Optimization methods
Lecture 2: Convex functions properties. Subdifferential and automatic differentiation

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Brief reminder of the last lecture

- Introduction and course details

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- Convex sets and their properties

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- Introduction and course details
- Convex sets and their properties
- Convex functions, how to recognize and construct them

Plan for today

- Matrix calculus

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- Non-differentiable convex functions and subdifferential

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- Matrix calculus
- Non-differentiable convex functions and subdifferential
- Automatic differentiation technique
- L-smooth convex functions
- More about strongly convex functions

Main definitions

Let $f : D \to E$, derivative related entity $\frac{\partial f}{\partial x} \in G$:

D	E	G	Name
$\mathbb{R}$	$\mathbb{R}$	$\mathbb{R}$	Derivative, $f'(x)$
$\mathbb{R}^n$	$\mathbb{R}$	$\mathbb{R}^n$	Gradient, $\frac{\partial f}{\partial x_i}$
$\mathbb{R}^n$	$\mathbb{R}^m$	$\mathbb{R}^{m \times n}$	Jacobi matrix, $\frac{\partial f_i}{\partial x_j}$
$\mathbb{R}^{m \times n}$	$\mathbb{R}$	$\mathbb{R}^{m \times n}$	$\frac{\partial f}{\partial x_{ij}}$

A square $n \times n$ matrix of second derivatives $\mathbf{H} = [h_{ij}]$ in the case of $f : \mathbb{R}^n \to \mathbb{R}$ is called hessian and has the following elements $h_{ij} = \frac{\partial^2 f}{\partial x_i \partial x_j}$.

Main technique

Matrix representation of function: $f(\mathbf{x}) = \mathbf{x}^\top \mathbf{A}\mathbf{x},\ \mathbf{A} \in \mathbf{S}^n$

$\downarrow$

Scalar representation: $f = \sum_{ij} a_{ij} x_i x_j$

$\xrightarrow{f'_k = \frac{\partial f}{\partial x_k}}$

Scalar representation of gradient: $f'_k(\mathbf{x}) = 2\sum_j a_{kj} x_j$

$\uparrow$

Matrix representation of gradient: $f'(\mathbf{x}) = 2\mathbf{A}\mathbf{x}$

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- There is another approach to compute gradients based on a set of rules
- We will discuss it in the webinar

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2. Trace of the matrix product: $f(\mathbf{X}) = \mathrm{trace}(\mathbf{X}^\top \mathbf{X})$

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- $h(\mathbf{x}) = \cos(\mathbf{x})$ elementwise, $g(\mathbf{u}) = \sum_i u_i$. Find $\frac{\partial f}{\partial \mathbf{x}}$

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Compressed sensing

$$\min \|\mathbf{x}\|_1$$
$$\text{s.t. } \mathbf{A}\mathbf{x} = \mathbf{b}$$

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- According to the FO criterion for convex function the following inequality holds:

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

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- If f is differentiable, then $\mathbf{a} = f'(\mathbf{x})$.
- What to do if f is non-differentiable?

Definitions

Subgradient

A vector $\mathbf{a}$ is called subgradient of a function $f : \mathcal{X} \to \mathbb{R}$ at a point $\mathbf{x}$, if

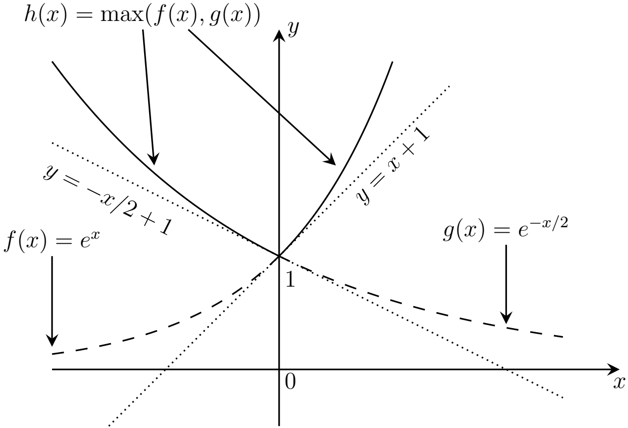
$$f(\mathbf{y}) - f(\mathbf{x}) \geq \langle \mathbf{a}, \mathbf{y} - \mathbf{x} \rangle$$

for all $\mathbf{y} \in \mathcal{X}$.

