Technische Hochschule **Rosenheim**

Analysis 2

Priv.-Doz. Dr. Sven-Joachim Kimmerle

Summer term 2022

Bachelor Applied Artificial Intelligence (AAI)

Outline

1. Introduction
   - Lecturer
   - Motivation
   - Administrative and organisational matters
2. Power series
3. Differentiation in Higher Dimensions
4. Integration in Higher Dimensions
5. Further Topics in Calculus
6. Summary - Outlook and Review

Lecturer: Sven-Joachim Kimmerle

- 2000: “Vordiplom” in Mathematics & “Vordiplom” in Physics (U Heidelberg)
- 2002: Maîtrise in Mathematics (U Paris 7, France)
- 2004: Diploma in Mathematics (U Heidelberg)
- 2004-2009: Research center MATHEON, Berlin
- 2009: PhD in Mathematics (HU Berlin)
- 2010: Toyota/U Ottawa, Ottawa, Canada
- 2011-2018: Postdoc & deputy professor, UniBw München, Neubiberg
- 2019: “Habilitation” in Mathematics (UniBw München, Neubiberg)
- Since 2018: Physical Software Solutions GmbH, Münsing & Ottobrunn
- Since 2021: Lecturer (part-time), TH Rosenheim

What do you expect from the lecture?

Aims of the course

Teaching mathematical basics (continued):

- Review of mathematics from Analysis 1 (& “school”)
- Completion of power series; Taylor series
- Fourier series
- Differentiation in higher dimensions
- Integration in higher dimensions
- Further topics: vector calculus, integral transformations (shortly)
- Mathematical thinking, techniques & working

In parallel this semester: Linear Algebra

- Systems of equations, matrices & vectors, eigenvalues, vector spaces, . . .

Administrative & organisational matters 1

4 SWS: ~ 2.67 hours lecture with ~ 1.33 hours exercise

- Lecture (2-3 hours per week)
  Thursday, 09:45-11:15 (every week) in A3.14
  Thursday, 11:45-13:15 (begin of the semester) in A3.14 with integrated exercises

  In presence (at least for the moment ...).
  Please wear masks at all times!

- 2 exercise groups:

  We start at the middle of the semester with 2 exercise groups instead of the 2nd lecture block.
  Thursday, 11:45-13:15 in A3.14
  Thursday, 13:45-15:15 in A3.14

  In presence

  Please register later for a group in the LC!

In case of (technical) issues, we wait for 20 minutes!

Administrative & organisational matters 2

- Presentations, exercises and other material can be found in the Learning Campus (LC)
  - learning-campus.th-rosenheim.de
  - → Department ANG
    → Mathematics
    → Analysis 2 (AAI - B2), SoSe 2022
  - shortly: “Analysis 2 AAI, 22”
  - login: KenneIch!

- Office hours & contact
  - After each lecture/exercise group or
  - some time Wednesday afternoons or on Thursday
  - by appointment by email:
    `sven-joachim.kimmerle@th-rosenheim.de`

Marking

- **Examination type**
  - Written exam: 90 min.
  - Auxiliary tools: 1 sheet (DIN A4) both sides, hand written with formulas, e.g.
  - No calculators (or smartphones etc.) will be permitted.
- **Homework and bonus system**
  - Marked homework (bonus), sometimes in groups up to 2
  - To hand-in each Friday morning online, discussion next Thursday

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Workload

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According to the module handbook for 5 ECTS we expect a workload of about 150 hours:

- 60 hours contact (in presence or virtual):
  $\sim$ 40 hours lecture, $\sim$ 20 hours exercise
- 90 hours independent study

Preliminaries:

- Good math skills from school or previous semesters
- Sound understanding of English
- Perseverance and endurance

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S.-J. Kimmerle

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Recommended literature

- James Stewart: *Calculus*. Brooks/Cole, 6th edition, 2009.
- J. Hass, C. Heil, M.D. Weir: *Thomas' Calculus: Early transcendentals*. Pearsons, 14th edition, 1999.

In German only:

- Forster, O.: *Analysis 1*. Springer-Spektrum, 11. Auflage, 2013.
- Forster, O.: *Analysis 2*. Springer-Spektrum, 11. Auflage, 2017.
- Forster, O.: *Analysis 3*. Springer-Spektrum, 8. Auflage, 2017.

Further literature and material (software, e.g.) will be given during the course.

Copying ban

All materials made available in this lecture have been protected by me with a password, which has only been made available to the registered participants of this course.
Any form of distribution is prohibited!

Sven-Joachim Kimmerle

Revision

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Power Series

We know the concepts of

functions,
sequences, and
series.

We are interested in series representing a function $f(x)$ at every x:

$$f(x) = \sum_{j=0}^{\infty} a_j (x - x_0)^j$$

For this purpose we need the concept of a sequence of functions at first.

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Sequences of Functions

A sequence of elements of $\mathbb{R}$ (cf. Analysis 1):

$$g : \mathbb{N} \to \mathbb{R},\ n \mapsto a_n =: g(n)$$

Definition (Sequences of Functions)

Let D be a set. A mapping

$$g : D \times \mathbb{N} \to \mathbb{R},\ (x, n) \mapsto f_n = f_n(x) =: g(x, n)$$

is called a **sequence** of functions $f_n : D \to \mathbb{R}$, $n \in \mathbb{N}$.

Other notations by writing the functions, e.g., are:

$$\{f_n\}_{n\in\mathbb{N}} = \{f_n\}_{n\geq 1} = \{f_1, f_2, f_3, \ldots, f_n, \ldots\}$$

The domain of definition D and the target area, here $\mathbb{R}$, have to be identical for all functions f_n.

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Example (Pointwise Convergence)

Consider $\{f_n\}_{n\in\mathbb{N}}$, $f_n : [0,2] \to \mathbb{R}$ with

$$f_n(x) = \begin{cases} n^2 x, & 0 \le x \le \frac{1}{n}, \\ 2n - n^2 x, & \frac{1}{n} \le x \le \frac{2}{n}, \\ 0, & \frac{2}{n} \le x \le 2. \end{cases}$$

This example exhibits that we may not swap the limit and the integral (another limit process) in general!

Pointwise Convergence

Definition (Pointwise Convergence)

Let D be a set. A sequence $\{f_n\}_{n \geq n_0}$ of functions $f_n : D \to \mathbb{R}$ is called **pointwise convergent** to a function $f : D \to \mathbb{R}$,
if and only if

$$\lim_{n\to\infty} f_n(x) = f(x) \quad \text{for any } x \text{ in } D.$$

Equivalently,

For any $x \in D$ and $\varepsilon > 0$
there exists a $N = N(x, \varepsilon) \geq n_0$ s.t.:

$$|f_n(x) - f(x)| < \varepsilon \quad \text{for any } x \text{ in } D \text{ and all } n \geq N.$$

Uniform Convergence

Definition (Uniform Convergence)

Let D be a set. A sequence $\{f_n\}_{n \geq n_0}$ of functions $f_n : D \to \mathbb{R}$ is called **uniformly convergent** to a function $f : D \to \mathbb{R}$,
if and only if

For any $x \in D$ and $\varepsilon > 0$
there exists a $N = N(\varepsilon) \geq n_0$ s.t.:

$$|f_n(x) - f(x)| < \varepsilon \quad \text{for any } x \text{ in } D \text{ and all } n \geq N.$$

Notice that N may depend only on ε but not on the point x.

Uniform convergence always implies pointwise convergence, the opposite is not true (see last example).

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Example Uniform Convergence

Let $x \in D = [0, 1)$. The sequence

$$\left\{ \frac{1}{2^{x+n}} \right\}_{n \in \mathbb{N}}$$

converges uniformly:

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Theorem (Uniform convergence preserves continuity)

Let $D \subseteq \mathbb{C}$ and $f_n : D \to \mathbb{C}$, $n \in \mathbb{N}$, a sequence of continuous functions,
that uniformly converge to a function $f : D \to \mathbb{C}$,

then f is continuous.

The limit of a uniformly convergent sequence of continuous functions,
is again continuous.

Example: Saw-tooth function

Uniform norm

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Definition (Uniform norm or sup norm)

Let D be a set and $f : D \to \mathbb{C}$.

We set

$$\|f\|_D := \sup_{x \in D} |f(x)|.$$

$\|\cdot\|_D$ defines a norm on D.

A function f is bounded iff $\|f\| < \infty$.

