Optimization Theory

Lecture 02

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Outline

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Matrix Calculus

Given differentiable $f : \mathbb{R}^{p\times q} \to \mathbb{R}$ and $\mathbf{X} \in \mathbb{R}^{p\times q}$, we define

$$\nabla f(\mathbf{X}) = \begin{bmatrix} \frac{\partial f(\mathbf{X})}{\partial x_{11}} & \dots & \frac{\partial f(\mathbf{X})}{\partial x_{1q}} \\ \vdots & \ddots & \vdots \\ \frac{\partial f(\mathbf{X})}{\partial x_{p1}} & \dots & \frac{\partial f(\mathbf{X})}{\partial x_{pq}} \end{bmatrix} \in \mathbb{R}^{p\times q} \quad \text{and} \quad \mathrm{d}\mathbf{X} = \begin{bmatrix} \mathrm{d}x_{11} & \dots & \mathrm{d}x_{1q} \\ \vdots & \ddots & \vdots \\ \mathrm{d}x_{p1} & \dots & \mathrm{d}x_{pq} \end{bmatrix} \in \mathbb{R}^{p\times q}.$$

We have

$$\mathrm{d}f(\mathbf{X}) = \sum_{i=1}^{p}\sum_{j=1}^{q} \frac{\partial f(\mathbf{X})}{\partial x_{ij}} \cdot \mathrm{d}x_{ij} = \langle \nabla f(\mathbf{X}), \mathrm{d}\mathbf{X} \rangle = \mathrm{tr}\big(\nabla f(\mathbf{X})^\top \mathrm{d}\mathbf{X}\big)$$

and

$$\mathrm{d}(\mathbf{XY}) = (\mathrm{d}\mathbf{X})\mathbf{Y} + \mathbf{X}\mathrm{d}\mathbf{Y}, \quad \mathrm{d}(\mathbf{AXB}) = \mathbf{A} \cdot \mathrm{d}\mathbf{X} \cdot \mathbf{B}$$

The Hessian

Suppose that $f : \mathbb{R}^n \to \mathbb{R}$ is a smooth function that takes as input a matrix $\mathbf{x} \in \mathbb{R}^n$ and returns a real value. Then the Hessian with respect to $\mathbf{x}$, written as $\nabla^2 f(\mathbf{x})$, which is defined as

$$\nabla^2 f(\mathbf{x}) = \begin{bmatrix} \dfrac{\partial^2 f(\mathbf{x})}{\partial x_1 \partial x_1} & \cdots & \dfrac{\partial^2 f(\mathbf{x})}{\partial x_1 \partial x_n} \\ \vdots & \ddots & \vdots \\ \dfrac{\partial^2 f(\mathbf{x})}{\partial x_n \partial x_1} & \cdots & \dfrac{\partial^2 f(\mathbf{x})}{\partial x_n \partial x_n} \end{bmatrix} \in \mathbb{R}^{n \times n}.$$

We write Taylor's expansion for multivariate function $f : \mathbb{R}^n \to \mathbb{R}$ as

$$f(\mathbf{x}) \approx f(\mathbf{a}) + \nabla f(\mathbf{a})^\top (\mathbf{x} - \mathbf{a}) + \frac{1}{2}(\mathbf{x} - \mathbf{a})^\top \nabla^2 f(\mathbf{a})(\mathbf{x} - \mathbf{a}).$$

Outline

Topology in Euclidean Space

Open set, closed set, bounded set and compact set:

1. A subset $\mathcal{C}$ of $\mathbb{R}^d$ is called open, if for every $\mathbf{x} \in \mathcal{C}$ there exists $\delta > 0$ such that the ball $\mathcal{B}_\delta(\mathbf{x}) = \{\mathbf{y} \in \mathbb{R}^d : \|\mathbf{y} - \mathbf{x}\|_2 \leq \delta\}$ is included in $\mathcal{C}$.
2. A subset $\mathcal{C}$ of $\mathbb{R}^d$ is called closed, if its complement $\mathcal{C}^{\mathrm{c}} = \mathbb{R}^d \backslash \mathcal{C}$ is open.
3. A subset $\mathcal{C}$ of $\mathbb{R}^d$ is called bounded, if there exists $r > 0$ such that $\|\mathbf{x}\|_2 < r$ for all $\mathbf{x} \in \mathcal{C}$.
4. A subset $\mathcal{C}$ of $\mathbb{R}^d$ is called compact, if it is both bounded and closed.

