Analysis III for engineering study programs

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

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Content of the course Analysis III.

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

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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)

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

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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

$$\begin{aligned} \frac{\partial f}{\partial x_i}(x^0) &:= \lim_{t \to 0} \frac{f(x^0 + te_i) - f(x^0)}{t} \\ &= \lim_{t \to 0} \frac{f(x_1^0, \dots, x_i^0 + t, \dots, x_n^0) - f(x_1^0, \dots, x_i^0, \dots, x_n^0)}{t} \end{aligned}$$

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 x⁰ the partial derivatives with respect to every variable x_i, i = 1,..., n exist and if the partial derivatives are continuous functions then we call f continuous partial differentiable or a C¹-function.

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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!

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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 x⁰ 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

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

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

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More rules on differentiation.

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

$$grad(\alpha f + \beta g) = \alpha \cdot grad f + \beta \cdot grad g$$

$$grad(f \cdot g) = g \cdot grad f + f \cdot grad g$$

$$grad\left(\frac{f}{g}\right) = \frac{1}{g^2}(g \cdot grad f - f \cdot grad g), \quad g \neq 0$$

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

where $x = (x_1, \ldots, x_n)$ 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

$$f_{x}(0,0) = f_{y}(0,0) = 0$$

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

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

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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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 $||x - x^0||_{\infty} < \varepsilon$, $\varepsilon > 0$ sufficiently small we write: $f(x) - f(x^0) = (f(x_1, \dots, x_{n-1}, x_n) - f(x_1, \dots, x_{n-1}, x_n^0))$ $+ (f(x_1, \dots, x_{n-1}, x_n^0) - f(x_1, \dots, x_{n-2}, x_{n-1}^0, x_n^0))$

+
$$(f(x_1, x_2^0, \dots, x_n^0) - f(x_1^0, \dots, x_n^0))$$

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 .

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Proof of the theorem (continuation).

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

$$\begin{aligned} f(\mathbf{x}) - f(\mathbf{x}^0) &= \frac{\partial f}{\partial x_n} (x_1, \dots, x_{n-1}, \xi_n) \cdot (x_n - x_n^0) \\ &+ \frac{\partial f}{\partial x_{n-1}} (x_1, \dots, x_{n-2}, \xi_{n-1}, x_n^0) \cdot (x_{n-1} - x_{n-1}^0) \end{aligned}$$

$$+ \quad \frac{\partial f}{\partial x_1}(\xi_1, x_2^0, \dots, x_n^0) \cdot (x_1 - x_1^0)$$

Using the boundedness of the partial derivatives

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

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

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

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,

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

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 C^k -function on D. Continuous functions f are called 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. $f_{xy}(0,0) \neq f_{yx}(0,0)$.

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

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

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

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!

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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

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

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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 $u(\mathbf{x}) = u(x_1, \ldots, x_n)$ 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):

$$\Delta u - \frac{1}{c^2} u_{tt} = 0 \quad (\text{wave equation})$$

$$\Delta u - \frac{1}{k} u_t = 0 \quad (\text{heat equation})$$

$$\Delta u = 0 \quad (\text{Laplace-equation or equation for the potential})$$

$$u = 0 \quad (\text{Laplace-equation or equation for the potential})$$
Ingenuin Gasser (Mathematik, UniHH) Analysis III for students in engineering 20/136

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

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

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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 $f = (f_1, \ldots, f_n)^T$ is a \mathcal{C}^k -function, then f is called \mathcal{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:

$$\operatorname{div} (\alpha f + \beta g) = \alpha \operatorname{div} f + \beta \operatorname{div} g \quad \text{for } f, g : D \to \mathbb{R}^n$$

 $\mathsf{div}\,(\varphi\cdot\mathsf{f}) \ = \ (\nabla\varphi,\mathsf{f})+\varphi\,\mathsf{div}\,\mathsf{f} \quad \mathsf{for}\;\varphi:D\to\mathbb{R},\mathsf{f}:D\to\mathbb{R}^n$

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

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

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

$$\operatorname{rot} f(x^{0}) := \left(\frac{\partial f_{3}}{\partial x_{2}} - \frac{\partial f_{2}}{\partial x_{3}}, \frac{\partial f_{1}}{\partial x_{3}} - \frac{\partial f_{3}}{\partial x_{1}}, \frac{\partial f_{2}}{\partial x_{1}} - \frac{\partial f_{1}}{\partial x_{2}} \right)^{T} \Big|_{x^{0}}$$

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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:

$$\operatorname{rot} (\alpha \, \mathbf{f} + \beta \, \mathbf{g}) = \alpha \operatorname{rot} \mathbf{f} + \beta \operatorname{rot} \mathbf{g}$$
$$\operatorname{rot} (\varphi \cdot \mathbf{f}) = (\nabla \varphi) \times \mathbf{f} + \varphi \operatorname{rot} \mathbf{f}$$

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

$$\mathsf{rot}\,(\nabla\varphi)=\mathsf{0}\,,$$

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

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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

$$|(\mathbf{x},\mathbf{x}^0) := \mathsf{A} \cdot (\mathbf{x} - \mathbf{x}^0)$$

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.

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

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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 $\langle a^T, x - x^0 \rangle$.

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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

$$\mathsf{J} \mathsf{f}(\mathsf{x}^{0}) = \begin{pmatrix} \frac{\partial f_{1}}{\partial x_{1}}(\mathsf{x}^{0}) & \dots & \frac{\partial f_{1}}{\partial x_{n}}(\mathsf{x}^{0}) \\ \vdots & & \vdots \\ \frac{\partial f_{m}}{\partial x_{1}}(\mathsf{x}^{0}) & \dots & \frac{\partial f_{m}}{\partial x_{n}}(\mathsf{x}^{0}) \end{pmatrix} = \begin{pmatrix} Df_{1}(\mathsf{x}^{0}) \\ \vdots \\ Df_{m}(\mathsf{x}^{0}) \end{pmatrix}$$

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

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

Therefore the function f is continuous at x^0 .

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Proof of b).

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

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

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

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

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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:

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

 \bullet 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.

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

We conclude

$$Jf(x) = gradf(x) = x^{T}(A^{T} + A)$$

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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 $\alpha f(x^0) + \beta g(x^0)$, and $\alpha, \beta \in \mathbb{R}$ 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

$$\mathsf{d}(\mathsf{g}\circ\mathsf{f})(\mathsf{x}^0)=\mathsf{d}\mathsf{g}(\mathsf{y}^0)\circ\mathsf{d}\mathsf{f}(\mathsf{x}^0)$$

and analoglously for the Jacobian matrix

$$\mathsf{J}(g\circ f)(x^0)=\mathsf{J}g(y^0)\cdot\mathsf{J}f(x^0)$$

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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

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

is differentiable in t_0 and we have for the derivative:

$$(f \circ h)'(t_0) = Jf(h(t_0)) \cdot Jh(t_0)$$

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

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

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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:

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

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(x⁰) describes the slope of f(x) in the direction of v.
- If f(x) is differentiable in x⁰, then all directional derivatives of f(x) in x⁰ exist. With h(t) = x⁰ + tv we have

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

This follows directely applying the chain rule.

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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 $f(\mathsf{x}^0) \in \mathbb{R}^n$ 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 $u = (r, \varphi)$ with r > 0 and $-\pi < \varphi < \pi$ and set

$$x = r \cos \varphi$$

$$y = r \sin \varphi$$

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

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Calculation of the partial derivatives.

For all $u \in U$ with $x = \Phi(u)$ the following relations hold $\Phi^{-1}(\Phi(u)) = u$ $J \Phi^{-1}(x) \cdot J \Phi(u) = I_n$ (chain rule) $J \Phi^{-1}(x) = (J \Phi(u))^{-1}$ Let $\tilde{f} : V \to \mathbb{R}$ 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

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

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

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

We calculate

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

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

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

The Jacobian-matrix is given by:

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

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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

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

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Chapter 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: 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 $heta \in (0,1)$ with

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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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

$$f(t) := \left(egin{array}{c} \cos t \ \sin t \end{array}
ight), \qquad t \in [0, \pi/2]$$

lt is

$$f(\pi/2) - f(0) = \begin{pmatrix} 0 \\ 1 \end{pmatrix} - \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} -1 \\ 1 \end{pmatrix}$$

and

$$\mathsf{f}'\left(heta \, rac{\pi}{2}
ight) \cdot \left(rac{\pi}{2} - 0
ight) = rac{\pi}{2} \, \left(egin{array}{c} -\sin(heta\pi/2) \ \cos(heta\pi/2) \end{array}
ight)$$

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

$$\|f(b) - f(a)\|_2 \leq \|Jf(a + \theta(b - a)) \cdot (b - a)\|_2$$

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

$$g(x) := (f(b) - f(a))^T f(x) \qquad (\text{scalar product!})$$

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

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

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

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

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
$$D_i^{\alpha_i} = \underbrace{D_i \dots D_i}_{\alpha_i - \text{mal}}$$
. We write
 $x^{\alpha} := x_1^{\alpha_1} x_2^{\alpha_2} \dots x_n^{\alpha_n}$ for $x = (x_1, \dots, x_n) \in \mathbb{R}^n$.

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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 \mathcal{C}^{m+1} -function and $x_0 \in D$. Then the Taylor-expansion holds true in $x \in D$

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

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

$$g(t) := f(\mathsf{x}_0 + t(\mathsf{x} - \mathsf{x}_0))$$

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

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

= $D_1 f(x_0) \cdot (x_1 - x_1^0) + \dots + D_n f(x_0) \cdot (x_n - x_n^0)$
= $\sum_{|\alpha|=1} \frac{D^{\alpha} f(x_0)}{\alpha!} \cdot (x - x_0)^{\alpha}$

Continuation of the derivation.

