *Hessian* matrix of f is defined by

$$\nabla^2 f = \begin{bmatrix} \frac{\partial^2 f}{\partial {x_1}^2} & \cdots & \frac{\partial^2 f}{\partial x_n \, \partial x_1} \\ \vdots & & \vdots \\ \frac{\partial^2 f}{\partial x_1 \, \partial x_n} & \cdots & \frac{\partial^2 f}{\partial {x_n}^2} \end{bmatrix}.$$

Note that the Hessian matrix of f is symmetric if all second order partial derivatives are continuous.

Taylor's Theorem

Suppose that $f \in C^3(S)$, where

$$S = \{x : a_j \le x_j \le b_j, j = 1, 2, \ldots, n\}.$$

Let $c = (c_1, c_2, \ldots, c_n)^T \in S$. For every $x \in S$,

$$f(x) \approx f(c) + \nabla f(c)^T (x - c) + \frac{1}{2}(x - c)^T \nabla^2 f(c)(x - c).$$

If we want to change the above approximate equality to an exact one, then

$$f(x) = f(c) + \nabla f(c)^T (x - c) + \frac{1}{2}(x - c)^T \nabla^2 f(\xi)(x - c),$$

where ξ is a point in the line segment linking x and c, but its exact location is unknown.

Example

For the function

$$f(x) = x_1^3 + 5x_1^2 x_2 + 7x_1 x_2^2 + 2x_2^3$$

where $x = (x_1, x_2)^T$, consider its approximate function values near the point $c = (-2, 3)^T$.

The gradient of this function is

$$\nabla f(x) = \begin{bmatrix} 3x_1^2 + 10x_1 x_2 + 7x_2^2 \\ 5x_1^2 + 14x_1 x_2 + 6x_2^2 \end{bmatrix}$$

and the Hessian matrix is

$$\nabla^2 f(x) = \begin{bmatrix} 6x_1 + 10x_2 & 10x_1 + 14x_2 \\ 10x_1 + 14x_2 & 14x_1 + 12x_2 \end{bmatrix}.$$

At the point c, $f, \nabla f$ and $\nabla^2 f$ become

$$f(c) = -20, \quad \nabla f(c) = \begin{bmatrix} 15 \\ -10 \end{bmatrix} \quad \text{and} \quad \nabla^2 f(c) = \begin{bmatrix} 18 & 22 \\ 22 & 8 \end{bmatrix}.$$

By Taylor's Theorem,

$$\begin{aligned} f(x) \quad &\approx \quad -20 + \begin{bmatrix} 15 & -10 \end{bmatrix} \begin{bmatrix} x_1 + 2 \\ x_2 - 3 \end{bmatrix} \\ &\quad + \frac{1}{2} \begin{bmatrix} x_1 + 2 & x_2 - 3 \end{bmatrix} \begin{bmatrix} 18 & 22 \\ 22 & 8 \end{bmatrix} \begin{bmatrix} x_1 + 2 \\ x_2 - 3 \end{bmatrix} \end{aligned}$$

Thus, for example,

$$f(-1.9, 3.2) \approx -19.81.$$

The true value is $f(-1.9, 3.2) = -19.755$. So the approximation is accurate to three digits.

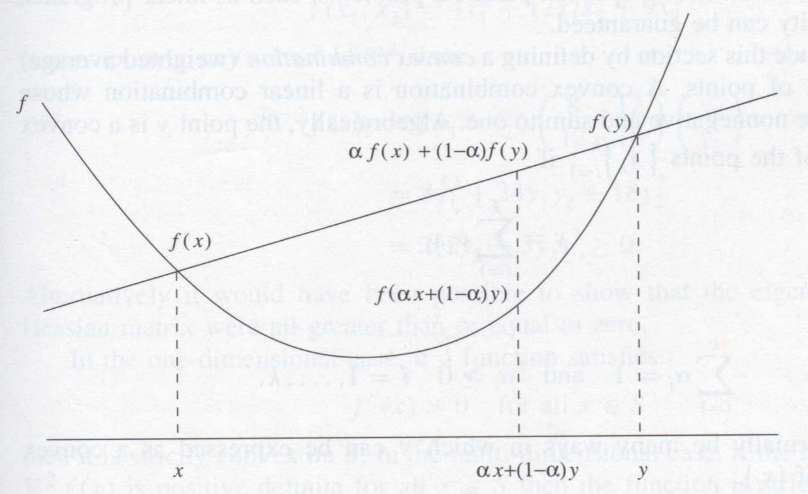
Definitions

A function $f(x)$ of a single real variable x, defined in an interval $[a, b]$, is a **convex function** if, for each pair of distinct values of x, say $\bar{x}$ and $\hat{x}$ in the interval, there holds

$$f(\lambda\bar{x} + (1-\lambda)\hat{x}) \leq \lambda f(\bar{x}) + (1-\lambda)f(\hat{x})$$

for all values of λ such that $0 < \lambda < 1$. It is a *strictly convex function* if $\leq$ can be replaced by $<$. It is a **concave function** (or a *strictly concave function*) if this statement holds when $\leq$ is replaced by $\geq$ (or by $>$).