When misunderstandings are excluded, we just write $\|f\|$ instead of $\|f\|_D$.

Uniform Norm and Uniform Convergence

By this notation we may reformulate the uniform convergence:

$$\{f_n\}_{n\in\mathbb{N}} \text{ converges uniformly on } D$$
$$\iff \lim_{n\to\infty} \|f_n - f\|_D = 0$$

Criterion for Uniform Convergence of a Series

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Theorem (Weierstrass Convergence Criterion)

Let $f_n : D \to \mathbb{C}$, $n \in \mathbb{N}$.
If

$$\sum_{n=0}^{\infty} \|f_n\|_D < \infty$$

then the series

$$\sum_{n=0}^{\infty} f_n$$

converges absolutely and uniformly on D to a function $F : D \to \mathbb{C}$.

Example: Convergence of a Power Series

The series

$$\sum_{n=1}^{\infty} \frac{\cos(nx)}{n^2}$$

converges uniformly on $\mathbb{R}$.

Power Series

Polynomials are among the functions that are easy to handle (e.g. for a machine).

Many other functions become manageable, when they are approximated by polynomials, i.e. as power series.

As for polynomials it is helpful to consider power series on $\mathbb{C}$ from the start.

Definition (Power Series)

Let $\{a_j\}_{j\in\mathbb{N}}$ be a complex sequence and $z_0 \in \mathbb{C}$.

Then

$$f(z) = \sum_{j=0}^{\infty} a_j(z - z_0)^j = a_0 + a_1(z - z_0) + a_2(z - z_0)^2 + \ldots$$

is called a **(complex) power series** with the **center** of the series z_0.

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Properties of Power Series I

The set of points z where the power series converges form a set $M \subseteq \mathbb{C}$.
Note that $z_0 \in M$.

By this the power series defines a function $f : M \to \mathbb{C}$.

The partial sums of power series are polynomials (multiply out!).

Power series have excellent properties of convergence.

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Theorem (Radius of Convergence)

Let

$$f(z) = \sum_{j=0}^{\infty} a_j (z - z_0)^j$$

be a complex power series.

Then exactly one of the following 2 cases holds:

- *There exists a $\rho \in \mathbb{R}_0^+$ s.t. the series converges absolutely for all $z \in O_\rho(z_0) = \{z \in \mathbb{C} \mid |z - z_0| < \rho\}$ and diverges for all z with $|z - z_0| > \rho$.*
- *The series converges absolutely for all $z \in \mathbb{C}$.*

$\rho \in \mathbb{R}_0^+ \cup \{+\infty\}$ is called **radius of convergence**,
$O_\rho(z_0)$ is called **circle of convergence**.

For $|z| = \rho$ no general statement on convergence/divergence is possible.

Computing a Radius of Convergence

Assume for a power series holds

$$\overline{\lim}_{j\to\infty} \sqrt[j]{|a_j|} = b \quad \text{or} \quad \lim_{j\to\infty} \left| \frac{a_{j+1}}{a_j} \right| = b,$$

where $b \in \mathbb{R}_0^+ \cup \infty$, then:

- If $b = 0$, then $\rho = +\infty$.
- If $b = +\infty$, then $\rho = 0$.
- If $0 < b$, then $\rho = \frac{1}{b}$.

The limes superior (or inferior) of the quotient is not helpful in general.

Example: Geometric Series

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Geometric series:

$$\sum_{j=0}^{\infty} z^n$$

Set $a_j = 1$ for all $j \in \mathbb{N}$ (and $z_0 = 0$).

Since $b = \lim_{j\to\infty} \sqrt[j]{a_j} = 1$, we find $\rho = \frac{1}{b} = 1$.

Thus we have (as expected) convergence for $|z| < 1$ and divergence for $|z| > 1$.

What happens for $|z| = 1$? Divergence, since we do not encounter a zero sequence z^n.

Moreover $\sum_{j=0}^{\infty} z^n = \frac{1}{1-z}$ for $|z| < 1$.

Properties of Power Series II

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Theorem (Addition & Scaling of Power Series)

Consider two power series
$f(z) = \sum_{n=0}^{\infty} a_n z^n$ *with radius of convergence* ρ_f *and*
$g(z) = \sum_{n=0}^{\infty} b_n z^n$ *with radius of convergence* ρ_g.

Then the sum/difference is given for all z *with* $|z| < \min(\rho_f, \rho_g)$ *by:*

$$\sum_{n=0}^{\infty} (a_n \pm b_n)\, z^n = \sum_{n=0}^{\infty} a_n z^n \pm \sum_{n=0}^{\infty} b_n z^n = f(z) \pm g(z)$$

Further, the scaling i.e. multiplication with a factor $c \in \mathbb{C}$ *is given for all* z *with* $|z| < \rho_f$ *by:*

$$\sum_{n=0}^{\infty} c a_n z^n = c \sum_{n=0}^{\infty} a_n z^n = c f(z).$$

Properties of Power Series III

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Theorem ((Cauchy) Product of Power Series)

Consider two power series
$f(z) = \sum_{n=0}^{\infty} a_n z^n$ *with radius of convergence* ρ_f *and*
$g(z) = \sum_{n=0}^{\infty} b_n z^n$ *with radius of convergence* ρ_g.

Then the product $f(z_1)g(z_2)$ *is given for all* z_1, z_2 *with* $|z_1|, |z_2| < \min(\rho_f, \rho_g)$ *by:*

$$f(z_1)g(z_2) = \sum_{n=0}^{\infty} \sum_{k=0}^{n} a_k b_{n-k} z_1^k z_2^{n-k}.$$

In particular, if $z = z_1 = z_2$*:*

$$f(z)g(z) = \sum_{n=0}^{\infty} \left(\sum_{k=0}^{n} a_k b_{n-k} \right) z^n.$$

The latter 2 theorems also hold for $f(z) = \sum_{n=0}^{\infty} a_n (z - z_0)^n$, $g(z) = \sum_{n=0}^{\infty} b_n (z - z_0)^n$ by a shift.

Continuity of Power Series

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Theorem (Series of polynomials are continuous)

Let

$$f(z) = \sum_{j=0}^{\infty} a_j (z - z_0)^j$$

be a complex power series with radius of convergence ρ.

Then the function

$$f : O_\rho(z_0) \to \mathbb{C} : z \mapsto \sum_{j=0}^{\infty} a_j (z - z_0)^j$$

is continuous.

More Examples: Exponential Series etc.

The series
for the exponential function and
for (co)sine, resp.,
have the radius of convergence $\rho = \infty$.

The latter 3 series yield a continuous function.

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Identity of Power Series

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Theorem (Identity Theorem for Power Series)

Let

$$f(z) = \sum_{j=0}^{\infty} a_j (z-\zeta)^j, \quad g(z) = \sum_{j=0}^{\infty} b_j (z-\zeta)^j$$

be complex power series, both with radius of convergence ρ.
Suppose there exists a series of points $z_n \in O_\rho(\zeta) \setminus \zeta$, $n \in \mathbb{N}$, *s.t.*

$$f(z_n) = g(z_n) \text{ for all } n \in \mathbb{N} \text{ and } \lim_{n\to\infty} z_n = \zeta,$$

then f *and* g *are identical, i.e.* $a_j = b_j$ *for all* $j \in \mathbb{N}$.

Remark: Power series may be extended from the real axis to the complex plane $\rightsquigarrow$ complex analysis ("Funktionentheorie").

Proof of the Identity Theorem

Proof:

Integration of Power Series

We know an example where the limit of f_n and the integration do not commutate.
But in case of uniform convergence we may swap the limit of the sequence and the integration:

Theorem (Commutation of integration and limit of a sequence)

Let $f_n : [a, b] \to \mathbb{R}$, $n \in \mathbb{N}$, a sequence of continuous functions.
Let $\{f_n\}_{n\in\mathbb{N}}$ be uniformly convergent on $[a, b]$ to $f : [a, b] \to \mathbb{R}$.

