Foundation of Computing and Mathematical Sciences — Optimization —

Tokyo Institute of Technology Dept. Mathematical and Computing Sciences MITUHIRO FUKUDA

Fall/Winter Semester of 2012

"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

Bibliography

- [DASPREMONT2008] A. d'Aspremont, "Smooth optimization with approximate gradient", SIAM Journal on Optimization 19 (2008), pp. 1171–1183.
- [GK2008] C. C. Gonzaga and E. W. Karas, "Fine tuning Nesterov's steepest descent algorithm for differentiable convex programming", *Mathematical Programming*, to appear.
- [LLM2006] G. Lan, Z. Lu, and R. D. C. Monteiro, "Primal-dual first-order methods with $\mathcal{O}(1/\varepsilon)$ iteration-complexity for cone programming", *Mathematical Programming*, **126** (2011), pp.1–29.
- [NESTEROV2004] Yu. Nesterov, Introductory Lecture on Convex Optimization: A Basic Course, (Kluwer Academic Publishers, Boston, 2004).
- [NESTEROV2005] Yu. Nesterov, "Smooth minimization of non-smooth functions", *Mathematical Programming* **103** (2005), pp. 127–152.
- [NESTEROV2005-2] Yu. Nesterov, "Excessive gap technique in nonsmooth convex minimization", SIAM Journal on Optimization 16 (2005), pp. 669–700.
- [NESTEROV2007] Yu. Nesterov, "Smoothing technique and its applications in semidefinite optimization", Mathematical Programming 110 (2007), pp. 245–259.
- [NESTERVO2009] Yu. Nesterov, "Primal-dual subgradient methods for convex problems", Mathematical Programming 120 (2009), pp. 221-259.
- [NOCEDAL2006] J. Nocedal and S. J. Wright, *Numerical Optimization*, 2nd edition, (Springer, New York, 2006).
- [TSENG2010] P. Tseng, "Approximation accuracy, gradient methods, and error bound for structured convex optimization", *Mathematical Programming* 12 (2010), pp. 263–295.
- [YUAN2010] Y.-X. Yuan, "A short note on the Q-linear convergence of the steepest descent method", Mathematical Programming 123 (2010), pp. 339–343.

Chapter 1

Nonlinear Optimization

1.1 General minimization problem and terminologies

Definition 1.1.1 We define the general minimization problem as follows

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

where $f : \mathbb{R}^n \to \mathbb{R}, f_j : \mathbb{R}^n \to \mathbb{R} \ (j = 1, 2, ..., m)$, 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

$$Q = \{ \boldsymbol{x} \in S \mid f_j(\boldsymbol{x}) \& 0, \ (j = 1, 2, \dots, m) \}.$$

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 $f(\mathbf{x}), f_j(\mathbf{x})$ 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 $f_j(\boldsymbol{x}) = \sum_{i=1}^n [\boldsymbol{a}]_{ji}[\boldsymbol{x}]_i + [\boldsymbol{b}]_j$ (j = 1, 2, ..., m), (1.1) is a linear constrained optimization problem.
 - In addition, if $f(\mathbf{x})$ is linear, (1.1) is a linear programming problem.
 - In addition, if $f(\mathbf{x})$ is quadratic, (1.1) is a quadratic programming problem.
- If $f(\boldsymbol{x})$, $f_j(\boldsymbol{x})$ (j = 1, 2, ..., 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 $f(\boldsymbol{x}^*) \leq f(\boldsymbol{x})$, $\forall \boldsymbol{x} \in Q$. Moreover, $f(\boldsymbol{x}^*)$ is called the global optimal value. \boldsymbol{x}^* is called a local optimal solution of (1.1) if there exists an open ball $B(\varepsilon) = \{\boldsymbol{x} \in \mathbb{R}^n \mid ||\boldsymbol{x} - \boldsymbol{x}^*|| < \varepsilon\} \subseteq Q$ such that $f(\boldsymbol{x}^*) \leq f(\boldsymbol{x}), \quad \forall \boldsymbol{x} \in B(\varepsilon)$. Moreover, $f(\boldsymbol{x}^*)$ 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: $I_k := I_{k-1} \cup (\boldsymbol{x}_k, \mathcal{O}(\boldsymbol{x}_k)).$
- **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 \bar{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 ε .

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 ε .

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 $f(\mathbf{x})$, and the gradient $f'(\mathbf{x})$.
- 3. The second-order oracle returns the value $f(\mathbf{x})$, $f'(\mathbf{x})$ and the Hessian $f''(\mathbf{x})$.

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.

$$\begin{cases} \text{minimize} & f(\boldsymbol{x}) \\ \text{subject to} & \boldsymbol{x} \in B_n = \{ \boldsymbol{x} \in \mathbb{R}^n \mid 0 \le [\boldsymbol{x}]_i \le 1, \ i = 1, 2, \dots, n \}. \end{cases}$$
(1.2)

To be coherent, we use the ℓ_{∞} -norm:

$$\|oldsymbol{x}\|_{\infty} = \max_{1 \leq i \leq n} |[oldsymbol{x}]_i|.$$

Let us also assume that $f(\mathbf{x})$ is Lipschitz continuous on B_n :

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

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 $(i_1, i_2, \dots, i_n) \in \{0, 1, \dots, p\}^n$.

- 2. Among all points $\boldsymbol{x}_{i_1,i_2,\ldots,i_n}$, find a point $\bar{\boldsymbol{x}}$ which has the minimal value for the objective function.
- 3. Return the pair $(\bar{\boldsymbol{x}}, f(\bar{\boldsymbol{x}}))$ as the result.