Calculation of g''(0) gives

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

$$= D_{11}f(x_0)(x_1 - x_1^0)^2 + D_{21}f(x_0)(x_1 - x_1^0)(x_2 - x_2^0) + \dots + D_{ij}f(x_0)(x_i - x_i^0)(x_j - x_j^0) + \dots + + D_{n-1,n}f(x_0)(x_{n-1} - x_{n-1}^0)(x_n - x_n^0) + D_{nn}f(x_0)(x_n - x_n^0)^2)$$

$$= \sum_{|\alpha|=2} \frac{D^{\alpha} f(\mathsf{x}_0)}{\alpha !} (\mathsf{x} - \mathsf{x}_0)^{\alpha} \qquad (\text{exchange theorem of Schwarz!})$$

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

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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)

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

and

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

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

- The calculation of T₂(x; x₀) requires the partial derivatives up to order 2.
- 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

$$T_2(\mathsf{x};\mathsf{x}_0) = 4z(x+y-2)$$

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Remarks to the remainder of a Taylor-expansion.

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

$$\mathcal{R}_m(\mathsf{x};\mathsf{x}_0) = \sum_{|\alpha|=m+1} \frac{D^{\alpha} f(\mathsf{x}_0 + \theta(\mathsf{x} - \mathsf{x}_0))}{\alpha!} (\mathsf{x} - \mathsf{x}_0)^{\alpha}$$

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

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

We conlude for the quality of the approximation of a 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 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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The matrix

$$Hf(x_0) := \begin{pmatrix} f_{x_1x_1}(x_0) & \dots & f_{x_1x_n}(x_0) \\ \vdots & & \vdots \\ f_{x_nx_1}(x_0) & \dots & f_{x_nx_n}(x_0) \end{pmatrix}$$

is called Hesse-matrix of f at x_0 .

Hesse-matrix = Jacobi-matrix of the gradient ∇f

The Taylor–expansion of a \mathcal{C}^3 –function can be written as

$$f(x) = f(x_0) + \operatorname{grad} f(x_0)(x - x_0) + \frac{1}{2}(x - x_0)^T Hf(x_0)(x - x_0) + O(||x - x_0||^3)$$

The Hesse-matrix of a C^2 -function is symmetric.

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Chapter 2. Applications of multivariate differential calculus

2.1 Extrem values of multivariate functions

Definition: Let $D \subset \mathbb{R}^n$, $f : D \to \mathbb{R}$ and $x^0 \in D$. Then at x^0 the function f has

- a global maximum if $f(x) \leq f(x^0)$ for all $x \in D$.
- a strict global maximum if $f(x) < f(x^0)$ for all $x \in D$.
- a local maximum if there exists an $\varepsilon > 0$ such that

$$f(\mathsf{x}) \leq f(\mathsf{x}^0)$$
 for all $\mathsf{x} \in D$ with $\|\mathsf{x} - \mathsf{x}^0\| < \varepsilon$.

• a strict local maximum if there exists an $\varepsilon > 0$ such that

$$f(x) < f(x^0)$$
 for all $x \in D$ with $||x - x^0|| < \varepsilon$.

Analogously we define the different forms of minima.

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Necessary conditions for local extrem values.

Theorem: If a C^1 -function f(x) has a local extrem value (minimum or maximum) at $x^0 \in D^0$, then

grad $f(x^0) = 0 \in \mathbb{R}^n$

Proof: For an arbitrary $v \in \mathbb{R}^n$, $v \neq 0$ the function

 $\varphi(t) := f(x^0 + tv)$

is differentiable in a neighborhood of $t^0 = 0$. $\varphi(t)$ has a local extrem value at $t^0 = 0$. We conclude:

$$\varphi'(0) = \operatorname{grad} f(x^0) v = 0$$

Since this holds true for all $v \neq 0$ we obtain

grad
$$f(x^0) = (0, ..., 0)^T$$

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Remarks to local extrem values.

Bemerkungen:

- Typically the condition grad $f(x^0) = 0$ gives a non-linear system of *n* equations for *n* unknowns for the calculation of $x = x^0$.
- The points x⁰ ∈ D⁰ with grad f(x⁰) = 0 are called stationary points of f.
 Stationary points are **not** necessarily local extram values. As an example take

$$f(x,y) := x^2 - y^2$$

with the gradient

$$\operatorname{\mathsf{grad}} f(x,y) = 2(x,-y)$$

and therefore with the only stationary point $x^0 = (0, 0)^T$. However, the point x^0 is a saddel point of f, i.e. in every neighborhood of x^0 there exist two points x^1 and x^2 with

$$f(x^1) < f(x^0) < f(x^2).$$

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Classification of stationary points.

Theorem: Let f(x) be a C^2 -function on D^0 and let $x^0 \in D^0$ be a stationary point of f(x), i.e. grad $f(x^0) = 0$.

a) necessary condition

If x^0 is a local extrem value of f, then:

 x^0 local minimum \Rightarrow H $f(x^0)$ positiv semidefinit

 x^0 local maximum $\Rightarrow Hf(x^0)$ negativ semidefinit

b) sufficient condition

If $H f(x^0)$ is positiv definit (negativ definit) then x^0 is a strict local minimum (maximum) of f.

If $H f(x^0)$ is indefinit then x^0 is a saddel point, i.e. in every neighborhood of x^0 there exist points x^1 and x^2 with $f(x^1) < f(x^0) < f(x^2)$.

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Proof of the theorem, part a).

Let x^0 be a local minimum. For $v\neq 0$ and $\varepsilon>0$ sufficiently small we conclude from the Taylor–expansion

$$f(\mathbf{x}^{0} + \varepsilon \mathbf{v}) - f(\mathbf{x}^{0}) = \frac{1}{2} (\varepsilon \mathbf{v})^{T} \mathsf{H} f(\mathbf{x}^{0} + \theta \varepsilon \mathbf{v}) (\varepsilon \mathbf{v}) \ge 0$$
(1)

with $\theta = \theta(\varepsilon, \mathsf{v}) \in (0, 1)$.

The gradient in the Taylor expansion grad $f(x^0) = 0$ vanishes since x^0 is stationary.

From (1) it follows

$$\mathsf{v}^{\mathsf{T}}\mathsf{H}\,f(\mathsf{x}^{0}+\theta\varepsilon\mathsf{v})\mathsf{v}\geq0\tag{2}$$

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Since f is a C^2 -function, the Hesse-matrix is a continuous map. In the limit $\varepsilon \to 0$ we conclude from (2),

$$v^T H f(x^0) v \ge 0$$

i.e. $H f(x^0)$ is positiv semidefinit.

Proof of the theorem, part b).

If $H f(x^0)$ is positiv definit, then H f(x) is positiv definit in a sufficiently small neighborhood $x \in K_{\varepsilon}(x^0) \subset D$ around x^0 . This follows from the continuity of the second partial derivatives.

For $\mathsf{x} \in \mathit{K}_{arepsilon}(\mathsf{x}^0)$, $\mathsf{x}
eq \mathsf{x}^0$ we have

$$f(x) - f(x^{0}) = \frac{1}{2}(x - x^{0})^{T} H f(x^{0} + \theta(x - x^{0}))(x - x^{0})$$

> 0

with $\theta \in (0, 1)$, i.e. f has a strict local minimum at x^0 .

If H $f(x^0)$ is indefinit, then there exist Eigenvectors v, w for Eigenvalues of H $f(x^0)$ with opposite sign with

$$v^T H f(x^0) v > 0$$
 $w^T H f(x^0) w < 0$

and thus x^0 is a saddel point.

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Remarks.

- A stationary point x⁰ with det Hf(x⁰) = 0 is called degenerate. The Hesse-matrix has an Eigenvalue λ = 0.
- If x⁰ is not degenerate, then there exist 3 cases for the Eigenvalues of Hf(x⁰):

all Eigenvalues are strictly positive $\Rightarrow x^0$ is a strict local min

all Eigenvalues are strictly negative $\Rightarrow x^0$ is a strict local ma

there are strictly positive and negative Eigenvalues $\Rightarrow x^0$ saddel point

• The following implications are true (but not the inverse)

 $\begin{array}{rcl} x^0 \mbox{ local minimum } & \Leftarrow & x^0 \mbox{ strict local minimum } \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$

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Further remarks.

 If f is a C³-function, x⁰ a stationary point of f and Hf(x⁰) positiv definit. Then the following estimate is true:

$$(\mathbf{x} - \mathbf{x}^0)^T \operatorname{Hf}(\mathbf{x}^0) (\mathbf{x} - \mathbf{x}^0) \geq \lambda_{\min} \cdot \|\mathbf{x} - \mathbf{x}^0\|^2$$

where λ_{\min} denoted the smallest Eigenvalue of the Hesse-matrix. Using the Taylor theorem we obtain:

$$\begin{array}{ll} f({\rm x}) - f({\rm x}^0) & \geq & \frac{1}{2} \lambda_{min} \|{\rm x} - {\rm x}^0\|^2 + R_3({\rm x};{\rm x}^0) \\ \\ & \geq & \|{\rm x} - {\rm x}^0\|^2 \left(\frac{\lambda_{min}}{2} - C \|{\rm x} - {\rm x}^0\|\right) \end{array}$$

with an appropriate constant C > 0.

The function f grows at least quadratically around x^0 .

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Example .

We consider the function

$$f(x,y) := y^2(x-1) + x^2(x+1)$$

and look for stationary points :

grad
$$f(x,y) = (y^2 + x(3x+2), 2y(x-1))^7$$

The condition grad f(x, y) = 0 gives two stationary points

$$x^0 = (0,0)^T$$
 und $x^1 = (-2/3,0)^T$.

The related Hesse-matrices of f at x^0 and x^1 are

$$\mathsf{H}f(\mathsf{x}^0)=\left(egin{array}{cc} 2 & 0 \\ 0 & -2 \end{array}
ight) \qquad {
m and} \qquad \mathsf{H}f(\mathsf{x}^1)=\left(egin{array}{cc} -2 & 0 \\ 0 & -10/3 \end{array}
ight)$$

The matrix $Hf(x^0)$ is indefinit, therefore x^0 is a saddel point. $Hf(x^1)$ is negative definit and thus x^1 is a strict local ein strenges maximum of f.