Geometric meaning of a convex function: for each pair of $x < y$, over the interval $[x, y]$, the line segment joining the two points $(x, f(x))$ and $(y, f(y))$ either lies above, or coincides with the curve of f.



Graph of a Convex Function

Convexity Test for a Function of a Single Variable by Its First Order Derivatives

Consider a single variable function $f(x)$ that is defined in an interval S and possesses continuous first order derivative at each point x in the interval. Then $f(x)$ is

- *Convex* if and only if for each $\bar{x} \in S$,

$$f(y) \geq f(\bar{x}) + f'(\bar{x})(y - \bar{x}), \quad \text{for any } y \in S;$$

- *Strictly convex* if and only if for each $\bar{x} \in S$,

$$f(y) > f(\bar{x}) + f'(\bar{x})(y - \bar{x}), \quad \text{for any } y \in S \text{ and } y \neq \bar{x};$$

- *Concave* if and only if for each $\bar{x} \in S$,

$$f(y) \leq f(\bar{x}) + f'(\bar{x})(y - \bar{x}), \quad \text{for} \;\; \text{any } y \in S;$$

- *Strictly concave* if and only if for each $\bar{x} \in S$,

$$f(y) < f(\bar{x}) + f'(\bar{x})(y - \bar{x}), \quad \text{for} \;\; \text{any } y \in S \text{ and } y \neq \bar{x};$$

We will prove these properties in Section 2.4.2 for multi-variable convex functions.

Geometric Meaning of the Convexity Test. For a single variable function $f(x)$ over an interval S, the tangent line to the graph of $f(x)$ at $\bar{x}$ is given by

$$\{(x, y) \mid y = f(\bar{x}) + f'(\bar{x})(x - \bar{x})\}.$$

Hence, the first conclusion here says that $f(x)$ is a convex function if and only if every tangent line to $f(x)$ lies on or below the graph of $f(x)$;

The second conclusion here says that $f(x)$ is a strictly convex function if and only if every tangent line to $f(x)$ lies below the graph of $f(x)$ and contact the graph only at the point of tangency;

It is easy to state the geometric meaning of the last two conclusions.

Convexity Test for a Function of a Single Variable by Its Second Order Derivatives

Consider a single variable function $f(x)$ that is defined in an interval S and possesses continuous second order derivative at each point x in the interval. Then $f(x)$ is

- *Convex* if and only if $f''(x) \geq 0$ for all x in S;
- *Strictly convex* if $f''(x) > 0$ for all x in S;
- *Concave* if and only if $f''(x) \leq 0$ for all x in S;
- *Strictly concave* if $f''(x) < 0$ for all x in S.

We also leave the proof to the multi-variable case.

Note that in the second (and also the fourth) conclusion above, there is no "only if", that is, $f''(x) > 0$ is only a sufficient condition for strictly convex, but not a necessary condition.

Example. Function $f(x) = x^4$ is a strictly convex function for all $x \in (-\infty, \infty)$, but $f''(0) = 0$. So,

$$f \text{ is strictly convex over } (-\infty, \infty) \not\Longrightarrow f''(x) > 0, \ \forall x \in (-\infty, \infty)$$

(because at $x = 0$, $f''(x) = 0$).

Definitions

A function of several variables $f(x)$, defined in a convex set S of $\Re^n$, is a *convex function* if, for each pair of distinct points in S, say

$$\bar{x} = (\bar{x}_1, \ldots, \bar{x}_n)^T, \quad \text{and} \quad \hat{x} = (\hat{x}_1, \ldots, \hat{x}_n)^T,$$

there holds

$$f(\lambda\bar{x} + (1-\lambda)\hat{x}) \leq \lambda f(\bar{x}) + (1-\lambda)f(\hat{x})$$

for all values of λ such that $0 < \lambda < 1$. It is a *strictly convex function* if $\leq$ can be replaced by $<$. It is a *concave function* (or a *strictly concave function*) if this statement holds when $\leq$ is replaced by $\geq$ (or by $>$).

