

# Analysis III for engineering study programs

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# Content of the course Analysis III.

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

# Chapter 1. Multi variable differential calculus

## 1.1 Partial derivatives

Let

$f(x_1, \dots, x_n)$  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  $T$  (temperature) can be expressed as a function of the others ( $R$  is the gas constant)

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

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

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

# 1.1. Partial derivatives

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

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

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

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

# Examples.

- Consider the function

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

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

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

Thus  $f$  is a  $\mathcal{C}^1$ -function.

- The function

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

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

# An engineering example.

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

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

The partial derivative

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

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

The partial derivative

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

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

# Rules for differentiation

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

$$\frac{\partial}{\partial x_i} (\alpha f(x) + \beta g(x)) = \alpha \frac{\partial f}{\partial x_i}(x) + \beta \frac{\partial g}{\partial x_i}(x)$$

$$\frac{\partial}{\partial x_i} (f(x) \cdot g(x)) = \frac{\partial f}{\partial x_i}(x) \cdot g(x) + f(x) \cdot \frac{\partial g}{\partial x_i}(x)$$

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

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

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

# Gradient and nabla-operator.

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

- We denote the **row vector**

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

as **gradient** of  $f$  at  $x^0$ .

- We denote the symbolic vector

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

as **nabla-operator**.

- Thus we obtain the **column vector**

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



## More rules on differentiation.

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

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

$$\text{grad}(f \cdot g) = g \cdot \text{grad} f + f \cdot \text{grad} g$$

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

### Examples:

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

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

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

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

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

# 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  $f : \mathbb{R}^2 \rightarrow \mathbb{R}$  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 differentiable 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  $(0, 0)$ :

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

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

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

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

and thus we have

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

# Boundedness of the derivatives implies continuity.

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

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

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

# Proof of the theorem.

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

$$\begin{aligned} f(x) - f(x^0) &= (f(x_1, \dots, x_{n-1}, x_n) - f(x_1, \dots, x_{n-1}, x_n^0)) \\ &+ (f(x_1, \dots, x_{n-1}, x_n^0) - f(x_1, \dots, x_{n-2}, x_{n-1}^0, x_n^0)) \\ &\vdots \\ &+ (f(x_1, x_2^0, \dots, x_n^0) - f(x_1^0, \dots, x_n^0)) \end{aligned}$$

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  $\xi_n$  between  $x_n$  and  $x_n^0$ .

## Proof of the theorem (continuation).

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

$$\begin{aligned}f(x) - f(x^0) &= \frac{\partial f}{\partial x_n}(x_1, \dots, x_{n-1}, \xi_n) \cdot (x_n - x_n^0) \\ &+ \frac{\partial f}{\partial x_{n-1}}(x_1, \dots, x_{n-2}, \xi_{n-1}, x_n^0) \cdot (x_{n-1} - x_{n-1}^0) \\ &\vdots \\ &+ \frac{\partial f}{\partial x_1}(\xi_1, x_2^0, \dots, x_n^0) \cdot (x_1 - x_1^0)\end{aligned}$$

Using the boundedness of the partial derivatives

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

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

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

## 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  $i_1, \dots, i_k \in \{1, \dots, n\}$ . Then we define recursively

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

# 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  $f(x_1, \dots, x_n) = \prod_{i=1}^n x_i^i$  we have  $\frac{\partial^n f}{\partial x_n \dots \partial x_1} = ?$



# Partial derivatives are not arbitrarily exchangeable.

**ATTENTION:** The order how to execute partial derivatives is in general **not** arbitrarily 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.  $f_{xy}(0, 0) \neq f_{yx}(0, 0)$ .

# Theorem of Schwarz on exchangeability.

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

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

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

## Idea of the proof:

Apply the mean value theorem twice.

## Conclusion:

If  $f$  is a  $\mathcal{C}^k$ -function, then we can exchange the differentiation in order to calculate partial derivatives up to order  $k$  **arbitrarily!**

## 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 exchangeable since  $f \in \mathcal{C}^3$ .

- 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):

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

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

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

# The Laplace operator.

The **Laplace-operator** or **Laplacian** is defined as

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

For a scalar function  $u(x) = u(x_1, \dots, x_n)$  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):

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

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

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

# Vector valued functions.

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

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

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

exist. The calculation is done componentwise

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

# Vectorfields.

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

## Examples of vectorfields:

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

**Definition:** Let  $f : D \rightarrow \mathbb{R}^n$  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

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

# Rules of computation and the rotation.

The following rules hold true:

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

$$\operatorname{div}(\varphi \cdot f) = (\nabla \varphi, f) + \varphi \operatorname{div} f \quad \text{for } \varphi : D \rightarrow \mathbb{R}, f : D \rightarrow \mathbb{R}^n$$

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

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

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

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

## Alternative notations and additional rules.

$$\operatorname{rot} f(\mathbf{x}) = \nabla \times f(\mathbf{x}) = \begin{vmatrix} \mathbf{e}_1 & \mathbf{e}_2 & \mathbf{e}_3 \\ \frac{\partial}{\partial x_1} & \frac{\partial}{\partial x_2} & \frac{\partial}{\partial x_3} \\ f_1 & f_2 & f_3 \end{vmatrix}$$

**Remark:** The following rules hold true:

$$\operatorname{rot}(\alpha f + \beta g) = \alpha \operatorname{rot} f + \beta \operatorname{rot} g$$

$$\operatorname{rot}(\varphi \cdot f) = (\nabla \varphi) \times f + \varphi \operatorname{rot} f$$

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

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

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



## 1.2 The total differential

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

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

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

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

i.e.

