

Advanced Mathematical Methods

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2 Multivariate Calculus

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Outline: Multivariate Calculus

- 2.1 Real valued and vector-valued functions
- 2.2 Derivatives
- 2.3 Differentiation of linear and quadratic forms
- 2.4 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

Online References

MIT course on Multivariable Calculus (Herbert Gross)

- ▶ Lecture 3: Directional Derivatives

MIT course on Multivariable Calculus (Denis Auroux)

- ▶ Session 34: The Chain Rule with More Variables
- ▶ Session 38: Directional Derivatives

2.1 Real valued and 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 **real-valued function (scalar function) of m variables** if $n = 1$ and a **vector-valued function (vector function) of m variables** if $n > 1$

Notation:

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

2.1 Real valued and vector-valued functions

We write:

$$\begin{aligned} \mathbf{F}(x_1, x_2 \cdots x_m) &= (F_1(x_1, x_2 \cdots, x_m), \cdots, F_n(x_1, x_2 \cdots, x_m)) \\ &\text{or} = (F_1(\mathbf{x}), \cdots, F_n(\mathbf{x})) \end{aligned}$$

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

2.1 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.

→ real-valued function of three variables defined on $U = \mathbb{R}^3$

▶ **Projection function:**

$F(x, y, z) = (x, y)$ 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

1.2 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

2.2 Derivatives

Partial Derivative:

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

Partial derivative (real-valued function)

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

if the limit exists.

2.2 Derivatives

Derivative of a function of several variables:

$$F : U \subseteq \mathbb{R}^m \rightarrow \mathbb{R}^n$$

$$DF(\mathbf{x}) = \begin{pmatrix} \frac{\partial F_1}{\partial x_1}(\mathbf{x}) & \frac{\partial F_1}{\partial x_2}(\mathbf{x}) & \dots & \frac{\partial F_1}{\partial x_m}(\mathbf{x}) \\ \frac{\partial F_2}{\partial x_1}(\mathbf{x}) & \frac{\partial F_2}{\partial x_2}(\mathbf{x}) & \dots & \frac{\partial F_2}{\partial x_m}(\mathbf{x}) \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial F_n}{\partial x_1}(\mathbf{x}) & \frac{\partial F_n}{\partial x_2}(\mathbf{x}) & \dots & \frac{\partial F_n}{\partial x_m}(\mathbf{x}) \end{pmatrix}$$

Provided that all partial derivatives exist at \mathbf{x}

2.2 Derivatives

The i – th column is the matrix

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

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

2.2 Derivatives

Gradient:

Consider the special case $f : U \subset \mathbb{R}^n \rightarrow \mathbb{R}$

Here $Df(\mathbf{x}) = [\frac{\partial f}{\partial x_1}, \dots, \frac{\partial f}{\partial x_n}]$ is a $1 \times n$ matrix

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

2.2 Derivatives

Higher order derivatives:

Suppose that $f : U \subset \mathbb{R}^n \rightarrow \mathbb{R}$ has second order continuous derivatives $\left(\frac{\partial^2 f}{\partial x_i \partial x_j} \right) (\mathbf{x}_0)$, for $i, j = 1, \dots, n$, at a point $\mathbf{x}_0 \in U$.

The **Hessian** of f is given as

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

2.3 Differentiation of linear and quadratic forms

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

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

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

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

2.4 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

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

where

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

2.4 Taylor series approximations

Multi-variable case

Theorem: First-order Taylor formula

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

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

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

2.4 Taylor series approximations

Multi-variable case

Theorem: Second-order Taylor formula

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

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

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