Analysis III for engineering study programs

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Technische Universität Hamburg–Harburg Wintersemester 2021/22

based on slides of Prof. Jens Struckmeier from Wintersemster 2020/21

Content of the course Analysis III.

- Partial derivatives, differential operators.
- 2 Vector fields, total differential, directional derivative.
- 3 Mean value theorems, Taylor's theorem.
- 4 Extrem values, implicit function theorem.
- Implicit rapresentaion of curves and surfces.
- **6** Extrem values under equality constraints.
- Newton-method, non-linear equations and the least squares method.
- Multiple integrals, Fubini's theorem, transformation theorem.
- Potentials, Green's theorem, Gauß's theorem.
- Green's formulas, Stokes's theorem.



Chapter 1. Multi variable differential calculus

1.1 Partial derivatives

Let

$$f(x_1,\ldots,x_n)$$
 a scalar function depending n variables

Example: The constitutive law of an ideal gas pV = RT.

Each of the 3 quantities p (pressure), V (volume) and T (emperature) can be expressed as a function of the others (R is the gas constant)

$$p = p(V, t) = \frac{RT}{V}$$

$$V = V(p, T) = \frac{RT}{p}$$

$$T = T(p, V) = \frac{pV}{R}$$

1.1. Partial derivatives

Definition: Let $D \subset \mathbb{R}^n$ be open, $f : D \to \mathbb{R}$, $x^0 \in D$.

• f is called partially differentiable in x^0 with respect to x_i if the limit

$$\frac{\partial f}{\partial x_{i}}(x^{0}) := \lim_{t \to 0} \frac{f(x^{0} + te_{i}) - f(x^{0})}{t}$$

$$= \lim_{t \to 0} \frac{f(x_{1}^{0}, \dots, x_{i}^{0} + t, \dots, x_{n}^{0}) - f(x_{1}^{0}, \dots, x_{i}^{0}, \dots, x_{n}^{0})}{t}$$

exists. e_i denotes the i-th unit vector. The limit is called partial derivative of f with respect to x_i at x^0 .

• If at every point x^0 the partial derivatives with respect to every variable $x_i, i = 1, \ldots, n$ exist and if the partial derivatives are **continuous functions** then we call f continuous partial differentiable or a \mathcal{C}^1 -function.

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Examples.

Consider the function

$$f(x_1, x_2) = x_1^2 + x_2^2$$

At any point $x^0 \in \mathbb{R}^2$ there exist both partial derivatives and both partial derivatives are continuous:

$$\frac{\partial f}{\partial x_1}(x^0) = 2x_1, \qquad \frac{\partial f}{\partial x_2}(x^0) = 2x_2$$

Thus f is a C^1 -function.

The function

$$f(x_1, x_2) = x_1 + |x_2|$$

at $x^0 = (0,0)^T$ is partial differentiable with respect to x_1 , but the partial derivative with respect to x_2 does **not** exist!

An engineering example.

The acoustic pressure of a one dimensional acoustic wave is given by

$$p(x,t) = A\sin(\alpha x - \omega t)$$

The partial derivative

$$\frac{\partial p}{\partial x} = \alpha A \cos(\alpha x - \omega t)$$

describes at a given time t the spacial rate of change of the pressure.

The partial derivative

$$\frac{\partial p}{\partial t} = -\omega A \cos(\alpha x - \omega t)$$

describes for a fixed position x the temporal rate of change of the acoustic pressure.

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Rules for differentiation

• Let f,g be differentiable with respect to x_i and $\alpha,\beta\in\mathbb{R}$, then we have the rules

$$\frac{\partial}{\partial x_{i}} \left(\alpha f(\mathbf{x}) + \beta g(\mathbf{x}) \right) = \alpha \frac{\partial f}{\partial x_{i}}(\mathbf{x}) + \beta \frac{\partial g}{\partial x_{i}}(\mathbf{x})$$

$$\frac{\partial}{\partial x_{i}} \left(f(\mathbf{x}) \cdot g(\mathbf{x}) \right) = \frac{\partial f}{\partial x_{i}}(\mathbf{x}) \cdot g(\mathbf{x}) + f(\mathbf{x}) \cdot \frac{\partial g}{\partial x_{i}}(\mathbf{x})$$

$$\frac{\partial}{\partial x_{i}} \left(\frac{f(\mathbf{x})}{g(\mathbf{x})} \right) = \frac{\frac{\partial f}{\partial x_{i}}(\mathbf{x}) \cdot g(\mathbf{x}) - f(\mathbf{x}) \cdot \frac{\partial g}{\partial x_{i}}(\mathbf{x})}{g(\mathbf{x})^{2}} \quad \text{for } g(\mathbf{x}) \neq 0$$

• An alternative notation for the partial derivatives of f with respect to x_i at x^0 is given by

$$D_i f(x^0)$$
 oder $f_{x_i}(x^0)$

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Gradient and nabla-operator.

Definition: Let $D \subset \mathbb{R}^n$ be an open set and $f: D \to \mathbb{R}$ partial differentiable.

We denote the row vector

$$\operatorname{grad} f(x^0) := \left(\frac{\partial f}{\partial x_1}(x^0), \dots, \frac{\partial f}{\partial x_n}(x^0)\right)$$

as gradient of f at x^0 .

• We denote the symbolic vector

$$\nabla := \left(\frac{\partial}{\partial x_1}, \dots, \frac{\partial}{\partial x_n}\right)^T$$

as nabla-operator.

Thus we obtain the column vector

$$\nabla f(\mathbf{x}^0) := \left(\frac{\partial f}{\partial x_1}(\mathbf{x}^0), \dots, \frac{\partial f}{\partial x_n}(\mathbf{x}^0)\right)^T$$

More rules on differentiation.

Let f and g be partial differentiable. Then the following rules on differentiation hold true:

$$\begin{array}{rcl} \operatorname{grad} \left(\alpha f + \beta g \right) & = & \alpha \cdot \operatorname{grad} f + \beta \cdot \operatorname{grad} g \\ \\ \operatorname{grad} \left(f \cdot g \right) & = & g \cdot \operatorname{grad} f + f \cdot \operatorname{grad} g \\ \\ \operatorname{grad} \left(\frac{f}{g} \right) & = & \frac{1}{g^2} \left(g \cdot \operatorname{grad} f - f \cdot \operatorname{grad} g \right), \quad g \neq 0 \end{array}$$

Examples:

• Let $f(x, y) = e^x \cdot \sin y$. Then:

$$\operatorname{grad} f(x,y) = (e^{x} \cdot \sin y, e^{x} \cdot \cos y) = e^{x} (\sin y, \cos y)$$

• For $r(x) := ||x||_2 = \sqrt{x_1^2 + \dots + x_n^2}$ we have

grad
$$r(x) = \frac{x}{r(x)} = \frac{x}{\|x\|_2}$$
 für $x \neq 0$,

where $x = (x_1, \dots, x_n)$ denotes a row vector.