Is there any subset of $\mathbb{R}^d$ that is both open and closed?

Topology in Euclidean Space

Interior, closure and boundary:

1. The interior of $\mathcal{C} \in \mathbb{R}^n$ is defined as

$$\mathcal{C}^\circ = \{\mathbf{y} \in \mathbb{R}^n : \text{there exist } \delta > 0 \text{ such that } \mathcal{B}_\delta(\mathbf{y}) \subseteq \mathcal{C}\}$$

2. The closure of $\mathcal{C} \in \mathbb{R}^n$ is defined as

$$\overline{\mathcal{C}} = \mathbb{R}^n \backslash (\mathbb{R}^n \backslash \mathcal{C})^\circ.$$

3. The boundary of $\mathcal{C} \in \mathbb{R}^n$ is defined as $\overline{\mathcal{C}} \backslash \mathcal{C}^\circ$.

Topology in General Case

In a metric space, an open set is a set that, along with every point $\mathbf{x}$, contains all points that are sufficiently near to $\mathbf{x}$.

The other concept also can be generalized in the similar way.

For example, the positive-definite matrices on $\mathbb{R}^{d\times d}$ with distance under spectral norm is open.

Convergence Rates

Assume the sequence $\{\mathbf{x}_k\}$ converges to $\mathbf{x}^*$. We define the errors

$$z_k = \|\mathbf{x}_k - \mathbf{x}^*\|$$

and suppose

$$\lim_{k \to +\infty} \frac{z_{k+1}}{z_k^r} = C \quad \text{for some } C \in \mathbb{R}.$$

Q-convergence rates:

1. linear: $r = 1$, $0 < C < 1$;
2. sublinear: $r = 1$, $C = 1$;
3. superlinear: $r = 1$, $C = 0$;
4. quadratic: $r = 2$.

Convergence Rates

Consider the example

$$x_k = 2^{-\lceil k/2 \rceil} + 1,$$

It should converge to $x^* = 0$ linearly, however,

$$\lim_{k \to +\infty} \frac{|x_{k+1} - x^*|}{|x_k - x^*|}$$

does not exist.

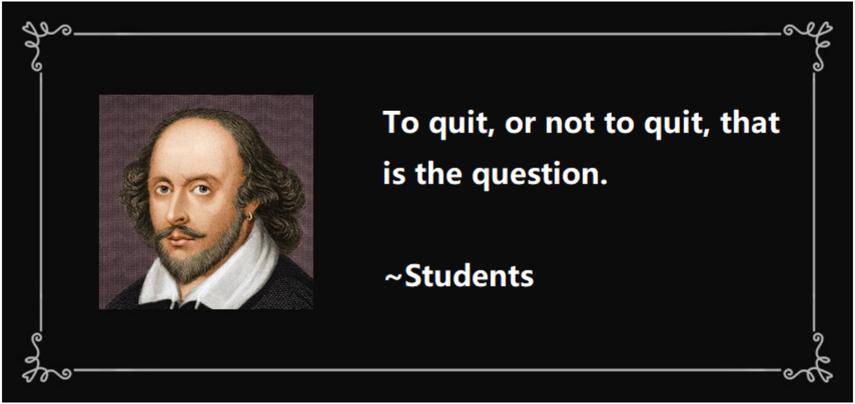
Convergence Rates

Suppose that $\{\mathbf{x}_k\}$ converges to $\mathbf{x}^*$. The sequence is said to converge R-linearly to $\mathbf{x}^*$ if there exists a sequence $\{\epsilon_k\}$ such that

$$\|\mathbf{x}_k - \mathbf{x}^*\| \leq \epsilon_k$$

for all k and $\{\epsilon_k\}$ converges Q-linearly to zero.