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Chapter 2. Applications of multivariate differential calculus

2.2 Implicitely defined functions

Aim: study the set of solutions of the system of *non-linear* equations of the form

$$g(x) = 0$$

with $g: D \to \mathbb{R}^m$, $D \subset \mathbb{R}^n$. I.e. we consider *m* equations for *n* unknowns with

Thus: there are less equations than unknowns.

We call such a system of equations underdetermined and the set of solutions $G \subset \mathbb{R}^n$ contains typically *infinitely* many points.

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Solvability of (non-linear) equations.

Question: can we **solve** the system g(x) = 0 with respect to certain unknowns, i.e. with respect to the last *m* variables x_{n-m+1}, \ldots, x_n ?

In other words: is there a function $f(x_1, \ldots, x_{n-m})$ with

$$g(\mathbf{x}) = 0 \quad \Longleftrightarrow \quad (x_{n-m+1}, \dots, x_n)^T = f(x_1, \dots, x_{n-m})$$

Terminology: "solve" means express the last *m* variables by the first n - m variables?

Other question: with respect to which *m* variables can we solve the system? Is the solution possible *globally* on the domain of definition *D*? Or only *locally* on a subdomain $\tilde{D} \subset D$?

Geometrical interpretation: The set of solution G of g(x) = 0 can be expressed (at least locally) as graph of a function $f : \mathbb{R}^{n-m} \to \mathbb{R}^m$.

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Example.

The equation for a circle

$$g(x,y) = x^2 + y^2 - r^2 = 0$$
 mit $r > 0$

defines an underdetermined non-linear system of equations since we have **two** unknowns (x, y), but only **one** scalar equation.

The equation for the circle can be solved locally and defines the four functions :

$$y = \sqrt{r^2 - x^2}, \quad -r \le x \le r$$
$$y = -\sqrt{r^2 - x^2}, \quad -r \le x \le r$$
$$x = \sqrt{r^2 - y^2}, \quad -r \le y \le r$$
$$x = -\sqrt{r^2 - y^2}, \quad -r \le y \le r$$

Example.

Let g be an affin-linear function, i.e. g has the form

$$g(x) = Cx + b$$
 for $C \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^m$

We split the variables x into two vectors

$$\mathbf{x}^{(1)} = (x_1, \dots, x_{n-m})^T \in \mathbb{R}^{n-m}$$
 and $\mathbf{x}^{(2)} = (x_{n-m+1}, \dots, x_n)^T \in \mathbb{R}^n$

Splitting of the matrix $\mathsf{C} = [\mathsf{B},\mathsf{A}]$ gives the form

$$g(x) = Bx^{(1)} + Ax^{(2)} + b$$

with $B \in \mathbb{R}^{m \times (n-m)}$, $A \in \mathbb{R}^{m \times m}$.

The system of equations g(x) = 0 can be solved (uniquely) with respect to the variables $x^{(2)}$, if A is regular. Then

$$g(x) = 0 \quad \iff \quad x^{(2)} = -A^{-1}(Bx^{(1)} + b) = f(x^{(1)})$$

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Question: How can we write the matrix A as dependent of g?

From the equation

$$\mathsf{g}(\mathsf{x}) = \mathsf{B}\mathsf{x}^{(1)} + \mathsf{A}\mathsf{x}^{(2)} + \mathsf{b}$$

we see that

$$\mathsf{A} = \frac{\partial \mathsf{g}}{\partial \mathsf{x}^{(2)}}(\mathsf{x}^{(1)},\mathsf{x}^{(2)})$$

holds, i.e. A is the Jacobian of the map

$$x^{(2)} \rightarrow g(x^{(1)},x^{(2)})$$

for fixed $x^{(1)}!$

We conclude: Solvability is given if the Jacobian is regular (invertible).

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Implicit function theorem.

Theorem: Let $g : D \to \mathbb{R}^m$ be a C^1 -function, $D \subset \mathbb{R}^n$ open. We denote the variables in D by (x, y) with $x \in \mathbb{R}^{n-m}$ und $y \in \mathbb{R}^m$. Let $Der(x^0, y^0) \in D$ be a solution of $g(x^0, y^0) = 0$.

If the Jacobi-matrix

$$\frac{\partial g}{\partial y}(x^0, y^0) := \begin{pmatrix} \frac{\partial g_1}{\partial y_1}(x^0, y^0) & \dots & \frac{\partial g_1}{\partial y_m}(x^0, y^0) \\ \vdots & & \vdots \\ \frac{\partial g_m}{\partial y_1}(x^0, y^0) & \dots & \frac{\partial g_m}{\partial y_m}(x^0, y^0) \end{pmatrix}$$

is regular, then there exist neighborhoods U of x^0 and V of y^0 , $U \times V \subset D$ and a uniquely determined continuous differentiable function $f: U \to V$ with

$$\mathsf{f}(\mathsf{x}^0) = \mathsf{y}^0 \quad \text{und} \quad \mathsf{g}(\mathsf{x},\mathsf{f}(\mathsf{x})) = 0 \quad \text{für alle } \mathsf{x} \in U$$

and

$$\mathsf{J}\,\mathsf{f}(\mathsf{x}) = -\left(\frac{\partial \mathsf{g}}{\partial \mathsf{y}}(\mathsf{x},\mathsf{f}(\mathsf{x}))\right)^{-1}\,\left(\frac{\partial \mathsf{g}}{\partial \mathsf{x}}(\mathsf{x},\mathsf{f}(\mathsf{x}))\right)$$

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Example.

For the equation of a circle $g(x, y) = x^2 + y^2 - r^2 = 0, r > 0$ we have at $(x^0, y^0) = (0, r)$

$$\frac{\partial g}{\partial x}(0,r) = 0, \quad \frac{\partial g}{\partial y}(0,r) = 2r \neq 0$$

Thus we can solve the equation of a circle in a neighborhod of (0, r) with respect to y:

$$f(x) = \sqrt{r^2 - x^2}$$

The derivative f'(x) can be calculated by implicit diffentiation:

$$g(x,y(x)) = 0 \implies g_x(x,y(x)) + g_y(x,y(x))y'(x) = 0$$

and therefore

$$2x + 2y(x)y'(x) = 0 \quad \Rightarrow \quad y'(x) = f'(x) = -\frac{x}{y(x)}$$

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Another example.

Consider the equation $g(x, y) = e^{y-x} + 3y + x^2 - 1 = 0$. It is

$$\frac{\partial g}{\partial y}(x,y) = e^{y-x} + 3 > 0$$
 for all $x \in \mathbb{R}$.

Therefore the equation con be solved for every $x \in \mathbb{R}$ with respect to y =: f(x)and f(x) is a continuous differentiable function. Implicit differentiation ives

$$e^{y-x}(y'-1) + 3y' + 2x = 0 \implies y' = \frac{e^{y-x} - 2x}{e^{y-x} + 3}$$

Differentiating again gives

$$e^{y-x}y'' + e^{y-x}(y'-1)^2 + 3y'' + 2 = 0 \implies y' = -\frac{2 + e^{y-x}(y'-1)^2}{e^{y-x} + 3}$$

But: Solving the equation with respect to y (in terms of elementary functions) is not possible in this case!

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general remark.

Implicit differentiation of a implicitely defined function

$$g(x,y) = 0, \quad \frac{\partial g}{\partial y} \neq 0$$

y = f(x), with $x, y \in \mathbb{R}$, gives

$$f'(x) = -\frac{g_x}{g_y}$$
$$f''(x) = -\frac{g_{xx}g_y^2 - 2g_{xy}g_xg_y + g_{yy}g_x^2}{g_y^3}$$

Therefore the opint x^0 is a stationary point of f(x) if

$$g(x^0, y^0) = g_x(x^0, y^0) = 0$$
 and $g_y(x^0, y^0) \neq 0$

And x^0 is a local maximum (minimum) if

$$\frac{g_{xx}(x^0, y^0)}{g_y(x^0, y^0)} > 0 \qquad \left(\text{ bzw. } \frac{g_{xx}(x^0, y^0)}{g_y(x^0, y^0)} < 0 \right)$$

Ingenuin Gasser (Mathematik, UniHH) Analysis III for students in engineering

Implicit representation of curves.

Consider the set of solutions of a scalar equation

$$g(x,y)=0$$

lf

$$\operatorname{\mathsf{grad}} g = (g_x, g_y) \neq 0$$

then g(x, y) defines locally a function y = f(x) or $x = \overline{f}(y)$.

Definition: A solution point (x^0, y^0) of the equation g(x, y) = 0 with

- grad $g(x^0, y^0) \neq 0$ is called regular point,
- grad $g(x^0, y^0) = 0$ is called singular point.

Example: Consider (again) the equation for a circle

$$g(x,y) = x^2 + y^2 - r = 0$$
 mit $r > 0$.

on the circle there are no singular points!

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Remarks:

a) If for a regular point (x^0, y^0) we have

$$g_x(\mathbf{x}^0) = 0$$
 und $g_y(\mathbf{x}^0) \neq 0$

then the set of solutions contains a horizontal tangent in x^0 .

b) If for a regular point (x^0, y^0) we have

$$g_{\scriptscriptstyle X}(\mathsf{x}^0)
eq 0$$
 und $g_{\scriptscriptstyle Y}(\mathsf{x}^0) = 0$

then the set of solutions contains a vertical tangent in x^0 .

c) If x^0 is a singular point, then the set of solutions is approximated at x^0 "in second order" by the following quadratic equation

$$g_{xx}(x^0)(x-x^0)^2 + 2g_{xy}(x^0)(x-x^0)(y-y^0) + g_{yy}(x^0)(y-y^0)^2 = 0$$

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Remarks.