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

# The total differential and the Jacobian matrix.

**Notation:** We call the linear map  $l$  the **differential** or the **total differential** of  $f(x)$  at the point  $x^0$ . We denote  $l$  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 vector and  $a(x - x^0)$  a scalar product  $\langle a^T, x - x^0 \rangle$ .

# Total and partial differentiability.

**Theorem:** Let  $f : D \rightarrow \mathbb{R}^m$ ,  $x^0 \in D \subset \mathbb{R}^n$ ,  $D$  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

$$Jf(x^0) = \begin{pmatrix} \frac{\partial f_1}{\partial x_1}(x^0) & \dots & \frac{\partial f_1}{\partial x_n}(x^0) \\ \vdots & & \vdots \\ \frac{\partial f_m}{\partial x_1}(x^0) & \dots & \frac{\partial f_m}{\partial x_n}(x^0) \end{pmatrix} = \begin{pmatrix} Df_1(x^0) \\ \vdots \\ Df_m(x^0) \end{pmatrix}$$

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

## Proof of a).

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

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

Thus we conclude

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

and we obtain

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

Therefore the function  $f$  is continuous at  $x^0$ .

## Proof of b).

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

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

We write

$$\begin{aligned} \frac{f(x) - f(x^0) - A \cdot (x - x^0)}{\|x - x^0\|_\infty} &= \frac{f(x^0 + te_i) - f(x^0)}{|t|} - \frac{tAe_i}{|t|} \\ &= \frac{t}{|t|} \cdot \left( \frac{f(x^0 + te_i) - f(x^0)}{t} - Ae_i \right) \\ &\rightarrow 0 \quad \text{as } t \rightarrow 0 \end{aligned}$$

Thus

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

# Examples.

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

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

- Consider the function  $f : \mathbb{R}^3 \rightarrow \mathbb{R}^2$  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

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

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

## Further examples.

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

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

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

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

We conclude

$$Jf(x) = \text{grad}f(x) = x^T (A^T + A)$$

# Rules for the differentiation.

## Theorem:

- a) **Linearität:** LET  $f, g : D \rightarrow \mathbb{R}^m$  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  $f : D \rightarrow \mathbb{R}^m$  be differentiable in  $x^0 \in D$ ,  $D$  open. Let  $g : E \rightarrow \mathbb{R}^k$  be differentiable in  $y^0 = f(x^0) \in E \subset \mathbb{R}^m$ ,  $E$  open. Then  $g \circ f$  is differentiable in  $x^0$ .

For the differentials it holds

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

and analogously for the Jacobian matrix

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



## Examples for the chain rule.

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

Then the composition

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

is differentiable in  $t_0$  and we have for the derivative:

$$\begin{aligned}(f \circ h)'(t_0) &= Jf(h(t_0)) \cdot Jh(t_0) \\ &= \operatorname{grad} f(h(t_0)) \cdot h'(t_0) \\ &= \sum_{k=1}^n \frac{\partial f}{\partial x_k}(h(t_0)) \cdot h'_k(t_0)\end{aligned}$$

# Directional derivative.

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

$$D_v f(x^0) := \lim_{t \rightarrow 0} \frac{f(x^0 + tv) - f(x^0)}{t}$$

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:

$$\begin{aligned} D_v f(x, y) &= \lim_{t \rightarrow 0} \frac{(x+t)^2 + (y+t)^2 - x^2 - y^2}{t} \\ &= \lim_{t \rightarrow 0} \frac{2xt + t^2 + 2yt + t^2}{t} \\ &= 2(x + y) \end{aligned}$$

## Remarks.

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

$$D_v f(x^0) = \frac{\partial f}{\partial x_i}(x^0)$$

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

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

This follows directly applying the chain rule.

# Properties of the gradient.

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

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

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

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

- 2) The gradient  $\text{grad } f(x^0)$  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

$$|D_v f(x^0)| = |(\text{grad } f(x^0), v)| \leq \|\text{grad } f(x^0)\|_2$$

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

# Curvilinear coordinates.

**Definition:** Let  $U, V \subset \mathbb{R}^n$  be open and  $\Phi : U \rightarrow V$  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  $\Phi^{-1} : V \rightarrow U$  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**  $x = (x, y)$ .

# Calculation of the partial derivatives.

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

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

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

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

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

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

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

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

# Notations.

We use the short notation

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

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

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

where

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

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

## Example: polar coordinates.

We consider polar coordinates

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

We calculate

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

and thus

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



# 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

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

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

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

## Example: spherical coordinates.

We consider spherical coordinates

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

The Jacobian–matrix is given by:

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

# Partial derivatives for spherical coordinates.

Calculating the partial derivatives gives

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

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

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

**Example:** calculation of the [Laplace-operator](#) in spherical coordinates

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

# Chapter 1. Multivariate differential calculus

## 1.3 Mean value theorems and Taylor expansion

**Theorem (Mean value theorem):** Let  $f : D \rightarrow \mathbb{R}$  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

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

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

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

**Proof:** We set

$$h(t) := f(a + t(b - a))$$

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

$$\begin{aligned} f(b) - f(a) &= h(1) - h(0) = h'(\theta) \cdot (1 - 0) \\ &= \text{grad } f(a + \theta(b - a)) \cdot (b - a) \end{aligned}$$