Outline



You can make the decision after the sections of convex analysis.

Convex Set

We say a set $\mathcal{C} \subseteq \mathbb{R}^n$ is convex if for all $\mathbf{x}, \mathbf{y} \in \mathcal{C}$ and $\alpha \in [0, 1]$, it holds that

$$\alpha \mathbf{x} + (1 - \alpha)\mathbf{y} \in \mathcal{C}.$$

Geometrically, a set $\mathcal{C}$ is convex means that the line-segment connecting any two points in $\mathcal{C}$ also belongs to $\mathcal{C}$.

Given any collection of convex sets (finite, countable or uncountable), their intersection is itself a convex set.

Projection

Given a closed and convex set $\mathcal{C} \subseteq \mathbb{R}^n$ and any point $\mathbf{y} \in \mathbb{R}^d$, we define the projection of $\mathbf{y}$ onto $\mathcal{C}$ in Euclidean norm as the point in $\mathcal{C}$ that is closest to $\mathbf{y}$ as

$$\mathrm{proj}_{\mathcal{C}}(\mathbf{y}) = \operatorname*{arg\,min}_{\mathbf{x}\in\mathcal{C}} \|\mathbf{y} - \mathbf{x}\|_2^2 \, .$$

Projection

Some properties of the projection:

1. The projection $\mathrm{proj}_{\mathcal{C}}(\mathbf{y})$ is uniquely defined.
2. If $\mathbf{y} \notin \mathcal{C}$, then $\mathbf{z} = \mathrm{proj}_{\mathcal{C}}(\mathbf{y})$ lies on the boundary of $\mathcal{C}$. The hyperplane

$$\{\mathbf{x} : \langle \mathbf{y} - \mathbf{z}, \mathbf{x} - \mathbf{z} \rangle = 0\}$$

separates $\mathbf{y}$ and $\mathcal{C}$ in that they lie on different sides, that is

$$\langle \mathbf{y} - \mathbf{z}, \mathbf{y} - \mathbf{z} \rangle > 0 \quad \text{and} \quad \langle \mathbf{y} - \mathbf{z}, \mathbf{x} - \mathbf{z} \rangle \leq 0$$

for any $\mathbf{x} \in \mathcal{C}$. It implies

$$\|\mathbf{x} - \mathbf{z}\|_2^2 \leq \|\mathbf{x} - \mathbf{y}\|_2^2$$

for any $\mathbf{x} \in \mathcal{C}$.

Outline

Convex Function

A function $f : \mathcal{C} \to \mathbb{R}$, defined on a convex set $\mathcal{C}$, is convex if it holds

$$f(\alpha \mathbf{x} + (1-\alpha)\mathbf{y}) \leq \alpha f(\mathbf{x}) + (1-\alpha) f(\mathbf{y})$$

for all $\mathbf{x}, \mathbf{y} \in \mathcal{C}$ and $\alpha \in [0,1]$.

Epigraph

The epigraph of a function $f : \mathcal{C} \to \mathbb{R}$ is defined as the set

$$\operatorname{epi} f \triangleq \{(\mathbf{x}, u) \in \mathcal{C} \times \mathbb{R} : f(\mathbf{x}) \leq u\}.$$

We say a function $f(\mathbf{x})$ is closed if its epigraph is closed.

Theorem

A function $f(\mathbf{x})$ is convex if and only if its epigraph is a convex set.

