Advanced Mathematical Methods

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2 Multivariate Calculus

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Outline: Multivariate Calculus

2.1 Recap: Differentiation rules

2.2 Real valued and vector-valued functions

2.3 Derivatives

2.4 Differentiation of linear and quadratic forms

2.5 Taylor series approximations

Readings

- Miroslav Lovric. *Vector Calculus*.
  Wiley, 2007, Chapter 2
- J. E. Marsden and A. J. Tromba. *Vector Calculus*.
  W H Freeman and Company, fifth edition, 2003, Chapters 2-3

2.1 Recap: Differentiation rules

Assume that functions $f(x), g(x)$ and $h(x)$ are once differentiable.

Basic rules:

1. $f(x) = x^a$ and $f'(x) = ax^{a-1}$
2. $f(x) = \frac{1}{x^a} = x^{-a}$ and $f'(x) = -ax^{-a-1}$
3. $f(x) = a^x$ and $f'(x) = \ln(a)a^x$
4. $f(x) = e^x$ and $f'(x) = e^x$

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2.1 Recap: Differentiation rules

Product rule

$$f(x) = g(x) \cdot h(x) \quad \text{and} \quad f'(x) = g'(x) \cdot h(x) + g(x) \cdot h'(x)$$

Chain rule

$$f(x) = g(h(x)) \quad \text{and} \quad f'(x) = g'(h(x)) \cdot h'(x)$$

Quotient rule

$$f(x) = \frac{g(x)}{h(x)} \quad \text{and} \quad f'(x) = \frac{g'(x) \cdot h(x) - g(x) \cdot h'(x)}{(h(x))^2}$$

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2.2 Real valued functions

A function whose domain is a subset U of $\mathbb{R}^m$, $m \geq 1$ and whose range is contained in $\mathbb{R}^n$ is called a **real-valued function (scalar function) of m variables** if $n = 1$

Notation:

- $f : U \subseteq \mathbb{R}^m \to \mathbb{R}$ describes a scalar function
- a scalar function assigns a unique *real number* $f(\boldsymbol{x}) = f(x_1, x_2 \cdots x_m)$ to each element $\boldsymbol{x} = (x_1, x_2 \cdots x_m)$ in its domain U

2.2 Vector-valued functions

A function whose domain is a subset U of $\mathbb{R}^m$, $m \geq 1$ and whose range is contained in $\mathbb{R}^n$ is called a **vector-valued function (vector function) of m variables** if $n > 1$

Notation:

- $\boldsymbol{F} : U \subseteq \mathbb{R}^m \to \mathbb{R}^n$ describes a vector function
- a vector function assigns a unique *vector* $\boldsymbol{F}(\boldsymbol{x}) = \boldsymbol{F}(x_1, x_2 \cdots x_m) \in \mathbb{R}^n$ to each $\boldsymbol{x} = (x_1, x_2 \cdots x_m) \in U$

2.2 Real valued and vector-valued functions

We write:

$$\boldsymbol{F}(x_1, x_2 \cdots x_m) = (F_1(x_1, x_2 \cdots, x_m), \cdots, F_n(x_1, x_2 \cdots, x_m))$$
$$\text{or} = (F_1(\boldsymbol{x}), \cdots, F_n(\boldsymbol{x}))$$

- $F_1 \cdots F_n$ are the **component functions** of $\boldsymbol{F}$ (and **real-valued functions** of $x_1 \cdots x_m$)

2.2 Real valued and vector-valued functions

Examples:

- **Distance function:**
  $f(x, y, z) = \sqrt{x^2 + y^2 + z^2}$ measures the distance from the point (x, y, z) to the origin.
  $\rightarrow$ real-valued function of three variables defined on $U = \mathbb{R}^3$
- **Projection function:**
  $\boldsymbol{F}(x, y, z) = (x, y)$ is a vector-valued function of three variables that assigns to every vector $(x, y, z) \in \mathbb{R}^3$ its projection (x, y) onto the xy-plane in

2.3 Derivatives

Open sets in $\mathbb{R}^m$:
A set $U \subseteq \mathbb{R}^m$ is **open** in $\mathbb{R}^m$ if and only if all of its points are interior points

2.3 Derivatives

Partial Derivative:
Let $f : U \subseteq \mathbb{R}^m \to \mathbb{R}$ be a real valued function of m variables $x_1, x_2 \cdots, x_m$ defined on an open set U in $\mathbb{R}^m$

Partial derivative (real-valued function)

$$\frac{\partial f}{\partial x_i}(x_1, x_2 \cdots, x_m) = \lim_{h \to 0} \frac{f(x_1, \cdots, x_i + h, \cdots, x_m) - f(x_1, \cdots, x_i, \cdots, x_m)}{h},$$

if the limit exists.