## Definition and example.

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

**Example for the mean value theorem:** Given a scalar function

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

It is

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

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

$$\text{grad } f \left( \theta \begin{pmatrix} \pi/2 \\ \pi/2 \end{pmatrix} \right) \cdot \begin{pmatrix} \pi/2 \\ \pi/2 \end{pmatrix} = 0$$

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

# Mean value theorem is only true for **scalar** functions.

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

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

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

It 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

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

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

# A mean value estimate for vector-valued functions.

**Theorem:** Let  $f : D \rightarrow \mathbb{R}^m$  be differentiable on an open set  $D \subset \mathbb{R}^n$ . Let  $a, b$  be 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

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

**Remark:** Another (weaker) form 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.

# Taylor series: notations.

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

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

Let

$$|\alpha| := \alpha_1 + \dots + \alpha_n \quad \alpha! := \alpha_1! \cdots \alpha_n!$$

Let  $f : D \rightarrow \mathbb{R}$  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

$$x^\alpha := x_1^{\alpha_1} x_2^{\alpha_2} \dots x_n^{\alpha_n} \quad \text{for } x = (x_1, \dots, x_n) \in \mathbb{R}^n.$$



# The Taylor theorem.

## Theorem: (Taylor)

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

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

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

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

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

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

# Derivation of the Taylor expansion.

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

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

and calculate the (univariate) Taylor–expansion **at  $t = 0$** . It is

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

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

$$\begin{aligned} g'(0) &= \left. \frac{d}{dt} f(x_1^0 + t(x_1 - x_1^0), x_2^0 + t(x_2 - x_2^0), \dots, x_n^0 + t(x_n - x_n^0)) \right|_{t=0} \\ &= D_1 f(x_0) \cdot (x_1 - x_1^0) + \dots + D_n f(x_0) \cdot (x_n - x_n^0) \\ &= \sum_{|\alpha|=1} \frac{D^\alpha f(x_0)}{\alpha!} \cdot (x - x_0)^\alpha \end{aligned}$$

# Continuation of the derivation.

Calculation of  $g''(0)$  gives

$$\begin{aligned}g''(0) &= \left. \frac{d^2}{dt^2} f(x_0 + t(x - x_0)) \right|_{t=0} = \left. \frac{d}{dt} \sum_{k=1}^n D_k f(x_0 + t(x - x_0)) (x_k - x_k^0) \right|_{t=0} \\&= D_{11} f(x_0) (x_1 - x_1^0)^2 + D_{21} f(x_0) (x_1 - x_1^0) (x_2 - x_2^0) \\&\quad + \dots + D_{ij} f(x_0) (x_i - x_i^0) (x_j - x_j^0) + \dots + \\&\quad + D_{n-1,n} f(x_0) (x_{n-1} - x_{n-1}^0) (x_n - x_n^0) + D_{nn} f(x_0) (x_n - x_n^0)^2 \\&= \sum_{|\alpha|=2} \frac{D^\alpha f(x_0)}{\alpha!} (x - x_0)^\alpha \quad (\text{exchange theorem of Schwarz!})\end{aligned}$$

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

# Proof of the Taylor theorem.

The function

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

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

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

In addition we have (by induction over  $k$ )

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

and

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

# Examples for the Taylor–expansion.

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

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

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

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

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

- 5 [Details on extra slide.](#)

# Remarks to the remainder of a Taylor–expansion.

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

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

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

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

We conclude 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

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

# The Hesse-matrix.

The matrix

$$Hf(x_0) := \begin{pmatrix} f_{x_1 x_1}(x_0) & \cdots & f_{x_1 x_n}(x_0) \\ \vdots & & \vdots \\ f_{x_n x_1}(x_0) & \cdots & f_{x_n x_n}(x_0) \end{pmatrix}$$

is called **Hesse-matrix** of  $f$  at  $x_0$ .

Hesse-matrix = Jacobi-matrix of the gradient  $\nabla f$

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

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

The Hesse-matrix of a  $\mathcal{C}^2$ -function is symmetric.

## 2.1 Extrem values of multivariate functions

**Definition:** Let  $D \subset \mathbb{R}^n$ ,  $f : D \rightarrow \mathbb{R}$  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

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

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

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

Analogously we define the different forms of minima.



# 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

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

**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:

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

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

$$\text{grad } f(x^0) = (0, \dots, 0)^T$$

# Remarks to local extrem values.

## Bemerkungen:

- Typically the condition  $\text{grad } f(x^0) = 0$  gives a **non-linear** system of  $n$  equations for  $n$  unknowns for the calculation of  $x = x^0$ .
- The points  $x^0 \in D^0$  with  $\text{grad } f(x^0) = 0$  are called **stationary points** of  $f$ . Stationary points are **not** necessarily local extrem values. As an example take

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

with the gradient

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

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

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

# Classification of stationary points.

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

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  $\Rightarrow H f(x^0)$  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 saddle point, i.e. in every neighborhood of  $x^0$  there exist points  $x^1$  and  $x^2$  with  $f(x^1) < f(x^0) < f(x^2)$ .