Then:

$$\int_a^b f(x)\,dx = \lim_{n\to\infty} \int_a^b f_n(x)\,dx.$$

Proof: Commutation of Integration & Limit

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- Check:
$$\int_a^b e^x\,dx = \int_a^b \sum_{j=0}^\infty \frac{x^j}{j!}\,dx = \sum_{j=0}^\infty \int_a^b \frac{x^j}{j!}\,dx = \sum_{j=0}^\infty \left[\frac{x^{j+1}}{(j+1)!}\right]_a^b = \left[\sum_{j=0}^\infty \frac{x^{j+1}}{(j+1)!}\right]_a^b = \left[\sum_{k=1}^\infty \frac{x^k}{k!}\right]_a^b = [e^x]_a^b$$
- Power series for the integral sine:

Differentiation of Power Series

We ask what are the conditions that the limit of f_n and the differentiation commutate.
We require the pointwise convergence of f_n and the uniform convergence of f_n':

Theorem (Commutation of differentiation and limit of a sequence)

Let $f_n : [a, b] \to \mathbb{R}$, $n \in \mathbb{N}$, a sequence of continuously differentiable functions, with derivatives $f_n' : [a, b] \to \mathbb{R}$.
Let $\{f_n\}_{n\in\mathbb{N}}$ be pointwise convergent on $[a, b]$ to
$f : [a, b] \to \mathbb{R}$ and
$\{f_n'\}_{n\in\mathbb{N}}$, be uniformly convergent on $[a, b]$.

Then f is differentiable and:

$$f'(x) = \lim_{n\to\infty} f_n'(x) \quad \text{for all } x \in [a, b].$$

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Proof.

Let $f^\star := \lim_{n\to\infty} f_n'$. According to the result from above $f^\star$ is continuous on $[a,b]$. Thus for all $x \in [a,b]$ there holds

$$f_n(x) = f_n(a) + \int_a^x f_n'(\xi)\,d\xi. \tag{1}$$

According to the last theorem

$$\int_a^x f_n'(\xi)\,d\xi \to \int_a^x f^\star(\xi)\,d\xi \text{ as } n \to \infty,$$

thus taking the limit on both sides of (1) yields

$$f(x) = f(a) + \int_a^x f^\star(\xi)\,d\xi.$$

By differentiation $f'(x) = f^\star(x)$ for any $x \in [a,b]$. □

(Counter-)Examples

- $$f_n(x) = \frac{1}{n}\sin(nx),\ n \in \mathbb{N}$$

- $$F(x) = \sum_{n=1}^{\infty} \frac{\cos(nx)}{n^2}$$

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Corollary

Suppose the power series

$$f(x) = \sum_{n=0}^{\infty} c_n (x - x_0)^n$$

converges on $I := (x_0 - \rho, x_0 + \rho)$, *where* $\rho > 0$ *is the radius of convergence.*

Then $f : I \to \mathbb{R}$ *is arbitrarily many times differentiable and:*

$$c_n = \frac{1}{n!} f^{(n)}(x_0)$$

Proof: Apply iteratively the theorem on commutation of differentiation and limits.

Taylor Series

In many applications “higher order” terms are neglected in order to find simpler or manageable formulas.

The base for this and for an estimate of the resulting error is the following theorem:

Theorem (Taylor theorem)

Let $f : [a, b] \to \mathbb{R}$ be an $n+1$-times continuously differentiable function.
Then for any two points x and x_0 in (a, b) there exists a number $\Theta_{x,x_0} \in (0, 1)$ such that

$$f(x) = \sum_{k=0}^{n} \frac{f^{(k)}(x_0)}{k!}(x - x_0)^k + \frac{f^{(n+1)}(x_0 + \Theta_{x,x_0} \cdot (x - x_0))}{(n+1)!}(x - x_0)^{n+1}.$$

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Taylor Polynomial & Remainder

Definition (Taylor Polynomial, Lagrange Form of the Remainder)

We call

$$T_n(f, x, x_0) = \sum_{k=0}^{n} \frac{f^{(k)}(x_0)}{k!}(x - x_0)^k$$

the **Taylor polynomial of n-th order** (not of n-th degree!) around the center x_0.

The term

$$\frac{f^{(n+1)}(x_0 + \Theta_{x,x_0} \cdot (x - x_0))}{(n+1)!}(x - x_0)^{n+1}$$

is called the **Lagrange form of the remainder**.

There are other forms of the remainder: Peano form, Cauchy form, ...

Examples for the Taylor Theorem

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Definition (Taylor Series)

Let $f : [a, b] \to \mathbb{R}$ be arbitrarily many times differentiable.

Then for $x \in [a, b]$ the power series

$$T(f, x, x_0) = \sum_{k=0}^{\infty} \frac{f^{(k)}(x_0)}{k!}(x - x_0)^k.$$

is called the **Taylor series** of the function f with the center x_0.

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Theorem (Convergence Criterion for Taylor Series)

The Taylor series $T(f, x, x_0)$ converges for a given $x \in [a, b]$ to $f(x)$

iff

$$\lim_{n \to \infty} R_n(f, x, x_0) = 0.$$

We are interested in an interval $[a, b]$ such that the remainder converges to 0 and this should happen “fast”.

Warning: There exist functions whose Taylor series represent the function in a single point only!

Maclaurin Series

An important special case: $x_0 = 0$.

Let f be as in the Taylor theorem and $0 \in (a, b)$. For any point $x \in (a, b)$ there exists a number $\Theta_x \in (0, 1)$ such that

$$f(x) = \sum_{k=0}^{n} \frac{f^{(k)}(0)}{k!} x^k + \frac{f^{(n+1)}(\Theta_x x)}{(n+1)!} x^{n+1}.$$

The corresponding series is called **Maclaurin series** of the function f:

$$M(f, x) = \sum_{k=0}^{\infty} \frac{f^{(k)}(0)}{k!} x^k.$$

Its center is $x_0 = 0$.

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A Taylor Series for the Logarithm

- $\ln(1+x) = \sum_{n=1}^{\infty} (-1)^{n-1} \frac{x^n}{n}$

- $\ln(2) = 1 - \frac{1}{2} + \frac{1}{3} - \frac{1}{4} + \frac{1}{5} - \dots$

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Fourier Series

Motivation:

- Periodic signals, image processing (jpeg/mpeg compression)
- Generation of signals by periodic means
- Harmonic oscillations, acoustics
- Periodic orbits
- Revolving motors

Many periodic functions may be approximated by a sum of trigonometric base functions as

$$1, \quad \cos(kx), \quad \sin(kx), \quad k \in \mathbb{N}$$

with suitable coefficients a_0, a_k, b_k.

Frequently, it may make sense to replace the finite sum by a series.

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Example: Rotational Force of an Engine I

A rotational force f (due to gas pressure and mass inertia) acts on the crankshaft of a single-cylinder two-stroke engine.

At the points $t_k = k \cdot \pi/8$, $k = 0, 1, \ldots, 15$, the following values of f_k were determined experimentally:

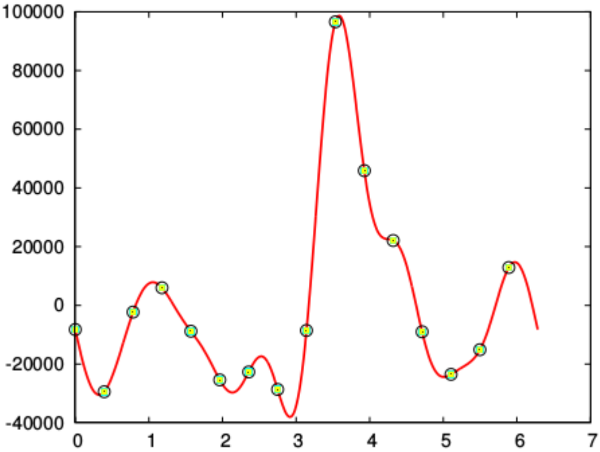
f_0	f_1	f_2	f_3	f_4	f_5
−8250	−29430	−2286	5974	−8829	−25408

f_6	f_7	f_8	f_9	f_{10}
−22681	−28655	−8564	96560	45862

f_{11}	f_{12}	f_{13}	f_{14}	f_{15}
22092	−9025	−23514	−15127	12880

Example: Rotational Force of an Engine II

The resulting trigonometric approximation of f looks as follows:



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Definition (Periodic function)

A function $f : \mathbb{R} \to \mathbb{C}$ is called T**-periodic**, if there exists a $T > 0$ s.t.

$$f(x+T) = f(x) \quad \text{for all } x \in \mathbb{R}.$$

T is called a **period** of f.

Note that a T-periodic function f is completely defined by its values on the interval $[0, T)$. Thus it is enough to consider f only on $[0, T)$.

Properties of Periodic Functions

Let f and g be T-periodic.