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Partial differentiability does not imply continuity.

Observation: A partial differentiable function (with respect to all coordinates) is not necessarily a continuous function.

Example: Consider the function $f: \mathbb{R}^2 \to \mathbb{R}$ defined as

$$f(x,y) := \begin{cases} \frac{x \cdot y}{(x^2 + y^2)^2} & : & \text{for } (x,y) \neq 0 \\ 0 & : & \text{for } (x,y) = 0 \end{cases}$$

The function is partial differntiable on the **entire** \mathbb{R}^2 and we have

$$f_x(0,0) = f_y(0,0) = 0$$

$$\frac{\partial f}{\partial x}(x,y) = \frac{y}{(x^2 + y^2)^2} - 4\frac{x^2y}{(x^2 + y^2)^3}, \quad (x,y) \neq (0,0)$$

$$\frac{\partial f}{\partial y}(x,y) = \frac{x}{(x^2 + y^2)^2} - 4\frac{xy^2}{(x^2 + y^2)^3}, \quad (x,y) \neq (0,0)$$

Example (continuation).

We calculate the partial derivatives at the origin (0,0):

$$\frac{\partial f}{\partial x}(0,0) = \lim_{t \to 0} \frac{f(t,0) - f(0,0)}{t} = \frac{\frac{t \cdot 0}{(t^2 + 0^2)^2} - 0}{t} = 0$$

$$\frac{\partial f}{\partial y}(0,0) = \lim_{t \to 0} \frac{f(0,t) - f(0,0)}{t} = \frac{\frac{0 \cdot t}{(0^2 + t^2)^2} - 0}{t} = 0$$

But: At (0,0) the function is **not** continuous since

$$\lim_{n \to \infty} f\left(\frac{1}{n}, \frac{1}{n}\right) = \frac{\frac{1}{n} \cdot \frac{1}{n}}{\left(\frac{1}{n} \cdot \frac{1}{n} + \frac{1}{n} \cdot \frac{1}{n}\right)^2} = \frac{\frac{1}{n^2}}{\frac{4}{n^4}} = \frac{n^2}{4} \to \infty$$

and thus we have

$$\lim_{(x,y)\to(0,0)} f(x,y) \neq f(0,0) = 0$$

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Boundedness of the derivatives implies continuity.

To guarantee the continuity of a partial differentiable function we need additional conditions on f.

Theorem: Let $D \subset \mathbb{R}^n$ be an open set. Let $f: D \to \mathbb{R}$ be partial differentiable in a neighborhood of $x^0 \in D$ and let the partial derivatives $\frac{\partial f}{\partial x_i}$, $i = 1, \ldots, n$, be bounded. Then f is continuous in x^0 .

Attention: In the previous example the partial derivatives are not bounded in a neighborhood of (0,0) since

$$\frac{\partial f}{\partial x}(x,y) = \frac{y}{(x^2 + y^2)^2} - 4\frac{x^2y}{(x^2 + y^2)^3} \quad \text{für } (x,y) \neq (0,0)$$

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Proof of the theorem.

For $\|\mathbf{x} - \mathbf{x}^0\|_{\infty} < \varepsilon$, $\varepsilon > 0$ sufficiently small we write:

$$f(x) - f(x^{0}) = (f(x_{1}, \dots, x_{n-1}, x_{n}) - f(x_{1}, \dots, x_{n-1}, x_{n}^{0}))$$

$$+ (f(x_{1}, \dots, x_{n-1}, x_{n}^{0}) - f(x_{1}, \dots, x_{n-2}, x_{n-1}^{0}, x_{n}^{0}))$$

$$\vdots$$

$$+ (f(x_{1}, x_{2}^{0}, \dots, x_{n}^{0}) - f(x_{1}^{0}, \dots, x_{n}^{0}))$$

For any difference on the right hand side we consider f as a function in one single variable:

$$g(x_n) - g(x_n^0) := f(x_1, \dots, x_{n-1}, x_n) - f(x_1, \dots, x_{n-1}, x_n^0)$$

Since f is partial differentiable g is differentiable and we can apply the mean value theorem on g:

$$g(x_n) - g(x_n^0) = g'(\xi_n)(x_n - x_n^0)$$

for an appropriate ξ_n between x_n and x_n^0 .

Proof of the theorem (continuation).

Applying the mean value theorem to every term in the right hand side we obtain

$$f(x) - f(x^{0}) = \frac{\partial f}{\partial x_{n}}(x_{1}, \dots, x_{n-1}, \xi_{n}) \cdot (x_{n} - x_{n}^{0})$$

$$+ \frac{\partial f}{\partial x_{n-1}}(x_{1}, \dots, x_{n-2}, \xi_{n-1}, x_{n}^{0}) \cdot (x_{n-1} - x_{n-1}^{0})$$

$$\vdots$$

$$+ \frac{\partial f}{\partial x_{1}}(\xi_{1}, x_{2}^{0}, \dots, x_{n}^{0}) \cdot (x_{1} - x_{1}^{0})$$

Using the boundedness of the partial derivatives

$$|f(x) - f(x^0)| \le C_1|x_1 - x_1^0| + \cdots + C_n|x_n - x_n^0|$$

for $\|\mathbf{x} - \mathbf{x}^0\|_{\infty} < \varepsilon$, we obtain the continuity of f at \mathbf{x}^0 since

$$f(x) \rightarrow f(x^0)$$
 für $||x - x^0||_{\infty} \rightarrow 0$

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Higher order derivatives.