Extended Arithmetic Operations

We shall define convex function with possibly infinite values, which leads to arithmetic calculations involving $+\infty$ and $-\infty$:

- $-(-\infty) = +\infty$
- $\alpha \pm (+\infty) = (+\infty) \pm \alpha = +\infty$ for $\alpha \in \mathbb{R}$,
- $\alpha \pm (-\infty) = (-\infty) \pm \alpha = -\infty$ for $\alpha \in \mathbb{R}$,
- $\alpha \cdot (\pm\infty) = (\pm\infty) \cdot \alpha = \pm\infty$ for $\alpha \in (0, +\infty)$
- $\alpha \cdot (\pm\infty) = (\pm\infty) \cdot \alpha = \mp\infty$ for $\alpha \in (-\infty, 0)$
- $\alpha/(\pm\infty) = 0$ for $\alpha \in (-\infty, +\infty)$
- $(\pm\infty)/\alpha = \pm\infty$ for $\alpha \in (0, +\infty)$
- $(\pm\infty)/\alpha = \mp\infty$ for $\alpha \in (-\infty, 0)$
- $\inf \emptyset = \infty, \ \ \sup \emptyset = -\infty$

The extended real number system $\overline{\mathbb{R}}$, defined as

$$[-\infty, +\infty] \qquad \text{or} \qquad \mathbb{R} \cup \{-\infty, +\infty\}.$$

Extended Arithmetic Operations

The expressions

$$(+\infty) - (+\infty), \quad (-\infty) + (+\infty), \quad \frac{+\infty}{-\infty} \quad \text{and} \quad \frac{-\infty}{+\infty}.$$

are undefined and are avoided.

In the context of convex analysis, we also define

$$0 \cdot \infty = \infty \cdot 0 = 0 \qquad \text{and} \qquad 0 \cdot (-\infty) = (-\infty) \cdot 0 = 0.$$

Proper Convex Function

One may extend a convex function with domain $\mathcal{C} \subset \mathbb{R}^d$ to a proper convex function

$$f_{\mathcal{C}}(\mathbf{x}) = \begin{cases} f(\mathbf{x}), & \text{if } \mathbf{x} \in \mathcal{C}, \\ +\infty, & \text{if } \mathbf{x} \notin \mathcal{C}. \end{cases}$$

We define

$$\operatorname{dom} f \triangleq \{\mathbf{x} : f(\mathbf{x}) < +\infty\}.$$

We say a convex function is proper if its domain is non-empty and its values are all larger than $-\infty$.

We say a function $f(\mathbf{x})$ on $\mathbb{R}^d$ is concave if $-f(\mathbf{x})$ is convex. Linear functions are both convex and concave.

Convex Function

Some properties of convex function:

1. Given any $\mathbf{g} : \mathbb{R}^d \to \mathbb{R}^k$ such that each component $g_j(\mathbf{x})$ is convex, then the set $\mathcal{C} = \{\mathbf{x} : \mathbf{g}(\mathbf{x}) \leq \mathbf{0}\}$ is convex.
2. The supremum over a family of convex functions is convex.
3. The positively weighted sum of convex functions is convex.
4. The partial minimization of a convex function is convex.
5. The composition of convex functions may not preserve convexity.

Indicator Function

Given a closed convex set $\mathcal{C} \in \mathbb{R}^d$, we can define a convex function $\mathbb{1}_{\mathcal{C}}(\mathbf{x})$ on $\mathbb{R}^d$, called the indicator function of $\mathcal{C}$ on $\mathbb{R}^d$, as

$$\mathbb{1}_{\mathcal{C}}(\mathbf{x}) \triangleq \begin{cases} 0, & \text{if } \mathbf{x} \in \mathcal{C}, \\ +\infty, & \text{if } \mathbf{x} \notin \mathcal{C}. \end{cases}$$

We may write $f_{\mathcal{C}}(\mathbf{x}) = f(\mathbf{x}) + \mathbb{1}_{\mathcal{C}}(\mathbf{x})$ and the problem

$$\min_{\mathbf{x} \in \mathcal{C}} f(\mathbf{x})$$

is equivalent to

$$\min_{\mathbf{x} \in \mathbb{R}^d} f(\mathbf{x}) + \mathbb{1}_{\mathcal{C}}(\mathbf{x}).$$

Closed Convex Function

We shall focus on closed functions in convex optimization.

