

# DATA8004: Optimization for Statistical Learning

Subject Lecturer: Man-Chung YUE

Lecture 1  
Overview  
Preliminary materials

# What is optimization?

- Optimization is a mathematical subject that studies techniques for finding “best” solutions/decisions.
- An optimization problem takes the form of minimizing (or maximizing) an objective function subject to constraints:

$$\begin{array}{ll}\text{Minimize} & f(x) \\ \text{subject to} & x \in \Omega.\end{array}$$

Here:

- ★  $x \in \mathbb{R}^n$  is called decision variables.
- ★  $f$  is called the objective function.
- ★  $\Omega \subseteq \mathbb{R}^n$  is called the constraint set / feasible set / feasible region.

## Example: Objectives

### Objective functions:

- Linear:  $f(x) = c^T x$  for some  $c \in \mathbb{R}^n$ .
- Quadratic:  $f(x) = \frac{1}{2}x^T Gx + c^T x + \beta$  for some  $c \in \mathbb{R}^n$ ,  $\beta \in \mathbb{R}$ , and symmetric matrix  $G \in \mathbb{R}^{n \times n}$ .

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### Note:

- The symmetry of  $G$  can be assumed without loss of generality. Indeed, if  $H \in \mathbb{R}^{n \times n}$  and  $x \in \mathbb{R}^n$ , then

$$x^T H x = x^T H^T x = \frac{1}{2} x^T (H^T + H) x.$$

- For  $f(x) = \frac{1}{2}x^T Gx + c^T x + \beta$  with  $G \in \mathbb{R}^{n \times n}$  being symmetric, it holds that

$$\nabla f(x) = Gx + c.$$

## Example: Constraints

The feasible set  $\Omega$  can be specified by one or more of the following constraints.

- **Equality constraints:**

- $x_1^2 + x_2^2 + \cdots + x_n^2 = 1$  (sphere).
- $x_1 + x_2 + \cdots + x_n = 1$  (hyperplane).
- In  $\mathbb{R}^3$ :  $x_3 = x_1^2 + x_2^2$  (paraboloid).

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- In  $\mathbb{R}^3$ :  $x_3 \geq x_1^2 + x_2^2$ .

- **Box constraint:**  $\ell \leq x \leq u$ , where  $\ell \in \mathbb{R}^n$  and  $u \in \mathbb{R}^n$ . This means

$$\ell_i \leq x_i \leq u_i \quad \forall i.$$

- The problem is said to be **unconstrained** if  $\Omega = \mathbb{R}^n$ .

# Infimum

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- $s \geq \ell$  for every  $s \in S$ ; and
- for every  $\zeta > \ell$  ( $\zeta \in \mathbb{R}$ ), one can find  $s \in S$  so that  $s < \zeta$ .

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- The existence and uniqueness of  $\inf S$  follow from the **completeness of  $\mathbb{R}$** .
- Roughly speaking,  $\ell = \inf S$  is the **largest number** that is smaller than everything in  $S$ . However, it is **not necessary that  $\ell \in S$ !**  
e.g.,  $\inf\{e^{-x} : x \in \mathbb{R}\} = 0$ , but there is no  $a \in \mathbb{R}$  so that  $e^{-a} = 0$ .

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e.g.,  $\inf\{e^{-x} : x \in \mathbb{R}\} = 0$ , but there is no  $a \in \mathbb{R}$  so that  $e^{-a} = 0$ .
- For optimization problems, we refer to the infimum of the set  $\{f(x) : x \in \Omega\}$  as the **optimal value**.  
e.g., “Minimize  $e^{-x}$  subject to  $x \in \mathbb{R}$ ” has optimal value 0.

# Norm

**Definition:** A function  $\|\cdot\| : \mathbb{R}^n \rightarrow \mathbb{R}$  is called a (vector) **norm** if

- $\|x\| \geq 0$  for all  $x \in \mathbb{R}^n$ .
- $\|x\| = 0$  if and only if  $x = 0$ .
- $\|\alpha x\| = |\alpha| \|x\|$  for any  $\alpha \in \mathbb{R}$  and  $x \in \mathbb{R}^n$ .
- $\|x + y\| \leq \|x\| + \|y\|$  for any  $x, y \in \mathbb{R}^n$ .