In the above definition, we consider two points, $\bar{x}$ and $\hat{x}$. In fact for a convex or concave function, we can also consider p points $x^1, x^2, \ldots, x^p$, here p is a positive integer. That is, if $f(x)$ is a convex function over a convex set S, then for any p points $x^1, x^2, \ldots, x^p$ in S,

$$f(\sum_{i=1}^{p} \lambda_i x^i) \leq \sum_{i=1}^{p} \lambda_i f(x^i)$$

for any $\lambda_1, \ldots, \lambda_p$ satisfying

$$\lambda_i \geq 0, \; i = 1, \ldots, p; \text{ and } \sum_{i=1}^{p} \lambda_i = 1.$$

This conclusion can be proved by induction. For example, consider the case of $p = 3$. Then we can assume that $\lambda_1, \lambda_2, \lambda_3 > 0$ (otherwise it reduces to the case of $p < 3$). As the conclusion is true when $p = 2$, we know that

$$
\begin{aligned}
& f(\lambda_1 x^1 + \lambda_2 x^2 + \lambda_3 x^3) \\
= \quad & f(\lambda_1 x^1 + [\lambda_2 + \lambda_3][\frac{\lambda_2}{\lambda_2 + \lambda_3} x^2 + \frac{\lambda_3}{\lambda_2 + \lambda_3} x^3]) \\
\leq \quad & \lambda_1 f(x^1) + (\lambda_2 + \lambda_3) f(\frac{\lambda_2}{\lambda_2 + \lambda_3} x^2 + \frac{\lambda_3}{\lambda_2 + \lambda_3} x^3) \\
\leq \quad & \lambda_1 f(x^1) + (\lambda_2 + \lambda_3)[\frac{\lambda_2}{\lambda_2 + \lambda_3} f(x^2) + \frac{\lambda_3}{\lambda_2 + \lambda_3} f(x^3)] \\
= \quad & \lambda_1 f(x^1) + \lambda_2 f(x^2) + \lambda_3 f(x^3).
\end{aligned}
$$

Hence the conclusion is true if $p = 3$.

Examples of Convex Functions

- **Example 1** The linear function

$$f(x) = a^T x + b, \quad a, x \in \Re^n, \; b \in \Re.$$

In fact

$$\begin{aligned} f(\lambda x + (1-\lambda)y) &= a^T(\lambda x + (1-\lambda)y) + b \\ &= \lambda(a^T x + b) + (1-\lambda)(a^T y + b) \\ &= \lambda f(x) + (1-\lambda) f(y). \end{aligned}$$

So, $f(x)$ is convex, but not strictly convex.

Question: is this $f(x)$ also concave?

- **Example 2** The quadratic function

$$f(x) = (a^T x)^2, \quad a, x \in \Re^n.$$

In fact as $0 < \lambda < 1$,

$$\begin{aligned} & f(\lambda x + (1-\lambda)y) - [\lambda f(x) + (1-\lambda) f(y)] \\ = \; & [a^T(\lambda x + (1-\lambda)y)]^2 - [\lambda (a^T x)^2 + (1-\lambda)(a^T y)^2] \\ = \; & -\lambda(1-\lambda)(a^T x - a^T y)^2 \\ \leq \; & 0. \end{aligned}$$

Hence f is a convex function.

Convexity Test for a Function of Multi-Variable by Its First Order Derivatives

Consider a multi-variable function $f(x)$ that is defined in a convex set $S \subseteq \Re^n$ and possesses continuous gradient at each point x in S. Then $f(x)$ is

- *Convex* if and only if for each $\bar{x} \in S$,

$$f(y) \geq f(\bar{x}) + \nabla f(\bar{x})^T (y - \bar{x}), \quad \text{for any } y \in S; \tag{1}$$

- *Strictly convex* if and only if for each $\bar{x} \in S$,

$$f(y) > f(\bar{x}) + \nabla f(\bar{x})^T (y - \bar{x}), \quad \text{for any } y \in S \text{ and } y \neq \bar{x}; \tag{2}$$

- *Concave* if and only if for each $\bar{x} \in S$,

$$f(y) \le f(\bar{x}) + \nabla f(\bar{x})^T (y - \bar{x}), \quad \text{for any } y \in S;$$

- *Strictly concave* if and only if for each $\bar{x} \in S$,

$$f(y) < f(\bar{x}) + \nabla f(\bar{x})^T (y - \bar{x}), \quad \text{for any } y \in S \text{ and } y \neq \bar{x};$$

Here we explain the first conclusion in detail (other conclusions can be proved similarly).

First, suppose $f(x)$ is convex. Then for any $y \in S$ and any $\lambda \in (0, 1]$,

$$f(\bar{x} + \lambda(y - \bar{x})) = f(\lambda y + (1 - \lambda)\bar{x}) \le \lambda f(y) + (1 - \lambda)f(\bar{x}),$$

hence

$$\frac{f(\bar{x} + \lambda(y - \bar{x})) - f(\bar{x})}{\lambda} \le f(y) - f(\bar{x}).$$

Using Taylor's formula on the left hand side, we have

$$\nabla f(\bar{x} + \xi(y - \bar{x}))^T (y - \bar{x}) \le f(y) - f(\bar{x}),$$

where ξ is a number between 0 and λ: $0 \le \xi \le \lambda$. Let $\lambda \to 0^+$ (hence $\xi \to 0^+$) and take limit, we obtain

$$\nabla f(\bar{x})^T (y - \bar{x}) \le f(y) - f(\bar{x}),$$

i.e.,the inequality (1) is true.

