# Foundation of Computing and Mathematical Sciences <br> - Optimization 

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"In our opinion, the main fact, which should be known to any person dealing with optimization models, is that in general optimization problems are unsolvable." - Yurii Nesterov

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## Chapter 1

## Nonlinear Optimization

### 1.1 General minimization problem and terminologies

Definition 1.1.1 We define the general minimization problem as follows

$$
\begin{cases}\operatorname{minimize} & f(\boldsymbol{x})  \tag{1.1}\\ \text { subject to } & f_{j}(\boldsymbol{x}) \& 0, \quad j=1,2, \ldots, m \\ & \boldsymbol{x} \in S,\end{cases}
$$

where $f: \mathbb{R}^{n} \rightarrow \mathbb{R}, f_{j}: \mathbb{R}^{n} \rightarrow \mathbb{R}(j=1,2, \ldots, m)$, the symbol \& could be $=, \geq$, or $\leq$, and $S \subseteq \mathbb{R}^{n}$.

Definition 1.1.2 The feasible set $Q$ of (1.1) is

$$
Q=\left\{\boldsymbol{x} \in S \mid f_{j}(\boldsymbol{x}) \& 0,(j=1,2, \ldots, m)\right\}
$$

In the following items we assume $S \equiv \mathbb{R}^{n}$.

- If $Q \equiv \mathbb{R}^{n}$, (1.1) is a unconstrained optimization problem.
- If $Q \subsetneq \mathbb{R}^{n}$, (1.1) is a constrained optimization problem.
- If all functionals $f(\boldsymbol{x}), f_{j}(\boldsymbol{x})$ are differentiable, (1.1) is a smooth optimization problem.
- If one of functionals $f(\boldsymbol{x}), f_{j}(\boldsymbol{x})$ is non-differentiable, (1.1) is a non-smooth optimization problem.
- If all constraints are linear $f_{j}(\boldsymbol{x})=\sum_{i=1}^{n}[\boldsymbol{a}]_{j i}[\boldsymbol{x}]_{i}+[\boldsymbol{b}]_{j}(j=1,2, \ldots, m),(1.1)$ is a linear constrained optimization problem.
- In addition, if $f(\boldsymbol{x})$ is linear, (1.1) is a linear programming problem.
- In addition, if $f(\boldsymbol{x})$ is quadratic, (1.1) is a quadratic programming problem.
- If $f(\boldsymbol{x}), f_{j}(\boldsymbol{x})(j=1,2, \ldots, m)$ are quadratic, (1.1) is a quadratically constrained quadratic programming problem.

Definition 1.1.3 $\boldsymbol{x}^{*}$ is called a global optimal solution of (1.1) if $f\left(\boldsymbol{x}^{*}\right) \leq f(\boldsymbol{x}), \quad \forall \boldsymbol{x} \in Q$. Moreover, $f\left(\boldsymbol{x}^{*}\right)$ is called the global optimal value. $\boldsymbol{x}^{*}$ is called a local optimal solution of (1.1) if there exists an open ball $B(\varepsilon)=\left\{\boldsymbol{x} \in \mathbb{R}^{n} \mid\left\|\boldsymbol{x}-\boldsymbol{x}^{*}\right\|<\varepsilon\right\} \subseteq Q$ such that $f\left(\boldsymbol{x}^{*}\right) \leq f(\boldsymbol{x}), \quad \forall \boldsymbol{x} \in B(\varepsilon)$. Moreover, $f\left(\boldsymbol{x}^{*}\right)$ is called a local optimal value.

## General Iterative Scheme

Input: A starting point $\boldsymbol{x}_{0}$ and an accuracy $\varepsilon>0$. Initialization: Set the iteration counter $k:=0$, and the information set $I_{-1}:=\emptyset$.

Main Loop

1. Call oracle $\mathcal{O}$ at $\boldsymbol{x}_{k}$.
2. Update the information set: $I_{k}:=I_{k-1} \cup\left(\boldsymbol{x}_{k}, \mathcal{O}\left(\boldsymbol{x}_{k}\right)\right)$.
3. Apply the rules of the method $\mathcal{M}$ to $I_{k}$ and compute $\boldsymbol{x}_{k+1}$.
4. Check stopping criterion $\mathcal{T}_{\varepsilon}$. If Yes, output $\overline{\boldsymbol{x}}$. Otherwise set $k:=k+1$ and go to Step 1.

Definition 1.1.4 The analytical complexity of a method is the number of calls of an oracle which is required to solve a problem $\mathcal{P}$ up to the given accuracy $\varepsilon$.