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**Note:**

- The following are some commonly used norms:
  - ★  $\ell_1$  norm:  $\|x\|_1 := \sum_{i=1}^n |x_i|$ .
  - ★  $\ell_2$  norm:  $\|x\|_2 := \sqrt{\sum_{i=1}^n |x_i|^2}$ .
  - ★  $\ell_\infty$  norm:  $\|x\|_\infty := \max_{1 \leq i \leq n} |x_i|$ .

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  - ★  $\ell_\infty$  norm:  $\|x\|_\infty := \max_{1 \leq i \leq n} |x_i|$ .
- For instance, if  $x = [3 \quad -4 \quad 5]^T$ , then  $\|x\|_1 = 12$ ,  $\|x\|_2 = \sqrt{50}$  and  $\|x\|_\infty = 5$ .

## Norm cont.

**Theorem 1.1:** Let  $\|\cdot\|$  be a norm. Then there exist positive numbers  $C_1$  and  $C_2$  so that for all  $x \in \mathbb{R}^n$ ,

$$C_1 \sum_{i=1}^n |x_i| \leq \|x\| \leq C_2 \sum_{i=1}^n |x_i|$$

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**Theorem 1.1:** Let  $\|\cdot\|$  be a norm. Then there exist positive numbers  $C_1$  and  $C_2$  so that for all  $x \in \mathbb{R}^n$ ,

$$C_1 \sum_{i=1}^n |x_i| \leq \|x\| \leq C_2 \sum_{i=1}^n |x_i|$$

**Proof:** We will only prove the **second inequality**. The first inequality is a consequence of **compactness** and is left as an exercise later.

To prove the **second inequality**, notice that for any  $x \in \mathbb{R}^n$ , we have

$$\|x\| = \left\| \sum_{i=1}^n x_i e_i \right\| \leq \sum_{i=1}^n \|x_i e_i\| = \sum_{i=1}^n |x_i| \|e_i\| \leq C_2 \sum_{i=1}^n |x_i|,$$

where  $C_2 := \max_{1 \leq i \leq n} \|e_i\|$ .

## Convergence and norm

**Definition:** Let  $\{x^k\} \subset \mathbb{R}^n$  be a sequence and  $x^* \in \mathbb{R}^n$ . We say that  $\lim_{k \rightarrow \infty} x^k = x^*$  if

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**Corollary 1.1:** Let  $\|\cdot\|$  be a norm,  $\{x^k\} \subset \mathbb{R}^n$  be a sequence and  $x^* \in \mathbb{R}^n$ . Then  $\lim_{k \rightarrow \infty} x^k = x^*$  if and only if  $\lim_{k \rightarrow \infty} \|x^k - x^*\| = 0$ .

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**Proof:** Note that  $\lim_{k \rightarrow \infty} x_i^k = x_i^*$  for all  $i$  is the same as  $\lim_{k \rightarrow \infty} |x_i^k - x_i^*| = 0$  for all  $i$ , which in turn is equivalent to

$$\lim_{k \rightarrow \infty} \sum_{i=1}^n |x_i^k - x_i^*| = 0.$$

The conclusion now follows from this and **Theorem 1.1**.

# Matrix norm

**Definition:** A function  $\|\cdot\| : \mathbb{R}^{n \times n} \rightarrow \mathbb{R}$  is called a **matrix norm** if

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- $\|\alpha A\| = |\alpha| \|A\|$  for any  $\alpha \in \mathbb{R}$  and  $A \in \mathbb{R}^{n \times n}$ .
- $\|A + B\| \leq \|A\| + \|B\|$  for any  $A, B \in \mathbb{R}^{n \times n}$ .
- $\|AB\| \leq \|A\| \|B\|$  for any  $A, B \in \mathbb{R}^{n \times n}$ .

## Matrix norm

The following theorem provides a large source of matrix norms.

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- The maximum is actually **attained** at some  $x$  satisfying  $\|x\| = 1$ . We will need this fact below.
- The attainment is due to **compactness** of the set  $\{x : \|x\| = 1\}$ : the continuous function  $x \mapsto \|Ax\|$  attains its maximum over the compact set  $\{x : \|x\| = 1\}$ .