Conversely, suppose (1) holds for every pair of points $(\bar{x}, y)$ in S. Now for any $u, v \in S$ and any $\lambda \in (0,1)$, let $w = \lambda u + (1-\lambda)v$. For the two pairs (w, u) and (w, v), by the condition (1),

$$f(u) - f(w) \geq \nabla f(w)^T(u - w),$$
$$f(v) - f(w) \geq \nabla f(w)^T(v - w).$$

Multiplying the first inequality by λ, multiplying the second one by $1-\lambda$, and then adding them, we obtain:

$$\lambda f(u) + (1-\lambda) f(v) - f(w) \geq \nabla f(w)^T[\lambda(u-w) + (1-\lambda)(v-w)] = 0,$$

which means that

$$f(w) = f(\lambda u + (1-\lambda)v) \leq \lambda f(u) + (1-\lambda) f(v).$$

Hence by definition f is a convex function.

The geometric meaning of these conclusions is similar to the single variable case. That is, in the two-dimensional case, $f(x)$ is a convex function if and only if every tangent plane to $f(x)$ lies on or below the surface of $f(x)$; and $f(x)$ is a strictly convex function if and only if every tangent plane to $f(x)$ lies below the surface of $f(x)$ and contact the surface only at the point of tangency.

Example 3 Let

$$f(x) = f(x_1, x_2) = x_1^2 + 2x_2^2.$$

Then

$$\nabla f(x) = (2x_1, 4x_2)^T.$$

Let $\bar{x} = (\bar{x}_1, \bar{x}_2)$, then for any $x = (x_1, x_2) \neq (\bar{x}_1, \bar{x}_2)$,

$$\begin{aligned} & f(x) - f(\bar{x}) - \nabla f(\bar{x})^T(x - \bar{x}) \\ = \;& x_1^2 + 2x_2^2 - \bar{x}_1^2 - 2\bar{x}_2^2 - (2\bar{x}_1, 4\bar{x}_2)^T(x_1 - \bar{x}_1, x_2 - \bar{x}_2) \\ = \;& x_1^2 + 2x_2^2 - \bar{x}_1^2 - 2\bar{x}_2^2 - 2\bar{x}_1(x_1 - \bar{x}_1) - 4\bar{x}_2(x_2 - \bar{x}_2) \\ = \;& [x_1^2 + \bar{x}_1^2 - 2x_1\bar{x}_1] + 2[x_2^2 + \bar{x}_2^2 - 2x_2\bar{x}_2] \\ = \;& (x_1 - \bar{x}_1)^2 + 2(x_2 - \bar{x}_2)^2 > 0 \end{aligned}$$

So, the inequality (2) holds, and hence $f(x)$ is a strictly convex function over $\mathcal{R}^2$.

Convexity Test for a Function of Multi-Variable by Its Second Order Derivatives

Consider a multi-variable function $f(x)$ that is defined in an convex set $S \subseteq \Re^n$ and possesses all continuous second order partial derivatives at each point x in S. Then $f(x)$ is

- *Convex* if and only if $\nabla^2 f(x)$ is positive semi-definite at all points of S;
- *Strictly convex* if $\nabla^2 f(x)$ is positive definite at all points of S.
- *Concave* if and only if $\nabla^2 f(x)$ is negative semi-definite at all points of S;
- *Strictly concave* if $\nabla^2 f(x)$ is negative definite at all points of S

In fact for Example 3, $\nabla^2 f(x) = \begin{bmatrix} 2 & 0 \\ 0 & 4 \end{bmatrix}$, which is positive definite everywhere. Hence this function is strictly convex. What are the Hessian matrices of the functions in Examples 1 and 2?

Definition

An $n \times n$ real symmetric matrix A is called positive semi-definite if

$$v^T A v \geq 0, \quad \text{for all non-zero vectors } v \in \Re^n.$$

A is *positive definite* if $\geq$ can be replaced by $>$.

We now can see that for a function f having continuous second order partial derivatives, **f is convex in a convex set S if and only if $\nabla^2 f(x)$ is positive semi-definite on S.**

First suppose $\nabla^2 f$ is positive semi-definite on S. Then at each $\bar{x} \in S$ and for any $y \in S$,

$$\begin{aligned} f(y) &= f(\bar{x}) + \nabla f(\bar{x})^T (y - \bar{x}) + \frac{1}{2}(y - \bar{x})^T \nabla^2 f(\xi)(y - \bar{x}) \\ &\geq f(\bar{x}) + \nabla f(\bar{x})^T (y - \bar{x}). \end{aligned}$$

Hence f is convex over the set S. In the above, ξ is a point between $\bar{x}$ and y. Hence $\xi \in S$, and $\nabla^2 f(\xi)$ is positive semi-definite.