1. All convex functions can be made closed by taking the closure of its epigraph.
2. In some pessimistic case, a closed convex function may not be continuous at the boundary of its domain. Consider the function

$$f(x, y) = \begin{cases} \frac{x^2}{y}, & (x, y) \neq (0, 0) \\ 0, & (x, y) = (0, 0) \end{cases}$$

   with domain $\{(x, y) : y > 0\} \cup \{(0, 0)\}$.
3. We will only consider problems where the optimal solution can be achieved at a point that is continuous.

Outline

Why do we love convex optimization?

Theorem

Let $f(\mathbf{x})$ be a convex function defined on a convex set $\mathcal{C}$ and $\mathbf{x}^*$ be a local solution of

$$\min_{\mathbf{x}\in\mathcal{C}} f(\mathbf{x}). \tag{1}$$

That is, there exist some $\delta > 0$ such that any $\hat{\mathbf{x}} \in \mathcal{B}_\delta(\mathbf{x}^*) \cap \mathcal{C}$ holds

$$f(\mathbf{x}^*) \leq f(\hat{\mathbf{x}}).$$

Then the local solution $\mathbf{x}^*$ is a global solution of problem (1).

First-Order Condition

Theorem

If a function f is differentiable on open set $\mathcal{C}$, then it is convex on $\mathcal{C}$ if and only if

$$f(\mathbf{y}) \geq f(\mathbf{x}) + \langle \nabla f(\mathbf{x}), \mathbf{y} - \mathbf{x} \rangle$$

hols for any $\mathbf{x}, \mathbf{y} \in \mathcal{C}$.

However, the gradient may not exist in general case.

Outline

Subgradient and Subdifferential

We say a vector $\mathbf{g} \in \mathbb{R}^d$ is a subgradient of a proper convex function $f : \mathbb{R}^d \to \mathbb{R}$ at $\mathbf{x} \in \operatorname{dom} f$ if

$$f(\mathbf{y}) \geq f(\mathbf{x}) + \langle \mathbf{g}, \mathbf{y} - \mathbf{x} \rangle$$

holds for any $\mathbf{y} \in \mathbb{R}^d$.

The set of subgradients at $\mathbf{x} \in \operatorname{dom} f$ is called the subdifferential of f at $\mathbf{x}$, defined as

$$\partial f(\mathbf{x}) \triangleq \left\{ \mathbf{g} : f(\mathbf{y}) \geq f(\mathbf{x}) + \langle \mathbf{g}, \mathbf{y} - \mathbf{x} \rangle \text{ holds for any } \mathbf{y} \in \mathbb{R}^d \right\}.$$

Examples of Subdifferential

1. The subdifferential of $f(x) = |x|$ at 0 is the set
$$\partial f(x) = [-1, 1].$$
What about the general norm?
2. The subdifferential of an indicator function $\mathbb{1}_{\mathcal{C}}(\mathbf{x})$ is
$$\partial \mathbb{1}_{\mathcal{C}}(\mathbf{x}) = \mathcal{N}_{\mathcal{C}}(\mathbf{x}),$$
where
$$\mathcal{N}_{\mathcal{C}}(\mathbf{x}) = \left\{\mathbf{g} \in \mathbb{R}^d : \langle \mathbf{g}, \mathbf{y} - \mathbf{x} \rangle \leq 0 \text{ for all } \mathbf{y} \in \mathcal{C}\right\}$$
is called the normal cone of $\mathcal{C}$ at $\mathbf{x}$.
3. If a convex function f is differentiable at $\mathbf{x}$, then
$$\partial f(\mathbf{x}) = \{\nabla f(\mathbf{x})\}.$$