Due to c) for $g_{xx}, g_{xy}, g_{yy} \neq 0$ we obtain: $\det Hg(x^0) > 0 \quad : \quad x^0 \text{ is an isolated point of the set of solutions}$ $\det Hg(x^0) < 0 \quad : \quad x^0 \text{ is a double point}$ $\det Hg(x^0) = 0 \quad : \quad x^0 \text{ is a return point or a cusp}$

Geometric interpretation:

- a) If det $Hg(x^0) > 0$, then both Eigenvalues of $Hg(x^0)$ are or strictly positiv or strictly negativ, i.e. x^0 is a strict local minimum or maximum of g(x).
- b) If det $Hg(x^0) < 0$, then both Eigenvalues of $Hg(x^0)$ have opposite sign, i.e. x^0 is a saddel point of g(x).
- c) If det $Hg(x^0) = 0$, then the stationary point x^0 of g(x) is degenerate.

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Example 1.

Consider the singular point $x^0 = 0$ of the implicit equation

$$g(x,y) = y^{2}(x-1) + x^{2}(x-2) = 0$$

Calculate the partial derivatives up to order 2:

 $g_{x} = y^{2} + 3x^{2} - 4x$ $g_{y} = 2y(x - 1)$ $g_{xx} = 6x - 4$ $g_{xy} = 2y$ $g_{yy} = 2(x - 1)$ $Hg(0) = \begin{pmatrix} -4 & 0 \\ 0 & -2 \end{pmatrix}$

Therefore $x^0 = 0$ is an isolated point.

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Example 2.

Consider the singular point $x^0 = 0$ of the implicit equation

$$g(x, y) = y^{2}(x - 1) + x^{2}(x + q^{2}) = 0$$

Calculate the partial derivatives up to order 2:

| g _× | = | $y^2 + 3x^2 + 2xq^2$ |
|-----------------|---|--|
| gy | = | 2y(x - 1) |
| g _{xx} | = | $6x + 2q^2$ |
| g _{×y} | = | 2 <i>y</i> |
| g _{yy} | = | 2(x - 1) |
| g(0) | = | $\left(\begin{array}{cc} 2q^2 & 0\\ 0 & -2 \end{array}\right)$ |

Therefore $x^0 = 0$ is an double point.

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Example 3.

Consider the singular point $x^0 = 0$ of the implicit equation

$$g(x, y) = y^{2}(x - 1) + x^{3} = 0$$

Calculate the partial derivatives up to order 2:

$$g_{x} = y^{2} + 3x^{2}$$

$$g_{y} = 2y(x-1)$$

$$g_{xx} = 6x$$

$$g_{xy} = 2y$$

$$g_{yy} = 2(x-1)$$

$$\lg(0) = \begin{pmatrix} 0 & 0 \\ 0 & -2 \end{pmatrix}$$

Therefore $x^0 = 0$ is a cusp (or a return point).

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Implicit representation of surfaces.

- The set of solutions of a scalar equation g(x, y, z) = 0 for grad g ≠ 0 is locally a surface in ℝ³.
- For the tangential in $x^0 = (x^0, y^0, z^0)^T$ with $g(x^0) = 0$ and grad $g(x^0) \neq 0^T$ we obtain by Taylor expanding (denoting $\Delta x^0 = x x^0$)

grad
$$g \cdot \Delta x^0 = g_x(x^0)(x-x^0) + g_y(x^0)(y-y^0) + g_z(x^0)(z-z_0) = 0$$

i.e. the gradient is vertical to the surface g(x, y, z) = 0.

• If for example $g_z(x^0) \neq 0$, then locally there exists a a representation at x^0 of the form

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

and for the partial derivatives of f(x, y) we obtain

$$\operatorname{\mathsf{grad}} f(x,y) = (f_x,f_y) = -\frac{1}{g_z}(g_x,g_y) = \left(-\frac{g_x}{g_z},\frac{g_y}{g_z}\right)$$

using the implicit function theorem.

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The inverted Problem.

Question: Given the set of equations

y = f(x)

with $f: D \to \mathbb{R}^n$, $D \subset \mathbb{R}^n$ open. Can we solve it with respect to x, i.e. can we **invert** the probem?

Theorem: (Inversion theorem)

Let $D \subset \mathbb{R}^n$ be open and $f: D \to \mathbb{R}^n$ a \mathcal{C}^1 -function. If the Jacobian-matrix $J f(x^0)$ is regular for an $x^0 \in D$, then there exist neighborhoods U and V of x^0 and $y^0 = f(x^0)$ such that f maps U on V bijectively.

The inverse function $f^{-1}: V \to U$ is also C^1 and for all $x \in U$ we have:

$$J f^{-1}(y) = (J f(x))^{-1}, \quad y = f(x)$$

Remark: We call f locally a C^1 -diffeomorphism.

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Chapter 2. Applications of multivariate differential calculus

2.3 Extrem value problems under constraints

Question: What is the size of a metallic cylindrical can in order to minimize the material amount by given volume?

Ansatz for solution: Let r > 0 be the radius and h > 0 the height of the can. Then

$$V = \pi r^2 h$$

$$O = 2\pi r^2 + 2\pi r h$$

Let $c \in \mathbb{R}_+$ be the given volume (with x := r, y := h),

$$f(x,y) = 2\pi x^2 + 2\pi xy$$
$$g(x,y) = \pi x^2 y - c = 0$$

Determine the minimum of the function f(x, y) on the set

$$G := \{(x,y) \in \mathbb{R}^2_+ \mid g(x,y) = 0\}$$

Solution of the constraint minimisation problem.

From $g(x, y) = \pi x^2 y - c = 0$ follows

$$y = \frac{c}{\pi x^2}$$

We plug this into f(x, y) and obtain

$$h(x) := 2\pi x^2 + 2\pi x \frac{c}{\pi x^2} = 2\pi x^2 + \frac{2c}{x}$$

Determine the minimum of the function h(x):

$$h'(x) = 4\pi x - \frac{2c}{x^2} = 0 \quad \Rightarrow \quad 4\pi x = \frac{2c}{x^2} \quad \Rightarrow \quad x = \left(\frac{c}{2\pi}\right)^{1/3}$$

Sufficient condition

$$h''(x) = 4\pi + \frac{4c}{x^3} \quad \Rightarrow \quad h''\left(\left(\frac{c}{\pi}\right)^{1/3}\right) = 12\pi > 0$$

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General formulation of the problem.

Determine the extrem values of the function $f:\mathbb{R}^n \to \mathbb{R}$ under the constraint

$$g(x) = 0$$

where $g : \mathbb{R}^n \to \mathbb{R}^m$. The constraints are

$$g_1(x_1,\ldots,x_n) = 0$$

$$\vdots$$

$$g_m(x_1,\ldots,x_n) = 0$$

Alternatively: Determine the extrem values of the function f(x) on the set

$$G:=\{\mathsf{x}\in\mathbb{R}^n\,|\,\mathsf{g}(\mathsf{x})=\mathsf{0}\}$$

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The Lagrange-function and the Lagrange-Lemma.

We define the Lagrange-function

$$F(\mathsf{x}) := f(\mathsf{x}) + \sum_{i=1}^m \lambda_i g_i(\mathsf{x})$$

and look for the extrem values of F(x) for fixed $\lambda = (\lambda_1, \ldots, \lambda_m)^T$.

The numbers λ_i , i = 1, ..., m are called Lagrange–multiplier.

Theorem: (Lagrange–Lemma) If x^0 minimizes (or maximizes) the Lagrange–function F(x) (for a fixed λ) on D and if $g(x^0) = 0$ holds, then x^0 is the minimum (or maximum) of f(x) on $G := \{x \in D \mid g(x) = 0\}$.

Proof: For an arbitrary $x \in D$ we have

$$f(\mathbf{x}^0) + \lambda^T \mathbf{g}(\mathbf{x}^0) \leq f(\mathbf{x}) + \lambda^T \mathbf{g}(\mathbf{x})$$

If we choose $x \in G$, then $g(x) = g(x^0) = 0$, thus $f(x^0) \le f(x)$.

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A necessary condition for local extrema.

Let f and g_i , i = 1, ..., m, C^1 -functions, then a necessary condition for an extrem value x^0 of F(x) is given by

$$\operatorname{grad} F(\mathsf{x}) = \operatorname{grad} f(\mathsf{x}) + \sum_{i=1}^m \lambda_i \operatorname{grad} g_i(\mathsf{x}) = 0$$

Together with the constraints g(x) = 0 we obtain a set of (non-linear) equations with (n + m) equations and (n + m) unknowns x and λ .

The solutions (x^0, λ^0) are the candidates for the extrem values, since these solutions satisfy the above necessary condition.

Alternatively: Define a Langrange-function

$$G(\mathbf{x}, \lambda) := f(\mathbf{x}) + \sum_{i=1}^{m} \lambda_i g_i(\mathbf{x})$$

and look for the extrem values of $G(x, \lambda)$ with respect to x and λ .

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Some remarks on sufficient conditions.

- We can formulate a sufficient condition:
 If the functions f and g are C²-functions and if the Hesse-matrix HF(x⁰) of the Lagrange-function is positiv (negativ) definit, then x⁰ is a strict local minimum (maximum) of f(x) on G.
- In most of the applications the necessary condition are **not** satisfied, allthough x⁰ is a strict local extremum.
- And from the indefinitness of the Hesse-matrix HF(x⁰) we cannot conclude, that x⁰ is not an extremum.
- We have a similar problem with the necessary condition which is obtained from the Hesse-matrix of the Lagrange-function G(x, λ) with respect to x and λ.

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An example of a minimisation problem with constraints.

We look for extrem values of f(x, y) := xy on the disc

$$K := \{ (x, y)^T \, | \, x^2 + y^2 \le 1 \}$$

Since the function f is continuous and $K \subset \mathbb{R}^2$ compact we conclude from the min-max-property the existence of global maxima and minima on K.

We consider first the interior K^0 of K, i.e. the open set

$$K^0 := \{ (x, y)^T \, | \, x^2 + y^2 < 1 \}$$

The necessary condition for an extrem value is given by

$$\operatorname{grad} f = (y, x) = 0$$

Thus the origin $x^0 = 0$ is a candidate for a (local) extrem value.

