Optimization Basic concepts

Instructor: Jin Zhang

Department of Mathematics
Southern University of Science and Technology
Spring 2023

Goals of this lecture

The general form of optimization:

$$\begin{aligned} \min \quad & f(x), \\ \text{subject to} \quad & x \in \Omega. \end{aligned}$$

We study the following topics:

- terminology
- types of minimizers
- optimality conditions 必要条件 & etc.

Unconstrained vs constrained optimization

$$\begin{aligned} \min \quad & f(x), \\ \text{subject to} \quad & x \in \Omega. \end{aligned}$$

Suppose $x \in \mathbb{R}^n$, Ω is called the feasible set.

- if $\Omega = \mathbb{R}^n$, then the problem is called unconstrained.
- otherwise, the problem is called constrained.

In general, more sophisticated techniques are needed to solve constrained problems.

(off the topic)

Later, we will study some nonsmooth analysis and algorithms that allow f to have the extended value, ∞. Then, we can write any constrained problem in the unconstrained form

$$\min f(x) + \iota_\Omega(x),$$

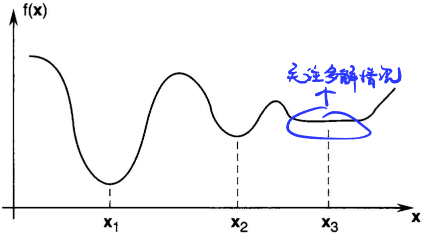
where the *indicator function* 示性函数. 利用函数的分段 s.t. Local $\Rightarrow$ Global

$$\iota_\Omega(x) = \begin{cases} 0, & x \in \Omega, \\ \infty, & x \notin \Omega. \end{cases}$$

The objective function $f(x) + \iota_\Omega(x)$ is nonsmooth.

Types of solutions

- x^* is a local minimizer if there is $\epsilon > 0$ such that $f(x) \geq f(x^*)$ for all $x \in \Omega \setminus \{x^*\}$ and $\|x - x^*\| < \epsilon$.
- x^* is a global minimizer if $f(x) \geq f(x^*)$ for all $x \in \Omega \setminus \{x^*\}$
- If "$\geq$" is replaced with "$>$", then they are strict local minimizer and strict global minimizer, respectively.



$Ax = b$

若高斯消元: $O(n^3)$

$Ax - b = 0$

$\Leftrightarrow \min \left(\frac{1}{2} x^T A x - b^T x\right)$

Figure: x_1: strict global minimizer; x_2: strict local minimizer; x_3: local minimizer

例. 单点是凸的.

- A set Ω is convex if $\lambda x+(1-\lambda)y \in \Omega$ for any $x,\ y \in \Omega$ and $\lambda \in [0,1]$.

- A function is convex if $\Leftrightarrow$ $epi(f) = \{(x,t) \mid f(x) \le t\}$ is convex set.

凸 convex.

f convex $\Rightarrow f(y) \ge f(x) + \nabla f(x)(y-x)$ for $\forall x, y$

? 相减. 求导

$$f(\lambda x+(1-\lambda)y) \le \lambda f(x) + (1-\lambda)f(y)$$

(用二分法???) 见下面

for a~~ny $x,\ y \in$~~ Ω and $\lambda \in [0,1]$.

A function is convex if and only if its epigraph is convex.

$F(y) = f(y) - f(x) + \nabla f(x)(y-x)$

- An optimization problem is convex if both the objective function and feasible set are convex. (and the constraint condition is convex)

$F'(y) = \nabla f(y) - \nabla f(x) = 0$

- **Theorem:** Any local minimizer of a convex optimization problem is a global minimizer.

$\Leftrightarrow \nabla f(y) = \nabla f(x) \Leftrightarrow y = x$

$F(y) \ge F(x) = 0.$ $\square$

Derivatives

- First-order derivative: row vector

$$Df \triangleq \left[\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \cdots, \frac{\partial f}{\partial x_n}\right].$$

- **Gradient** of $\nabla f = (Df)^T$, which is a column vector.