Definition 1.1.5 The arithmetical complexity of a method is the total number of arithmetic operations (including the work of the oracle and the method) which is required to solve a problem $\mathcal{P}$ up to the given accuracy $\varepsilon$.

## Assumption 1.1.6 (Local black box)

1. The only information available for the numerical scheme is the answer of the oracle.
2. The oracle is local, that is, a small variation of the problem far enough from the test point $\boldsymbol{x}$ does not change the answer at $\boldsymbol{x}$.

## Definition 1.1.7

1. The zero-order oracle returns the value $f(\boldsymbol{x})$.
2. The first-order oracle returns the value $f(\boldsymbol{x})$, and the gradient $f^{\prime}(\boldsymbol{x})$.
3. The second-order oracle returns the value $f(\boldsymbol{x}), f^{\prime}(\boldsymbol{x})$ and the Hessian $f^{\prime \prime}(\boldsymbol{x})$.

### 1.2 Complexity bound for a global optimization problem on the unit box

Consider one of the simplest problems in optimization, that is, minimizing a function in the $n$-dimensional box.

$$
\begin{cases}\text { minimize } & f(\boldsymbol{x})  \tag{1.2}\\ \text { subject to } & \boldsymbol{x} \in B_{n}=\left\{\boldsymbol{x} \in \mathbb{R}^{n} \mid 0 \leq[\boldsymbol{x}]_{i} \leq 1, i=1,2, \ldots, n\right\} .\end{cases}
$$

### 1.2. COMPLEXITY BOUND FOR A GLOBAL OPTIMIZATION PROBLEM ON THE UNIT BOX7

To be coherent, we use the $\ell_{\infty}$-norm:

$$
\|\boldsymbol{x}\|_{\infty}=\max _{1 \leq i \leq n}\left|[\boldsymbol{x}]_{i}\right| .
$$

Let us also assume that $f(\boldsymbol{x})$ is Lipschitz continuous on $B_{n}$ :

$$
|f(\boldsymbol{x})-f(\boldsymbol{y})| \leq L\|\boldsymbol{x}-\boldsymbol{y}\|_{\infty}, \quad \forall \boldsymbol{x}, \boldsymbol{y} \in B_{n} .
$$

Let us define a very simple method to solve (1.2), the uniform grid method.
Given a positive integer $p>0$,

1. Form $(p+1)^{n}$ points

$$
\boldsymbol{x}_{i_{1}, i_{2}, \ldots, i_{n}}=\left(\frac{i_{1}}{p}, \frac{i_{2}}{p}, \ldots, \frac{i_{n}}{p}\right)^{T}
$$

where $\left(i_{1}, i_{2}, \ldots, i_{n}\right) \in\{0,1, \ldots, p\}^{n}$.
2. Among all points $\boldsymbol{x}_{i_{1}, i_{2}, \ldots, i_{n}}$, find a point $\overline{\boldsymbol{x}}$ which has the minimal value for the objective function.
3. Return the pair $(\overline{\boldsymbol{x}}, f(\overline{\boldsymbol{x}}))$ as the result.

Theorem 1.2.1 Let $f^{*}$ be the global optimal value for (1.2). Then the uniform grid method yields

$$
f(\overline{\boldsymbol{x}})-f^{*} \leq \frac{L}{2 p}
$$

Proof: Let $\boldsymbol{x}^{*}$ be a global optimal solution. Then there are coordinates $\left(i_{1}, i_{2}, \ldots, i_{n}\right)$ such that $\boldsymbol{x} \equiv \boldsymbol{x}_{i_{1}, i_{2}, \ldots, i_{n}} \leq \boldsymbol{x}^{*} \leq \boldsymbol{x}_{i_{1}+1, i_{2}+1, \ldots, i_{n}+1} \equiv \boldsymbol{y}$. Observe that $[\boldsymbol{y}]_{i}-[\boldsymbol{x}]_{i}=1 / p$ for $i=1,2, \ldots, n$ and $\left[\boldsymbol{x}^{*}\right]_{i} \in\left[[\boldsymbol{x}]_{i},[\boldsymbol{y}]_{i}\right](i=1,2, \ldots, n)$.
Consider $\hat{\boldsymbol{x}}=(\boldsymbol{x}+\boldsymbol{y}) / 2$ and form a new point $\tilde{\boldsymbol{x}}$ as:

$$
[\tilde{\boldsymbol{x}}]_{i}= \begin{cases}{[\boldsymbol{y}]_{i},} & \text { if }\left[\boldsymbol{x}^{*}\right]_{i} \geq[\hat{\boldsymbol{x}}]_{i} \\ {[\boldsymbol{x}]_{i},} & \text { otherwise }\end{cases}
$$