Conversely, assume f is convex over S. We will see that $\nabla^2 f(x)$ must be positive semi-definite on S.

In fact if it is not true, then $\nabla^2 f$ is not positive semi-definite at some point $\bar{x}$ in S, which means that there exists a vector $z \neq 0$ such that

$$z^T \nabla^2 f(\bar{x}) z < 0.$$

As $\nabla^2 f$ is continuous, it means that for all ξ near $\bar{x}$, $z^T \nabla^2 f(\xi) z < 0$. Now consider $f(\bar{x} + \lambda z)$ for very small positive λ,

$$\begin{aligned} f(\bar{x} + \lambda z) &= f(\bar{x}) + \lambda \nabla f(\bar{x})^T z + \frac{1}{2}\lambda^2 z^T \nabla^2 f(\xi) z \\ &< f(\bar{x}) + \lambda \nabla f(\bar{x})^T z, \end{aligned}$$

where ξ is between $\bar{x}$ and $\bar{x} + \lambda z$, and hence near $\bar{x}$. The above inequality is against the convexity of f. Therefore, $\nabla^2 f(x)$ must be p.s.d. over S.

Eigenvalue Test

A real symmetric matrix A is positive semi-definite if and only if all its eigenvalues are non-negative, i.e., all the solutions, λ, to the equation $|A - \lambda I| = 0$ are real and non-negative.

Similarly, A is positive definite if and only if all its eigenvalues are positive.

Principle Minor Test

A real symmetric matrix A is positive semi-definite if and only if all its principal minors are non-negative, i.e.

$$a_{11} \geq 0, \quad \begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} \geq 0, \quad \cdots, \quad \begin{vmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & & \vdots \\ a_{n1} & \cdots & a_{nn} \end{vmatrix} \geq 0.$$

Similarly, A is positive definite if and only if all its principal minors are positive.

2.5.2 Negative Definite Matrices

Definition

An $n \times n$ real symmetric matrix A is called *negative semi-definite* if

$$v^T A v \leq 0, \quad \text{for all non-zero vectors } v \in \Re^n.$$

A is *negative definite* if $\leq$ can be replaced by $<$.

Eigenvalue Test

A real symmetric matrix A is negative semi-definite if and only if all its eigenvalues are non-positive.

Similarly, A is negative definite if and only if all its eigenvalues are negative.

Principle Minor Test

A real symmetric matrix A is negative definite if and only if its principal minors alternate in sign starting with a minus sign:

$$a_{1,1} < 0, \quad \begin{vmatrix} a_{1,1} & a_{1,2} \\ a_{2,1} & a_{2,2} \end{vmatrix} > 0, \quad \cdots$$

$$\begin{vmatrix} a_{1,1} & \cdots & a_{1,2k-1} \\ \vdots & & \vdots \\ a_{2k-1,1} & \cdots & a_{2k-1,2k-1} \end{vmatrix} < 0, \quad \begin{vmatrix} a_{1,1} & \cdots & a_{1,2k} \\ \vdots & & \vdots \\ a_{2k,1} & \cdots & a_{2k,2k} \end{vmatrix} > 0, \quad \cdots.$$

2.5.3 Indefinite Matrices

An $n \times n$ real symmetric matrix A is said to be *indefinite* if the matrix A is neither positive semi-definite nor negative semi-definite.

2.6 Some Properties of Convex Function

- If $f(x)$ and $g(x)$ are two convex functions defined on a convex set $S \subseteq \Re^n$, then $f(x) + g(x)$ is also a convex function in S; Moreover, if at least one of $f(x)$ and $g(x)$ is strictly convex, then $f(x) + g(x)$ is a strictly convex function;
- If $f(x)$ is a convex function over a convex set S, then $\alpha f(x)$ is a convex function if $\alpha > 0$ and a concave function if $\alpha < 0$;
- If $f(x)$ is a convex function defined on a convex set $S \subseteq \Re^n$ and $g(u)$ is a single variable function which is convex and increasing on $\Re$, then $h(x) \equiv g(f(x))$ is convex on S.

We now explain the last property. For any $y, z \in S$, as f is convex, for any $\lambda \in [0,1]$,

$$f(\lambda y + (1-\lambda)z) \leq \lambda f(y) + (1-\lambda)f(z).$$

Since g is increasing,

$$\begin{aligned} g(f(\lambda y + (1-\lambda)z)) &\leq g(\lambda f(y) + (1-\lambda)f(z)) \\ &\leq \lambda g(f(y)) + (1-\lambda)g(f(z)), \end{aligned}$$

i.e.,

$$h(\lambda y + (1-\lambda)z) \leq \lambda h(y) + (1-\lambda)h(z).$$

So, $h(x)$ is a convex function.