- Then $\alpha f + \beta g$ is T-periodic for any $\alpha, \beta \in \mathbb{C}$.
- Then there holds for all $c \in \mathbb{R}$:

$$\int_c^{c+T} f(x)\,dx = \int_0^T f(x)\,dx.$$

- Then the function $\tilde{f} : \mathbb{R} \to \mathbb{C}$, defined by

$$\tilde{f}(x) := f\left(\frac{T}{2\pi}x\right)$$

  is 2π-periodic, since:

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Definition (Fourier Series)

The function series

$$F(x) := \frac{a_0}{2} + \sum_{k=1}^{\infty} a_k \cos(k\omega x) + b_k \sin(k\omega x) \quad \text{with } \omega := \frac{2\pi}{T}$$

is called **Fourier series.** The coefficients $a_0, a_1, \ldots$ and $b_1, b_2, \ldots$ are called **Fourier coefficients.** The representation of a function by its Fourier series is called **Fourier** (or harmonic) **analysis.** The finite sum is called **Fourier sum**:

$$F_n(x) := \frac{a_0}{2} + \sum_{k=1}^{n} a_k \cos(k\omega x) + b_k \sin(k\omega x).$$

Computing Fourier Coefficients

Theorem (Fourier)

Assume a T-periodic function f may be represented as a Fourier series

$$F(x) := \frac{a_0}{2} + \sum_{k=1}^{\infty} a_k \cos(k\omega x) + b_k \sin(k\omega x) \quad \text{with } \omega := \frac{2\pi}{T},$$

then the Fourier coefficients are given by

$$a_0 = \frac{2}{T} \int_0^T f(x)\, dx,$$
$$a_k = \frac{2}{T} \int_0^T f(x) \cos(k\omega x)\, dx,$$
$$b_k = \frac{2}{T} \int_0^T f(x) \sin(k\omega x)\, dx.$$

Symmetry & Fourier Coefficients

The following symmetries may be exploited when computing Fourier coefficients, $k \in \mathbb{N}$:

- If f is an odd function, i.e. $f(x) = -f(-x)$ for all $x \in \mathbb{R}$, then

$$b_k = \frac{2}{T}\int_0^T f(x)\sin(k\omega x)\,dx = \frac{4}{T}\int_0^{T/2} f(x)\sin(k\omega x)\,dx,$$

$$a_k = \frac{2}{T}\int_0^T f(x)\cos(k\omega x)\,dx = \qquad = 0.$$

- If f is an even function, i.e. $f(x) = f(-x)$ for all $x \in \mathbb{R}$, then

$$b_k = \frac{2}{T}\int_0^T f(x)\sin(k\omega x)\,dx = \qquad = 0,$$

$$a_k = \frac{2}{T}\int_0^T f(x)\cos(k\omega x)\,dx = \frac{4}{T}\int_0^{T/2} f(x)\cos(k\omega x)\,dx.$$

Example: Saw-tooth Function revisited

Warning: In general $f(x) \neq F(x)$ for all $x \in \mathbb{R}$!

Gibbs phenomenon: overshooting & undershooting (up to 18% for large n) at points of discontinuity

Revision: Trigonometric Functions

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Definition (Cosine and sine)

For $x \in \mathbb{R}$ we define:

$$\cos(x) := \operatorname{Re}(\exp(ix))$$
$$\sin(x) := \operatorname{Im}(\exp(ix))$$

We see that the Euler formula holds:

$$\exp(ix) = \cos(x) + i\sin(x), \quad x \in \mathbb{R}$$

Complex Representation

By the complex exponential function we may rewrite

$$F(x) = \sum_{k=-\infty}^{\infty} c_k \exp(ik\omega x) \quad \text{with } \omega := \frac{2\pi}{T}$$

where the complex Fourier coefficient c_k, $k \in \mathbb{Z}$, is given by

$$c_k = \frac{1}{T} \int_0^T f(x) \exp(-ik\omega x)\, dx.$$

Note that the limit is to be understood symmetrically:

$$\sum_{k=-\infty}^{\infty} c_k \exp(ik\omega x) := \lim_{n\to\infty} \sum_{k=-n}^{n} c_k \exp(ik\omega x).$$

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Theorem (Orthonormality Relations)

If $m, n \in \mathbb{N}$, then:

$$\frac{2}{T}\int_0^T \sin(m\omega x)\sin(n\omega x)\,dx = \delta_{m,n},$$

$$\frac{2}{T}\int_0^T \cos(m\omega x)\cos(n\omega x)\,dx = \delta_{m,n},$$

$$\frac{2}{T}\int_0^T \sin(m\omega x)\cos(n\omega x)\,dx = 0,$$

and if $m, n \in \mathbb{Z}$, then:

$$\frac{1}{T}\int_0^T \exp(im\omega x)\exp(-in\omega x)\,dx = \delta_{m,n}.$$

Piecewise Continuous Differentiability

Definition (Piecewise Continuously Differentiable Function)

Let $f : \mathbb{R} \to \mathbb{R}$ with

(i) Only at a finite number of **singularities** the function f is not continuously differentiable.

(ii) At any singularity x_0 there exist the following one-sided limits:

$$f(x_0+) := \lim_{x \to x_0+} f(x) \qquad f(x_0-) := \lim_{x \to x_0-} f(x),$$
$$f'(x_0+) := \lim_{x \to x_0+} f'(x) \qquad f'(x_0-) := \lim_{x \to x_0-} f'(x).$$

Then f is called **piecewise continuously differentiable.**

Discontinuities are singularities, but not any singularity is a discontinuity.

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Convergence of Fourier Series

Theorem (Convergence of Fourier Series)

Let $f : \mathbb{R} \to \mathbb{R}$ be a periodic function that is piecewise continuously differentiable. Then:

- *The Fourier series F converges at any x that is not a singularity to f.*
- *At any singularity x_0 the Fourier series converges to the "mean value" of the jump*

$$\frac{1}{2}\left(f(x_0+)+f(x_0-)\right).$$

- *In any compact interval that does not contain a discontinuity, the convergence of F to f is uniform.*

Note that there exist periodic, continuous functions, whose Fourier series does not converge to f!

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Let f and g be piecewise continuous, periodic functions with Fourier series $F = \sum_{k=-\infty}^{\infty} c_k \exp(ik\omega x)$, $G = \sum_{k=-\infty}^{\infty} d_k \exp(ik\omega x)$, resp. There holds:

- For any $\alpha, \beta \in \mathbb{R}$:

$$\alpha F(x) + \beta G(x) = \sum_{k=-\infty}^{\infty} (\alpha c_k + \beta d_k) \exp(ik\omega x)$$

- $F(-x) = \sum_{k=-\infty}^{\infty} c_{-k} \exp(ik\omega x)$
- For any $\alpha \in \mathbb{R}$

$$F(\alpha x) = \sum_{k=-\infty}^{\infty} c_k \exp(ik\omega\alpha x)$$

- For any $\alpha \in \mathbb{R}$

$$F(\alpha + x) = \sum_{k=-\infty}^{\infty} (c_k \exp(ik\omega\alpha)) \exp(ik\omega x)$$

Properties of Fourier Series II

Let f be a piecewise continuously differentiable, periodic function with Fourier series $F = \sum_{k=-\infty}^{\infty} c_k \exp(ik\omega x)$. There holds:

- The Fourier series F' represents f':

$$F'(x) = \sum_{k=-\infty}^{\infty} (ik\omega c_k) \exp(ik\omega x)$$

- $F(-x) = \sum_{k=-\infty}^{\infty} c_{-k} \exp(ik\omega x)$
- Suppose $c_0 = 0$, then the Fourier series $\tilde{F} := \int F(\xi)\, d\xi$ represents $\tilde{f} := \int f(\xi)\, d\xi$:

$$\tilde{F}(x) = \frac{1}{T} \int_0^T \tilde{f}(\xi)\, d\xi + \sum_{k=-\infty, k\neq 0}^{\infty} \frac{c_k}{ik\omega} \exp(ik\omega x)$$

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Discrete Fourier Transform: Interpolation

Problem (General Interpolation Task)

For a given function $g : \mathbb{R} \to \mathbb{R}$ with given points

$$(x_j, g(x_j)), \quad j = 1, \ldots, n,$$

we search for a function p, s.t. the graph of p goes through these given points.

p is chosen within a class of reasonable (and manageable) functions, e.g.

- *the class of real polynomials,*
- *the class of trigonometric polynomials in case of $T-$periodic functions.*

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In the later case we consider a function $g : [0, 2\pi] \to \mathbb{R}$, periodically extended with $T = 2\pi$.