Definition: Let f be a scalar function and partial differentiable on an open set $D \subset \mathbb{R}^n$. If the partial derivatives are differentiable we obtain (by differentiating) the partial derivatives of second order of f with

$$\frac{\partial^2 f}{\partial x_j \partial x_i} := \frac{\partial}{\partial x_j} \left(\frac{\partial f}{\partial x_i} \right)$$

Example: Second order partial derivatives of a function f(x, y):

$$\frac{\partial^2 f}{\partial x^2} = \frac{\partial}{\partial x} \left(\frac{\partial f}{\partial x} \right), \quad \frac{\partial^2 f}{\partial y \partial x} = \frac{\partial}{\partial y} \left(\frac{\partial f}{\partial x} \right), \quad \frac{\partial^2 f}{\partial x \partial y}, \quad \frac{\partial^2 f}{\partial y^2}$$

Let $i_1, \ldots, i_k \in \{1, \ldots, n\}$. Then we define recursively

$$\frac{\partial^k f}{\partial x_{i_k} \partial x_{i_{k-1}} \dots \partial x_{i_1}} := \frac{\partial}{\partial x_{i_k}} \left(\frac{\partial^{k-1} f}{\partial x_{i_{k-1}} \partial x_{i_{k-2}} \dots \partial x_{i_1}} \right)$$

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Higher order derivatives.

Definition: The function f is called k-times partial differentiable, if all derivatives of order k,

$$\frac{\partial^k f}{\partial x_{i_k} \partial x_{i_{k-1}} \dots \partial x_{i_1}} \qquad \text{for all } i_1, \dots, i_k \in \{1, \dots, n\},$$

exist on D.

Alternative notation:

$$\frac{\partial^k f}{\partial x_{i_k} \partial x_{i_{k-1}} \dots \partial x_{i_1}} = D_{i_k} D_{i_{k-1}} \dots D_{i_1} f = f_{x_{i_1} \dots x_{i_k}}$$

If all the derivatives of k-th order are continuous the function f is called k-times continuous partial differentiable or called a \mathcal{C}^k -function on D. Continuous functions f are called \mathcal{C}^0 -functions.

Example: For the function
$$f(x_1, ..., x_n) = \prod_{i=1}^n x_i^i$$
 we have $\frac{\partial^n f}{\partial x_n ... \partial x_1} = ?$

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Partial derivaratives are not arbitrarely exchangeable.

ATTENTION: The order how to execute partial derivatives is in general not arbitrarely exchangeable!

Example: For the function

$$f(x,y) := \begin{cases} xy \frac{x^2 - y^2}{x^2 + y^2} & : & \text{for } (x,y) \neq (0,0) \\ 0 & : & \text{for } (x,y) = (0,0) \end{cases}$$

we calculate

$$f_{xy}(0,0) = \frac{\partial}{\partial y} \left(\frac{\partial f}{\partial x}(0,0) \right) = -1$$

 $f_{yx}(0,0) = \frac{\partial}{\partial x} \left(\frac{\partial f}{\partial y}(0,0) \right) = +1$

i.e. $f_{xy}(0,0) \neq f_{yx}(0,0)$.

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Theorem of Schwarz on exchangeablity.

Satz: Let $D \subset \mathbb{R}^n$ be open and let $f: D \to \mathbb{R}$ be a \mathcal{C}^2 -function. Then it holds

$$\frac{\partial^2 f}{\partial x_i \partial x_i}(x_1, \dots, x_n) = \frac{\partial^2 f}{\partial x_i \partial x_i}(x_1, \dots, x_n)$$

for all $i, j \in \{1, ..., n\}$.

Idea of the proof:

Apply the men value theorem twice.

Conclusion:

If f is a C^k -function, then we can exchange the differentiation in order to calculate partial derivatives up to order k arbitrarely!

Example for the exchangeability of partial derivatives.

Calculate the partial derivative of third order f_{xyz} for the function

$$f(x, y, z) = y^2 z \sin(x^3) + (\cosh y + 17e^{x^2})z^2$$

The order of execution is exchangealbe since $f \in C^3$.

• Differentiate first with respect to z:

$$\frac{\partial f}{\partial z} = y^2 \sin(x^3) + 2z(\cosh y + 17e^{x^2})$$

• Differentiate then f_z with respect to x (then $\cosh y$ disappears):

$$f_{zx} = \frac{\partial}{\partial x} \left(y^2 \sin(x^3) + 2z(\cosh y + 17e^{x^2}) \right)$$
$$= 3x^2 y^2 \cos(x^3) + 68xze^{x^2}$$

• For the partial derivative of f_{zx} with respect to y we obtain

$$f_{xyz} = 6x^2y\cos(x^3)$$

The Laplace operator.

The Laplace-operator or Laplacian is defined as

$$\Delta := \sum_{i=1}^{n} \frac{\partial^2}{\partial x_i^2}$$

For a scalar function $u(x) = u(x_1, ..., x_n)$ we have

$$\Delta u = \sum_{i=1}^{n} \frac{\partial^{2} u}{\partial x_{i}^{2}} = u_{x_{1}x_{1}} + \dots + u_{x_{n}x_{n}}$$

Examples of important partial differential equations of second order (i.e. equations containing partial derivatives up to order two):

$$\Delta u - rac{1}{c^2} u_{tt} = 0$$
 (wave equation)
$$\Delta u - rac{1}{k} u_t = 0$$
 (heat equation)

 $\Delta u = 0$ (Laplace-equation or equation for the potential)

Vector valued functions.

Definition: Let $D \subset \mathbb{R}^n$ be open and let $f: D \to \mathbb{R}^m$ be a vector valued function.

The function f is called partial differentiable on $x^0 \in D$, if for all i = 1, ..., n the limits

$$\frac{\partial f}{\partial x_i}(x^0) = \lim_{t \to 0} \frac{f(x^0 + te_i) - f(x^0)}{t}$$

exist. The calculation is done componentwise

$$\frac{\partial f}{\partial x_i}(x^0) = \begin{pmatrix} \frac{\partial f_1}{\partial x_i} \\ \vdots \\ \frac{\partial f_m}{\partial x_i} \end{pmatrix} \quad \text{for } i = 1, \dots, n$$

Vectorfields.

Definition: If m = n the function $f: D \to \mathbb{R}^n$ is called a vectorfield on D. If every (coordinate-) function $f_i(x)$ of $f = (f_1, \dots, f_n)^T$ is a C^k -function, then f is called C^k -vectorfield.

Examples of vectorfields:

- velocity fields of liquids or gases;
- elektromagnetic fields;
- temperature gradients in solid states.