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**Property 5:** By the definition of  $\|\cdot\|$ , we have for all  $x$  with  $\|x\| = 1$  that

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Consider any  $x \neq 0$ . Then  $\|\frac{x}{\|x\|}\| = 1$  and hence  $\|A\frac{x}{\|x\|}\| \leq \|A\|$ . Thus,  $\|Ax\| \leq \|A\|\|x\|$  for any  $x \neq 0$ , and hence for all  $x$  since the inequality holds trivially for  $x = 0$ .

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Then

$$\|AB\| = \max_{\|x\|=1} \|A(Bx)\| \leq \max_{\|x\|=1} \|A\| \|Bx\| = \|A\| \|B\|.$$

## Example 1

**Example:** The following functions are matrix norms:

- $\|A\|_1 = \max_j \sum_{i=1}^n |a_{ij}|$  (maximum of the  $\ell_1$  norms of columns).  
Moreover, this is an **induced matrix norm**:

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- $\|A\|_F = \sqrt{\sum_{i=1}^n \sum_{j=1}^n |a_{ij}|^2}$ . This is known as the Fröbenius norm.

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- $\|A\|_\infty = \max\{3, 7\} = 7.$
- $\|A\|_F = \sqrt{1^2 + 2^2 + 3^2 + 4^2} = \sqrt{30}.$

## Lower Semicontinuity

**Definition:** A function  $f : \Omega \rightarrow \mathbb{R}$  is said to be **lower semicontinuous** at a point  $x \in \Omega$  if for any sequence  $\{x^k\}$  converging to  $x$ , it holds that

$$f(x) \leq \liminf_{i \rightarrow \infty} f(x^k).$$

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**Example:**

- The following function is lower semicontinuous:

$$f(x) = \begin{cases} x^2 & \text{if } x \leq 0, \\ x^2 + 1 & \text{if } x > 0. \end{cases}$$

- But the following function is not lower semicontinuous:

$$f(x) = \begin{cases} x^2 & \text{if } x < 0, \\ x^2 + 1 & \text{if } x \geq 0. \end{cases}$$

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**Theorem 1.3: (Bolzano-Weierstrass)**

Let  $\Omega \subset \mathbb{R}^n$  be bounded. If  $\{x^k\} \subseteq \Omega$ , then there exists a convergent subsequence  $\{x^{k_i}\}$ , i.e., for some  $x^* \in \mathbb{R}^n$ , we have

$$\lim_{i \rightarrow \infty} x^{k_i} = x^*.$$

**Note:** A closed and bounded set in  $\mathbb{R}^n$  is called a **compact set**.

## Existence of minimizers

**Theorem 1.4:** (Existence of minimizers)

Let  $\Omega \subset \mathbb{R}^n$  be a nonempty compact set and  $f : \Omega \rightarrow \mathbb{R}$  be lower semicontinuous on  $\Omega$ . Then  $f$  achieves its infimum value over  $\Omega$ , i.e., there exists  $x^* \in \Omega$  so that  $f(x^*) = \inf\{f(x) : x \in \Omega\}$ .

**Proof:** Let  $\ell := \inf\{f(x) : x \in \Omega\}$  and let  $\{\lambda_k\} \subset \mathbb{R}$  be a strictly decreasing sequence converging to  $\ell$ .

By the definition of infimum, for each  $\lambda_k$ ,  $k = 1, 2, \dots$ , there exists  $x^k \in \Omega$  so that

$$\ell \leq f(x^k) < \lambda_k.$$

Since  $\{x^k\} \subseteq \Omega$  and  $\Omega$  is bounded, by Bolzano-Weierstrass theorem there exists a subsequence  $\{x^{k_i}\}$  converging to some  $x^* \in \mathbb{R}^n$ . Since  $\{x^{k_i}\}$  is itself a sequence in  $\Omega$  and  $\Omega$  is closed,  $x^* \in \Omega$ . Thus,

$$\ell \leq f(x^*) \leq \liminf_{i \rightarrow \infty} f(x^{k_i}) \leq \lim_{i \rightarrow \infty} \lambda_{k_i} = \ell,$$

showing that  $f$  achieves  $\ell$  at  $x^* \in \Omega$ .