It is clear that $\left|[\tilde{\boldsymbol{x}}]_{i}-\left[\boldsymbol{x}^{*}\right]_{i}\right| \leq 1 /(2 p)$ for $i=1,2, \ldots, n$. Then $\left\|\tilde{\boldsymbol{x}}-\boldsymbol{x}^{*}\right\|_{\infty}=\max _{1 \leq i \leq n} \mid[\tilde{\boldsymbol{x}}]_{i}-$ $\left[\boldsymbol{x}^{*}\right]_{i} \mid \leq 1 /(2 p)$. Since $\tilde{\boldsymbol{x}}$ belongs to the grid,

$$
f(\overline{\boldsymbol{x}})-f\left(\boldsymbol{x}^{*}\right) \leq f(\tilde{\boldsymbol{x}})-f\left(\boldsymbol{x}^{*}\right) \leq L\left\|\tilde{\boldsymbol{x}}-\boldsymbol{x}^{*}\right\|_{\infty} \leq L /(2 p) .
$$

Let us define our goal

$$
\text { Find } \boldsymbol{x} \in B_{n} \text { such that } f(\boldsymbol{x})-f^{*}<\varepsilon
$$

Corollary 1.2.2 The analytical complexity of the problem (1.2) for the uniform grid method is at most

$$
\left(\left\lfloor\frac{L}{2 \varepsilon}\right\rfloor+2\right)^{n}
$$

Proof: Take $p=\lfloor L /(2 \varepsilon)\rfloor+1$. Then, $p>L /(2 \varepsilon)$ and from the previous theorem, $f(\overline{\boldsymbol{x}})-f\left(\boldsymbol{x}^{*}\right) \leq L /(2 p)<\varepsilon$. Observe that we constructed $(p+1)^{n}$ points.

Consider the class of problems $\mathcal{C}$ defined as follows:

| Model: | $\min \boldsymbol{x} \in B_{n} f(\boldsymbol{x})$ |
| :--- | :--- |
|  | $f(\boldsymbol{x})$ is $\ell_{\infty}$-Lipschitz continuous on $B_{n}$. |
| Oracle: | zero-order local black box (only function values) |
| Approximate solution: | Find $\overline{\boldsymbol{x}} \in B_{n}$ such that $f(\overline{\boldsymbol{x}})-f^{*}<\varepsilon$ |

Theorem 1.2.3 For $\varepsilon<\frac{L}{2}$, the analytical complexity of class of problems $\mathcal{C}$ using zeroorder methods is at least $\left(\left\lfloor\frac{L}{2 \varepsilon}\right\rfloor\right)^{n}$.

Proof: Let $p=\left\lfloor\frac{L}{2 \varepsilon}\right\rfloor$ (which is $\geq 1$ from the hypothesis).
Suppose that there is a method which requires $N<p^{n}$ calls of the oracle to solve the problem $\mathcal{P}$.

Then, there is a point $\hat{\boldsymbol{x}} \in B_{n}=\left\{\boldsymbol{x} \in \mathbb{R}^{n} \mid 0 \leq[\boldsymbol{x}]_{i} \leq 1, i=1,2, \ldots, n\right\}$ where there is no test points in the interior of $B \equiv\{\boldsymbol{x} \mid \hat{\boldsymbol{x}} \leq \boldsymbol{x} \leq \hat{\boldsymbol{x}}+\boldsymbol{e} / p\}$ where $\boldsymbol{e}=(1,1, \ldots, 1)^{T} \in \mathbb{R}^{n}$.

Let $\boldsymbol{x}^{*}=\hat{\boldsymbol{x}}+\boldsymbol{e} /(2 p)$ and consider the function $\bar{f}(\boldsymbol{x})=\min \left\{0, L\left\|\boldsymbol{x}-\boldsymbol{x}^{*}\right\|_{\infty}-\varepsilon\right\}$. Clearly, $\bar{f}$ is $\ell_{\infty}$-Lipschitz continuous with constant $L$ and its global minimum is $-\varepsilon$. Moreover, $\bar{f}(\boldsymbol{x})$ is non-zero valued only inside the box $B^{\prime}=\left\{\boldsymbol{x} \mid\left\|\boldsymbol{x}-\boldsymbol{x}^{*}\right\|_{\infty} \leq \varepsilon / L\right\}$.

Since $2 p \leq L / \varepsilon, B^{\prime} \subseteq B=\left\{\boldsymbol{x} \mid\left\|\boldsymbol{x}-\boldsymbol{x}^{*}\right\|_{\infty} \leq 1 /(2 p)\right\}$.
Therefore, $\bar{f}(\boldsymbol{x})$ is equal to zero to all test points of our method and the accuracy of the $\operatorname{method}$ is $\varepsilon$.