Subdifferential

All subgradients of a function f at a point $\mathbf{x}$ is called subdifferential of f in $\mathbf{x}$ and is denoted by $\partial f(\mathbf{x})$.

Geometric interpretation



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- The answer is $\partial f(0) = [-1, 1]$

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Theorem

A convex function f is differentiable at $\mathbf{x}$ if $\partial f(\mathbf{x}) = \{\mathbf{a}\}$. If function f is differentiable, then $\partial f(\mathbf{x}) = \{f'(\mathbf{x})\}$.

Main theorems

Moreau-Rockafellar theorem

Let $f_i(\mathbf{x})$ be convex functions defined on the convex sets $\mathcal{X}_i,\ i = 1, \ldots, n$. If $\bigcap\limits_{i=1}^{n} \operatorname{int}(\mathcal{X}_i) \neq \varnothing$ then a function $f(\mathbf{x}) = \sum\limits_{i=1}^{n} a_i f_i(\mathbf{x}),\ a_i > 0$ is subdifferentiable in a set $\mathcal{X} = \bigcap\limits_{i=1}^{n} \mathcal{X}_i$ and $\partial_{\mathcal{X}} f(\mathbf{x}) = \sum\limits_{i=1}^{n} a_i \partial_{\mathcal{X}_i} f_i(\mathbf{x})$.

Subdifferential of a maximum

If $f(\mathbf{x}) = \max\limits_{i=1,\ldots,m} (f_i(\mathbf{x}))$, where $f_i(\mathbf{x})$ are convex, then

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How to compute subdifferential

- Definition

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- Gradient, hessian and Jacobi matrix

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- Compositions of functions

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- Gradient, hessian and Jacobi matrix
- Compositions of functions
- Subdifferentials and how to compute them

From chain rule to `autodiff`[1]

Motivating example

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- Every function f_i has to compute not only its own value but also the result of product $\mathbf{J}_i$ by given vector

Backward mode or backpropagation

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- Every f_i has to compute not only its own value but also multiplication of $\mathbf{J}_i^\top$ by vector

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Implementation

- Choose element f_k
- Assign $\mathbf{u} = \mathbf{e}_k$, where $\mathbf{e}_k$ is the k-th orth
- Multiply recursively $\mathbf{u}^\top \mathbf{J}_L \dots \mathbf{J}_2 \mathbf{J}_1$ from left to right
- Compute f firstly, and after product from above. Therefore, we have to make two sweeps over computational graph
- Every f_i has to compute not only its own value but also multiplication of $\mathbf{J}_i^\top$ by vector

If $m = 1$, then $\mathbf{u} = 1$ and the result of backward mode differentiation equals to gradient!

Forward vs backward modes

Computational complexity

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Different implementations can significantly optimize all computations!

Example

Given function $f(x_1, x_2) = \cos^2(x_1 + x_2^3)$. Find $\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}$

$$f(x_1, x_2) = f_1(f_2(f_3(x_1, f_4(x_2))))$$

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- Compute $\frac{\partial f}{\partial x_2}$
- $w_1 = x_1$, $w_2 = x_2$
- $\frac{\partial w_1}{\partial x_1} = 0$, $\frac{\partial w_2}{\partial x_2} = 1$
- $w_3 = 3w_2^2 \frac{\partial w_2}{\partial x_2}$
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Why this is good idea?

- No storing of full hessian, therefore less memory is needed
- The choice of the modes in computing of gradient and hessian by vector product is based on the input/output dimensions of f and f'

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- Chain rule leads to autodiff technique
- Forward mode vs backward mode
- Typical use cases and issues

L-smooth function

Definition

Let $L > 0$. A function f is called L-smooth if it is differentiable and satisfies

$$\|f'(\mathbf{x}) - f'(\mathbf{y})\|_2 \leq L\|\mathbf{x} - \mathbf{y}\|_2.$$

Descent lemma

Let f be an L-smooth function. Then for any $\mathbf{x}, \mathbf{y}$

$$f(\mathbf{y}) \leq f(\mathbf{x}) + \langle f'(\mathbf{x}), \mathbf{y} - \mathbf{x}\rangle + \frac{L}{2}\|\mathbf{y} - \mathbf{x}\|_2^2$$