- A gradient represents the slope of the tangent of the graph of function. It gives the linear approximation of f at a point. It points toward the greatest rate of increase.

minimize $\Leftrightarrow$ 负梯度方向

(减少最快方向)

理论 + 实践. "step" $\leftarrow$ locally.

- **Hessian** (i.e., second-derivative) of f:

$$F(x) \triangleq D^2 f(x) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2}(x) & \cdots & \frac{\partial^2 f}{\partial x_n \partial x_1}(x) \\ \vdots & & \vdots \\ \frac{\partial^2 f}{\partial x_1 \partial x_n}(x) & \cdots & \frac{\partial^2 f}{\partial x_n^2}(x) \end{bmatrix}$$

  which is a symmetric matrix.

- For one-dimensional function $f(x)$ where $x \in \mathbb{R}$, it reduces to $f''(x)$.
- $F(x)$ is the Jacobian of $\nabla f(x)$, that is, $F(x) = J(\nabla f(x))$.
- Alternative notation: $H(x)$ and $\nabla^2 f(x)$ are also used for Hessian.

  二次逼近.

- A Hessian gives a quadratic approximation of f at a point.
- Gradient and Hessian are local properties that help us recognize local solutions and determine a direction to move at toward the next point.

convex

differentiable $f: \mathbb{R}^n \to \mathbb{R}$

$$f\left(\frac{x+y}{2}\right) \le \frac{1}{2} f(x) + \frac{1}{2} f(y).$$

$h = y - x$

$$f(y) \ge f(x) + \nabla f(x)^T (y-x) \quad \forall\, x, y$$

$$f\left(x + \frac{h}{2}\right) \le \frac{1}{2} f(x) + \frac{1}{2} f(x+h) - f(x)$$

$- f(x)$

$$f(x+h) - f(x) \ge \frac{f(x+\frac{h}{2}) - f(x)}{1/2}$$

$\forall\, k \in \mathbb{Z}^+$.

$$\ge \frac{f(x+\frac{h}{4}) - f(x)}{1/4} \ge \cdots \ge \frac{f(x+\frac{h}{2^k}) - f(x)}{1/2^k}$$

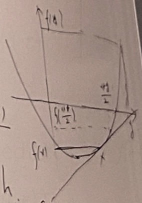
$$\frac{f(x+th) - f(x)}{t}$$

$$f(x+h) - f(x) \ge f'(x; h) = \nabla f(x)^T h$$

$$f(x + t(y-x)) \le (1-t) f(x) + t f(y)$$

$0 < t < 1$

$$f(y) \ge f(x) + \frac{f(x+t(y-x)) - f(x)}{t} \qquad t \to 0^+$$



Example

Consider

$$f(x_1, x_2) = x_1^3 + x_1^2 - x_1 x_2 + x_2^2 + 5x_1 + 8x_2 + 4$$

Then,

$$\nabla f(x) = \begin{bmatrix} 3x_1^2 + 2x_1 - x_2 + 5 \\ -x_1 + 2x_2 + 8 \end{bmatrix} \in \mathbb{R}^2$$

and

$$F(x) = \begin{bmatrix} 6x_1 + 2 & -1 \\ -1 & 2 \end{bmatrix} \in \mathbb{R}^{2\times 2}$$

Observation: if f is a quadratic function (remove x_1^3 in the above example), $\nabla f(x)$ is a linear vector and $F(x)$ is a symmetric constant matrix for any x.

Taylor expansion

Suppose $\phi \in \mathcal{C}^m$ (m times continuously differentiable). The Taylor expansion of ϕ at a point a is

$$\phi(a+h) = \phi(a) + \phi'(a)h + \frac{\phi''(a)}{2!}h^2 + \cdots + \frac{\phi^m(a)}{m!}h^m + o(h^m).$$

There are other ways to write the last two terms.