## 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

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

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

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

From (1) it follows

$$v^T H f(x^0 + \theta \varepsilon v) v \geq 0 \quad (2)$$

Since  $f$  is a  $\mathcal{C}^2$ –function, the Hesse–matrix is a **continuous** map. In the limit  $\varepsilon \rightarrow 0$  we conclude from (2),

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

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

## Proof of the theorem, part b).

If  $Hf(x^0)$  is positiv definit, then  $Hf(x)$  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  $x \in K_\varepsilon(x^0)$ ,  $x \neq x^0$  we have

$$\begin{aligned} f(x) - f(x^0) &= \frac{1}{2}(x - x^0)^T Hf(x^0 + \theta(x - x^0))(x - x^0) \\ &> 0 \end{aligned}$$

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

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

$$v^T Hf(x^0)v > 0 \quad w^T Hf(x^0)w < 0$$

and thus  $x^0$  is a saddle point.

# Remarks.

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

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

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

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

- The following implications are true (**but not the inverse**)

$x^0$  local minimum  $\Leftarrow x^0$  strict local minimum

$\Downarrow$

$\Uparrow$

$Hf(x^0)$  positiv semidefinit  $\Leftarrow Hf(x^0)$  positiv definit

## Further remarks.

- If  $f$  is a  $C^3$ -function,  $x^0$  a stationary point of  $f$  and  $Hf(x^0)$  positiv definit. Then the following estimate is true:

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

where  $\lambda_{min}$  denoted the **smallest** Eigenvalue of the Hesse-matrix.

Using the Taylor theorem we obtain:

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

with an appropriate constant  $C > 0$ .

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

## Example .

We consider the function

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

and look for stationary points :

$$\text{grad } f(x, y) = (y^2 + x(3x + 2), 2y(x - 1))^T$$

The condition  $\text{grad } f(x, y) = 0$  gives two stationary points

$$x^0 = (0, 0)^T \quad \text{und} \quad x^1 = (-2/3, 0)^T.$$

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

$$Hf(x^0) = \begin{pmatrix} 2 & 0 \\ 0 & -2 \end{pmatrix} \quad \text{and} \quad Hf(x^1) = \begin{pmatrix} -2 & 0 \\ 0 & -10/3 \end{pmatrix}$$

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



## 2.2 Implicitly defined functions

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

$$g(x) = 0$$

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

$$m < n.$$

**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.

# 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  $x_{n-m+1}, \dots, x_n$ ?

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

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

**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  $f : \mathbb{R}^{n-m} \rightarrow \mathbb{R}^m$ .

## Example.

The equation for a circle

$$g(x, y) = x^2 + y^2 - r^2 = 0 \quad \text{mit } r > 0$$

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 :

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

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

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

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

## Example.

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

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

We split the variables  $x$  into two vectors

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

Splitting of the matrix  $C = [B, A]$  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

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

## Continuation of the example.

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

From the equation

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

we see that

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

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).

# Implicit function theorem.

**Theorem:** Let  $g : D \rightarrow \mathbb{R}^m$  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  $\text{Der } (x^0, y^0) \in D$  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  $f : U \rightarrow V$  with

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

and

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

## 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 neighborhood of  $(0, r)$  with respect to  $y$ :

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

The derivative  $f'(x)$  can be calculated by **implicit differentiation**:

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

and therefore

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

## Another example.

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

It is

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

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

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

Differentiating again gives

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

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



## general remark.

Implicit differentiation of a implicitly 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 point  $x^0$  is a **stationary** point of  $f(x)$  if

$$g(x^0, y^0) = g_x(x^0, y^0) = 0 \quad \text{and} \quad g_y(x^0, y^0) \neq 0$$

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

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

# Implicit representation of curves.

Consider the set of solutions of a scalar equation

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

If

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

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

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

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

**Example:** Consider (again) the equation for a circle

$$g(x, y) = x^2 + y^2 - r = 0 \quad \text{mit } r > 0.$$

on the circle there are **no** singular points!

# Horizontal and vertical tangents.

## Remarks:

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

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

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

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

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

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**

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

# Remarks.

Due to c) for  $g_{xx}, g_{xy}, g_{yy} \neq 0$  we obtain:

$\det Hg(x^0) > 0$  :  $x^0$  is an **isolated point** of the set of solutions

$\det Hg(x^0) < 0$  :  $x^0$  is a **double point**

$\det Hg(x^0) = 0$  :  $x^0$  is a **return point** or a **cuspl**

## Geometric interpretation:

- 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  $g(x)$ .
- 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  $g(x)$ .
- If  $\det Hg(x^0) = 0$ , then the stationary point  $x^0$  of  $g(x)$  is **degenerate**.

## 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**.

## 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:

$$g_x = y^2 + 3x^2 + 2xq^2$$

$$g_y = 2y(x - 1)$$

$$g_{xx} = 6x + 2q^2$$

$$g_{xy} = 2y$$

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

$$Hg(0) = \begin{pmatrix} 2q^2 & 0 \\ 0 & -2 \end{pmatrix}$$

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

## 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:

$$g_x = y^2 + 3x^2$$

$$g_y = 2y(x - 1)$$

$$g_{xx} = 6x$$

$$g_{xy} = 2y$$

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

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

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

# Implicit representation of surfaces.

- The set of solutions of a scalar equation  $g(x, y, z) = 0$  for  $\text{grad } g \neq 0$  is *locally* a **surface** in  $\mathbb{R}^3$ .
- For the **tangential** in  $x^0 = (x^0, y^0, z^0)^T$  with  $g(x^0) = 0$  and  $\text{grad } g(x^0) \neq 0^T$  we obtain by Taylor expanding (denoting  $\Delta x^0 = x - x^0$ )

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

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

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

using the implicit function theorem.