Proof of descent lemma

- The fundamental theorem of calculus

$$f(\mathbf{y}) - f(\mathbf{x}) = \int_0^1 \langle f'(\mathbf{x} + t(\mathbf{y} - \mathbf{x})), \mathbf{y} - \mathbf{x} \rangle dt$$

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- $|f(\mathbf{y}) - f(\mathbf{x}) - \langle f'(\mathbf{x}), \mathbf{y} - \mathbf{x} \rangle| \leq \int_0^1 |\langle f'(\mathbf{x} + t(\mathbf{y} - \mathbf{x})) - f'(\mathbf{x}), \mathbf{y} - \mathbf{x} \rangle| dt \leq \int_0^1 \|f'(\mathbf{x} + t(\mathbf{y} - \mathbf{x})) - f'(\mathbf{x})\| \|\mathbf{y} - \mathbf{x}\| dt$

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- $\int_0^1 \|f'(\mathbf{x} + t(\mathbf{y} - \mathbf{x})) - f'(\mathbf{x})\| \|\mathbf{y} - \mathbf{x}\| dt \leq \int_0^1 tL \|\mathbf{y} - \mathbf{x}\|_2^2 dt = \frac{L}{2} \|\mathbf{y} - \mathbf{x}\|_2^2$

Example

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- $\|\mathbf{A}\|_2$ is indeed the smallest smooth parameter

Second order characteristic

Claim

Let $f : \mathbb{R}^n \to \mathbb{R}$ is twice continuously differentiable, then for given $L > 0$ the following claims are equivalent

- f is L-smooth
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- $f(\lambda \mathbf{x} + (1 - \lambda) \mathbf{y}) \geq \lambda f(\mathbf{x}) + (1 - \lambda) f(\mathbf{y}) - \frac{L}{2} \lambda (1 - \lambda) \|\mathbf{x} - \mathbf{y}\|_2^2$ for any pair $\mathbf{x}, \mathbf{y}$

Strongly convex function

Definition: reminder

Function $f : \mathcal{X} \subset \mathbb{R}^n \to \mathbb{R}$ is called **strongly** convex with constant $m > 0$, if $\mathcal{X}$ is convex set and $\forall \mathbf{x}_1, \mathbf{x}_2 \in \mathcal{X}$ и $\alpha \in [0, 1]$ we have:

$$f(\alpha \mathbf{x}_1 + (1-\alpha)\mathbf{x}_2) \leq \alpha f(\mathbf{x}_1) + (1-\alpha) f(\mathbf{x}_2) - \frac{m}{2}\alpha(1-\alpha)\|\mathbf{x}_1 - \mathbf{x}_2\|_2^2$$

Uniqueness of minimizer

If function f is strictly convex, then its minimizer is unique.

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- Then if we take λ sufficiently close to 1, we get a contradiction with the assumption that $\mathbf{x}_2$ is a minimizer

Facts about strongly convex functions

Claim

The following conditions are all equivalent to the strong convexity of a differentiable function f

- $f(\mathbf{y}) \geq f(\mathbf{x}) + \langle f'(\mathbf{x}), \mathbf{y} - \mathbf{x} \rangle + \frac{m}{2} \|\mathbf{y} - \mathbf{x}\|_2^2$
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Implications of strong conveity

If function f is strongly convex, then

- $\frac{1}{2}\|f'(\mathbf{x})\|_2^2 \geq m(f(\mathbf{x}) - f(\mathbf{x}^*))$
- $\|f'(\mathbf{x}) - f'(\mathbf{y})\|_2 \geq m\|\mathbf{x} - \mathbf{y}\|_2$

Summary on the convex functions properties

- Criterion of L-smoothness of convex function

Summary on the convex functions properties

- Criterion of L-smoothness of convex function
- Properties and facts about strongly convex functions

Summary on the convex functions properties

- Criterion of L-smoothness of convex function
- Properties and facts about strongly convex functions
- Why these characteristics of convex functions are important?