Let

$$x_0 = 0, x_1 = \frac{2\pi}{n}, \ldots, x_{n-1} = (n-1)\frac{2\pi}{n}, x_n = 2\pi.$$

We search for a trigonometric polynomial

$$p_n(x) := \sum_{k=0}^{n-1} c_k \exp(ikx)$$

such that

$$p_n(x_j) = g(x_j) \quad \text{for } j = 0, \ldots, n-1.$$

Remark: Due to the periodicity, we have $g(x_0) = g(x_n)$.

By inserting:

$$\sum_{k=0}^{n-1} \exp(ikx_j) c_k = g(x_j) \quad \text{for } j = 0, \ldots, n-1.$$

This is a linear equation system (LES) with coefficient matrix

$$f_{jk} = \exp\left(2\pi ik\frac{j}{n}\right) = \zeta^{jk} \quad \text{with } \zeta := \exp\left(2\pi i\frac{1}{n}\right).$$

Fourier Matrix

This motivates the definition of the so-called **Fourier matrix** :

$$F_n = (f_{ij})_{i,j=1,\ldots,n}$$

Properties of the Fourier matrix:

- F_n is symmetric
- $\frac{1}{\sqrt{n}} F_n$ is unitary, i.e. $\left(\frac{1}{\sqrt{n}} F_n\right)^{-1} = \overline{\left(\frac{1}{\sqrt{n}} F_n\right)}^{\top}$ (details later in LA)

Thus, we may rewrite the LES

$$F_n \begin{pmatrix} c_1 \\ \vdots \\ c_n \end{pmatrix} = \begin{pmatrix} g(x_1) \\ \vdots \\ g(x_n) \end{pmatrix}$$

that uniquely determines the trigonometric polynomial p_n by

$$\begin{pmatrix} c_1 \\ \vdots \\ c_n \end{pmatrix} = \frac{1}{n} \overline{F}_n^{\top} \begin{pmatrix} g(x_1) \\ \vdots \\ g(x_n) \end{pmatrix}$$

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The mapping

$$\mathbb{C}^n \to \mathbb{C}^n, v \mapsto F_n v$$

is called **discrete Fourier transform (DFT)**, i.e.

$$(F_n v)_j = \sum_{k=0}^{n-1} v_k \exp\left(2\pi i \frac{jk}{n}\right).$$

This may be interpreted as a discretization of the (continuous) Fourier transform (at the end of lecture).

The inverse DFT solves the trigonometric interpolation problem.

By an algorithm, called **fast Fourier transform (FFT)** the DFT may be computed with only "few" operations!

Example: Fourier Matrix

Let $v^\top = \left(1, -1, 0, 1\right)$.

Compute

$$F_4 \, v =$$

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Image & Audio-Video Compression

An image with decreasing quality from the left to the right. (Source: Wikipedia)

Typical standards: `jpeg`, `mpeg`

An important step (among others) in these data compression methods is the discrete Fourier cosine transform that maps into the frequency domain.

Theoretically, this step is invertible, i.e. without loss of information possible.

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Outlook Fourier Analysis

At the end of a lecture (if time permits) we will have a short look at

- (Continuous) Fourier transform
- Laplace transform
- Short-time Fourier transform
- Wavelet

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Differential Calculus in $\mathbb{R}^n$

In Analysis 1 we have discussed differentiation of functions of 1 variable.

Now we consider a real-valued function in several variables

$$f : D \subseteq \mathbb{R}^n \to \mathbb{R}$$
$$\mathbf{x} = (x_1, \ldots, x_n)^\top \mapsto f(x_1, \ldots, x_n) = f(\mathbf{x})$$

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Differential Calculus in $\mathbb{R}^n$

In Analysis 1 we have discussed differentiation of functions of 1 variable.

Now we consider a real-valued function in several variables

$$f : D \subseteq \mathbb{R}^n \to \mathbb{R}$$
$$\mathbf{x} = (x_1, \dots, x_n)^\top \mapsto f(x_1, \dots, x_n) = f(\mathbf{x})$$

Later we are going to extend the differential calculus to vector-valued functions (of several variables)

$$f : D \subseteq \mathbb{R}^n \to \mathbb{R}^m$$
$$\mathbf{x} = (x_1, \dots, x_n)^\top \mapsto (f_1(x_1, \dots, x_n), \dots, f_m(x_1, \dots, x_n))^\top$$

Special Case: n = 2

A real-valued function in 2 variables

$$f : D \subseteq \mathbb{R}^2 \to \mathbb{R}$$
$$\mathbf{x} = (x_1, x_2)^\top \mapsto f(x_1, x_2)$$

We may plot the function value as 3rd coordinate over the real plane $\mathbb{R}^2$.
The graph of f is a subset of $\mathbb{R}^3$: a "landscape" or "mountains".

Contour Line, Equipotential Surface, ...

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Definition (Level set)

We define the **level set** of a function $f : D \subseteq \mathbb{R}^n \to \mathbb{R}$, $(x_1, \ldots, x_n)^\top \mapsto f(x_1, \ldots, x_n)$ for the function value $c \in \mathbb{R}$ as the set

$$N_c := \{\mathbf{x} \in D \,|\, f(\mathbf{x}) = c\}.$$

The structure of N_c may be "complicated", it might also be the empty set.

For $n = 2$ the level set is called a contour line or level curve (though it may be an area, e.g.),
for $n = 3$ the level set is called an equipotential surface (though it may be a solid, e.g.).

Partial Function: Definition

A partial function is a "cross section"-function that is obtained by freezing all but 1 variables, e.g. x_i:

$$g_i : D_i \subseteq \mathbb{R} \to \mathbb{R}$$
$$x_i \mapsto f(a_1, \dots, a_{i-1}, x_i, a_{i+1}, \dots, a_n),$$

with $(a_1, \dots, a_{i-1}, x_i, a_{i+1}, \dots, a_n) \in D$ for all $x_i \in D_i$, $a_1, \dots, a_{i-1}, a_{i+1}, \dots, a_n$ fixed.

Partial Function: Example

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

Partial Derivatives: Definition

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Definition (Partial derivative)

Let $f : D \subseteq \mathbb{R}^n \to \mathbb{R}$, $\mathbf{x} = (x_1, \ldots, x_n)^\top \mapsto f(x_1, \ldots, x_n)$ and $a \in D$, D an open set.

If the derivative of the partial function

$$x_i \mapsto f(a_1, \ldots, a_{i-1}, x_i, a_{i+1}, \ldots, a_n)$$

exists at $x_i = a_i$,
then we call it the **partial derivative** of f w.r.t. x_i at a.

We write:

$$\frac{\partial f}{\partial x_i}(\mathbf{a}) \quad \text{or} \quad f'_{x_i}(\mathbf{a}) \quad \text{or} \quad \ldots$$

We say f is **partially differentiable** in $\mathbf{a}$, if all $\frac{\partial f}{\partial x_i}(\mathbf{a})$ exist.
We say f is partially differentiable in $E \subseteq D$, if f is partially differentiable at any $\mathbf{a} \in E$.

Partial Derivatives: Gradient

We assume that f is partially differentiable in D.
It is convenient to arrange the (first) partial derivatives in a vector.

We define the **gradient** of $f : D \subseteq \mathbb{R} \to \mathbb{R}$ as the column vector (function):

$$\nabla f(\mathbf{x}) := \begin{pmatrix} \frac{\partial f}{\partial x_1}(\mathbf{x}) \\ \vdots \\ \frac{\partial f}{\partial x_i}(\mathbf{x}) \\ \vdots \\ \frac{\partial f}{\partial x_n}(\mathbf{x}) \end{pmatrix}$$

The gradient is

- orthogonal to level sets and
- points into the direction of the steepest ascent.

Partial Derivatives: Examples

Higher Partial Derivatives: Definition

Partial derivatives w.r.t. some x_j are again functions of x_1, x_2, ..., x_n and, again, we may search for partial derivatives w.r.t. some x_i, yielding **second partial derivatives.** $(i, j = 1, \ldots, n)$

We write:

$$\frac{\partial}{\partial x_i}\frac{\partial f}{\partial x_j}(\mathbf{a}) \quad \text{or} \quad \frac{\partial^2}{\partial x_i \partial x_j} f(\mathbf{a}) \quad \text{or} \quad f''_{x_i,x_j}(\mathbf{a}) \quad \text{or} \quad f''_{i,j}(\mathbf{a}) \quad \ldots$$

In 2d with $(x, y) = (x_1, x_2)$ this reads, e.g.:

$$\frac{\partial}{\partial x}\frac{\partial f}{\partial y}(\mathbf{a}) \quad \text{or} \quad \frac{\partial^2}{\partial x \partial y} f(\mathbf{a}) \quad \text{or} \quad f''_{x,y}(\mathbf{a}) \quad \text{or} \quad f''_{1,2}(\mathbf{a}) \quad \ldots$$

Higher Partial Derivatives: Hesse Matrix

We assume that f is $2x$ partially differentiable in D. Again it is convenient to order the second partial derivatives in a (quadratic) matrix.