# The inverted Problem.

**Question:** Given the set of equations

$$y = f(x)$$

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

**Theorem:** ([Inversion theorem](#))

Let  $D \subset \mathbb{R}^n$  be open and  $f : D \rightarrow \mathbb{R}^n$  a  $\mathcal{C}^1$ -function. If the Jacobian-matrix  $Jf(x^0)$  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  $f^{-1} : V \rightarrow U$  is also  $\mathcal{C}^1$  and for all  $x \in U$  we have:

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

**Remark:** We call  $f$  locally a  $\mathcal{C}^1$ -**diffeomorphism**.

# 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

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

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

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

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

# General formulation of the problem.

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

$$g(x) = 0$$

where  $g : \mathbb{R}^n \rightarrow \mathbb{R}^m$ .

The constraints are

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

$$\vdots$$

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

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

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

# The Lagrange–function and the Lagrange–Lemma.

We define the **Lagrange–function**

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

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

The numbers  $\lambda_i$ ,  $i = 1, \dots, m$  are called **Lagrange–multiplier**.

**Theorem: (Lagrange–Lemma)** If  $x^0$  minimizes (or maximizes) the Lagrange–function  $F(x)$  (for a fixed  $\lambda$ ) 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

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

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

# A necessary condition for local extrema.

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

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

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  $\lambda$ .

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

**Alternatively:** Define a Lagrange-function

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

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

## Some remarks on sufficient conditions.

- 1 We can formulate a **sufficient** condition:  
If the functions  $f$  and  $g$  are  $\mathcal{C}^2$ -functions and if the Hesse-matrix  $HF(x^0)$  of the Lagrange-function is positiv (negativ) definit, then  $x^0$  is a strict local minimum (maximum) of  $f(x)$  on  $G$ .
- 2 In most of the applications the necessary condition are **not** satisfied, although  $x^0$  is a strict local extremum.
- 3 And from the indefinitness of the Hesse-matrix  $HF(x^0)$  we **cannot** conclude, that  $x^0$  is not an extremum.
- 4 We have a similar problem with the necessary condition which is obtained from the Hesse-matrix of the Lagrange-function  $G(x, \lambda)$  with respect to  $x$  **and**  $\lambda$ .

# An example of a minimisation problem with constraints.

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

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

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

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

The necessary condition for an extrem value is given by

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

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



## continuation of the example.

The Hesse-matrix at the origin is given by

$$Hf(0) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

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

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

# 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 solutions

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

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

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

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

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

# Lagrange–multiplier–rule.

**Satz:** Let  $f, g_1, \dots, g_m : D \rightarrow \mathbb{R}$  be  $\mathcal{C}^1$ -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**

$$\text{rang} \left( Jg(x^0) \right) = m$$

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

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

the following **first order necessary condition** holds true:

$$\text{grad} F(x^0) = 0$$

# 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  $\lambda_1, \dots, \lambda_m$  be the related Lagrange-multiplier. Then the Hesse-matrix  $HF(x^0)$  of the Lagrange-function is **positiv semi-definit** on the tangential space

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

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

2) Let the regularity condition for a point  $x^0 \in G$  be satisfied. If there exist Lagrange-multiplier  $\lambda_1, \dots, \lambda_m$ , 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  $g(x) = 0$ .

## 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

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

From the necessary condition we obtain the non-linear system

$$-2x + 8 = -2\lambda x$$

$$-2y = -2\lambda y$$

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

## 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

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

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

## Another example.

Determine the local extrem values of

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

on the intersection of the cylinder surface

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

with the plane

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

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

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

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

# Continuation of the example.

The Jacobi-matrix

$$Jg(x) = \begin{pmatrix} 2x & 2y & 0 \\ 1 & 0 & 1 \end{pmatrix}$$

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

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

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

$$2 + \lambda_2 = 0$$

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

$$x + z = 1$$



## 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

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

## Completion if the example.

The possible extrem values are

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

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

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

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

We calculate the related function 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 and the point  $(x, y, z) = (0, -\sqrt{2}, 1)$  a minimum.

## 2.4 the Newton–method

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

$$f(x) = 0$$

- We already know the **fixed-point iteration**

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

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

- 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.

# The construction of the Newton method.

**Starting point:** Let  $\mathcal{C}^1$ -function  $f : D \rightarrow \mathbb{R}^n$ ,  $D \subset \mathbb{R}^n$  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

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

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

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

# The Newton–method as algorithm.

The **Newton–method** can be formulated as algorithm.

**Algorithm** (**Newton–method**):

**(1) FOR**  $k = 0, 1, 2, \dots$

**(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  $\Delta x^k$  is called **Newton–correction**.
- The Newton–method is **scaling-invariant**.

# Scaling-invariance of the Newton–method.

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

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

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  $g$  coincide.

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

# Local convergence of the Newton–method.

**Theorem:** Let  $f : D \rightarrow \mathbb{R}^n$  be a  $\mathcal{C}^1$ -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  $Jf(x)$  be regular for  $x \in D$ , and suppose the **Lipschitz–condition**

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

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

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

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

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

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

# The damped Newton–method.

## Additional observations:

- 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**  $k = 0, 1, 2, \dots$

**(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**  $\lambda_k$ ?



# Choice of the damping parameter.

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

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

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

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

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

**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

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

# 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**  $\|f(x^k)\|_2 > \|f(x^k + \lambda_k \Delta x^k)\|_2$  **THEN**

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

**ELSE**

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

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

- $\lambda_k := \mu$

**END**

# Chapter 3. Integration in higher dimensions

## 3.1 Area integrals

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

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

$$V = \int_D f(x) dx$$

**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.

# 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

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

i.e.  $D$  is compact cuboid (rectangle).