We may consider the condition to further strengthen the last property to a strictly convex function, that is, under what conditions, $h(x) \equiv g(f(x))$ is strictly convex?

Example Show that

$$h(x_1, x_2, x_3) = e^{x_1^2 + x_2^2 + x_3^2}$$

is a convex function in $\Re^3$.

Let $f(x) = x_1^2 + x_2^2 + x_3^2$ and $g(u) = e^u$ for $x \in \Re^3$ and $u \in \Re$. As

$$\nabla^2 f(x) = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{bmatrix}$$

which is positive definite, $f(x)$ is strictly convex. On the other hand, as

$$g''(u) = e^u > 0 \text{ for every } u,$$

$g(u)$ is also strictly convex. Also, g is an increasing function. Therefore, $h(x)$ is a convex function. In fact it is strictly convex.

Example Show that

$$f(x_1, x_2) = x_1^2 - 4x_1x_2 + 5x_2^2 - \ln x_1x_2$$

is a strictly convex function on $S = \{x \in \Re^2 \mid x_1 > 0, x_2 > 0\}$. Let

$$g(x_1, x_2) = x_1^2 - 4x_1x_2 + 5x_2^2$$

and

$$h(x_1, x_2) = -\ln x_1x_2 = -\ln x_1 - \ln x_2.$$

Hence

$$f(x_1, x_2) = g(x_1, x_2) + h(x_1, x_2).$$

We now consider convexity of g and h respectively.

As

$$\nabla^2 g(x) = \begin{bmatrix} 2 & -4 \\ -4 & 10 \end{bmatrix}$$

is positive definite, $g(x)$ is strictly convex. Let

$$\phi(t) = -\ln t, \quad t > 0.$$

As $\phi''(t) = \frac{1}{t^2} > 0$, $\phi(t)$ is a strictly convex function for all $t > 0$. So, $h(x) = \phi(x_1) + \phi(x_2)$ is strictly convex on S.

Therefore, f is a strictly convex function.

General Optimization Problems

$$\begin{array}{ll} \min & f(x) \\ \text{s.t.} & x \in S \subset \Re^n. \end{array}$$

Weierstrass Theorem

A continuous function $f(x)$ defined on a **compact set** S has a minimum point in S.

Local Minimizers

A point $x^* \in S$ is said to be a local minimizer (or local minimum point) of f over S if there is an $\varepsilon > 0$ such that $f(x) \geq f(x^*)$ for all $x \in S \cap N_\varepsilon(x^*)$, where $N_\varepsilon(x^*)$ is the ε-neighborhood of x^*.

If $f(x) > f(x^*)$ for all $x \in S \cap N_\varepsilon(x^*)$ and $x \neq x^*$, then x^* is said to be a strict local minimizer of f over S.

Global Minimizers

A point $x^* \in S$ is said to be a global minimizer (or global minimum point) of f over S if $f(x) \geq f(x^*)$ for all $x \in S$.

If $f(x) > f(x^*)$ for all $x \in S$ and $x \neq x^*$, then x^* is said to be a strict global minimizer of f over S.

Remarks

- It is preferred to find a global minimizer when formulating an optimization problem.
- In most situations, however, optimization theory and methodologies only enable us to locate local minimum points or stationary points.

Recall that a point x^* is called a **stationary point** of f if $\nabla f(x^*) = 0$.

Minimum Point for Convex Functions

For a convex function $f(x)$ defined on a convex set S, its minimum points have the following nice properties.

- Every stationary point is a global minimizer.
  Let $\bar{x}$ be a stationary point of f, i.e., $\nabla f(\bar{x}) = 0$. Then for every $y \in S$,

$$f(y) \geq f(\bar{x}) + \nabla f(\bar{x})^T (y - \bar{x}) = f(\bar{x}).$$

  Hence $\bar{x}$ is the global minimizer of f over the convex set S.
- Every local minimizer of f is also a global minimizer of f over the convex set S.

Suppose x^* is a local minimizer of f. Then there is a small $r > 0$ such that for every $x \in S$ satisfying $\|x - x^*\| < r$, $f(x^*) \leq f(x)$. We now consider an arbitrary $y \in S$. As S is a convex set, the line segment $\{x^* + \lambda(y - x^*) \mid 0 \leq \lambda \leq 1\}$ joining x^* and y is in S. We choose a sufficiently small positive $\bar{\lambda} < 1$ such that $\|\bar{\lambda}(y - x^*)\| < r$. Thus,

$$\begin{aligned} f(x^*) &\leq f(x^* + \bar{\lambda}(y - x^*)) \\ &= f(\bar{\lambda}y + (1 - \bar{\lambda})x^*) \\ &\leq \bar{\lambda}f(y) + (1 - \bar{\lambda})f(x^*). \end{aligned}$$

It follows that

$$\bar{\lambda}f(x^*) \leq \bar{\lambda}f(y),$$

i.e., $f(x^*) \leq f(y)$. As y can be any point in S, x^* is a global minimizer of f over the convex set S.