2.3 Derivatives

Derivative of a function of several variables:
$\boldsymbol{F} : U \subseteq \mathbb{R}^m \to \mathbb{R}^n$

$$D\boldsymbol{F}(x) = \begin{pmatrix} \frac{\partial F_1}{\partial x_1}(\boldsymbol{x}) & \frac{\partial F_1}{\partial x_2}(\boldsymbol{x}) & \dots & \frac{\partial F_1}{\partial x_m}(\boldsymbol{x}) \\ \frac{\partial F_2}{\partial x_1}(\boldsymbol{x}) & \frac{\partial F_2}{\partial x_2}(\boldsymbol{x}) & \dots & \frac{\partial F_2}{\partial x_m}(\boldsymbol{x}) \\ \vdots & \vdots & & \vdots \\ \frac{\partial F_n}{\partial x_1}(\boldsymbol{x}) & \frac{\partial F_n}{\partial x_2}(\boldsymbol{x}) & \dots & \frac{\partial F_n}{\partial x_m}(\boldsymbol{x}) \end{pmatrix}$$

Provided that all partial derivatives exist at $\boldsymbol{x}$

2.3 Derivatives

The $i - th$ column is the matrix

$$\frac{\partial \boldsymbol{F}}{\partial x_i}(\boldsymbol{x}) = \boldsymbol{F}_{x_i}(\boldsymbol{x}) = \begin{pmatrix} \frac{\partial F_1}{\partial x_j}(\boldsymbol{x}) \\ \frac{\partial F_2}{\partial x_i}(\boldsymbol{x}) \\ \vdots \\ \frac{\partial F_n}{\partial x_i}(\boldsymbol{x}) \end{pmatrix}$$

which consists of partial derivatives of the component functions $F_1, \cdots, F_n$ with respect to the same variable x_i, evaluated at $\boldsymbol{x}$

2.3 Derivatives

Gradient:
Consider the special case $f : U \subset \mathbb{R}^n \to \mathbb{R}$
Here $Df(\boldsymbol{x}) = [\frac{\partial f}{\partial x_1}, \cdots, \frac{\partial f}{\partial x_n}]$ is a $1 \times n$ matrix

We can form the corresponding vector $(\frac{\partial f}{\partial x_1}, \cdots, \frac{\partial f}{\partial x_n})$, called the **gradient** of f and denoted by ∇f.

2.3 Derivatives

Higher order derivatives:
Suppose that $f : U \subset \mathbb{R}^n \to \mathbb{R}$ has second order continuous derivatives $\left(\frac{\partial^2 f}{\partial x_i \partial x_j}\right)(\boldsymbol{x}_0)$, for $i, j = 1, \cdots, n$, at a point $\boldsymbol{x}_0 \in U$.
The **Hessian of** f is given as

$$\begin{pmatrix} \frac{\partial^2 f}{\partial x_1 \partial x_1} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \vdots & & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \cdots & \frac{\partial^2 f}{\partial x_n \partial x_n} \end{pmatrix}$$

2.4 Differentiation of linear and quadratic forms

For a given $n \times 1$ vector $\boldsymbol{a}$ and any $n \times 1$ vector $\boldsymbol{x}$, consider the real-valued linear function $f(\boldsymbol{x}) = \boldsymbol{a}'\boldsymbol{x}$. The derivative of f with respect to $\boldsymbol{x}$ is

$$\frac{\partial f(\boldsymbol{x})}{\partial \boldsymbol{x}} = \boldsymbol{a}'.$$

For a quadratic form $Q(\boldsymbol{x}) = \boldsymbol{x}'\boldsymbol{A}\boldsymbol{x}$ the derivative of Q with respect to $\boldsymbol{x}$ is

$$\frac{\partial Q(\boldsymbol{x})}{\partial \boldsymbol{x}} = 2\boldsymbol{x}'\boldsymbol{A}.$$

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2.5 Taylor series approximations

Single-variable case

Suppose that at least $k+1$ derivatives of a function $f(x)$ exist and are continuous in a neighborhood of x_0. Taylor's theorem asserts that

$$f(x_0 + h) = \sum_{i=0}^{k} \frac{f^{(k)}(x_0)}{i!} h^i + R_k(x_0, h)$$

where

$$R_k(x_0, h) = \int_{x_0}^{x_0+h} \frac{(x_0 + h - \tau)^k}{k!} f^{(k+1)}(\tau) d\tau.$$

2.5 Taylor series approximations

Multi-variable case

Theorem: First-order Taylor formula

Let $f : U \subset \mathbb{R}^n \to \mathbb{R}$ be differentiable at $\boldsymbol{x}_0 \in U$. Then

$$f(\boldsymbol{x}_0 + \boldsymbol{h}) = f(\boldsymbol{x}_0) + \sum_{i=1}^{n} h_i \frac{\partial f}{\partial x_i}(\boldsymbol{x}_0) + R_1(\boldsymbol{x}_0, \boldsymbol{h}),$$

where $R_1(\boldsymbol{x}_0, \boldsymbol{h})/d(h) \to 0$ as $\boldsymbol{h} \to 0$ in $\mathbb{R}^n$.

2.5 Taylor series approximations

Multi-variable case

Theorem: Second-order Taylor formula

Let $f : U \subset \mathbb{R}^n \to \mathbb{R}$ have continuous partial derivatives of third order. Then

$$\begin{aligned} f(\boldsymbol{x}_0 + \boldsymbol{h}) &= f(\boldsymbol{x}_0) + \sum_{i=1}^{n} h_i \frac{\partial f}{\partial x_i}(\boldsymbol{x}_0) \\ &\quad + \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} h_i h_j \frac{\partial^2 f}{\partial x_i \partial x_j}(\boldsymbol{x}_0) + R_2(\boldsymbol{x}_0, \boldsymbol{h}), \end{aligned}$$

where $R_2(\boldsymbol{x}_0, \boldsymbol{h})/d(h)^2 \to 0$ as $\boldsymbol{h} \to 0$.