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continuation of the example.

The Hesse-matrix at the origin is given by

$$\mathsf{H}f(0)=\left(egin{array}{cc} 0 & 1 \ 1 & 0 \end{array}
ight)$$

and is indefinit. Thus x^0 is a saddel point.

Therefore the extrem values have to be on the boundary which is represented by a constraint equation:

$$g(x, y) = x^2 + y^2 - 1 = 0$$

Therefore we look for the extrem values of f(x, y) = xy under the constraint g(x, y) = 0.

The Lagrange-function is given by

$$F(x,y) = xy + \lambda(x^2 + y^2 - 1)$$

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Completion of the example.

We obtain the non-linear system of equations

$$y + 2\lambda x = 0$$

$$x + 2\lambda y = 0$$

$$x^{2} + y^{2} = 1$$

with the four solution

$$\lambda = \frac{1}{2} \quad : \quad \mathbf{x}^{(1)} = (\sqrt{1/2}, -\sqrt{1/2})^{\mathsf{T}} \quad \mathbf{x}^{(2)} = (-\sqrt{1/2}, \sqrt{1/2})^{\mathsf{T}}$$
$$\lambda = -\frac{1}{2} \quad : \quad \mathbf{x}^{(3)} = (\sqrt{1/2}, \sqrt{1/2})^{\mathsf{T}} \quad \mathbf{x}^{(4)} = (-\sqrt{1/2}, -\sqrt{1/2})^{\mathsf{T}}$$

Minima and Maxima can be concluded from the values of the function

$$f(\mathbf{x}^{(1)}) = f(\mathbf{x}^{(2)}) = -1/2$$
 $f(\mathbf{x}^{(3)}) = f(\mathbf{x}^{(4)}) = 1/2$

i.e. minima are $x^{(1)}$ and $x^{(2)},$ maxima are $x^{(3)}$ and $x^{(4)}.$

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Satz: Let $f, g_1, \ldots, g_m : D \to \mathbb{R}$ be C^1 -functions, und let $x^0 \in D$ a local extrem value of f(x) under the constraint g(x) = 0. In addition let the regularity condition

$$\operatorname{rang}\left(\operatorname{\mathsf{J}g}(\operatorname{\mathsf{x}}^0)
ight)=m$$

hold true. Then there exist Lagrange–multiplier $\lambda_1, \ldots, \lambda_m$, such that for the Lagrange function

$$F(\mathsf{x}) := f(\mathsf{x}) + \sum_{i=1}^{m} \lambda_i g_i(\mathsf{x})$$

the following first order necessary condition holds true:

grad
$$F(x^0) = 0$$

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Necessary condition of second order and sufficient condition.

Theorem: 1) Let $x^0 \in D$ a local minimum of f(x) under the constraint g(x) = 0, let the regularity condition be satisfied and let $\lambda_1, \ldots, \lambda_m$ be the related Lagrange–multiplier. Then the Hesse–matrix $HF(x^0)$ of the Lagrange–function is positiv semi-definit on the tangential space

$$TG(\mathsf{x}^0) := \{\mathsf{y} \in \mathbb{R}^n \,|\, \mathsf{grad}\, g_i(\mathsf{x}^0) \cdot \mathsf{y} = 0 \text{ for } i = 1, \dots, m\}$$

i.e. it is $y^T HF(x^0) y \ge 0$ for all $y \in TG(x^0)$.

2) Let the regularity condition for a point $x^0 \in G$ be staisfied. If there exist Lagrange–multiplier $\lambda_1, \ldots, \lambda_m$, such that x^0 is a stationary point of the related Lagrange–function. Let the Hesse–matrix $HF(x^0)$ be positiv definit on the tangential space $TG(x^0)$, i.e. it holds

$$y^T HF(x^0) y > 0 \quad \forall y \in TG(x^0) \setminus \{0\},$$

then x^0 is a strict local minimum of f(x) under the constraint g(x) = 0.

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Example.

Determine the global maximum of the function

$$f(x,y) = -x^2 + 8x - y^2 + 9$$

under the constraint

$$g(x, y) = x^2 + y^2 - 1 = 0$$

The Lagrange-function is given by

$$F(x) = -x^{2} + 8x - y^{2} + 9 + \lambda(x^{2} + y^{2} - 1)$$

From the necessary condition we obtain the non-linear system

$$-2x + 8 = -2\lambda x$$
$$-2y = -2\lambda y$$
$$x^{2} + y^{2} = 1$$

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Continuation of the example.

From the necessary condition we obtain the non-linear system

$$-2x + 8 = -2\lambda x$$
$$-2y = -2\lambda y$$
$$x^{2} + y^{2} = 1$$

The first equation gives $\lambda \neq 1$. Using this in the second equation we get y = 0. From the third equation we obtain $x = \pm 1$.

Therefore the two points (x, y) = (1, 0) and (x, y) = (-1, 0) are candidates for a global maximum. Since

$$f(1,0) = 16$$
 $f(-1,0) = 0$

the global maximum of f(x, y) under the constraint g(x, y) = 0 is given at the point (x, y) = (1, 0).

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Another example.

Determine the local extrem values of

$$f(x, y, z) = 2x + 3y + 2z$$

on the intersection of the cylinder surface

$$M_Z := \{ (x, y, z)^T \in \mathbb{R}^3 \, | \, x^2 + y^2 = 2 \}$$

with the plane

$$E := \{ (x, y, z)^T \in \mathbb{R}^3 \, | \, x + z = 1 \}$$

Reformulation: Determine the extrem values of the function f(x, y, z) under the constraint

$$g_1(x, y, z)$$
 := $x^2 + y^2 - 2 = 0$
 $g_2(x, y, z)$:= $x + z - 1 = 0$

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Continuation of the example.

The Jacobi-matrix

$$\mathsf{Jg}(\mathsf{x}) = \left(\begin{array}{rrr} 2x & 2y & 0\\ 1 & 0 & 1\end{array}\right)$$

has rank 2, i.e. we can determine extrem values using the Lagrange-function:

$$F(x, y, z) = 2x + 3y + 2z + \lambda_1(x^2 + y^2 - 2) + \lambda_2(x + z - 1)$$

The necessary condition gives the non-linear system

$$2 + 2\lambda_1 x + \lambda_2 = 0$$

$$3 + 2\lambda_1 y = 0$$

$$2 + \lambda_2 = 0$$

$$x^2 + y^2 = 2$$

$$x + z = 1$$

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Continuation of the example.

The necessary condition gives the non-linear system

$$2 + 2\lambda_1 x + \lambda_2 = 0$$

$$3+2\lambda_1 y = 0$$

$$2+\lambda_2 = 0$$

$$x^2 + y^2 = 2$$

$$x+z = 1$$

From the first and the third equation it follows

$$2\lambda_1 x = 0$$

From the second equation it follows $\lambda_1 \neq 0$, i.e. x = 0. Thus we have possible extrem values

$$(x, y, z) = (0, \sqrt{2}, 1)$$
 $(x, y, z) = (0, -\sqrt{2}, 1)$

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Completion if the example.

The possible extrem values are

$$(x, y, z) = (0, \sqrt{2}, 1)$$
 $(x, y, z) = (0, -\sqrt{2}, 1)$

and lie on the cylinder surface M_Z of the cylinder Z with

$$Z = \{(x, y, z)^T \in \mathbb{R}^3 | x^2 + y^2 \le 2\}$$
$$M_Z = \{(x, y, z)^T \in \mathbb{R}^3 | x^2 + y^2 = 2\}$$

We calculate the related functiuon values

$$f(0, \sqrt{2}, 1) = 3\sqrt{2} + 2$$

$$f(0, -\sqrt{2}, 1) = -3\sqrt{2} + 2$$

Thus the point $(x, y, z) = (0, \sqrt{2}, 1)$ is a maximum an the point $(x, y, z) = (0, -\sqrt{2}, 1)$ a minimum.

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Chapter 2. Applications of multivariate differential calculus

2.4 the Newton-method

Aim: We look for the zero's of a function $f: D \to \mathbb{R}^n$, $D \subset \mathbb{R}^n$:

f(x) = 0

• We already know the fixed-point iteration

$$\mathsf{x}^{k+1} := \Phi(\mathsf{x}^k)$$

with starting point x^0 and iteration map $\Phi : \mathbb{R}^n \to \mathbb{R}^n$.

• Convergence results are given by the Banach Fixed Point Theorem.

Advantage: this method is derivative-free.

Disadvantages:

- the numerical scheme converges to slow (only linear),
- there is no unique iteratin map.

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The construction of the Newton method.

Starting point: Let C^1 -function $f: D \to \mathbb{R}^n$, $D \subset \mathbb{R}^n$ open.

We look for a zero of f, i.e. a $x^* \in D$ with

$$f(x^{*}) = 0$$

Construction of the Newton-method:

The Taylor–expansion of f(x) at x^0 is given by

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

Setting $x = x^*$ we obtain

$$\mathsf{Jf}(\mathsf{x}^0)(\mathsf{x}^*-\mathsf{x}^0)\approx-\mathsf{f}(\mathsf{x}^0)$$

An approximative solution for x^* is given by $x^1,\,x^1\approx x^*,$ the solution of the linear system of equations

$$Jf(x^{0})(x^{1}-x^{0}) = -f(x^{0})$$

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The Newton-method as algorithm.

The Newton-method can be formulated as algorithm.

Algorithm (Newton-method): (1) FOR k = 0, 1, 2, ...(2a) Solve $Jf(x^k) \cdot \Delta x^k = -f(x^k)$; (2b) Set $x^{k+1} = x^k + \Delta x^k$;

- In every Newton-step we solve a set of linear equations.
- The solution Δx^k is called Newton-correction.
- The Newton-method is scaling-invariant.

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Scaling-invariance of the Newton-method.