We define the **Hesse matrix** of $f : D \subseteq \mathbb{R} \to \mathbb{R}$ as the quadratic matrix (function):

$$H_f(\mathbf{x}) := \begin{pmatrix} \frac{\partial^2}{\partial x_1 \partial x_1} f(\mathbf{x}) & \dots & \dots & \frac{\partial^2}{\partial x_1 \partial x_n} f(\mathbf{x}) \\ \vdots & \frac{\partial^2}{\partial x_i \partial x_j} f(\mathbf{x}) & \ddots & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ \frac{\partial^2}{\partial x_n \partial x_1} f(\mathbf{x}) & \dots & \dots & \frac{\partial^2}{\partial x_n \partial x_n} f(\mathbf{x}) \end{pmatrix}$$

In 2d with $(x, y) = (x_1, x_2)$ this reads, e.g.:

$$H_f(x, y) := \begin{pmatrix} \frac{\partial^2}{\partial x \partial x} f(x, y) & \frac{\partial^2}{\partial x \partial y} f(x, y) \\ \frac{\partial^2}{\partial y \partial x} f(x, y) & \frac{\partial^2}{\partial y \partial y} f(x, y) \end{pmatrix}$$

Schwarz-Clairaut Theorem

According to the Schwarz-Clairaut theorem there holds:

Suppose f is defined on a disk $D \subseteq \mathbb{R}^2$ with $(x_0, y_0) \in D$.
If $\frac{\partial^2 f}{\partial x \partial y}$ and $\frac{\partial^2 f}{\partial y \partial x}$ are both continuous on D,
then $\frac{\partial^2 f}{\partial x \partial y} = \frac{\partial^2 f}{\partial y \partial x}$.

This shows that the Hesse matrix is symmetric.

Higher Partial Derivatives: Examples

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Limits and Continuity in $\mathbb{R}^n$

Let $D \subseteq \mathbb{R}^n$.

- ε-neighbourhood of $\mathbf{a} \in \mathbb{R}^n$:

$$U_\varepsilon(\mathbf{a}) := \left\{ \mathbf{x} \in \mathbb{R}^n \,\middle|\, \|\mathbf{x} - \mathbf{a}\|_2 := \sqrt{\sum_{i=1}^{n} (x_i - a_i)^2} < \varepsilon \right\}$$

- $\mathbf{a} \in D$ is called an **interior point** of D $:\Longleftrightarrow$ there exists $U_\epsilon(\mathbf{a})$ with $U_\epsilon(\mathbf{a}) \subseteq D$.
- A set D is called **open** $:\Longleftrightarrow$ any point of D is an interior point. A set D is called **closed** $:\Longrightarrow \mathbb{R}^n \setminus D$ is open.
- $\mathbf{b} \in \mathbb{R}^n$ is called a **boundary point** of D $:\Longrightarrow$ for all $U_\varepsilon(\mathbf{b})$ holds, there exists a $\mathbf{x}, \mathbf{y} \in U_\varepsilon(\mathbf{b})$ with $\mathbf{x} \in D$ and $\mathbf{y} \notin D$. The set ∂D of all boundary points $\mathbf{b}$ is called **boundary** of D.

Examples, see blackboard

Revision/Definition: Limits and Continuity

Let $f : \mathbb{R}^n \subseteq D \to \mathbb{R}^m$, $\mathbf{a} \in D \cup \partial D$.

$$\lim_{\mathbf{x}\to\mathbf{a}} f(\mathbf{x}) = c \in \mathbb{R}^m :\Longleftrightarrow$$

for all $\varepsilon > 0$ exists $U_\varepsilon(\mathbf{a}) : \|f(\mathbf{x}) - c\| \leq \varepsilon$ for all $\mathbf{x} \in D \cap U_\varepsilon(\mathbf{a})$.

f is called **continuous** in $\mathbf{a} \in D :\Longleftrightarrow \lim_{\mathbf{x}\to\mathbf{a}} f(\mathbf{x}) = f(\mathbf{a})$.
f is called continuous in $D :\Longleftrightarrow f$ is continuous for all $\mathbf{a} \in D$.

Example: For $n = 2, m = 1$, f is continuous means that there are no “jumps” or “ridges”.

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Pathologic Example for (Dis)continuity in 2d

Functions of severable variables exhibit phenomena that we do not encounter in 1d:

Consider $f : \mathbb{R}^2 \to \mathbb{R}$,

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

A limit in 2d has to hold for any “path” $(x,y) \to (x_0,y_0)$.
It is not enough to consider each coordinate separately!

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Summary - Outlook and Review

In this subsection we consider the total differentiability, a stronger requirement than partial differentiability.

Moreover, we consider expansions of functions of several variables.

Applications:

- Linear approximation of functions, tangent planes
- Taylor series for several variables

Here we consider:

$$f : D \subseteq \mathbb{R}^n \to \mathbb{R}^m$$

$$\mathbf{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} \mapsto \begin{pmatrix} f_1(\mathbf{x}) \\ \dots \\ f_m(\mathbf{x}) \end{pmatrix} = \begin{pmatrix} f_1(x_1, \dots, x_n) \\ \dots \\ f_m(x_1, \dots, x_n) \end{pmatrix}$$

Analysis 2

S.-J. Kimmerle

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Definition (Total differentiability)

$f : \mathbb{R}^n \supseteq D \to \mathbb{R}^m$ is called **totally differentiable** (or linearly approximable) in $\mathbf{x} \in D$,

if there exists a matrix $A \in \mathbb{R}^{m \times n}$,
such that for all $\mathbf{x}$ in a neighbourhood $U(\mathbf{x}_0)$, $\mathbf{x}_0 \in D$,

$$f(\mathbf{x}) = f(\mathbf{x}_0) + A \cdot (\mathbf{x} - \mathbf{x}_0) + R(\mathbf{x} - \mathbf{x}_0),$$

where

$$R : \mathbb{R}^n \supseteq U(\mathbf{x}_0) \to \mathbb{R}^m \text{ with } \lim_{\|\mathbf{x}-\mathbf{x}_0\| \to 0} \frac{R(\mathbf{x} - \mathbf{x}_0)}{\|\mathbf{x} - \mathbf{x}_0\|} = 0.$$

f is called totally differentiable in E, if this holds for all $\mathbf{x} \in E \subseteq D$.

Jacobi Matrix

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If f is totally differentiable, then

- f is continuous
- all f_i, $i = 1, \ldots, m$, are continuously partially differentiable
- the matrix A is uniquely determined by the so-called **Jacobi matrix**

$$J_f(\mathbf{x}) := \begin{pmatrix} \frac{\partial f_1}{\partial x_1}(\mathbf{x}) & \ldots & \ldots & \frac{\partial f_1}{\partial x_n}(\mathbf{x}) \\ \vdots & \ddots & \frac{\partial f_i}{\partial x_j}(\mathbf{x}) & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1}(\mathbf{x}) & \ldots & \ldots & \frac{\partial f_m}{\partial x_n}(\mathbf{x}) \end{pmatrix}$$

Special case $m = 1$: transposed gradient

We also write $D_f(\mathbf{x}) = J_f(\mathbf{x})$, indicating this is the general form of the derivative (as a matrix).

Linearization

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Theorem (Tangent plane)

Let $D \subseteq \mathbb{R}^2$, $f : D \to \mathbb{R}$ totally differentiable and $(x_0, y_0) \in D$.