# Positive semidefinite matrices

**Definition:** (Positive semidefinite matrices)

Let  $A \in \mathbb{R}^{n \times n}$  be symmetric. We say that  $A$  is positive semidefinite if  $x^T A x \geq 0$  for all  $x \in \mathbb{R}^n$ .

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**Example:** The matrix

$$A = \begin{bmatrix} 3 & 1 \\ 1 & 2 \end{bmatrix}$$

is positive semidefinite. To see this, note that

$$\begin{aligned} x^T A x &= 3x_1^2 + 2x_1 x_2 + 2x_2^2 \\ &= 2x_1^2 + (x_1 + x_2)^2 + x_2^2 \geq 0. \end{aligned}$$

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**Question:** Easier way to test for positive semidefiniteness?

## Positive semidefinite matrices cont.

**Theorem 1.5:** Let  $A \in \mathbb{R}^{n \times n}$  be **symmetric**. The following statements are equivalent.

1. All eigenvalues of  $A$  are **nonnegative**.
2. There exists  $M \in \mathbb{R}^{n \times n}$  so that  $A = M^T M$ .
3.  $A$  is **positive semidefinite**.

**Theorem 1.5 proof sketch:**

(1)  $\Rightarrow$  (2): Since  $A$  is symmetric, there exist an **orthogonal matrix**  $U$  and a **diagonal matrix**  $D$  so that  $A = UDU^T$ .

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Since all eigenvalues of  $A$  are **nonnegative**, we have  $D_{ii} \geq 0$  for all  $i$ .

Let  $W \in \mathbb{R}^{n \times n}$  be the matrix so that

$$W_{ij} = \begin{cases} \sqrt{D_{ii}} & \text{if } i = j, \\ 0 & \text{otherwise.} \end{cases}$$

## Positive semidefinite matrices cont.

Theorem 1.5 proof sketch cont.:

Then  $W = W^T$  and

$$A = U(WW)U^T = (WU^T)^T(WU^T).$$

Thus, (2) holds with  $M = WU^T$ .

## Positive semidefinite matrices cont.

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(2)  $\Rightarrow$  (3): Let  $x \in \mathbb{R}^n$  and  $y := Mx$ . Then

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(3)  $\Rightarrow$  (1): Let  $\lambda$  be an eigenvalue of  $A$  with a corresponding eigenvector  $v$ , i.e.,

$$v \neq 0 \text{ and } Av = \lambda v.$$

Then  $v^T v > 0$  and

$$\lambda v^T v = v^T Av \geq 0.$$

Thus, it follows that  $\lambda \geq 0$ .

# Positive definite matrices

**Definition:** A symmetric matrix  $A \in \mathbb{R}^{n \times n}$  is called **positive definite** if  $x^T Ax > 0$  for all  $x \in \mathbb{R}^n \setminus \{0\}$ .

**Notation:**  $A \succ 0$ .

**Theorem 1.6:** For a symmetric matrix  $A \in \mathbb{R}^{n \times n}$ , the following statements are equivalent:

- All eigenvalues of  $A$  are **positive**.
- There exists an **invertible** matrix  $M \in \mathbb{R}^{n \times n}$  so that  $A = M^T M$ .
- $A$  is **positive definite**.

**Note:** Let  $A \succ 0$ , then

- $A^{-1} \succ 0$  and  $\lambda_{\min}(A) = \inf\{x^T Ax : \|x\|_2 = 1\}$ .
- $\|A\|_2 = \lambda_{\max}(A) = [\lambda_{\min}(A^{-1})]^{-1}$ .

# Block matrix multiplication

Let  $A \in \mathbb{R}^{m \times n}$  and  $B \in \mathbb{R}^{n \times p}$  be **partitioned** so that

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \text{ and } B = \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix},$$

where

- $A_{11} \in \mathbb{R}^{m_1 \times n_1}$ ,  $A_{12} \in \mathbb{R}^{m_1 \times n_2}$ ,  $A_{21} \in \mathbb{R}^{m_2 \times n_1}$  and  $A_{22} \in \mathbb{R}^{m_2 \times n_2}$ ;
- $B_{11} \in \mathbb{R}^{n_1 \times p_1}$ ,  $B_{12} \in \mathbb{R}^{n_1 \times p_2}$ ,  $B_{21} \in \mathbb{R}^{n_2 \times p_1}$  and  $B_{22} \in \mathbb{R}^{n_2 \times p_2}$ .