Theorem: the Newton-method is invariant under linear transformations of the form

$$f(x) \rightarrow g(x) = Af(x)$$
 for $A \in \mathbb{R}^{n \times n}$ regular,

i.e. the iterates for f and g are identical.

Proof: Constructing the Newton–method for g(x), then the Newton–correction is given by

$$\begin{aligned} \Delta x^{k} &= -(Jg(x^{k}))^{-1} \cdot g(x^{k}) \\ &= -(AJf(x^{k}))^{-1} \cdot Af(x^{k}) \\ &= -(Jf(x^{k}))^{-1} \cdot A^{-1}A \cdot f(x^{k}) \\ &= -(Jf(x^{k}))^{-1} \cdot f(x^{k}) \end{aligned}$$

and thus the Newton-correction of f and g conincide.

Using the same starting point x^0 we obtain the same iterates x^k .

Local convergence of the Newton-method.

Theorem: Let $f: D \to \mathbb{R}^n$ be a C^1 -function, $D \subset \mathbb{R}^n$ open and convex. Let $x^* \in D$ a zero of f, i.e. $f(x^*) = 0$.

Let the Jacobi–matrix $\mathsf{Jf}(\mathsf{x})$ be regular for $\mathsf{x} \in D,$ and suppose the Lipschitz–condition

$$\|(\mathsf{Jf}(\mathsf{x})^{-1}(\mathsf{Jf}(\mathsf{y})-\mathsf{Jf}(\mathsf{x}))\|\leq L\|\mathsf{y}-\mathsf{x}\|\qquad\text{for all $\mathsf{x},\mathsf{y}\in D$,}$$

holds true with L > 0. Then the Newton–method is well defined for all starting points $x^0 \in D$ with

$$\|\mathbf{x}^0 - \mathbf{x}^*\| < \frac{2}{L} =: r \text{ and } K_r(\mathbf{x}^*) \subset D$$

with $x^k \in K_r(x^*)$, k = 0, 1, 2, ..., and the Newton-iterates x^k converge quadratically to x^* , i.e.

$$\|\mathbf{x}^{k+1} - \mathbf{x}^*\| \le \frac{L}{2} \|\mathbf{x}^k - \mathbf{x}^*\|^2$$

 x^* is the unique zero of f(x) within the ball $K_r(x^*)$.

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The damped Newton-method.

Additional obserrvations:

- The Newton-method converges quadratically, but only locally.
- Global convergence can be obtained if applicable by a damping term:

Algorithm (Damped Newton-method): (1) FOR k = 0, 1, 2, ...(2a) Solve $Jf(x^k) \cdot \Delta x^k = -f(x^k)$; (2b) Set $x^{k+1} = x^k + \lambda_k \Delta x^k$;

Frage: How should we choose the damping parameters λ_k ?

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Choice of the damping paramter.

Strategy: Use a testfunction T(x) = ||f(x)|| such that

 $T(\mathbf{x}) \geq 0, \quad \forall \mathbf{x} \in D$

$$T(x) = 0 \Leftrightarrow f(x) = 0$$

Choose $\lambda_k \in (0, 1)$ such that the sequence $T(x^k)$ decreases strictly monotonically, i.e.

$$\|f(x^{k+1})\| < \|f(x^k)\|$$
 für $k \ge 0$.

Close to the solution x^* we should choose $\lambda_k = 1$ to guarantee (local) quadratic convergence.

The following Theorem guarantees the existence of damping parameters.

Theorem: Let f a C^1 -function on the open and convex set $D \subset \mathbb{R}^n$. For $x^k \in D$ with $f(x^k) \neq 0$ there exists a $\mu_k > 0$ such that

$$\|\mathbf{f}(\mathbf{x}^k + \lambda \Delta x^k)\|_2^2 < \|\mathbf{f}(\mathbf{x}^k)\|_2^2$$
 for all $\lambda \in (0, \mu_k)$.

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Damping strategy.

For the **initial iteration** k = 0: Choose $\lambda_0 \in \{1, \frac{1}{2}, \frac{1}{4}, \dots, \lambda_{min}\}$ as big as possible such that

 $\|f(x^0)\|_2 > \|f(x^0 + \lambda_0 \Delta x^0)\|_2$

holds. For subsequent iterations k > 0: Set $\lambda_k = \lambda_{k-1}$.

IF $\|\mathbf{f}(\mathbf{x}^k)\|_2 > \|\mathbf{f}(\mathbf{x}^k + \lambda_k \Delta \mathbf{x}^k)\|_2$ THEN

- $\mathbf{x}^{k+1} := \mathbf{x}^k + \lambda_k \Delta \mathbf{x}^k$
- $\lambda_k := 2\lambda_k$, falls $\lambda_k < 1$.

ELSE

• Determine $\mu = \max\{\lambda_k/2, \lambda_k/4, \dots, \lambda_{\min}\}$ with

$$\|\mathbf{f}(\mathbf{x}^k)\|_2 > \|\mathbf{f}(\mathbf{x}^k + \lambda_k \Delta \mathbf{x}^k)\|_2$$

• $\lambda_k := \mu$

END

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3.1 Area integrals

Given a function $f: D \to \mathbb{R}$ with domain of definiton $D \subset \mathbb{R}^n$.

Aim: Calculate the volume under the graph of f(x):

$$V = \int_D f(\mathsf{x}) d\mathsf{x}$$

Remember (Analysis II): Riemann–Integral of a function f on the interval [a, b]:

$$I = \int_{a}^{b} f(x) dx$$

The integral *I* is defined as limit of Riemann upper– and lower-sums, if the limits exist and coincide.

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Construction of area integrals.

Procedure: Same as in the one dimensional case.

But: the domain of definition *D* is more complex.

Starting point: consider the case of two variables n = 2 and a domain of definition $D \subset \mathbb{R}^2$ of the form

$$D = [a_1, b_1] imes [a_2, b_2] \subset \mathbb{R}^2$$

i.e. *D* is compact cuboid (rectangle). Let $f: D \to \mathbb{R}$ be a bounded function.

Definition: We call $Z = \{(x_0, x_1, \dots, x_n), (y_0, y_1, \dots, y_m)\}$ a partition of the cuboid $D = [a_1, b_1] \times [a_2, b_2]$ if it holds

$$a_1 = x_0 < x_1 < \cdots < x_n = b_1$$

$$a_2 = y_0 < y_1 < \cdots < y_m = b_2$$

Z(D) denotes the set of partitions of D.

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Partitions and Riemann sums.

Definition:

• The fineness of a partition $Z \in Z(D)$ is given by

$$\|Z\| := \max_{i,j} \{|x_{i+1} - x_i|, |y_{j+1} - y_j|\}$$

• For a given partition Z the sets

$$Q_{ij} := [x_i, x_{i+1}] \times [y_j, y_{j+1}]$$

are called the subcuboid of the partition Z. The volume of the subcuboid Q_{ij} is given by

$$vol(Q_{ij}) := (x_{i+1} - x_i) \cdot (y_{j+1} - y_j)$$

• For arbitrary points $x_{ij} \in Q_{ij}$ of the subcuboids we call

$$R_f(Z) := \sum_{i,j} f(\mathsf{x}_{ij}) \cdot \mathsf{vol}(Q_{ij})$$

a Riemann sum of the partition Z.

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Riemann upper and lower sums.

Definition:

In analogy to the integral for the univariate case we call for a partition \boldsymbol{Z}

$$U_f(Z) := \sum_{i,j} \inf_{\mathbf{x} \in Q_{ij}} f(\mathbf{x}) \cdot \operatorname{vol}(Q_{ij})$$
$$O_f(Z) := \sum_{i,j} \sup_{\mathbf{x} \in Q_{ij}} f(\mathbf{x}) \cdot \operatorname{vol}(Q_{ij})$$

the Riemann lower sum and the Riemann upper sum of f(x), respectively.

Remark:

A Riemann sum for the partition Z lies always between the lower and the upper sum of that partition i.e.

$$U_f(Z) \leq R_f(Z) \leq O_f(Z)$$

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Remark.

If a partition Z_2 is obtained from a partition Z_1 by adding additional intermediate points x_i and/or y_j , then

 $U_f(Z_2) \ge U_f(Z_1)$ and $O_f(Z_2) \le O_f(Z_1)$

For arbitrary two partitions Z_1 and Z_2 we always have:

 $U_f(Z_1) \leq O_f(Z_2)$

Question: what happens to the lower and upper sums in the limit $||Z|| \rightarrow 0$:

$$U_f := \sup\{U_f(Z) : Z \in Z(D)\}$$
$$O_f := \inf\{O_f(Z) : Z \in Z(D)\}$$

Observation: Both values U_f and O_f exist since lower and upper sum are monoton and bounded.

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Riemann upper and lower integrals.

Definition:

• The Riemann lower and upper integral of a function f(x) on D is given by

$$\int_{\underline{D}} f(\mathbf{x}) d\mathbf{x} := \sup\{U_f(Z) : Z \in \mathsf{Z}(D)\}$$
$$\int_{\overline{D}} f(\mathbf{x}) d\mathbf{x} := \inf\{O_f(Z) : Z \in \mathsf{Z}(D)\}$$

The function f(x) is called Riemann-integrable on D, if lower and upper integral conincide. The Riemann-integral of f(x) on D is then given by

$$\int_{D} f(\mathbf{x}) d\mathbf{x} := \int_{\underline{D}} f(\mathbf{x}) d\mathbf{x} = \int_{\overline{D}} f(\mathbf{x}) d\mathbf{x}$$

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Up to now we habe "only" considered the case of two variables:

$$f: D \to \mathbb{R}, \qquad D \in \mathbb{R}^2$$

In higher dimensions, n > 2, the procedure is the same.

Notation: for n = 2 and n = 3

$$\int_D f(x,y) dx dy \quad \text{bzw.} \quad \int_D f(x,y,z) dx dy dz$$

or

$$\iint_D f(x,y) dx dy \quad \text{bzw.} \quad \iiint_D f(x,y,z) dx dy dz$$

respectively.

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Elementary properties of the integral.