Definition: Let $f: D \to \mathbb{R}^n$ be a partial differentiable vector field. The divergence on $x \in D$ is defined as

$$\operatorname{div} f(x^0) := \sum_{i=1}^n \frac{\partial f_i}{\partial x_i}(x^0)$$

or

$$\operatorname{div} f(x) = \nabla^T f(x) = (\nabla, f(x))$$

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Rules of computation and the rotation.

The following rules hold true:

$$\begin{array}{lcl} \operatorname{div} \big(\alpha\, \mathsf{f} + \beta\, \mathsf{g}\big) & = & \alpha\, \operatorname{div}\, \mathsf{f} + \beta\, \operatorname{div}\, \mathsf{g} & \text{for}\, \mathsf{f}, \mathsf{g} : D \to \mathbb{R}^n \\ \\ \operatorname{div} \big(\varphi \cdot \mathsf{f}\big) & = & \big(\nabla \varphi, \mathsf{f}\big) + \varphi\, \operatorname{div}\, \mathsf{f} & \text{for}\, \varphi : D \to \mathbb{R}, \mathsf{f} : D \to \mathbb{R}^n \end{array}$$

Remark: Let $f:D\to\mathbb{R}$ be a \mathcal{C}^2 -function, then for the Laplacian we have

$$\Delta f = \operatorname{div}(\nabla f)$$

Definition: Let $D \subset \mathbb{R}^3$ open and $f: D \to \mathbb{R}^3$ a partial differentiable vector field. We define the rotation as

$$\mathsf{rot}\; \mathsf{f}(\mathsf{x}^0) := \left(\frac{\partial f_3}{\partial x_2} - \frac{\partial f_2}{\partial x_3}, \frac{\partial f_1}{\partial x_3} - \frac{\partial f_3}{\partial x_1}, \frac{\partial f_2}{\partial x_1} - \frac{\partial f_1}{\partial x_2}\right)^T \bigg|_{\mathsf{x}^0}$$

Alternative notations and additional rules.

$$\operatorname{rot} f(x) = \nabla \times f(x) = \begin{vmatrix} e_1 & e_2 & e_3 \\ \frac{\partial}{\partial x_1} & \frac{\partial}{\partial x_2} & \frac{\partial}{\partial x_3} \\ f_1 & f_2 & f_3 \end{vmatrix}$$

Remark: The following rules hold true:

$$\begin{split} \operatorname{rot} \left(\alpha \operatorname{f} + \beta \operatorname{g} \right) &= & \alpha \operatorname{rot} \operatorname{f} + \beta \operatorname{rot} \operatorname{g} \\ \\ \operatorname{rot} \left(\varphi \cdot \operatorname{f} \right) &= & \left(\nabla \varphi \right) \times \operatorname{f} + \varphi \operatorname{rot} \operatorname{f} \end{split}$$

Remark: Let $D \subset \mathbb{R}^3$ and $\varphi : D \to \mathbb{R}$ be a \mathcal{C}^2 -function. Then

$$rot (\nabla \varphi) = 0,$$

using the exchangeability theorem of Schwarz. I.e. gradient fileds are rotation-free everywhere.

Chapter 1. Multivariate differential calculus

1.2 The total differential

Definition: Let $D \subset \mathbb{R}^n$ open, $x^0 \in D$ and $f: D \to \mathbb{R}^m$. The function f(x) is called differentiable in x^0 (or totally differentiable in x_0), if there exists a linear map

$$I(x,x^0) := A \cdot (x - x^0)$$

with a matrix $A \in \mathbb{R}^{m \times n}$ which satisfies the following approximation property

$$f(x) = f(x^0) + A \cdot (x - x^0) + o(\|x - x^0\|)$$

i.e.

$$\lim_{x \to x^0} \frac{f(x) - f(x^0) - A \cdot (x - x^0)}{\|x - x^0\|} = 0.$$

The total differential and the Jacobian matrix.

Notation: We call the linear map I the differential or the total differential of f(x) at the point x^0 . We denote I by $df(x^0)$.

The related matrix A is called Jacobi–matrix of f(x) at the point x^0 and is denoted by $Jf(x^0)$ (or $Df(x^0)$ or $f'(x^0)$).

Remark: For m = n = 1 we obtain the well known relation

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + o(|x - x_0|)$$

for the derivative $f'(x_0)$ at the point x_0 .

Remark: In case of a scalar function (m = 1) the matrix A = a is a row vextor and $a(x - x^0)$ a scalar product $\langle a^T, x - x^0 \rangle$.



Total and partial differentiability.

Theorem: Let $f: D \to \mathbb{R}^m$, $x^0 \in D \subset \mathbb{R}^n$, D open.

- a) If f(x) is differentiable in x^0 , then f(x) is continuous in x^0 .
- b) If f(x) is differentiable in x^0 , then the (total) differential and thus the Jacobi-matrix are uniquely determined and we have

$$\mathsf{Jf}(\mathsf{x}^0) = \left(\begin{array}{ccc} \frac{\partial f_1}{\partial \mathsf{x}_1}(\mathsf{x}^0) & \dots & \frac{\partial f_1}{\partial \mathsf{x}_n}(\mathsf{x}^0) \\ \vdots & & \vdots \\ \frac{\partial f_m}{\partial \mathsf{x}_1}(\mathsf{x}^0) & \dots & \frac{\partial f_m}{\partial \mathsf{x}_n}(\mathsf{x}^0) \end{array} \right) = \left(\begin{array}{c} Df_1(\mathsf{x}^0) \\ \vdots \\ Df_m(\mathsf{x}^0) \end{array} \right)$$

c) If f(x) is a C^1 -function on D, then f(x) is differentiable on D.

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Proof of a).

If f is differentiable in x^0 , then by definition

$$\lim_{x \to x^0} \frac{f(x) - f(x^0) - A \cdot (x - x^0)}{\|x - x^0\|} = 0$$

Thus we conclude

$$\lim_{x \to x^0} \|f(x) - f(x^0) - A \cdot (x - x^0)\| = 0$$

and we obtain

$$\begin{split} \|f(x) - f(x^0)\| & \leq & \|f(x) - f(x^0) - A \cdot (x - x^0)\| + \|A \cdot (x - x^0)\| \\ & \to & 0 & \text{as } x \to x^0 \end{split}$$

Therefore the function f is continuous at x^0 .



Proof of b).