Then the points (x, y, z) of the tangent plane in (x_0, y_0) are described by the equation

$$z = f(x_0, y_0) + \nabla f(x_0, y_0)^\top \begin{pmatrix} x - x_0 \\ y - y_0 \end{pmatrix}$$

$$=$$

The tangent plane is locally the optimal (affine-)linear approximation for f. The plane consists out of all tangents.
In the general case the linear approximation reads

$$f(\mathbf{x}) \approx f(\hat{\mathbf{x}}) + D_f(\hat{\mathbf{x}})(\mathbf{x} - \hat{\mathbf{x}}).$$

Tangent Plane as Linear Approximation

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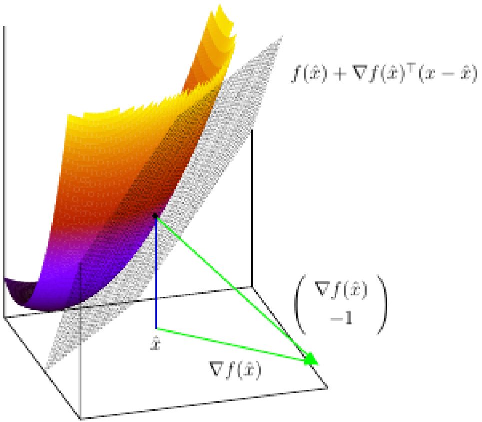
In 2d: tangent plane



Tangent Plane: Example

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Chain Rule (Simple Case)

Let $\mathbf{x} : \mathbb{R} \supseteq (a, b) \to D$ differentiable in $t \in (a, b)$,
$f : \mathbb{R}^n \supseteq D \to \mathbb{R}$ (totally) diff.able in $\mathbf{s} := \mathbf{x}(t) \in D$, D open,

then

$$f \circ \mathbf{x} : (a, b) \to \mathbb{R},\ t \mapsto f(\mathbf{s}) = f(\mathbf{x}(t))$$

is totally differentiable in t and

$$\frac{d}{dt} f(\mathbf{x}(t)) = \nabla f(\mathbf{x}(t))^\top \dot{\mathbf{x}}(t).$$

Chain Rule (General Case)

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Let $g : \mathbb{R}^p \supseteq E \to D$ (totally) diff.able in $\mathbf{t} \in E$, E open, $f : \mathbb{R}^n \supseteq D \to \mathbb{R}^m$ (totally) diff.able in $\mathbf{s} := g(\mathbf{t}) \in D$, D open,

then

$$f \circ g : E \to \mathbb{R}^m, \mathbf{t} \mapsto f(\mathbf{s}) = f(g(\mathbf{t}))$$

is totally differentiable in $\mathbf{t}$ and

$$D_{f \circ g}(\mathbf{t}) = D_f(\mathbf{x}(\mathbf{t}))\, D_g(\mathbf{t}).$$

Application: Coordinate Transformation I

Example (Polar Coordinates in $\mathbb{R}^2$)

Cartesian coordinates $(x, y) \in \mathbb{R}^2$
Polar coordinates $(r, \phi) \in [0, \infty) \times (-\pi, \pi]$

Consider $f : \mathbb{R}^2 \to \mathbb{R}, (x, y) \mapsto f(x, y)$ and
$F : [0, \infty) \times (-\pi, \pi], (r, \phi) \mapsto F(r, \phi) := f(r\cos(\phi), r\sin(\phi))$.

How do I transform the derivative when changing coordinates?

Let the change of coordinates be described by

$$g : \mathbb{R}^2 \to [0, \infty) \times (-\pi, \pi], \begin{pmatrix} r \\ \phi \end{pmatrix} \mapsto \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} r\cos(\phi) \\ r\sin(\phi) \end{pmatrix}.$$

By the chain rule, we compute $D_F = D_f \cdot D_g = \ldots$

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Application: Coordinate Transformation II

$$D_F = D_f \cdot D_g =$$

Directional Derivative

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The **directional derivative** $D_d f(\mathbf{x}) = f'(\mathbf{x}; \mathbf{d})$ of a continuously differentiable function $f : \mathbb{R}^n \to \mathbb{R}$ at $\mathbf{x} \in \mathbb{R}^n$ in direction $\mathbf{d} \in \mathbb{R}^n$ is defined as

$$D_d f(x) := \lim_{t \downarrow 0} \frac{f(\mathbf{x} + t\mathbf{d}) - f(\mathbf{x})}{t}.$$

Properties:

- If $\mathbf{d} = \mathbf{e_i}$, the unit vector of coordinate i, then $D_d f = \frac{\partial f}{\partial x_i}(\mathbf{x})$.
- If f is continuously differentiable, then $D_d f(\mathbf{x}) = \nabla f(\mathbf{x})^\top \mathbf{d}$.
- If $D_d f(\mathbf{x}) = \nabla f(\mathbf{x})^\top \mathbf{d} < 0$, then **d** is a **direction of descent**, i.e.

$$f(\mathbf{x} + \alpha \mathbf{d}) < f(\mathbf{x}) \quad \text{for all } \alpha \in (0, \overline{\alpha}].$$

Taylor expansion

- If f differentiable,
  then f may be approximated in a neighbourhood of $\hat{\mathbf{x}}$ by an affine-linear function as

$$f(\mathbf{x}) = f(\hat{\mathbf{x}}) + \nabla f(\hat{\mathbf{x}})^\top(\mathbf{x} - \hat{\mathbf{x}}) + R(\|\mathbf{x} - \hat{\mathbf{x}}\|),$$

where

$$\lim_{\mathbf{x}\to\hat{\mathbf{x}}} \frac{R(\|\mathbf{x} - \hat{\mathbf{x}}\|)}{\|\mathbf{x} - \hat{\mathbf{x}}\|} = 0$$

or with $t \in \mathbb{R}$, $\mathbf{d} \in \mathbb{R}^n$, $\xi_t \in (0, t)$, resp.,

$$f(\hat{\mathbf{x}} + t\mathbf{d}) = f(\hat{\mathbf{x}}) + t\,\nabla f(\hat{\mathbf{x}} + \xi_t\mathbf{d})^\top\mathbf{d}.$$

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Taylor Expansion II

- If f 2times differentiable,
  then f may be approximated in a neighbourhood of $\hat{\mathbf{x}}$ by a quadratic function as

$$f(\mathbf{x}) = f(\hat{\mathbf{x}}) + \nabla f(\hat{\mathbf{x}})^\top (\mathbf{x} - \hat{\mathbf{x}}) + \frac{1}{2}(\mathbf{x} - \hat{\mathbf{x}})^\top H_f(\hat{\mathbf{x}})(\mathbf{x} - \hat{\mathbf{x}}) + R(\|\mathbf{x} - \hat{\mathbf{x}}\|^2)$$

  or, resp.,

$$f(\hat{\mathbf{x}} + t\mathbf{d}) = f(\hat{\mathbf{x}}) + t\,\nabla f(\hat{\mathbf{x}})^\top \mathbf{d} + \frac{t^2}{2}\mathbf{d}^\top H_f(\hat{\mathbf{x}} + \xi_t \mathbf{d})\mathbf{d}.$$

Taylor Expansion - Example

Approximate around $(\hat{x}_1, \hat{x}_2) = (0, 0)$ the function

$$f(x_1, x_2) = \exp(x_1) \ln(1 + x_2).$$

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Error Analysis

Instead of the (usually unknown) real values

$$\hat{\mathbf{x}} = (\hat{x}_1, \ldots, \hat{x}_n)^\top$$

we measure approximate values

$$\mathbf{x} = (x_1, \ldots, x_n)^\top.$$

The measurement errors (uncertainty, observational deviations)

$$\Delta x_i := x_i - \hat{x}_i, 1, \ldots, n,$$

yield an error for the value of a function $f : \mathbb{R}^n \to \mathbb{R}$

$$\Delta f(\mathbf{x}) := f(\mathbf{x}) - f(\hat{\mathbf{x}}) \approx \nabla f(\hat{\mathbf{x}})^\top (\mathbf{x} - \hat{\mathbf{x}})$$

or in absolute values

Propagation of Uncertainty

Suppose

$$|\Delta f(\mathbf{x})| \leq \sum_{i=1}^{n} \left| \frac{\partial f}{\partial x_i}(\hat{\mathbf{x}}) \right| |\Delta x_i| \,.$$

If the “scattering” of errors is known as $|x_i| \leq S_i$, then the absolute maximal error S reads

$$|\Delta f(\mathbf{x})| \leq S := \sum_{i=1}^{n} \left| \frac{\partial f}{\partial x_i}(\hat{\mathbf{x}}) \right| S_i.$$

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Propagation of Uncertainty - Example

Given: measurement of 2 time intervals
$x = (20 \pm 0.1)[ms]$ and $y = (15 \pm 0.1)[ms]$

Searched for: maximal error of time difference $x - y$

Solution: Set $f : \mathbb{R}^2 \to \mathbb{R}$, $(x, y) \mapsto f(x, y) = x - y$.

$$\nabla f(x, y) = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

Absolute maximal error:

$$S = \left|\frac{\partial f}{\partial x}(20, 15)\right| \cdot 0.1 + \left|\frac{\partial f}{\partial y}(20, 15)\right| \cdot 0.1 = 0.2\,[ms]$$

Relative maximal error:

$$\frac{S}{|f(20, 15)|} = \frac{0.2}{5} = 4\%.$$

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Error Analysis - Rules of Thumbs

Sum or difference:
Absolute maximal error is sum of maximal errors of inputs

Product or quotient:
Relative maximal error is sum of relative errors of inputs

Remark:
More realistic for an error estimation is a stochastic error analysis (Gaussian propagation of uncertainty)
$\rightsquigarrow$ stochastics lecture

Optimization in Higher Dimensions

As an application we consider again the problem of minimizing a given function

$$f : \mathbb{R}^n \to \mathbb{R}$$

but now with n variables $\mathbf{x} = (x_1, x_2, \ldots, x_n)^\top \in \mathbb{R}^n$.