Example: Consider $x, d \in \mathbb{R}^n$ and $f \in \mathcal{C}^2$. Define $\phi(\alpha) = f(\underbrace{x}_{\text{当前点}} + \underbrace{\alpha}_{\text{step size}} \overset{\text{direction}}{\underline{d}})$. Then,

$$\begin{aligned}
\phi'(\alpha) &= \nabla f(x+\alpha d)^T d \\
\phi''(\alpha) &= dF(x+\alpha d)^T d
\end{aligned}$$

Hence,

$$\begin{aligned}
f(x+\alpha d) &= f(x) + (\nabla f(x)^T d)\alpha + o(\alpha) \\
&= f(x) + (\nabla f(x)^T d)\alpha + \frac{dF(x)^T d}{2}\alpha^2 + o(\alpha^2).
\end{aligned}$$

Feasible direction

- A vector $d \in \mathbb{R}^n$ is a feasible direction at $x \in \Omega$ if $d \neq 0$ and $x + \alpha d \in \Omega$ for some small $\alpha > 0$. (It is possible that d is an infeasible step, that is, $x + d \notin \Omega$. But if there is some room in Ω to move from x toward d, then d is a feasible direction.)

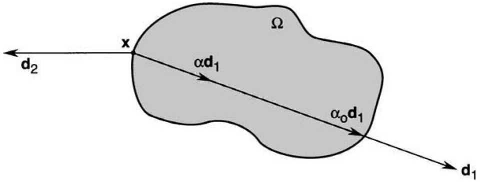


Figure: d_1 is feasible, d_2 is infeasible

- If $\Omega = \mathbb{R}^n$ or x lies in the interior of Ω, then any $d \in \mathbb{R}^n \setminus \{0\}$ is a feasible direction
- Feasible directions are introduced to establish optimality conditions, especially for points on the boundary of a constrained problem

First-order necessary condition

Let $\mathcal{C}^1$ be the set of continuously differentiable functions.

Theorem

First-Order Necessary Condition (FONC). *Let Ω be a subset of $\mathbb{R}^n$ and $f \in \mathcal{C}^1$ a real-value function on Ω. If x^* is a local minimizer of f over Ω, then for any feasible direction d at x^*, we have*

$$d^T \nabla f(x^*) \geq 0.$$

Proof: Let d by any feasible direction. First-order Taylor expansion:

$$f(x^* + \alpha d) = f(x^*) + \alpha d^T \nabla f(x^*) + o(\alpha).$$

If $d^T \nabla f(x^*) < 0$, which does not depend on α, then $f(x^* + \alpha d) < f(x^*)$ for all sufficiently small $\alpha > 0$ (that is, all $\alpha \in (0, \bar{\alpha})$ for some $\bar{\alpha} > 0$). This is a contradiction since x^* is a local minimizer. ∎

Corollary

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

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

Proof: Since any $d \in \mathbb{R}^n \setminus \{0\}$ is a feasible direction, we can set $d = -\nabla f(x^*)$. We have $d^T \nabla f(x^*) = -\|\nabla f(x^*)\|2 \geq 0$. Since $\|\nabla f(x^*)\|^2 \geq 0$, we have $\|\nabla f(x^*)\|^2 = 0$ and thus $\nabla f(x^*) = 0$. ■

Comment: This condition also reduces the problem

$$\min \ f(x)$$

to solving the equation

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

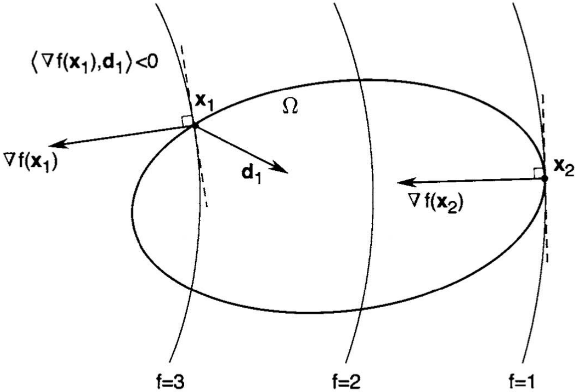


Figure: x_1 fails to satisfy the FONC; x_2 satisfies the FONC

Second-order necessary condition

In FONC, there are two possibilities

- $d^T \nabla f(x^*) > 0$;
- $d^T \nabla f(x^*) = 0$.