Let $x = x^0 + te_i$, $|t| < \varepsilon$, $i \in \{1, ..., n\}$. Since f in differentiable at x^0 , we have

$$\lim_{x\rightarrow x^0}\frac{f(x)-f(x^0)-A\cdot(x-x^0)}{\|x-x^0\|_\infty}=0$$

We write

$$\frac{f(x) - f(x^0) - A \cdot (x - x^0)}{\|x - x^0\|_{\infty}} = \frac{f(x^0 + te_i) - f(x^0)}{|t|} - \frac{tAe_i}{|t|}$$

$$= \frac{t}{|t|} \cdot \left(\frac{f(x^0 + te_i) - f(x^0)}{t} - Ae_i\right)$$

$$\to 0 \quad \text{as } t \to 0$$

Thus

$$\lim_{t\to 0}\frac{\mathsf{f}(\mathsf{x}^0+t\mathsf{e}_i)-\mathsf{f}(\mathsf{x}^0)}{t}=\mathsf{Ae}_i \qquad i=1,\ldots,n$$

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Examples.

• Consider the scalar function $f(x_1, x_2) = x_1 e^{2x_2}$. Then the Jacobian is given by:

$$Jf(x_1,x_2) = Df(x_1,x_2) = e^{2x_2}(1,2x_1)$$

• Consider the function $f: \mathbb{R}^3 \to \mathbb{R}^2$ defined by

$$f(x_1, x_2, x_3) = \begin{pmatrix} x_1 x_2 x_3 \\ \sin(x_1 + 2x_2 + 3x_3) \end{pmatrix}$$

The Jacobian is given by

$$\mathsf{Jf}(x_1, x_2, x_3) = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \frac{\partial f_1}{\partial x_3} \\ \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \frac{\partial f_2}{\partial x_3} \end{pmatrix} = \begin{pmatrix} x_2 x_3 & x_1 x_3 & x_1 x_2 \\ \\ \cos(s) & 2\cos(s) & 3\cos(s) \end{pmatrix}$$

with $s = x_1 + 2x_2 + 3x_3$.

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Further examples.

• Let f(x) = Ax, $A \in \mathbb{R}^{m \times n}$ and $x \in \mathbb{R}^n$. Then

$$Jf(x) = A$$
 for all $x \in \mathbb{R}^n$

• Let $f(x) = x^T A x = \langle x, Ax \rangle$, $A \in \mathbb{R}^{n \times n}$ and $x \in \mathbb{R}^n$. Then we have

$$\frac{\partial f}{\partial x_i} = \langle e_i, Ax \rangle + \langle x, Ae_i \rangle$$
$$= e_i^T Ax + x^T Ae_i$$
$$= x^T (A^T + A)e_i$$

We conclude

$$\mathsf{J} f(\mathsf{x}) = \mathsf{grad} f(\mathsf{x}) = \mathsf{x}^\mathsf{T} (\mathsf{A}^\mathsf{T} + \mathsf{A})$$

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Rules for the differentiation.

Theorem:

a) **Linearität:** LET f, g : $D \to \mathbb{R}^m$ be differentiable in $x^0 \in D$, D open. Then α f(x^0) + β g(x^0), and α , $\beta \in \mathbb{R}$ are differentiable in x^0 and we have

$$d(\alpha f + \beta g)(x^0) = \alpha df(x^0) + \beta dg(x^0)$$
$$J(\alpha f + \beta g)(x^0) = \alpha Jf(x^0) + \beta Jg(x^0)$$

b) Chain rule: Let $f: D \to \mathbb{R}^m$ be differentiable in $x^0 \in D$, D open. Let $g: E \to \mathbb{R}^k$ be differentiable in $y^0 = f(x^0) \in E \subset \mathbb{R}^m$, E open. Then $g \circ f$ is differentiable in x^0 .

For the differentials it holds

$$d(g\circ f)(x^0)=dg(y^0)\circ df(x^0)$$

and analoglously for the Jacobian matrix

$$J(g\circ f)(x^0)=Jg(y^0)\cdot Jf(x^0)$$

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Examples for the chain rule.

Let $I \subset \mathbb{R}$ be an intervall. Let $h: I \to \mathbb{R}^n$ be a curve, differentiable in $t_0 \in I$ with values in $D \subset \mathbb{R}^n$, D open. Let $f: D \to \mathbb{R}$ be a scalar function, differentiable in $x^0 = h(t_0)$.

Then the composition

$$(f \circ h)(t) = f(h_1(t), \dots, h_n(t))$$

is differentiable in t_0 and we have for the derivative:

$$(f \circ \mathsf{h})'(t_0) = \mathsf{J}f(\mathsf{h}(t_0)) \cdot \mathsf{J}\mathsf{h}(t_0)$$

$$= \mathsf{grad}f(\mathsf{h}(t_0)) \cdot \mathsf{h}'(t_0)$$

$$= \sum_{k=1}^n \frac{\partial f}{\partial x_k}(\mathsf{h}(t_0)) \cdot h_k'(t_0)$$

Directional derivative.

Definition: Let $f: D \to \mathbb{R}$, $D \subset \mathbb{R}^n$ open, $x^0 \in D$, and $v \in \mathbb{R} \setminus \{0\}$ a vector. Then

$$D_{v} f(x^{0}) := \lim_{t \to 0} \frac{f(x^{0} + tv) - f(x^{0})}{t}$$

is called the directional derivative (Gateaux-derivative) of f(x) in the direction of v.

Example: Let $f(x, y) = x^2 + y^2$ and $v = (1, 1)^T$. Then the directional derivative in the direction of v is given by:

$$D_{v} f(x,y) = \lim_{t \to 0} \frac{(x+t)^{2} + (y+t)^{2} - x^{2} - y^{2}}{t}$$
$$= \lim_{t \to 0} \frac{2xt + t^{2} + 2yt + t^{2}}{t}$$
$$= 2(x+y)$$

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Remarks.

• For $v = e_i$ the directional derivative in the direction of v is given by the partial derivative with respect to x_i :

$$D_{v} f(x^{0}) = \frac{\partial f}{\partial x_{i}}(x^{0})$$

- If v is a unit vector, i.e. ||v|| = 1, then the directional derivative $D_v f(x^0)$ describes the slope of f(x) in the direction of v.
- If f(x) is differentiable in x^0 , then all directional derivatives of f(x) in x^0 exist. With $h(t) = x^0 + tv$ we have

$$D_{\mathsf{v}} f(\mathsf{x}^0) = \frac{d}{dt} (f \circ \mathsf{h})|_{t=0} = \operatorname{\mathsf{grad}} f(\mathsf{x}^0) \cdot \mathsf{v}$$

This follows directely applying the chain rule.



