

Optimization methods
Lecture 2: Convex functions properties.
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

- ▶ L -smooth convex functions

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- ▶ More about strongly convex functions

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- ▶ More about strongly convex functions
- ▶ Matrix calculus: brief reminder
- ▶ Automatic differentiation technique

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

- ▶ Consider $f(\mathbf{x}) = \frac{1}{2}\mathbf{x}^\top \mathbf{A}\mathbf{x} - \mathbf{b}^\top \mathbf{x}$, where $\mathbf{A} \in \mathbf{S}^n$

Example

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$$\|\mathbf{A}\mathbf{x} - \mathbf{b} - \mathbf{A}\mathbf{y} + \mathbf{b}\|_2 \leq \|\mathbf{A}\|_2 \|\mathbf{x} - \mathbf{y}\|_2$$

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- ▶ Assume f is L -smooth, then consider the vector \mathbf{z} such that $\|\mathbf{z}\|_2 = 1$ and $\|\mathbf{A}\mathbf{z}\|_2 = \|\mathbf{A}\|_2$

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

Second order characteristic

Claim

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

- ▶ f is L -smooth
- ▶ $\|f''(\mathbf{x})\|_2 \leq L$ for any \mathbf{x}

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- ▶ $f(\mathbf{y}) \geq f(\mathbf{x}) + \langle f'(\mathbf{x}), \mathbf{y} - \mathbf{x} \rangle + \frac{1}{2L} \|f'(\mathbf{x}) - f'(\mathbf{y})\|_2^2$ for any pair \mathbf{x}, \mathbf{y}

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Strongly convex function

Definition: reminder

Function $f : \mathcal{X} \subset \mathbb{R}^n \rightarrow \mathbb{R}$ 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 convexity

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?

What are the next parts?

- ▶ Matrix calculus
- ▶ Automatic differentiation

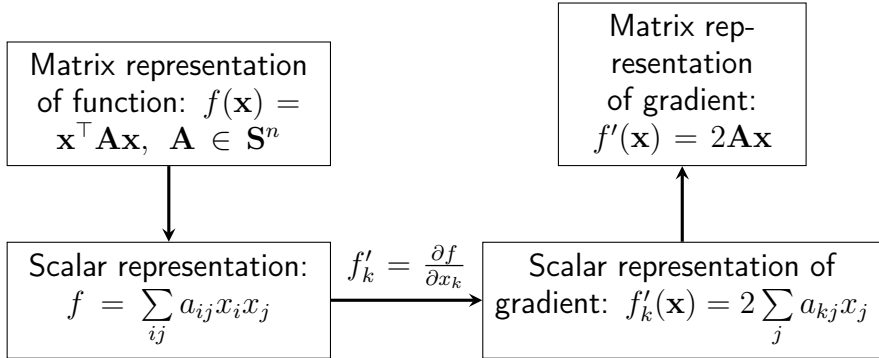
Main definitions

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

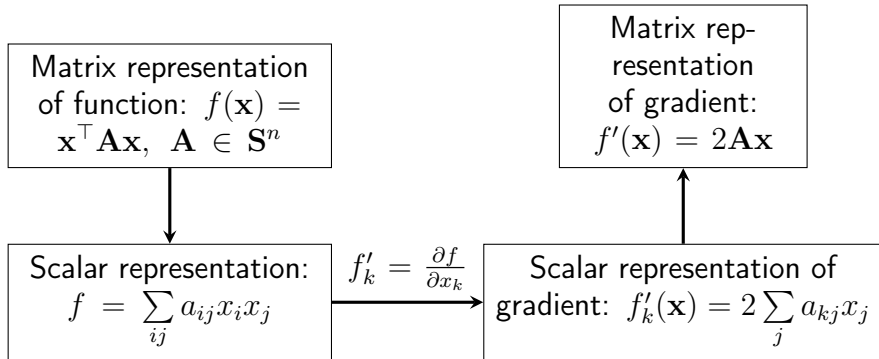
| D | E | G | Name |
|---------------------------|----------------|---------------------------|----------------------------------------------------|
| \mathbb{R} | \mathbb{R} | \mathbb{R} | Derivative, $f'(x)$ |
| \mathbb{R}^n | \mathbb{R} | \mathbb{R}^n | Gradient, $\frac{\partial f}{\partial x_i}$ |
| \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} | $\mathbb{R}^{m \times n}$ | $\frac{\partial^2 f}{\partial x_i \partial x_j}$ |

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

Main technique



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- ▶ There is another approach to compute gradients based on a set of rules
- ▶ You can use it if you are sure

Composition of functions: scalar case

- Let $f(\mathbf{x}) = g(u(\mathbf{x}))$, then $f'(\mathbf{x}) = \frac{\partial g}{\partial u} \frac{\partial u}{\partial \mathbf{x}}$

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1. ℓ_2 vector norm: $f(\mathbf{x}) = \|\mathbf{x}\|_2$
2. Trace of the matrix product: $f(\mathbf{X}) = \text{trace}(\mathbf{X}^\top \mathbf{X})$

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Compressed sensing

$$\begin{aligned} \min_{\mathbf{x}} \quad & \|\mathbf{x}\|_1 \\ \text{s.t.} \quad & \mathbf{Ax} = \mathbf{b} \end{aligned}$$

Summary on matrix calculus

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- ▶ Chain rule helps a lot

From chain rule to autodiff¹

Motivating example

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Compute $\frac{\partial f_i}{\partial x_k}$ for all i and fixed k , i.e. compute the j -th column of matrix \mathbf{J}_f

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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

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

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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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Forward mode

- ▶ Compute $\frac{\partial f}{\partial x_2}$
- ▶ $w_1 = x_1, w_2 = x_2$
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- ▶ $w_0 = 1$
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- ▶ Chain rule leads to autodiff technique
- ▶ Forward mode vs backward mode
- ▶ Typical use cases and issues