Then it holds that

$$AB = \begin{bmatrix} A_{11}B_{11} + A_{12}B_{21} & A_{11}B_{12} + A_{12}B_{22} \\ A_{21}B_{11} + A_{22}B_{21} & A_{21}B_{12} + A_{22}B_{22} \end{bmatrix}.$$

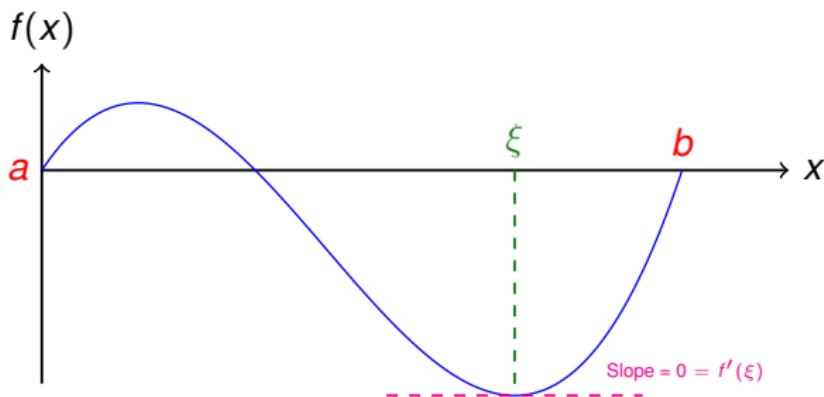
**Roughly speaking**, whenever the sizes match, matrix blocks can be multiplied as if they were numbers.

# Mean value theorem

Theorem 1.7. (Rolle's mean value theorem)

Let  $f$  be continuous on  $[a, b]$  and differentiable in  $(a, b)$ . If  $f(b) = f(a)$ , then there exists  $\xi \in (a, b)$  so that

$$f'(\xi) = 0.$$



# Taylor's theorem

**Theorem 1.8.** (Taylor's theorem with remainder term)

Suppose that  $f$  is  $(n + 1)$  times differentiable on an open interval containing  $[a, b]$ . Then

$$\begin{aligned}f(b) &= f(a) + f'(a)(b - a) + \frac{f''(a)}{2!}(b - a)^2 + \cdots + \frac{f^{(n)}(a)}{n!}(b - a)^n \\&\quad + \frac{f^{(n+1)}(\xi)}{(n+1)!}(b - a)^{n+1}\end{aligned}$$

for some  $\xi \in (a, b)$ .

## Taylor's theorem cont.

Proof of Theorem 1.8.: Define

$$T_n(x) = f(a) + f'(a)(x - a) + \frac{f''(a)}{2!}(x - a)^2 + \cdots + \frac{f^{(n)}(a)}{n!}(x - a)^n$$

and define  $K$  so that

$$f(b) = T_n(b) + K(b - a)^{n+1}.$$

## Taylor's theorem cont.

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We need to show that  $K$  is given by  $\frac{f^{(n+1)}(\xi)}{(n+1)!}$  for some  $\xi \in (a, b)$ .

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To this end, consider

$$g(x) = f(x) - T_n(x) - K(x - a)^{n+1}.$$

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To this end, consider

$$g(x) = f(x) - T_n(x) - K(x - a)^{n+1}.$$

Note:  $g(a) = 0$  and  $g(b) = 0$ . Thus, Rolle's mean value theorem gives the existence of  $a < \xi_1 < b$  with  $g'(\xi_1) = 0$ .

## Taylor's theorem cont.

Proof of Theorem 1.8. cont.:

Note that

$$\begin{aligned}g'(x) &= f'(x) - T'_n(x) - K(n+1)(x-a)^n \\&= f'(x) - f'(a) - f''(a)(x-a) - \cdots - \frac{f^{(n)}(a)}{(n-1)!}(x-a)^{n-1} \\&\quad - K(n+1)(x-a)^n.\end{aligned}$$

Hence  $g'(a) = g'(\xi_1) = 0$ . Thus, again by **Rolle's mean value theorem**, there exists  $a < \xi_2 < \xi_1$  so that  $g''(\xi_2) = 0$ .