Theorem:

a) Linearity

$$\int_{D} (\alpha f(\mathbf{x}) + \beta g(\mathbf{x})) d\mathbf{x} = \alpha \int_{D} f(\mathbf{x}) d\mathbf{x} + \beta \int_{D} g(\mathbf{x}) d\mathbf{x}$$

b) Monotonicity

If $f(x) \leq g(x)$ for all $x \in D$, then:

$$\int_D f(\mathbf{x}) d\mathbf{x} \le \int_D g(\mathbf{x}) d\mathbf{x}$$

c) Positivity

If for all $x \in D$ the relation $f(x) \ge 0$ holds, i.e. f(x) is non-negativ, then

$$\int_D f(\mathsf{x}) d\mathsf{x} \ge 0$$

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Additional properties of the integral.

Theorem:

a) Let D_1 , D_2 and D be cuboids, $D = D_1 \cup D_2$ and $vol(D_1 \cap D_2) = 0$, then f(x) is on D integrable if and only if f(x) is integrable on D_1 and D_2 . And we have

$$\int_D f(x)dx = \int_{D_1} f(x)dx + \int_{D_2} f(x)dx$$

b) The following estimate holds for the integral

$$\int_D f(x) dx \bigg| \leq \sup_{x \in D} |f(x)| \cdot \operatorname{vol}(D)$$

c) Riemann criterion

f(x) is integrable on D if and only if :

$$\forall \varepsilon > 0 \quad \exists Z \in Z(D) \quad : \quad O_f(Z) - U_f(Z) < \varepsilon$$

Fubini's theorem.

Theorem: (Fubini's theorem) Let $f : D \to \mathbb{R}$ be integrable, $D = [a_1, b_1] \times [a_2, b_2]$ be a cuboid. If the integrals

$$F(x) = \int_{a_2}^{b_2} f(x, y) dy$$
 und $G(y) = \int_{a_1}^{b_1} f(x, y) dx$

exist for all $x \in [a_1, b_1]$ and $y \in [a_2, b_2]$, respectively, then

$$\int_{D} f(\mathbf{x}) d\mathbf{x} = \int_{a_1}^{b_1} \int_{a_2}^{b_2} f(\mathbf{x}, \mathbf{y}) d\mathbf{y} d\mathbf{x}$$
$$\int_{D} f(\mathbf{x}) d\mathbf{x} = \int_{a_2}^{b_2} \int_{a_1}^{b_1} f(\mathbf{x}, \mathbf{y}) d\mathbf{x} d\mathbf{y}$$

holds true.

Importance:

Fubini's theorem allows to reduce higher-dimensional integrals to one-dimensional integrals.

Given the cuboid $D = [0,1] \times [0,2]$ and the function

$$f(x,y)=2-xy$$

We will show that continuous functions are integrable on cuboids. Thus we can apply Fubini's theorem:

$$\int_{D} f(x)dx = \int_{0}^{2} \int_{0}^{1} f(x,y)dxdy = \int_{0}^{2} \left[2x - \frac{x^{2}y}{2}\right]_{x=0}^{x=1} dy$$
$$= \int_{0}^{2} \left(2 - \frac{y}{2}\right)dy = \left[2y - \frac{y^{2}}{4}\right]_{y=0}^{y=2} = 3$$

Remark: Fubini's theorem requires the integrability of f(x). The existence of the two integrals F(x) and G(y) does **not** guarantee the integrability of f(x)!

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Definition: Let $D \subset \mathbb{R}^n$ compact and $f : D \to \mathbb{R}$ bounded. We set

$$f^*(\mathsf{x}) := \left\{ egin{array}{ccc} f(\mathsf{x}) & : & ext{if } \mathsf{x} \in D \ 0 & : & ext{if } \mathsf{x} \in \mathbb{R}^n \setminus D \end{array}
ight.$$

In particular for f(x) = 1 we call $f^*(x)$ the characteristic function of D. The characteristic function of D is called $\mathcal{X}_D(x)$.

Let Q be the smallest cuboid with $D \subset Q$. The function f(x) is called integrable on D, if $f^*(x)$ is integrable on Q. We set

$$\int_D f(\mathsf{x})d\mathsf{x} := \int_Q f^*(\mathsf{x})d\mathsf{x}$$

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Measurability and null sets.

Definition: The compact set $D \subset \mathbb{R}^n$ is called measurable, if the integral

$$\operatorname{vol}(D) := \int_D 1 d\mathsf{x} = \int_Q \mathcal{X}_D(\mathsf{x}) d\mathsf{x}$$

exists. We call vol(D) the volume of D in \mathbb{R}^n .

The compact set D is called null set, if D is measurable and if vol(D) = 0 holds. Remark:

• If D a cuboid, then Q = D and thus

$$\int_D f(x)dx = \int_Q f^*(x)dx = \int_Q f(x)dx$$

i.e. the introduced concepts of integrability coincide.

- Cuboids are measurable sets.
- vol(D) is the volume of the cuboid on \mathbb{R}^n .

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Three more properties of integration.

We have the following theorems for integrals in higher dimensions.

Theorem: Let $D \subset \mathbb{R}^n$ be compact. *D* is measurable if and only if the boundary ∂D of *D* is a null set.

Theorem: Let $D \subset \mathbb{R}^n$ be compact and measurable. Let $f : D \to \mathbb{R}$ be continuous. Then f(x) is integrable on D.

Theorem: (Mean value theorem) Let $D \subset \mathbb{R}^n$ be compact, connected and measurable, and let $f : D \to \mathbb{R}$ be continuous, then there exist a point $\xi \in D$ with

$$\int_D f(\mathsf{x})d\mathsf{x} = f(\xi) \cdot \mathsf{vol}(D)$$

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Definition:

• A subset $D \subset \mathbb{R}^2$ is called "normal" area, there exist continuous functions g, h and \tilde{g}, \tilde{h} with

$$D = \{(x, y) \mid a \le x \le b \text{ und } g(x) \le y \le h(x)\}$$

and

$$D = \{(x, y) \mid \tilde{a} \le y \le \tilde{b} \text{ und } \tilde{g}(y) \le x \le \tilde{h}(y)\}$$

respectively.

 \bullet A subset $D \subset \mathbb{R}^3$ is called "normal" area , if there is a representation

$$D = \{ (x_1, x_2, x_3) \mid a \le x_i \le b, g(x_i) \le x_j \le h(x_i)$$

and $\varphi(x_i, x_j) \le x_k \le \psi(x_i, x_j) \}$

with a permutation (i, j, k) of (1, 2, 3) and continuos functions g, h, φ and ψ .

Definition: A subset $D \subset \mathbb{R}^n$ is called projectable in the direction x_i , $i \in \{1, \ldots, n\}$, if there exist a measurable set $B \subset \mathbb{R}^{n-1}$ and continuous functions φ, ψ such that

$$D = \{ \mathbf{x} \in \mathbb{R}^n \mid \tilde{\mathbf{x}} = (x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_n)^T \in B$$

und $\varphi(\tilde{\mathbf{x}}) \le x_i \le \psi(\tilde{\mathbf{x}}) \}$

Remark:

- Projectable sets are measurable sets. Since "normal" areas are projectable, "normal" areas are measurable.
- Often the area of integration *D* can be represented by a union of finite many "normal" areas. Such areas are then also measurable.

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Integration on "normal" areas and projectable sets.

Theorem: If f(x) is a continuous function on a "normal" area

$$D = \{ (x, y) \in \mathbb{R}^2 : a \leq x \leq b \text{ and } g(x) \leq y \leq h(x) \}$$

then we have

$$\int_D f(x) dx = \int_a^b \int_{g(x)}^{h(x)} f(x, y) dy dx$$

Analogous relations hold in higher dimensions: If $D \subset \mathbb{R}^n$ is a projectable set in the direction x_i , i.e. D has a representation of the form

$$D = \{ \mathbf{x} \in \mathbb{R}^n \mid \tilde{\mathbf{x}} = (x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_n)^T \in B$$

and $\varphi(\tilde{\mathbf{x}}) \le x_i \le \psi(\tilde{\mathbf{x}}) \}$

then it holds

$$\int_D f(\mathbf{x}) d\mathbf{x} = \int_B \left(\int_{\varphi(\tilde{\mathbf{x}})}^{\psi(\tilde{\mathbf{x}})} f(\mathbf{x}) dx_i \right) d\tilde{\mathbf{x}}$$

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Example.

Given a function

$$f(x,y) := x + 2y$$

Calculate the integral on the area bounded by two parabolas

$$D:=\{(x,y)\mid \ -1\leq x\leq 1 \ ext{und} \ x^2\leq y\leq 2-x^2\}$$

The set D is a "normal" area and f(x, y) is continuous. Thus

$$\int_{D} f(x,y)dx = \int_{-1}^{1} \left(\int_{x^{2}}^{2-x^{2}} (x+2y)dy \right) dx = \int_{-1}^{1} \left[xy + y^{2} \right]_{x^{2}}^{2-x^{2}} dx$$
$$= \int_{-1}^{1} (x(2-x^{2}) + (2-x^{2})^{2} - x^{3} - x^{4})dx$$
$$= \int_{-1}^{1} (-2x^{3} - 4x^{2} + 2x + 4)dx = \frac{16}{3}$$

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Example.