In the first case, $f(x^* + \alpha d) > f(x^*)$ for all sufficiently small $\alpha > 0$.
In the second case, the vanishing $d^T \nabla f(x^*)$ allows us to check higher-order derivatives.

Let $\mathcal{C}^2$ be the set of twice continuously differentiable functions.

Theorem

Second-Order Necessary Condition (SONC). *Let $\Omega \subset \mathbb{R}^n$, $f \in \mathcal{C}^2$ 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*

$$d^T F(x^*) d \geq 0,$$

where F is the Hessian of f.

Proof: Assume that $\exists$ a feasible direction d with $d^T \nabla f(x^*) = 0$ and $d^T F(x^*) d < 0$. By 2nd-order Taylor expansion (with a vanishing 1st order term), we have

$$f(x^* + \alpha d) = f(x^*) + \frac{d^T F(x^*) d}{2} \alpha^2 + o(\alpha^2),$$

where by our assumption $d^T F(x^*) d < 0$. Hence, for all sufficiently small $\alpha > 0$, we have $f(x^* + \alpha d) < f(x^*)$, which contradicts that x^* is a local minimizer. ■

Corollary

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

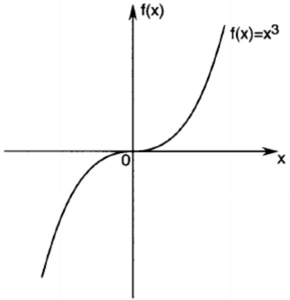
$$\nabla f(x^*) d = 0,$$

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

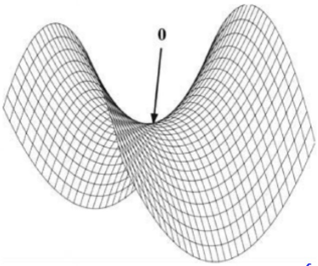
$$d^T F(x^*) d \geq 0.$$

The necessary conditions are not sufficient

Counter examples



$f(x) = x^3$, $f'(x) = 3x^2$, $f''(x) = 6x$



不定

$H = \begin{pmatrix} 2 & 0 \\ 0 & -2 \end{pmatrix}$

$f(x) = x_1^2 - x_2^2$

$\mathbf{0}$ is a saddle point: $\nabla f(\mathbf{0}) = \mathbf{0}$ but neither a local minimizer nor maximizer

By SONC, $\mathbf{0}$ is not a local minimizer!

Second-order sufficient condition

Let $\mathcal{C}^2$ be the set of twice continuously differentiable functions.

Theorem

Second-Order Sufficient Condition (SOSC), Interior point. *Let $f \in \mathcal{C}^2$ be defined on a region in which x^* is an interior point. Suppose that*

1. $\nabla f(x^*) = 0$;
2. $F(x^*) > 0$.

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

Comments:

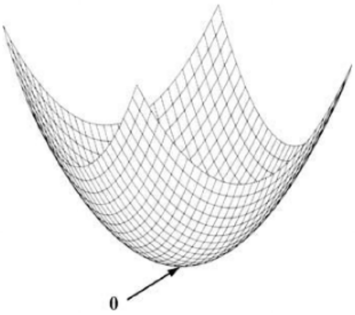
- part 2 states $F(x^*)$ is positive definite: $x^T F(x^*) x > 0$ for $x \neq 0$.
- the condition is not necessary for strict local minimizer.

Proof: For any $d \neq 0$ and $\|d\| = 1$, we have $d^T F(x^*) d \geq \lambda_{\min}(F(x^*)) > 0$. Use the 2nd order Taylor expansion

特征值.

$$f(x^* + \alpha d) = f(x^*) + \frac{\alpha^2}{2} d^T F(x^*) d + o(\alpha^2) \geq f(x^*) + \frac{\alpha^2}{2} \lambda_{\min}(F(x^*)) + o(\alpha^2).$$

Then, $\exists \bar{\alpha} > 0$, regardless of d, such that $f(x^* + \alpha d) > f(x^*)$, $\alpha \in (0, \bar{\alpha})$. ■



Graph of $f(x) = x_1^2 + x_2^2$

The point 0 satisfies the SOSC.