If the number of calls of the oracle is less than $p^{n}$, the accuracy can not be better than $\varepsilon$.

Theorem 1.2.3 supports our initial claim that the general optimization problem are unsolvable.

Example 1.2.4 Consider a problem defined by the following parameters. $L=2, n=10$, and $\varepsilon=0.01(1 \%)$.

```
lower bound (L/(2\varepsilon))\mp@subsup{)}{}{n}\quad: 1020}\mathrm{ calls of the oracle
complexity of the oracle : at least n arithmetic operations
total complexity : 1021 arithmetic operations
CPU : 1GHz or 109 arithmetic operations per second
total time : 10 12 seconds
one year : \leq < 2.2 < 107}\mathrm{ seconds
we need : \geq10000 years
```

- If we change $n$ by $n+1$, the analytical complexity estimate is multiplied by 100 .
- If we multiply $\varepsilon$ by 2 , the arithmetic complexity is reduced by 1000 .

We know from Corollary 1.2.2 that the analytical complexity for the uniform grid method is $(\lfloor L /(2 \varepsilon)\rfloor+2)^{n}$. Theorem 1.2 .3 showed that any method with zero-order oracle requires at least $(\lfloor L /(2 \varepsilon)\rfloor)^{n}$ calls to have a better performance that $\varepsilon$. If for instance we take $\varepsilon=\mathcal{O}(L / n)$, these two bounds coincide up to a constant factor. In this sense, the uniform grid method is an optimal method for $\mathcal{C}$.

### 1.3 Optimality conditions for unconstrained minimization problems

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

$$
f(\boldsymbol{y})=f(\overline{\boldsymbol{x}})+\left\langle f^{\prime}(\overline{\boldsymbol{x}}), \boldsymbol{y}-\overline{\boldsymbol{x}}\right\rangle+o(\|\boldsymbol{y}-\overline{\boldsymbol{x}}\|),
$$

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

$$
\lim _{r \rightarrow 0} \frac{1}{r} o(r)=0, o(0)=0
$$

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

$$
\Delta(\boldsymbol{s})=\lim _{\alpha \rightarrow 0} \frac{1}{\alpha}[f(\overline{\boldsymbol{x}}+\alpha \boldsymbol{s})-f(\overline{\boldsymbol{x}})]
$$

Since $f(\overline{\boldsymbol{x}}+\alpha \boldsymbol{s})-f(\overline{\boldsymbol{x}})=\alpha\left\langle f^{\prime}(\overline{\boldsymbol{x}}), \boldsymbol{s}\right\rangle+o(\|\alpha \boldsymbol{s}\|)$, we have $\Delta(\boldsymbol{s})=\left\langle f^{\prime}(\overline{\boldsymbol{x}}), \boldsymbol{s}\right\rangle$.
Using the Cauchy-Schwartz inequality $-\|\boldsymbol{x}\|\|\boldsymbol{y}\| \leq\langle\boldsymbol{x}, \boldsymbol{y}\rangle \leq\|\boldsymbol{x}\|\|\boldsymbol{y}\|$,

$$
\Delta(s)=\left\langle f^{\prime}(\overline{\boldsymbol{x}}), s\right\rangle \geq-\left\|f^{\prime}(\overline{\boldsymbol{x}})\right\| .
$$

Choosing the direction $\overline{\boldsymbol{s}}=-f^{\prime}(\overline{\boldsymbol{x}}) /\left\|f^{\prime}(\overline{\boldsymbol{x}})\right\|$,

$$
\Delta(\bar{s})=-\left\langle f^{\prime}(\overline{\boldsymbol{x}}), \frac{f^{\prime}(\overline{\boldsymbol{x}})}{\left\|f^{\prime}(\overline{\boldsymbol{x}})\right\|}\right\rangle=-\left\|f^{\prime}(\overline{\boldsymbol{x}})\right\| .
$$

Thus, the direction $-f^{\prime}(\overline{\boldsymbol{x}})$ is the direction of the fastest local decrease of $f(\boldsymbol{x})$ at point $\overline{\boldsymbol{x}}$.