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Hence  $g'(a) = g'(\xi_1) = 0$ . Thus, again by Rolle's mean value theorem, there exists  $a < \xi_2 < \xi_1$  so that  $g''(\xi_2) = 0$ .

Proceeding inductively, there exist  $a < \xi_n < \xi_{n-1} < \cdots < \xi_1 < b$  so that

$$g'(\xi_1) = g''(\xi_2) = \cdots = g^{(n)}(\xi_n) = 0.$$

## Taylor's theorem cont.

**Proof of Theorem 1.8. cont.**: Finally, notice that

$$\begin{aligned}g^{(n)}(x) &= f^{(n)}(x) - T_n^{(n)}(x) - K(n+1)!(x-a) \\&= f^{(n)}(x) - f^{(n)}(a) - K(n+1)!(x-a).\end{aligned}$$

## Taylor's theorem cont.

**Proof of Theorem 1.8. cont.**: Finally, notice that

$$\begin{aligned}g^{(n)}(x) &= f^{(n)}(x) - T_n^{(n)}(x) - K(n+1)!(x-a) \\&= f^{(n)}(x) - f^{(n)}(a) - K(n+1)!(x-a).\end{aligned}$$

Since  $g^{(n)}(a) = g^{(n)}(\xi_n) = 0$ , **Rolle's mean value theorem** gives the existence of  $\xi_{n+1} \in (a, \xi_n) \subset (a, b)$  such that

$$0 = g^{(n+1)}(\xi_{n+1}) = f^{(n+1)}(\xi_{n+1}) - K(n+1)!,$$

which gives

$$K = \frac{f^{(n+1)}(\xi_{n+1})}{(n+1)!}.$$

## Gradient and Hessian

- Let  $f \in C^1(\mathbb{R}^n)$ . Its gradient at an  $x \in \mathbb{R}^n$  is

$$\nabla f(x) := \begin{bmatrix} \frac{\partial f}{\partial x_1}(x) \\ \frac{\partial f}{\partial x_2}(x) \\ \vdots \\ \frac{\partial f}{\partial x_n}(x) \end{bmatrix}.$$

- Let  $f \in C^2(\mathbb{R}^n)$ . Its Hessian at an  $x \in \mathbb{R}^n$  is

$$\nabla^2 f(x) := \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2}(x) & \frac{\partial^2 f}{\partial x_2 \partial x_1}(x) & \cdots & \frac{\partial^2 f}{\partial x_n \partial x_1}(x) \\ \frac{\partial^2 f}{\partial x_1 \partial x_2}(x) & \cdots & \cdots & \frac{\partial^2 f}{\partial x_n \partial x_2}(x) \\ \vdots & \ddots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_1 \partial x_n}(x) & \cdots & \cdots & \frac{\partial^2 f}{\partial x_n^2}(x) \end{bmatrix}.$$

**Note:** Since  $f \in C^2(\mathbb{R}^n)$ , we have  $\frac{\partial^2 f}{\partial x_i \partial x_j} = \frac{\partial^2 f}{\partial x_j \partial x_i}$  for all  $i$  and  $j$ .

# High-dimensional Taylor's theorem

Theorem 1.9. (Taylor's theorem in  $\mathbb{R}^n$  with remainder term)

- Let  $f \in C^1(\mathbb{R}^n)$ ,  $x$  and  $y \in \mathbb{R}^n$ . Then there exists  $\xi \in \{(1-s)x + sy : s \in (0, 1)\}$  such that

$$f(y) = f(x) + [\nabla f(\xi)]^T (y - x).$$

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**Proof sketch:** Consider the function  $\psi(t) := f((1-t)x + ty)$ . Observe that  $\psi$  is  $C^1$  (resp.  $C^2$ ) if  $f$  is so.

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$$\psi'(t) = [\nabla f((1-t)x + ty)]^T (y - x), \quad \psi''(t) = (y - x)^T [\nabla^2 f((1-t)x + ty)] (y - x).$$

Now apply Taylor's theorem in 1 dimension to  $\psi$ .

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You do not need to follow this convention in your writings.