- If a strictly convex function $f(x)$ over a convex set S has a global minimizer, then it must be the unique global minimizer (i.e., there is no other global minimizer).
  Suppose x^* is a global minimizer on S, then for any $y \in S$, $y \neq x^*$, as f is strictly convex, we can obtain from the above reasoning that

$$f(x^*) \leq f(\bar{\lambda}y + (1-\bar{\lambda})x^*) < \bar{\lambda}f(y) + (1-\bar{\lambda})f(x^*)$$

  for any $\bar{\lambda}$ such that $0 < \bar{\lambda} < 1$. Therefore,

$$f(x^*) < f(y), \text{ for every } y \in S, y \neq x^*,$$

  which means that x^* is the unique global minimizer over S.

For most optimization problems, we fail to obtain an explicit analytic solution, and must use numerical method to get it by a sequence of computation. Such methods are often called iterative methods.

A General Scheme of an Iterative Solution Procedure

Step 1. Start from a feasible solution $x \in S$.

Step 2. Check if the stopping criteria (such as the optimality conditions) are met.
If the answer is YES, stop.
If the answer is NO, continue.

Step 3. Move to a better feasible solution and return to Step 2.

Feasible Directions

Along any given direction, the objective function can be regarded as a function of a single variable.

Given $x \in S$, a vector $d \in \Re^n$ is a *feasible direction* at x if there is an $\bar{\alpha} > 0$ such that $x + \alpha d \in S$ for all α such that $0 \leq \alpha \leq \bar{\alpha}$.

2.8 Appendix 1 - Gradients and Hessians for Linear and Quadratic Functions

2.8.1 Linear Function

Let

$$f(x) = a^T x = (a_1, a_2, \ldots, a_n) \begin{bmatrix} x_1 \\ x_2 \\ \cdot \\ \cdot \\ x_n \end{bmatrix}.$$

Then,

$$\frac{\partial f}{\partial x_1} = a_1, \quad \frac{\partial f}{\partial x_2} = a_2, \ \ldots, \ \frac{\partial f}{\partial x_n} = a_n.$$

So,

$$\nabla f(x) = a, \text{ and } \nabla^2 f(x) = 0.$$

Let

$$h(x) = \frac{1}{2} x^T A x,$$

where A is an $n \times n$ symmetric matrix. Then

$$h(x) = \frac{1}{2} \sum_{i,j=1}^{n} a_{ij} x_i x_j,$$

and the following terms of $h(x)$ contain x_1:

$$\frac{1}{2}(a_{11} x_1^2 + \sum_{j \neq 1} a_{1j} x_1 x_j + \sum_{i \neq 1} a_{i1} x_i x_1).$$

Hence,

$$
\begin{aligned}
\frac{\partial h}{\partial x_1} &= \frac{1}{2}\left(2a_{11}x_1 + \sum_{j\neq 1} a_{1j}x_j + \sum_{i\neq 1} a_{i1}x_i\right) \\
&= a_{11}x_1 + \sum_{j\neq 1} a_{1j}x_j \text{ (note that } a_{i1} = a_{1i}\text{)} \\
&= \sum_{j=1}^{n} a_{1j}x_j .
\end{aligned}
$$

Similarly,

$$
\frac{\partial h}{\partial x_2} = \sum_{j=1}^{n} a_{2j}x_j, \quad \cdots \quad , \frac{\partial h}{\partial x_n} = \sum_{j=1}^{n} a_{nj}x_j .
$$

Therefore,

$$
\nabla h(x) = Ax.
$$

For $i, j = 1, \ldots, n$, from

$$\frac{\partial h}{\partial x_i} = \sum_{k=1}^{n} a_{ik} x_k$$

we know that

$$\frac{\partial^2 h}{\partial x_i \partial x_j} = a_{ij}.$$

Hence,

$$\nabla^2 h(x) = A.$$

Let us return to **Example 2**:

$$f(x) = (a^T x)^2, \quad a, x \in \Re^n.$$

What are $\nabla f(x)$ and $\nabla^2 f(x)$?