Theorem 1.3.1 (First-order necessary optimality condition) Let $\boldsymbol{x}^{*}$ be a local minimum of the differentiable function $f(\boldsymbol{x})$. Then

$$
f^{\prime}\left(\boldsymbol{x}^{*}\right)=\mathbf{0}
$$

Proof: Let $\boldsymbol{x}^{*}$ be the local minimum of $f(\boldsymbol{x})$. Then, there is $r>0$ such that for all $\boldsymbol{y}$ with $\left\|\boldsymbol{y}-\boldsymbol{x}^{*}\right\| \leq r, f(\boldsymbol{y}) \geq f\left(\boldsymbol{x}^{*}\right)$.
Since $f$ is differentiable,

$$
f(\boldsymbol{y})=f\left(\boldsymbol{x}^{*}\right)+\left\langle f^{\prime}\left(\boldsymbol{x}^{*}\right), \boldsymbol{y}-\boldsymbol{x}^{*}\right\rangle+o\left(\left\|\boldsymbol{y}-\boldsymbol{x}^{*}\right\|\right) \geq f\left(\boldsymbol{x}^{*}\right) .
$$

Dividing by $\left\|\boldsymbol{y}-\boldsymbol{x}^{*}\right\|$, and taking the limit $\boldsymbol{y} \rightarrow \boldsymbol{x}^{*}$,

$$
\left\langle f^{\prime}\left(\boldsymbol{x}^{*}\right), \boldsymbol{s}\right\rangle \geq 0, \quad \forall \boldsymbol{s}, \quad\|\boldsymbol{s}\|=1
$$

Consider the opposite direction $\boldsymbol{- s}$, and then we conclude that

$$
\left\langle f^{\prime}\left(\boldsymbol{x}^{*}\right), \boldsymbol{s}\right\rangle=0, \quad \forall \boldsymbol{s}, \quad\|\boldsymbol{s}\|=1
$$

Choosing $\boldsymbol{s}=\boldsymbol{e}_{i} \quad(i=1,2, \ldots, n)$, we conclude that $f^{\prime}\left(\boldsymbol{x}^{*}\right)=0$.
Corollary 1.3.2 Let $\boldsymbol{x}^{*}$ be a local minimum of a differentiable function $f(\boldsymbol{x})$ subject to linear equality constraints

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

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

$$
f^{\prime}\left(\boldsymbol{x}^{*}\right)=\boldsymbol{A}^{T} \boldsymbol{\lambda}^{*} .
$$

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

$$
\boldsymbol{x}=\boldsymbol{x}(\boldsymbol{t}) \equiv \boldsymbol{x}^{*}+\sum_{i=1}^{k} t_{i} \boldsymbol{u}_{i}, \quad \boldsymbol{t} \in \mathbb{R}^{k} .
$$

Moreover, the point $\boldsymbol{t}=\mathbf{0}$ is the local minimal solution of the function $\phi(\boldsymbol{t})=f(\boldsymbol{x}(\boldsymbol{t}))$.
From Theorem 1.3.1, $\phi^{\prime}(\mathbf{0})=\mathbf{0}$. That is,

$$
\frac{d \phi}{d t_{i}}(\mathbf{0})=\left\langle f^{\prime}\left(\boldsymbol{x}^{*}\right), \boldsymbol{u}_{i}\right\rangle=0, \quad i=1,2, \ldots, k
$$

Now there is $\boldsymbol{t}^{*}$ and $\boldsymbol{\lambda}^{*}$ such that

$$
f^{\prime}\left(\boldsymbol{x}^{*}\right)=\sum_{i=1}^{k} t_{i}^{*} \boldsymbol{u}_{i}+\boldsymbol{A}^{T} \boldsymbol{\lambda}^{*}
$$

For each $i=1,2, \ldots, k$,

$$
\left\langle f^{\prime}\left(\boldsymbol{x}^{*}\right), \boldsymbol{u}_{i}\right\rangle=t_{i}^{*}=0 .
$$

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

$$
f^{\prime}(\boldsymbol{y})=f^{\prime}(\overline{\boldsymbol{x}})+f^{\prime \prime}(\overline{\boldsymbol{x}})(\boldsymbol{y}-\overline{\boldsymbol{x}})+\boldsymbol{o}(\|\boldsymbol{y}-\overline{\boldsymbol{x}}\|),
$$

where $\boldsymbol{o}(r)$ is such that $\lim _{r \rightarrow 0}\|\boldsymbol{o}(r)\| / r=0$ and $\boldsymbol{o}(0)=0$.
Theorem 1.3.3 (Second-order necessary optimality condition) Let $\boldsymbol{x}^{*}$ be a local minimum of a twice continuously differentiable function $f(\boldsymbol{x})$. Then

$$
f^{\prime}\left(\boldsymbol{x}^{*}\right)=0, \quad f^{\prime \prime}\left(\boldsymbol{x}^{*}\right) \succeq \boldsymbol{O} .
$$