Let  $f : D \rightarrow \mathbb{R}$  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

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

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

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

# 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

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

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

$$R_f(Z) := \sum_{i,j} f(x_{ij}) \cdot \text{vol}(Q_{ij})$$

a **Riemann sum** of the partition  $Z$ .

# Riemann upper and lower sums.

## Definition:

In analogy to the integral for the univariate case we call for a partition  $Z$

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

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

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.

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

## 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

$$U_f(Z_2) \geq U_f(Z_1) \quad \text{and} \quad O_f(Z_2) \leq O_f(Z_1)$$

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  $\|Z\| \rightarrow 0$ :

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

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

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

# Riemann upper and lower integrals.

## Definition:

- ① The **Riemann lower and upper integral** of a function  $f(x)$  on  $D$  is given by

$$\int_{\underline{D}} f(x) dx := \sup\{U_f(Z) : Z \in \mathcal{Z}(D)\}$$

$$\int_{\overline{D}} f(x) dx := \inf\{O_f(Z) : Z \in \mathcal{Z}(D)\}$$

- ② The function  $f(x)$  is called **Riemann-integrable** on  $D$ , if lower and upper intergral conincide. The **Riemann-integral** of  $f(x)$  on  $D$  is then given by

$$\int_D f(x) dx := \int_{\underline{D}} f(x) dx = \int_{\overline{D}} f(x) dx$$



## Remark.

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

$$f : D \rightarrow \mathbb{R}, \quad D \in \mathbb{R}^2$$

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.

# Elementary properties of the integral.

## Theorem:

### a) Linearity

$$\int_D (\alpha f(x) + \beta g(x)) dx = \alpha \int_D f(x) dx + \beta \int_D g(x) dx$$

### b) Monotonicity

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

$$\int_D f(x) dx \leq \int_D g(x) dx$$

### c) Positivity

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

$$\int_D f(x) dx \geq 0$$

# Additional properties of the integral.

## Theorem:

- a) Let  $D_1$ ,  $D_2$  and  $D$  be cuboids,  $D = D_1 \cup D_2$  and  $\text{vol}(D_1 \cap D_2) = 0$ , 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

$$\left| \int_D f(x) dx \right| \leq \sup_{x \in D} |f(x)| \cdot \text{vol}(D)$$

- c) **Riemann criterion**

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

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

# Fubini's theorem.

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

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

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

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

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

holds true.

## Importance:

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

## Example.

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:

$$\begin{aligned} \int_D f(x, y) dx dy &= \int_0^2 \int_0^1 f(x, y) dx dy = \int_0^2 \left[ 2x - \frac{x^2 y}{2} \right]_{x=0}^{x=1} dy \\ &= \int_0^2 \left( 2 - \frac{y}{2} \right) dy = \left[ 2y - \frac{y^2}{4} \right]_{y=0}^{y=2} = 3 \end{aligned}$$

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

# The characteristic function.

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

$$f^*(x) := \begin{cases} f(x) & : \text{if } x \in D \\ 0 & : \text{if } x \in \mathbb{R}^n \setminus D \end{cases}$$

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

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

# Measurability and null sets.

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

$$\text{vol}(D) := \int_D 1 dx = \int_Q \chi_D(x) dx$$

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

The compact set  $D$  is called **null set**, if  $D$  is measurable and if  $\text{vol}(D) = 0$  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.
- $\text{vol}(D)$  is the volume of the cuboid on  $\mathbb{R}^n$ .

## 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  $\partial D$  of  $D$  is a null set.

**Theorem:** Let  $D \subset \mathbb{R}^n$  be compact and measurable. Let  $f : D \rightarrow \mathbb{R}$  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  $f : D \rightarrow \mathbb{R}$  be continuous, then there exist a point  $\xi \in D$  with

$$\int_D f(x) dx = f(\xi) \cdot \text{vol}(D)$$

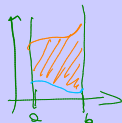


# "Normal" areas.

## Definition:

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

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



and

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

respectively.

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

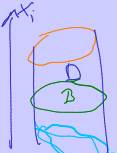
$$D = \{(x_1, x_2, x_3) \mid a \leq x_i \leq b, g(x_i) \leq x_j \leq h(x_i)$$

$$\text{and } \varphi(x_i, x_j) \leq x_k \leq \psi(x_i, x_j) \}$$

with a permutation  $(i, j, k)$  of  $(1, 2, 3)$  and continuous functions  $g, h, \varphi$  and  $\psi$ .