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

$$f(\bar{\boldsymbol{x}}) - f^* \le \frac{L}{2p}.$$

Proof: Let \mathbf{x}^* be a global optimal solution. Then there are coordinates (i_1, i_2, \ldots, i_n) such that $\mathbf{x} \equiv \mathbf{x}_{i_1, i_2, \ldots, i_n} \leq \mathbf{x}^* \leq \mathbf{x}_{i_1+1, i_2+1, \ldots, i_n+1} \equiv \mathbf{y}$. Observe that $[\mathbf{y}]_i - [\mathbf{x}]_i = 1/p$ for $i = 1, 2, \ldots, n$ and $[\mathbf{x}^*]_i \in [[\mathbf{x}]_i, [\mathbf{y}]_i]$ $(i = 1, 2, \ldots, n)$.

Consider $\hat{\boldsymbol{x}} = (\boldsymbol{x} + \boldsymbol{y})/2$ and form a new point $\tilde{\boldsymbol{x}}$ as:

$$[\tilde{\boldsymbol{x}}]_i = \left\{ egin{array}{cc} [\boldsymbol{y}]_i, & ext{if } [\boldsymbol{x}^*]_i \geq [\hat{\boldsymbol{x}}]_i \ [\boldsymbol{x}]_i, & ext{otherwise.} \end{array}
ight.$$

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

$$f(\bar{\boldsymbol{x}}) - f(\boldsymbol{x}^*) \le f(\tilde{\boldsymbol{x}}) - f(\boldsymbol{x}^*) \le L \|\tilde{\boldsymbol{x}} - \boldsymbol{x}^*\|_{\infty} \le L/(2p).$$

Let us define our goal

Find
$$\boldsymbol{x} \in B_n$$
 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, $f(\bar{\boldsymbol{x}}) - f(\boldsymbol{x}^*) \leq L/(2p) < \varepsilon$. 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 ℓ_{∞} -Lipschitz continuous on B_n .
Oracle:	zero-order local black box (only function values)
Approximate solution:	Find $\bar{\boldsymbol{x}} \in B_n$ such that $f(\bar{\boldsymbol{x}}) - f^* < \varepsilon$

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

Proof: Let $p = \lfloor \frac{L}{2\varepsilon} \rfloor$ (which is ≥ 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 $\hat{\boldsymbol{x}} \in B_n = \{\boldsymbol{x} \in \mathbb{R}^n \mid 0 \leq [\boldsymbol{x}]_i \leq 1, i = 1, 2, ..., n\}$ where there is no test points in the <u>interior</u> of $B \equiv \{\boldsymbol{x} \mid \hat{\boldsymbol{x}} \leq \boldsymbol{x} \leq \hat{\boldsymbol{x}} + \boldsymbol{e}/p\}$ where $\boldsymbol{e} = (1, 1, ..., 1)^T \in \mathbb{R}^n$.

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

Since $2p \leq L/\varepsilon$, $B' \subseteq B = \{ \boldsymbol{x} \mid \| \boldsymbol{x} - \boldsymbol{x}^* \|_{\infty} \leq 1/(2p) \}.$

Therefore, $\bar{f}(\boldsymbol{x})$ is equal to zero to all test points of our method and the accuracy of the method is ε .

If the number of calls of the oracle is less than p^n , the accuracy can not be better than ε .

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 $(L/(2\varepsilon))^n$:	10^{20} calls of the oracle
complexity of the oracle	:	at least n arithmetic operations
total complexity	:	10^{21} arithmetic operations
CPU	:	1 GHz or 10^9 arithmetic operations per second
total time	:	10^{12} seconds
one year	:	$\leq 3.2 \times 10^7$ seconds
we need	:	≥ 10000 years

- If we change n by n + 1, the analytical complexity estimate is multiplied by 100.
- If we multiply ε 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 $(|L/(2\varepsilon)|+2)^n$. Theorem 1.2.3 showed that any method with zero-order oracle requires at least $(|L/(2\varepsilon)|)^n$ calls to have a better performance that ε . 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* C.

Optimality conditions for unconstrained minimiza-1.3tion problems

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

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

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 $\|s\| = 1$. Consider the local decrease 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 $f(\bar{\boldsymbol{x}} + \alpha \boldsymbol{s}) - f(\bar{\boldsymbol{x}}) = \alpha \langle f'(\bar{\boldsymbol{x}}), \boldsymbol{s} \rangle + o(\|\alpha \boldsymbol{s}\|)$, we have $\Delta(\boldsymbol{s}) = \langle f'(\bar{\boldsymbol{x}}), \boldsymbol{s} \rangle$. Using the Cauchy-Schwartz inequality $-\|\boldsymbol{x}\|\|\boldsymbol{y}\| \leq \langle \boldsymbol{x}, \boldsymbol{y} \rangle \leq \|\boldsymbol{x}\|\|\boldsymbol{y}\|$,

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

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

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

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

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

Since f is differentiable,

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

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

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

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

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

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

Corollary 1.3.2 Let x^* be a local minimum of a differentiable function f(x) subject to linear equality constraints

$$oldsymbol{x} \in \mathcal{L} \equiv \{oldsymbol{x} \in \mathbb{R}^n \mid oldsymbol{A}oldsymbol{x} = oldsymbol{b}\}
eq \emptyset,$$

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

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

Moreover, the point $\mathbf{t} = \mathbf{0}$ is the local minimal solution of the function $\phi(\mathbf{t}) = f(\mathbf{x}(\mathbf{t}))$. From Theorem 1.3.1, $\phi'(\mathbf{0}) = \mathbf{0}$. 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.

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

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

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

Theorem 1.3.3 (Second-order necessary optimality condition) Let x^* be a local minimum of a twice continuously differentiable function f(x). Then

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