Properties of the gradient.

Theorem: Let $D \subset \mathbb{R}^n$ open, $f: D \to \mathbb{R}$ differentiable in $x^0 \in D$. Then we have

a) The gradient vector grad $f(x^0) \in \mathbb{R}^n$ is orthogonal in the level set

$$N_{x^0} := \{ x \in D \mid f(x) = f(x^0) \}$$

In the case of n=2 we call the level sets contour lines, in n=3 we call the level sets equipotential surfaces.

2) The gradient grad $f(x^0)$ gives the direction of the steepest slope of f(x) in x^0 .

Idea of the proof:

- a) application of the chain rule.
- b) for an arbitrary direction v we conclude with the Cauchy–Schwarz inequality

$$|D_{v} f(x^{0})| = |(\operatorname{grad} f(x^{0}), v)| \le \|\operatorname{grad} f(x^{0})\|_{2}$$

Equality is obtained for $v = \text{grad } f(x^0) / \|\text{grad } f(x^0)\|_2$.

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Curvilinear coordinates.

Definition: Let $U, V \subset \mathbb{R}^n$ be open and $\Phi: U \to V$ be a \mathcal{C}^1 -map, for which the Jacobimatrix $J\Phi(u^0)$ is regular (invertible) at every $u^0 \in U$.

In addition there exists the inverse map $\Phi^{-1}:V\to U$ and the inverse map is also a \mathcal{C}^1 -map.

Then $x = \Phi(u)$ defines a coordinate transformation from the coordinates u to x.

Example: Consider for n=2 the polar coordinates $\mathbf{u}=(r,\varphi)$ with r>0 and $-\pi<\varphi<\pi$ and set

$$x = r \cos \varphi$$

$$y = r \sin \varphi$$

with the cartesian coordinates x = (x, y).



Calculation of the partial derivatives.

For all $u \in U$ with $x = \Phi(u)$ the following relations hold

$$\Phi^{-1}(\Phi(u)) = u$$

$$J \Phi^{-1}(x) \cdot J \Phi(u) = I_n \quad \text{(chain rule)}$$

$$J \Phi^{-1}(x) = (J \Phi(u))^{-1}$$

Let $\widetilde{f}:V \to \mathbb{R}$ be a given function. Set

$$f(\mathsf{u}) := \tilde{f}(\Phi(\mathsf{u}))$$

the by using the chain rule we obtain

$$\frac{\partial f}{\partial u_i} = \sum_{j=1}^n \frac{\partial \tilde{f}}{\partial x_j} \frac{\partial \Phi_j}{\partial u_i} =: \sum_{j=1}^n g^{ij} \frac{\partial \tilde{f}}{\partial x_j}$$

with

$$g^{ij} := \frac{\partial \Phi_j}{\partial u_i}, \qquad \mathsf{G}(\mathsf{u}) := (g^{ij}) = (\mathsf{J}\,\Phi(\mathsf{u}))^T$$

Notations.

We use the short notation

$$\frac{\partial}{\partial u_i} = \sum_{j=1}^n g^{ij} \frac{\partial}{\partial x_j}$$

Analogously we can express the partial derivatives with respect to x_i by the partial derivatives with respect to u_i

$$\frac{\partial}{\partial x_i} = \sum_{j=1}^n g_{ij} \frac{\partial}{\partial u_j}$$

where

$$(g_{ij}) := (g^{ij})^{-1} = (J \Phi)^{-T} = (J \Phi^{-1})^{T}$$

We obtain these relations by applying the chain rule on Φ^{-1} .

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Example: polar coordinates.

We consider polar coordinates

$$x = \Phi(u) = \begin{pmatrix} r\cos\varphi \\ r\sin\varphi \end{pmatrix}$$

We calculate

$$\mathsf{J}\,\Phi(\mathsf{u}) = \left(\begin{array}{cc} \cos\varphi & -r\sin\varphi\\ \sin\varphi & r\cos\varphi \end{array}\right)$$

and thus

$$(g^{ij}) = \begin{pmatrix} \cos \varphi & \sin \varphi \\ \\ -r \sin \varphi & r \cos \varphi \end{pmatrix} \qquad (g_{ij}) = \begin{pmatrix} \cos \varphi & -\frac{1}{r} \sin \varphi \\ \\ \sin \varphi & \frac{1}{r} \cos \varphi \end{pmatrix}$$

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Partial derivatives for polar coordinates.

The calculation of the partial derivatives gives

$$\frac{\partial}{\partial x} = \cos \varphi \frac{\partial}{\partial r} - \frac{1}{r} \sin \varphi \frac{\partial}{\partial \varphi}$$
$$\frac{\partial}{\partial y} = \sin \varphi \frac{\partial}{\partial r} + \frac{1}{r} \cos \varphi \frac{\partial}{\partial \varphi}$$

Example: Calculation of the Laplacian-operator in polar coordinates

$$\frac{\partial^{2}}{\partial x^{2}} = \cos^{2}\varphi \frac{\partial^{2}}{\partial r^{2}} - \frac{\sin(2\varphi)}{r} \frac{\partial^{2}}{\partial r \partial \varphi} + \frac{\sin^{2}\varphi}{r^{2}} \frac{\partial^{2}}{\partial \varphi^{2}} + \frac{\sin(2\varphi)}{r^{2}} \frac{\partial}{\partial \varphi} + \frac{\sin^{2}\varphi}{r} \frac{\partial}{\partial r}$$

$$\frac{\partial^{2}}{\partial y^{2}} = \sin^{2}\varphi \frac{\partial^{2}}{\partial r^{2}} + \frac{\sin(2\varphi)}{r} \frac{\partial^{2}}{\partial r \partial \varphi} + \frac{\cos^{2}\varphi}{r^{2}} \frac{\partial^{2}}{\partial \varphi^{2}} - \frac{\sin(2\varphi)}{r^{2}} \frac{\partial}{\partial \varphi} + \frac{\cos^{2}\varphi}{r} \frac{\partial}{\partial r}$$

$$\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} = \frac{\partial^2}{\partial r^2} + \frac{1}{r^2} \frac{\partial^2}{\partial \varphi^2} + \frac{1}{r} \frac{\partial}{\partial r}$$

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Example: spherical coordinates.

