Optimization Theory

Lecture 02

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Matrix Calculus

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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

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

We have

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

and

$$d(XY) = (dX)Y + XdY, \quad d(AXB) = A \cdot dX \cdot B$$

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

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

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

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

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Topology in Euclidean Space

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

- 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 C of \mathbb{R}^d is called closed, if its complement $C^c = \mathbb{R}^d \backslash C$ is open.
- **3** A subset C of \mathbb{R}^d is called bounded, if there exists r > 0 such that $\|\mathbf{x}\|_2 < r$ for all $\mathbf{x} \in C$.
- **③** A subset 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 $C \in \mathbb{R}^n$ is defined as

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

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

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.

Matrix Calculus

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Convergence Rates

Assume the sequence $\{x_k\}$ converges to 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;
- superlinear: r = 1, C = 0;
- 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 $\{x_k\}$ converges to x^* . The sequence is said to converge R-linearly to x^* if there exists a sequence $\{\epsilon_k\}$ such that

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

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