Calculate the volume of the rotational paraboloid

$$V := \{(x, y, z)^T \mid x^2 + y^2 \le 1 \text{ and } x^2 + y^2 \le z \le 1\}$$

Representation of V as "normal" area

$$V = \{(x, y, z)^{\mathsf{T}} \mid -1 \le x \le 1, \ -\sqrt{1 - x^2} \le y \le \sqrt{1 - x^2} \text{ and } x^2 + y^2 \le z \le 1\}$$

Then we have

$$\operatorname{vol}(V) = \int_{-1}^{1} \int_{-\sqrt{1-x^{2}}}^{\sqrt{1-x^{2}}} \int_{x^{2}+y^{2}}^{1} dz dy dx = \int_{-1}^{1} \int_{-\sqrt{1-x^{2}}}^{\sqrt{1-x^{2}}} (1-x^{2}-y^{2}) dy dx$$
$$= \int_{-1}^{1} \left[(1-x^{2})y - \frac{y^{3}}{3} \right]_{y=-\sqrt{1-x^{2}}}^{y=\sqrt{1-x^{2}}} dx = \frac{4}{3} \int_{-1}^{1} (1-x^{2})^{3/2} dx$$
$$= \frac{1}{3} \left[x(\sqrt{1-x^{2}})^{3} + \frac{3}{2}x\sqrt{1-x^{2}} + \frac{3}{2}\operatorname{arcsin}(x) \right]_{-1}^{1} = \frac{\pi}{2}$$

Definition: Let $D \subset \mathbb{R}^n$ be a compact and measurable set. We call $Z = \{D_1, \ldots, D_m\}$ an universal partition of D, if the sets D_k are compact, measurable and connected and if

$$igcup_{j=1}^m D_j = D$$
 and $orall i
eq j : D^0_i \cap D^0_j = \emptyset$

We call

$$\mathsf{diam}(D_j) := \mathsf{sup} \{ \|\mathsf{x} - \mathsf{y}\| \, | \, \mathsf{x}, \mathsf{y} \in D_j \}$$

the diameter of the set D_j and

$$|Z\|:=\max\left\{\operatorname{\mathsf{diam}}(D_j) \mid j=1,\ldots,m
ight\}$$

the fineness of the universal partition Z.

Riemann sums for universal partitions.

For a continuous function $f: D \to \mathbb{R}$ we define the Riemann sums

$$R_f(Z) = \sum_{j=1}^m f(x^j) \operatorname{vol}(D_j)$$

with arbitrary $x^j \in D_j$, $j = 1, \ldots, m$.

Theorem: For any sequence $(Z_k)_{k\in\mathbb{N}}$ of universal partitons of D with $||Z_k|| \to 0$ (as $k \to \infty$) and for ony sequence of related Riemann sums $R_f(Z_k)$ we have

$$\lim_{k\to\infty}R_f(Z_k)=\int_Df(x)dx$$

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An important application of the area integrals is the calculation of the centers (of mass) of areas and solids.

Definition: Let $D \subset \mathbb{R}^2$ (or \mathbb{R}^3) be a measurable set and $\rho(x), x \in D$, a given mass density. Then the center (of mass) of the area (or the solid) D is given by

$$\mathsf{x}_{\mathsf{s}} := \frac{\int_D \rho(\mathsf{x}) \mathsf{x} d\mathsf{x}}{\int_D \rho(\mathsf{x}) d\mathsf{x}}$$

The numerator integral (over a vector valued function) is intended componentwise (and gives as result a vector).

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Example.

Calculate the center of mass of the pyramid P

$$P := \left\{ (x, y, z)^T \mid \max(|y|, |z|) \leq \frac{ax}{2h}, \quad 0 \leq x \leq h
ight\}$$

Calculate the volume of P under assumption of constant mass density

$$\operatorname{vol}(P) = \int_0^h \int_{-\frac{ax}{2h}}^{\frac{ax}{2h}} \int_{-\frac{ax}{2h}}^{\frac{ax}{2h}} dz \, dy \, dx$$

$$= \int_0^h \int_{-\frac{ax}{2h}}^{\frac{ax}{2h}} \frac{ax}{h} dy dx$$

$$= \int_0^h \left(\frac{ax}{h}\right)^2 dx = \frac{1}{3}a^2h$$

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Continuation of the example.

and
$$\int_{0}^{h} \int_{-\frac{ax}{2h}}^{\frac{ax}{2h}} \int_{-\frac{ax}{2h}}^{\frac{ax}{2h}} \begin{pmatrix} x \\ y \\ z \end{pmatrix} dz dy dx = \int_{0}^{h} \int_{-\frac{ax}{2h}}^{\frac{ax}{2h}} \begin{pmatrix} \frac{ax^{2}}{h} \\ \frac{axy}{h} \\ 0 \end{pmatrix} dy dx$$
$$= \int_{0}^{h} \begin{pmatrix} \frac{a^{2}x^{3}}{h^{2}} \\ 0 \\ 0 \end{pmatrix} dx$$
$$= \begin{pmatrix} \frac{1}{4}a^{2}h^{2} \\ 0 \\ 0 \end{pmatrix}$$

The center of mass of P lies in the point $x_s = (\frac{3}{4}h, 0, 0)^T$.

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Another important application of area integrals is the calculation of moments of inertia of areas and solids.

Definition: (moments of inertia with respect to an axis) Let $D \subset \mathbb{R}^2$ (or \mathbb{R}^3) be a measurable set, $\rho(x)$ denotes for $x \in D$ a mass density and r(x) the distance of the point $x \in D$ from the given axis of rotation.

Then the moment of inertia of D with respect to this axis is given by

$$\Theta := \int_D \rho(\mathsf{x}) r^2(\mathsf{x}) d\mathsf{x}$$

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Example.

We calculate the moment of inertia of a homogeneous cylinder

$$Z := \left\{ (x, y, z)^T : x^2 + y^2 \le r^2, -1/2 \le z \le 1/2 \right\}$$

with respect to the x-axis assuming a constant density ρ .

$$\Theta = \int_{Z} \rho(y^{2} + z^{2}) d(x, y, z) = \rho \int_{Z} (y^{2} + z^{2}) d(x, y, z)$$
$$= \rho \int_{-r}^{r} \int_{-\sqrt{r^{2} - x^{2}}}^{\sqrt{r^{2} - x^{2}}} \int_{-l/2}^{l/2} (y^{2} + z^{2}) dz dy dx$$
$$= \rho \int_{-r}^{r} \int_{-\sqrt{r^{2} - x^{2}}}^{\sqrt{r^{2} - x^{2}}} (ly^{2} + \frac{l^{3}}{12}) dy dx$$

$$= \rho \frac{\pi l r^2}{12} (3r^2 + l^2)$$

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Aim: A generalisation of the (one dimensional) rule of substitution

$$\int_{\varphi(a)}^{\varphi(b)} f(x) \, dx = \int_{a}^{b} f(\varphi(t)) \varphi'(t) \, dt$$

Theorem: (Theorem of transformation) Let $\Phi : U \to \mathbb{R}^n$, $U \subset \mathbb{R}^n$ be open and a \mathcal{C}^1 -map. Let $D \subset U$ be a compact, measurable set such that Φ is a \mathcal{C}^1 -diffeomorphisms on D^0 . Then $\Phi(D)$ is compact and measurable and for any continuous function $f : \Phi(D) \to \mathbb{R}$ the rule of transformation

$$\int_{\Phi(D)} f(\mathsf{x}) d\mathsf{x} = \int_D f(\Phi(\mathsf{u})) |\det \mathsf{J}\Phi(\mathsf{u})| \, d\mathsf{u}$$

holds.

Remark: Note that the rule of transformation requires the bijectivety of Φ only on the inertior D^0 of D – not on the boundary $\partial D!$

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Example.

Calculate the center of mass of a homogeneous spherical octant

$$V = \{(x, y, z,)^T \mid x^2 + y^2 + z^2 \le 1 \text{ und } x, y, z \ge 0\}$$

It is easier to calculate the center of mass using spherical coordinates Kugelkoordinaten:

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} r\cos\varphi\cos\psi \\ r\sin\varphi\cos\psi \\ r\sin\psi \end{pmatrix} = \Phi(r,\varphi,\psi)$$

The transformation is defined on \mathbb{R}^3 and with

$$D = [0,1] \times \left[0,\frac{\pi}{2}\right] \times \left[0,\frac{\pi}{2}\right]$$

we have $\Phi(D) = V$. It is Φ on D^0 a C^1 -diffeomorphisms with

$$\det \mathsf{J}\Phi(\mathbf{r},\varphi,\psi)=\mathbf{r}^2\cos\psi$$

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According to the theorem of transformation it follows

$$\operatorname{vol}(V) = \int_{V} dx = \int_{0}^{1} \int_{0}^{\pi/2} \int_{0}^{\pi/2} r^{2} \cos \psi d\psi d\varphi dr = \frac{\pi}{6}$$

and

$$\operatorname{vol}(V) \cdot x_{s} = \int_{V} x \, dx = \int_{0}^{1} \int_{0}^{\pi/2} \int_{0}^{\pi/2} (r \cos \varphi \cos \psi) \, r^{2} \cos \psi \, d\psi \, d\varphi \, dr$$
$$= \int_{0}^{1} r^{3} \, dr \cdot \int_{0}^{\pi/2} \cos \varphi \, d\varphi \cdot \int_{0}^{\pi/2} \cos^{2} \psi \, d\psi = \frac{\pi}{16}$$

The it follows $x_s = \frac{3}{8}$.

In Analogy we calculate $y_s = z_s = \frac{3}{8}$.

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The Theorem of Steiner.

Theorem: (Theorem of Steiner) For the moment of inertia of a homogeneous solid K with total mass m with respect to a given axis of rotation A we have

$$\Theta_A = md^2 + \Theta_S$$

S is the axis through to center of mass of the solid K parallel to the axis A and d the distance of the center of mass x_s from the axis A.

Idea of the proof: Set $x := \Phi(u) = x_s + u$. Then with the unit vector a in direction of the axis A

$$\begin{split} \Theta_{A} &= \rho \int_{K} (\langle \mathbf{x}, \mathbf{x} \rangle - \langle \mathbf{x}, \mathbf{a} \rangle^{2}) d\mathbf{x} \\ &= \rho \int_{D} (\langle \mathbf{x}_{s} + \mathbf{u}, \mathbf{x}_{s} + \mathbf{u} \rangle - \langle \mathbf{x}_{s} + \mathbf{u}, \mathbf{a} \rangle^{2}) d\mathbf{x} \end{split}$$

where

$$D:=\{x-x_s\,|\,x\in K\}$$

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