We consider spherical coordinates

$$x = \Phi(u) = \begin{pmatrix} r\cos\varphi\cos\theta \\ r\sin\varphi\cos\theta \\ r\sin\theta \end{pmatrix}$$

The Jacobian-matrix is given by:

$$J\Phi(u) = \begin{pmatrix} \cos\varphi\cos\theta & -r\sin\varphi\cos\theta & -r\cos\varphi\sin\theta \\ \sin\varphi\cos\theta & r\cos\varphi\cos\theta & -r\sin\varphi\sin\theta \\ \sin\theta & 0 & r\cos\theta \end{pmatrix}$$

Partial derivatives for spherical coordinates.

Calculating the partial derivatives gives

$$\frac{\partial}{\partial x} = \cos \varphi \cos \theta \frac{\partial}{\partial r} - \frac{\sin \varphi}{r \cos \theta} \frac{\partial}{\partial \varphi} - \frac{1}{r} \cos \varphi \sin \theta \frac{\partial}{\partial \theta}$$

$$\frac{\partial}{\partial y} = \sin \varphi \cos \theta \frac{\partial}{\partial r} + \frac{\cos \varphi}{r \cos \theta} \frac{\partial}{\partial \varphi} - \frac{1}{r} \sin \varphi \sin \theta \frac{\partial}{\partial \theta}$$

$$\frac{\partial}{\partial z} = \sin \theta \frac{\partial}{\partial r} + \frac{1}{r} \cos \theta \frac{\partial}{\partial \theta}$$

Example: calculation of the Laplace-operator in spherical coordinates

$$\Delta = \frac{\partial^2}{\partial r^2} + \frac{1}{r^2 \cos^2 \theta} \frac{\partial^2}{\partial \varphi^2} + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2} + \frac{2}{r} \frac{\partial}{\partial r} - \frac{\tan \theta}{r^2} \frac{\partial}{\partial \theta}$$



Kapitel 1. Multivariate differential calculus

1.3 Mean value theorems and Taylor expansion

Theorem (Mean value theorem): Let $f: D \to \mathbb{R}$ be a scalar differentiable function on an open set $D \subset \mathbb{R}^n$. Let $a, b \in D$ be points in D such that the connecting line segment

$$[a,b] := \{a + t(b-a) | t \in [0,1]\}$$

lies entirely in D. Then there exits a number $\theta \in (0,1)$ with

$$f(b) - f(a) = \operatorname{grad} f(a + \theta(b - a)) \cdot (b - a)$$

Proof: We set

$$h(t) := f(\mathsf{a} + t(\mathsf{b} - \mathsf{a}))$$

with the mean value theorem for a single variable and the chain rules we conclude

$$f(b) - f(a) = h(1) - h(0) = h'(\theta) \cdot (1 - 0)$$

= grad $f(a + \theta(b - a)) \cdot (b - a)$

Definition and example.

Definition: If the condition $[a,b] \subset D$ holds true for **all** points $a,b \in D$, then the set D is called **convex**.

Example for the mean value theorem: Given a scalar function

$$f(x, y) := \cos x + \sin y$$

It is

$$f(0,0) = f(\pi/2, \pi/2) = 1 \quad \Rightarrow \quad f(\pi/2, \pi/2) - f(0,0) = 0$$

Applying the mean value theorem there exists a $\theta \in (0,1)$ with

$$\operatorname{grad} f\left(\theta\left(\begin{array}{c}\pi/2\\\pi/2\end{array}\right)\right)\cdot\left(\begin{array}{c}\pi/2\\\pi/2\end{array}\right)=0$$

Indeed this is true for $\theta = \frac{1}{2}$.

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Mean value theorem is only true for scalar functions.

Attention: The mean value theorem for multivariate functions is only true for scalar functions but in general not for vector—valued functions!

Examples: Consider the **vector-valued** Function

$$f(t) := \begin{pmatrix} \cos t \\ \sin t \end{pmatrix}, \qquad t \in [0, \pi/2]$$

It is

$$\mathsf{f}(\pi/2) - \mathsf{f}(0) = \left(\begin{array}{c} 0 \\ 1 \end{array}\right) - \left(\begin{array}{c} 1 \\ 0 \end{array}\right) = \left(\begin{array}{c} -1 \\ 1 \end{array}\right)$$

and

$$\mathsf{f}'\left(\theta\,\frac{\pi}{2}\right)\cdot\left(\frac{\pi}{2}-0\right) = \frac{\pi}{2}\,\left(\begin{array}{c} -\sin(\theta\pi/2) \\ \cos(\theta\pi/2) \end{array}\right)$$

BUT: the vectors on the right hand side have lenght $\sqrt{2}$ and $\pi/2$!

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A mean value estimate for vector-valued functions.

Theorem: Let $f: D \to \mathbb{R}^m$ be differentiable on an open set $D \subset \mathbb{R}^n$. Let a, b bei points in D with $[a,b] \subset D$. Then there exists a $\theta \in (0,1)$ with

$$\|f(b) - f(a)\|_2 \le \|J f(a + \theta(b - a)) \cdot (b - a)\|_2$$

Idea of the proof: Application of the mean value theorem to the scalar function g(x) definid as

$$g(x) := (f(b) - f(a))^T f(x)$$
 (scalar product!)

Remark: Another (weaker) for of the mean value estimate is

$$\|f(b) - f(a)\| \le \sup_{\xi \in [a,b]} \|Jf(\xi)\| \cdot \|(b-a)\|$$

where $\|\cdot\|$ denotes an arbitrary vector norm with related matrix norm.

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Taylor series: notations.