In fact

$$f(x) = (a^T x)^2 = a^T x a^T x = x^T a a^T x = \frac{1}{2} x^T A x,$$

where $A = 2aa^T$. So,

$$\nabla f(x) = Ax = 2aa^T x = 2(a^T x)a,$$

and

$$\nabla^2 f(x) = A = 2aa^T.$$

2.9 Appendix 2 - Gradients and Hessians for Product and Composite Functions

2.9.1 Product Function

Let

$$f(x) = g(x)h(x),$$

where $x = (x_1, x_2, \ldots, x_n)$, and suppose that $g(x)$ and $h(x)$ are both continuously differentiable. We need to calculate $\nabla f(x)$ and $\nabla^2 f(x)$. We know that

$$\frac{\partial f}{\partial x_1} = \frac{\partial g}{\partial x_1} h(x) + \frac{\partial h}{\partial x_1} g(x)$$
$$\cdots\cdots\cdots$$
$$\frac{\partial f}{\partial x_n} = \frac{\partial g}{\partial x_n} h(x) + \frac{\partial h}{\partial x_n} g(x).$$

Hence

$$\nabla f(x) = h(x)\nabla g(x) + g(x)\nabla h(x).$$

2.9.1 Product Function

For $\nabla^2 f$, it can be verified that

$$\nabla^2 f(x) = h(x)\nabla^2 g(x) + g(x)\nabla^2 h(x) + \nabla g(x)\nabla h(x)^T + \nabla h(x)\nabla g(x)^T.$$

Note that

$$\nabla g(x)\nabla h(x)^T = \begin{bmatrix} \frac{\partial g}{\partial x_1} \\ \cdot \\ \cdot \\ \cdot \\ \frac{\partial g}{\partial x_n} \end{bmatrix} \begin{bmatrix} \frac{\partial h}{\partial x_1} & \cdot & \cdot & \cdot & \frac{\partial h}{\partial x_n} \end{bmatrix}$$

is an $n \times n$ matrix, and so is $\nabla h(x)\nabla g(x)^T$.

2.9.1 Product Function

Example Consider the function

$$f(x) = (a^T x)(b^T x),$$

where $a, b, x \in R^n$.

We can let $g(x) = a^T x$, $h(x) = b^T x$, and use the above general formula:

$$\begin{aligned} \nabla f(x) &= h(x)\nabla g(x) + g(x)\nabla h(x) \\ &= (b^T x)a + (a^T x)b. \end{aligned}$$

Since $\nabla^2 g(x) = \nabla^2 h(x) = 0$ (zero matrix),

$$\begin{aligned} \nabla^2 f(x) &= \nabla g(x)\nabla h(x)^T + \nabla h(x)\nabla g(x)^T \\ &= ab^T + ba^T. \end{aligned}$$

2.9.2 Composite Function - Chain Rule

Suppose

$$y = g(x) = g(x_1, x_2, \ldots, x_n)$$

and

$$x_i = x_i(t_1, t_2, \ldots, t_m), \quad i = 1, \ldots, n$$

where g is a continuously differential function of $x \in R^n$, and each x_i is a continuously differentiable function of $t = (t_1, \ldots, t_m)$. By the chain rule, we know that

$$\begin{aligned}
\frac{\partial y}{\partial t_1} &= \frac{\partial g}{\partial x_1}\frac{\partial x_1}{\partial t_1} + \cdots + \frac{\partial g}{\partial x_n}\frac{\partial x_n}{\partial t_1} \\
&\vdots \\
\frac{\partial y}{\partial t_m} &= \frac{\partial g}{\partial x_1}\frac{\partial x_1}{\partial t_m} + \cdots + \frac{\partial g}{\partial x_n}\frac{\partial x_n}{\partial t_m}.
\end{aligned}$$

So,

$$\begin{bmatrix} \frac{\partial y}{\partial t_1} \\ \cdot \\ \cdot \\ \cdot \\ \frac{\partial y}{\partial t_m} \end{bmatrix} = \begin{bmatrix} \frac{\partial x_1}{\partial t_1} & \cdots & \frac{\partial x_n}{\partial t_1} \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \frac{\partial x_1}{\partial t_m} & \cdots & \frac{\partial x_n}{\partial t_m} \end{bmatrix} \begin{bmatrix} \frac{\partial g}{\partial x_1} \\ \cdot \\ \cdot \\ \cdot \\ \frac{\partial g}{\partial x_n} \end{bmatrix},$$

i.e.,

$$\nabla y(t) = \nabla x(t) \nabla g(x),$$

where the matrix

$$\nabla x(t) = [\nabla x_1(t), \cdots, \nabla x_n(t)].$$

Example Let

$$\begin{aligned} y &= x_1^2 - x_1 x_2, \\ x_1 &= t_1 + 2t_2, \\ x_2 &= t_1^2 + t_2. \end{aligned}$$

Then, by the chain rule,

$$\begin{aligned} \nabla y(t) &= \nabla x(t) \nabla y(x) \\ &= \begin{bmatrix} 1 & 2t_1 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} 2x_1 - x_2 \\ -x_1 \end{bmatrix} \\ &= \begin{bmatrix} 1 & 2t_1 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} 2(t_1 + 2t_2) - (t_1^2 + t_2) \\ -(t_1 + 2t_2) \end{bmatrix}. \end{aligned}$$