Roles of optimality conditions

- **Recognize a solution:** given a candidate solution, check optimality conditions to verify it is a solution.
- **Measure the quality** of an approximate solution: measure how ¡°close¡± a point is to being a solution
- **Develop algorithms:** reduce an optimization problem to solving a (nonlinear) equation (finding a root of the gradient).

Later, we will see other forms of optimality conditions and how they lead to equivalent subproblems, as well as algorithms

Quiz questions

$(1,2)\begin{pmatrix} x \\ y \end{pmatrix} = 3$ $x+2y=3$ $y=-\frac{1}{2}x+\frac{3}{2}$

$(1,-\frac{1}{2})$ 线的方向.

1. Show that for $\Omega = \{x \in \mathbb{R}^n : Ax = b\}$, $d \neq 0$ is a feasible direction at $x \in \Omega$ if and only if $Ad = 0$. $Ax_1 = b$ $Ax_2 = b \Leftrightarrow A(x_1 - x_2) = 0 \Leftrightarrow Ad = 0.$
2. Show that for any unconstrained quadratic program, which has the form

$\nabla f(x^*) = 0$

$d^T F(x^*) d \geq 0$

$$\min\ f(x) = \frac{1}{2}x^T Qx - b^T x.$$

if x^* satisfies the second-order necessary condition, then x^* is a global minimizer.

3. Show that for any unconstrained quadratic program with $Q \geq 0$ (Q is symmetric and positive semi-definite), x^* is a global minimizer if and only if x^* satisfies the first-order necessary condition. That is, the problem is equivalent to solving $Qx = b$.
4. Consider $\min\ c^T x$, subject to $x \in \Omega$. Suppose that $c \neq 0$ and the problem has a global minimizer. Can the minimizer lie in the interior of Ω?

Quiz (Lecture 2)

1. *Proof.*

$$\begin{aligned}
& d \text{ is a feasible direction at } \overline{x} \in \Omega \\
\Longleftrightarrow\ & \overline{x} + \alpha d \in \Omega \text{ dose hold for some small } \alpha > 0 \\
\Longleftrightarrow\ & A(\overline{x} + \alpha d) = b \text{ holds for some small } \alpha > 0 \\
\Longleftrightarrow\ & Ad = 0.(\text{since } \overline{x} \in \Omega \text{ implies} A\overline{x} = b).
\end{aligned}$$

□

2. *Proof.* Obviously, $\bigtriangledown f(x) = Qx - b$ and $\bigtriangledown^2 f(x) = Q$ hold for any $x \in R^n$.
Notice another trivial fact that the feasible set Ω of the program is R^n, hence any point $x \in R^n$ is a interior point of R^n.
Based on the above and SONC, $Qx^* - b = 0$ and $Q \succeq 0$ hold since x^* satisfies the SONC [Interior Case].
Now back to objective function, for any $x \in R^n$

$$\begin{aligned}
f(x) &= f(x^* + (x - x^*)) \\
&= \frac{1}{2}(x^* + (x - x^*))^T Q(x^* + (x - x^*)) - b^T(x^* + (x - x^*) \\
&= \frac{1}{2}x^T Qx - b^T x + (x - x^*)^T Q(x - x^*) + (x - x^*)^T(Qx^* - b) \\
&= f(x^*) + (x - x^*)^T Q(x - x^*) + (x - x^*)^T(Qx^* - b) \\
&\geq f(x^*).
\end{aligned}$$

The last inequality holds since $Qx^* - b = 0$ and $Q \succeq 0$.
Hence, x^* is a global minimizer.

□

3. *Proof.* On the one hand, if $Qx^* = b$, by $Q2$, we know x^* is a global minimizer since $Q \succeq 0$ has been mentioned in the statement of this question.
On the other hand, if x^* is a global minimizer, then x^* is a local minimizer, hence x^* satisfies the FONC by Theorem [FONC].

□

4. *Proof.* According to Theorem [FONC], "the minimizer lies in the interior of Ω" implies $c = 0$. It's a contradiction.

□