# Projectable sets.

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


$$D = \{ x \in \mathbb{R}^n \mid \tilde{x} = (x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_n)^T \in B \\ \text{und } \varphi(\tilde{x}) \leq x_i \leq \psi(\tilde{x}) \}$$

## 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.

# 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

$$D = \{ x \in \mathbb{R}^n \mid \tilde{x} = (x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_n)^T \in B \\ \text{and } \varphi(\tilde{x}) \leq x_i \leq \psi(\tilde{x}) \}$$

then it holds

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

## Example.

Given a function

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

Calculate the integral on the area bounded by two parabolas

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

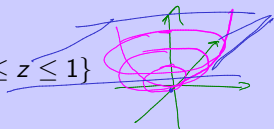
The set  $D$  is a "normal" area and  $f(x, y)$  is continuous. Thus

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

# Example.

Calculate the volume of the rotational paraboloid

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



Representation of  $V$  as "normal" area

$$V = \{(x, y, z)^T \mid \underbrace{-1 \leq x \leq 1}_{f(x)}, \underbrace{-\sqrt{1-x^2} \leq y \leq \sqrt{1-x^2}}_{h(x)}, \text{ and } \underbrace{x^2 + y^2 \leq z \leq 1}_{\varphi(x, y)}\}_{k(x)}$$

Then we have

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

# Integration over arbitrary domains.

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

$$\bigcup_{j=1}^m D_j = D \quad \text{and} \quad \forall i \neq j : D_i \cap D_j = \emptyset.$$

We call

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

the **diameter** of the set  $D_j$  and

$$\|Z\| := \max \{ \text{diam}(D_j) \mid j = 1, \dots, m \}$$

the **fineness** of the universal partition  $Z$ .

# Riemann sums for universal partitions.

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

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

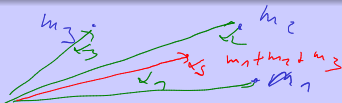
with arbitrary  $x^j \in D_j$ ,  $j = 1, \dots, m$ .

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

$$\lim_{k \rightarrow \infty} R_f(Z_k) = \int_D f(x) dx$$

it suffices to have a sequence  $(\epsilon_k)_{k \in \mathbb{N}}$ ,  $\|Z_k\| \xrightarrow{k \rightarrow \infty} 0$

# Center (of mass) of areas and solids.



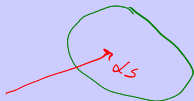
An important **application** of the area integrals is the calculation of the **centers (of mass)** of areas and solids.

**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

$$x_s = \frac{\sum_i m_i}{\sum_i m_i} = \frac{\sum_i m_i x_i}{\sum_i m_i}$$

$$x_s = \frac{\int_D \rho(x) dx}{\int_D \rho(x) dx} = \frac{\int_D \rho(x) x dx}{\int_D \rho(x) dx}$$

$$x_s := \frac{\int_D \rho(x) x dx}{\int_D \rho(x) dx}$$

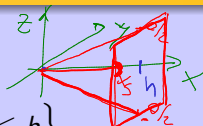


The numerator integral (over a vector valued function) is intended componentwise (and gives as result a vector).



## Example.

Calculate the center of mass of the pyramid  $P$



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

Calculate the volume of  $P$  under assumption of constant mass density  $\rho=1$

$$\begin{aligned} \text{vol}(P) &= \int_0^h \int_{-\frac{ax}{2h}}^{\frac{ax}{2h}} \int_{-\frac{ax}{2h}}^{\frac{ax}{2h}} dz \, dy \, dx \\ &= \int_0^h \int_{-\frac{ax}{2h}}^{\frac{ax}{2h}} \frac{ax}{h} dy \, dx \\ &= \int_0^h \left( \frac{ax}{h} \right)^2 dx = \frac{1}{3} a^2 h \end{aligned}$$

# 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  $x_s = \left(\frac{3}{4}h, 0, 0\right)^T = \frac{\begin{pmatrix} \frac{1}{4} a^2 h^2 \\ 0 \\ 0 \end{pmatrix}}{\frac{1}{2} h a^2}$

# Moments of inertia of areas and solids.



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

$$\Theta = \sum_{i=1}^3 m_i r_i^2$$

**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

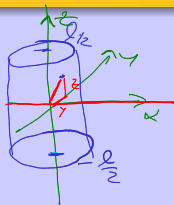
$$\Theta := \int_D \rho(x) r^2(x) dx$$

# Example.

We calculate the moment of inertia of a  <sup>$\rho = \text{constant}$</sup>  homogeneous cylinder

$$Z := \{ (x, y, z)^T : x^2 + y^2 \leq r^2, -l/2 \leq z \leq l/2 \}$$

with respect to the x-axis assuming a constant density  $\rho$ .



$$\begin{aligned} \Theta &= \int_Z \rho (y^2 + z^2) d(x, y, z) = \rho \int_Z (y^2 + z^2) d(x, y, z) \\ &= \rho \int_{-r}^r \int_{-\sqrt{r^2-x^2}}^{\sqrt{r^2-x^2}} \int_{-l/2}^{l/2} (y^2 + z^2) dz dy dx \\ &= \rho \int_{-r}^r \int_{-\sqrt{r^2-x^2}}^{\sqrt{r^2-x^2}} \left( ly^2 + \frac{l^3}{12} \right) dy dx \\ &= \rho \frac{\pi l r^2}{12} (3r^2 + l^2) \end{aligned}$$

# The theorem of transformation.

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

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

*f vector field*

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

$$\int_{\Phi(D)} f(x) dx = \int_D f(\Phi(u)) |\det J\Phi(u)| du$$

holds.

**Remark:** Note that the rule of transformation requires the bijectivity of  $\Phi$  only on the interior  $D^0$  of  $D$  – not on the boundary  $\partial D$ !