We define the multi-index $\alpha \in \mathbb{N}_0^n$ as

$$\alpha := (\alpha_1, \ldots, \alpha_n) \in \mathbb{N}_0^n$$

Let

$$|\alpha| := \alpha_1 + \dots + \alpha_n$$
 $\alpha! := \alpha_1! \cdot \dots \cdot \alpha_n!$

Let $f:D\to\mathbb{R}$ be $|\alpha|$ times continuous differentiable. Then we set

$$D^{\alpha} = D_1^{\alpha_1} D_2^{\alpha_2} \dots D_n^{\alpha_n} = \frac{\partial^{|\alpha|} f}{\partial x_1^{\alpha_1} \dots \partial x_n^{\alpha_n}},$$

where
$$D_i^{\alpha_i} = \underbrace{D_i \dots D_i}_{\alpha_i - \mathsf{mal}}$$
. We write

$$\mathsf{x}^{\alpha} := \mathsf{x}_1^{\alpha_1} \, \mathsf{x}_2^{\alpha_2} \dots \mathsf{x}_n^{\alpha_n} \qquad \text{for } \mathsf{x} = (\mathsf{x}_1, \dots, \mathsf{x}_n) \in \mathbb{R}^n.$$

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The Taylor theorem.

Theorem: (Taylor)

Let $D \subset \mathbb{R}^n$ be open and convex. Let $f: D \to \mathbb{R}$ be a \mathbb{C}^{m+1} -function and $x_0 \in D$. Then the Taylor–expansion holds true in $x \in D$

$$f(x) = T_m(x; x_0) + R_m(x; x_0)$$

$$T_m(x; x_0) = \sum_{|\alpha| \le m} \frac{D^{\alpha} f(x_0)}{\alpha!} (x - x_0)^{\alpha}$$

$$R_m(x; x_0) = \sum_{|\alpha| = m+1} \frac{D^{\alpha} f(x_0 + \theta(x - x_0))}{\alpha!} (x - x_0)^{\alpha}$$

for an appropriate $\theta \in (0,1)$.

Notation: In the Taylor–expansion we denote $T_m(x; x_0)$ Taylor–polynom of degree m and $R_m(x; x_0)$ Lagrange–remainder.

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Derivation of the Taylor expansion.

We define a scalar function in one single variable $t \in [0,1]$ as

$$g(t) := f(x_0 + t(x - x_0))$$

and calculate the (univariate) Taylor-expansion at t = 0. It is

$$g(1) = g(0) + g'(0) \cdot (1-0) + rac{1}{2} g''(\xi) \cdot (1-0)^2 \quad ext{for a } \xi \in (0,1).$$

The calculation of g'(0) is given by the chain rule

$$g'(0) = \frac{d}{dt} f(x_1^0 + t(x_1 - x_1^0), x_2^0 + t(x_2 - x_2^0), \dots, x_n^0 + t(x_n - x_n^0)) \Big|_{t=0}$$

$$= D_1 f(x_0) \cdot (x_1 - x_1^0) + \dots + D_n f(x_0) \cdot (x_n - x_n^0)$$

$$= \sum_{|\alpha|=1} \frac{D^{\alpha} f(x_0)}{\alpha!} \cdot (x - x_0)^{\alpha}$$

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Continuation of the derivation.

Calculation of g''(0) gives

$$g''(0) = \frac{d^2}{dt^2} f(x_0 + t(x - x_0)) \Big|_{t=0} = \frac{d}{dt} \sum_{k=1}^n D_k f(x^0 + t(x - x^0)) (x_k - x_k^0) \Big|_{t=0}$$

$$= D_{11} f(x_0) (x_1 - x_1^0)^2 + D_{21} f(x_0) (x_1 - x_1^0) (x_2 - x_2^0)$$

$$+ \dots + D_{ij} f(x_0) (x_i - x_i^0) (x_j - x_j^0) + \dots +$$

$$+ D_{n-1,n} f(x_0) (x_{n-1} - x_{n-1}^0) (x_n - x_n^0) + D_{nn} f(x_0) (x_n - x_n^0)^2)$$

$$= \sum_{|\alpha|=2} \frac{D^{\alpha} f(x_0)}{\alpha!} (x - x_0)^{\alpha} \quad \text{(exchange theorem of Schwarz!)}$$

Continuation: Proof of the Taylor–formula by (mathematical) induction!

Proof of the Taylor theorem.

The function

$$g(t) := f(x^0 + t(x - x^0))$$

is (m+1)-times continuous differentiable and we have

$$g(1) = \sum_{k=0}^m rac{g^{(k)}(0)}{k!} + rac{g^{(m+1)}(heta)}{(m+1)!} \quad ext{for a } heta \in [0,1].$$

In addition we have (by induction over k)

$$\frac{g^{(k)}(0)}{k!} = \sum_{|\alpha|=k} \frac{D^{\alpha} f(x^0)}{\alpha!} (x - x^0)^{\alpha}$$

and

$$\frac{g^{(m+1)}(\theta)}{(m+1)!} = \sum_{|\alpha|=m+1} \frac{D^{\alpha} f(x^0 + \theta(x - x^0))}{\alpha!} (x - x^0)^{\alpha}$$

Examples for the Taylor-expansion.

• Calculate the Taylor–polynom $T_2(x; x_0)$ of degree 2 of the function

$$f(x, y, z) = x y^2 \sin z$$

at
$$(x, y, z) = (1, 2, 0)^T$$
.

- **2** The calculation of $T_2(x; x_0)$ requires the partial derivatives up to order 2.
- **3** These derivatives have to be evaluated at $(x, y, z) = (1, 2, 0)^T$.
- The result is $T_2(x; x_0)$ in the form

$$T_2(x;x_0)=4z(x+y-2)$$

Details on extra slide.



Remarks to the remainder of a Taylor-expansion.

Remark: The remainder of a Taylor–expansion contains **all** partial derivatives of order (m+1):

$$R_m(\mathbf{x}; \mathbf{x}_0) = \sum_{|\alpha|=m+1} \frac{D^{\alpha} f(\mathbf{x}_0 + \theta(\mathbf{x} - \mathbf{x}_0))}{\alpha!} (\mathbf{x} - \mathbf{x}_0)^{\alpha}$$

If all these derivative are bounded by aconstant C in a neighborhood of x_0 then the estimate for the remainder hold true

$$|R_m(x;x_0)| \le \frac{n^{m+1}}{(m+1)!} C ||x-x_0||_{\infty}^{m+1}$$

We conclude for the quality of the approximation of a \mathcal{C}^{m+1} -function by the Taylor-polynom

$$f(x) = T_m(x; x_0) + O(||x - x_0||^{m+1})$$

Special case m=1: For a \mathcal{C}^2 -function f(x) we obtain

$$f(x) = f(x^0) + \operatorname{grad} f(x^0) \cdot (x - x^0) + O(\|x - x^0\|^2).$$

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