# Example.

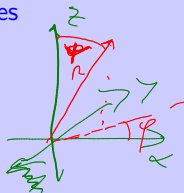
Calculate the center of mass of a  <sup>$\rho=1$</sup> homogeneous spherical octant

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



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  $\Phi$  on  $D^0$  a  $\mathcal{C}^1$ -diffeomorphism with

$$\det J\Phi(r, \varphi, \psi) = r^2 \cos \psi$$

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \phi(r, \varphi, \psi) = \begin{pmatrix} r \cos \varphi \cos \psi \\ r \sin \varphi \cos \psi \\ r \sin \psi \end{pmatrix} \quad 0 \leq \varphi \leq \pi$$

$$|J\phi| = \begin{vmatrix} c_\varphi c_\psi & -r s_\varphi c_\psi & -r c_\varphi s_\psi \\ s_\varphi c_\psi & r c_\varphi c_\psi & -r s_\varphi s_\psi \\ s_\psi & 0 & r c_\psi \end{vmatrix} = r^2 (c_\varphi^2 c_\psi^3 + s_\varphi^2 c_\psi^3 + c_\varphi^2 s_\psi^2 c_\psi + s_\varphi^2 s_\psi^2 c_\psi)$$

$$= r^2 (c_\psi^3 + s_\psi^2 c_\psi) = r^2 c_\psi = r^2 \cos \psi$$

$$z \geq 0 \quad 0 \leq \psi \leq \frac{\pi}{2} \quad \cos \psi \geq 0$$

# Continuation of the example.

According to the theorem of transformation it follows

$$\text{vol}(V) = \int_V dx = \int_0^1 \int_0^{\pi/2} \int_0^{\pi/2} \underbrace{r^2 \cos \psi}_{\text{Jacobian}} d\psi d\varphi dr = \frac{\pi}{6}$$

*Fubini*

and

$$\begin{aligned} \text{vol}(V) \cdot \underline{x_s} &= \int_V \underline{x} dx = \int_0^1 \int_0^{\pi/2} \int_0^{\pi/2} \underbrace{(r \cos \varphi \cos \psi)}_{\text{Jacobian}} \underbrace{r^2 \cos \psi}_{\text{Jacobian}} d\psi d\varphi dr \\ &\stackrel{\text{Fubini}}{=} \int_0^1 r^3 dr \cdot \int_0^{\pi/2} \cos \varphi d\varphi \cdot \int_0^{\pi/2} \cos^2 \psi d\psi = \frac{\pi}{16} \end{aligned}$$

The it follows  $x_s = \frac{3}{8}$ .  $= \frac{\frac{\pi}{16}}{\frac{\pi}{6}}$

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



# 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

$$\Theta_A = \underline{md^2} + \underline{\Theta_S}$$

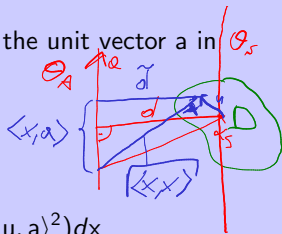
$S$  is the axis through to center of mass of the solid  $K$  parallel to the axis  $A$  and  $d$  the distance of the center of mass  $x_s$  from the axis  $A$ .

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

$$\begin{aligned} \Theta_A &= \rho \int_K (\underbrace{\langle x, x \rangle - \langle x, a \rangle^2}_{d^2}) dx \\ &= \rho \int_D (\langle x_s + u, x_s + u \rangle - \langle x_s + u, a \rangle^2) dx \end{aligned}$$

where

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



# Chapter 3. Integration over general areas

## 3.2 Line integrals

We already had a definition of a **line integral of a scalar field** for a piecewise  $C^1$ -curve  $c : [a, b] \rightarrow D$ ,  $D \subset \mathbb{R}^n$ , and a continuous **scalar** function  $f : D \rightarrow \mathbb{R}$

$$\int_c f(x) ds := \int_a^b f(c(t)) \|\dot{c}(t)\| dt$$

where  $\|\cdot\|$  denotes the Euklidian norm.

**Generalisation:** Line integrals of **vector valued** functions, i.e.

$$\int_c f(x) dx := ?$$

**Application:** A point mass is moving along  $c(t)$  in a force field  $f(x)$ .

**Question:** How much **physical** work has to be done along the curve?

# Line integral on vector fields.

**Definition:** For a continuous vector field  $f : D \rightarrow \mathbb{R}^n$ ,  $D \subset \mathbb{R}^n$  open, and a piecewise  $\mathcal{C}^1$ -curve  $c : [a, b] \rightarrow D$  we define the **line integral on vector fields** by

$$\int_c f(x) dx := \int_a^b \langle f(c(t), \dot{c}(t)) \rangle dt$$

**Derivation:** Approximate the curve by piecewise linear line segments with corners  $c(t_i)$ , where

$$Z = \{a = t_0 < t_1 < \dots < t_m = b\}$$

is a partition of the interval  $[a, b]$ .

Then the workload along the curve  $c(t)$  in the force field  $f(x)$  is approximately given by :

$$A \approx \sum_{i=0}^{m-1} \langle f(c(t_i)), c(t_{i+1}) - c(t_i) \rangle$$

## Continuation of the derivation.

Thus:

$$\begin{aligned} A &\approx \sum_{j=1}^n \sum_{i=0}^{m-1} f_j(c(t_i))(c_j(t_{i+1}) - c_j(t_i)) \\ &= \sum_{j=1}^n \sum_{i=0}^{m-1} f_j(c(t_i)) \dot{c}_j(\tau_{ij})(t_{i+1} - t_i) \end{aligned}$$

For a sequence of partitions  $Z$  with  $\|Z\| \rightarrow 0$  the left side converges to the above defined [line integral on vector fields](#).

**Remarks:** For a closed curve  $c(t)$ , i.e.  $c(a) = c(b)$ , we use the notation

$$\oint_c f(x) dx$$