For simplicity, we consider the case without restrictions (constraints) on $\mathbf{x}$.
The (local) conditions derived in this subsection hold in the interior of a domain, but not on boundaries.

Note that maximization problems for $g : \mathbb{R}^n \to \mathbb{R}$ are equivalent to minimization problems where $f = -g$.

Unrestricted Optimization for any $n \in \mathbb{N}$

We consider

Problem (Unrestricted optimization problem (UOP))

Minimize $f(x)$ *subject to the constraint* $x \in \mathbb{R}^n$.

Thereby let $f : \mathbb{R}^n \to \mathbb{R}$ *an at least 1x (better 2x) differentiable function.*

Idea:
Search at first for local minima (from which one obtains global extrema under certain conditions).

Aims:
Necessary conditions
Sufficient conditions
Wish: necessary & sufficient conditions

Remark:

Numerical methods are mostly based on necessary conditions.

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Revision/Outlook: Definite Matrices

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Matrices do not have signs, but:

Definition (Definiteness of a Matrix)

Let $H \in \mathbb{R}^{n \times n}$ and $v \in \mathbb{R}^n \setminus \mathbf{0}$.

$$\text{If } v^\top H v \left\{ \begin{array}{c} > \\ < \\ \geq \\ \leq \end{array} \right\} 0 \text{ for all } v, \text{ then } H \text{ is } \left\{ \begin{array}{c} \textbf{positive definite} \\ \textbf{negative definite} \\ \textbf{positive semi-definite} \\ \textbf{negative semi-definite} \end{array} \right. .$$

If $v^\top H v > 0$ for some v and $v^\top H v < 0$ for another v (i.e. H is neither positive semi-definite nor negative semi-definite), then H is **indefinite**.
If $v^\top H v = 0$ for some v, then H is **singular**.

For functions in several variables, the Hessian plays the role of the 2nd derivative.
The definiteness of the Hessian generalizes the sign of the 2nd derivative of a function in 1 variable.

Revision/Outlook: Definite Matrices - Examples

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Necessary Condition of 1st Order

Theorem (Necessary Condition of 1st Order)

Let $f : \mathbb{R}^n \to \mathbb{R}$ be continuously differentiable and $\hat{\mathbf{x}} \in \mathbb{R}^n$ a local minimum of f.

Then there holds

$$\nabla f(\hat{\mathbf{x}}) = \mathbf{0}.$$

Definition (Stationary Point)

Any point $\mathbf{x} \in \mathbb{R}^n$ with $\nabla f(\mathbf{x}) = \mathbf{0}$ is called a **stationary point** of $f : \mathbb{R}^n \to \mathbb{R}$.

Stationary points are not automatically minima, but candidates for (local) minima!

Most numerical methods try to approximate stationary points.

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Theorem (Necessary Condition of 2nd Order)

Let $f : \mathbb{R}^n \to \mathbb{R}$ be 2x continuously differentiable and $\hat{\mathbf{x}} \in \mathbb{R}^n$ a local minimum of f.

Then the Hessian

$$H_f(\hat{\mathbf{x}})$$

is positive semi-definite.

In case $n = 1$ we have

$$f''(\hat{x}) \geq 0.$$

Likewise, this condition only yields potential candidates for a (local) minimum.

Sufficient Condition of 2nd Order

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Theorem (Sufficient Condition of 2nd Order)

Let $f : \mathbb{R}^n \to \mathbb{R}$ be 2x continuously differentiable and $\hat{\mathbf{x}} \in \mathbb{R}^n$ a stationary point of f with positive definite Hessian.

Then $\hat{\mathbf{x}}$ is a strict local minimum of f.

In case $n = 1$ we assume that

$$f''(\hat{x}) > 0.$$

This allows us to decide whether a candidate $\hat{\mathbf{x}}$ that fulfills necessary conditions (1st or 2nd order) is indeed a local minimum.

Revision: Gradient

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- The **gradient** of a function $f : \mathbb{R}^n \to \mathbb{R}$ at a point $\mathbf{x} = (x_1, \ldots, x_n)^\top \in \mathbb{R}^n$ is defined as a column vector

$$\nabla f(x_1, \ldots, x_n) := \begin{pmatrix} \frac{\partial f}{\partial x_1}(x_1, \ldots, x_n) \\ \vdots \\ \frac{\partial f}{\partial x_n}(x_1, \ldots, x_n) \end{pmatrix}.$$

In case $n = 1$ the gradient is the 1st derivative of f at point x, shortly $f'(x)$.

Illustratively, the gradient describes the steepest ascent.

The gradient is orthogonal on level curves.

Revision: Hessian

- The **Hessian** of a function f at a point $\mathbf{x}$ is defined as the quadratic matrix

$$H_f(x_1,\dots,x_n) = H_f(\mathbf{x}) := \begin{pmatrix} \frac{\partial^2 f}{\partial x_1 \partial x_1}(\mathbf{x}) & \dots & \frac{\partial^2 f}{\partial x_1 \partial x_n}(\mathbf{x}) \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1}(\mathbf{x}) & \dots & \frac{\partial^2 f}{\partial x_n \partial x_n}(\mathbf{x}) \end{pmatrix}.$$

  In case $n = 1$ the Hessian ist the 2nd derivative of f at a point x, shortly $f''(x)$.

  Illustratively, the Hessian describes the local curvature of a function.

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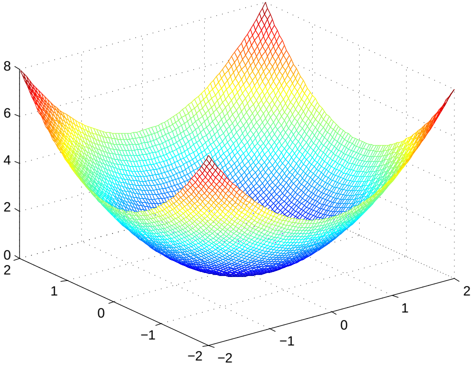
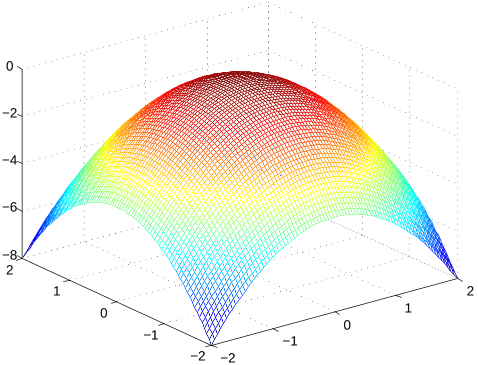
Hessian in 2d - Example 1



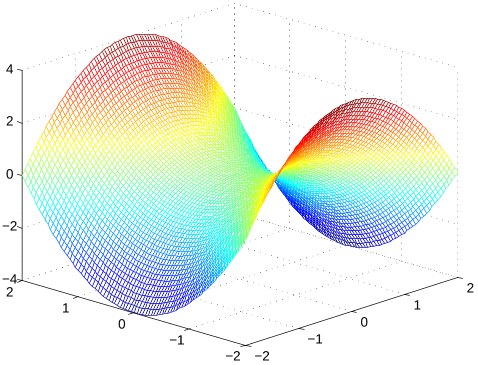
$$f(x_1, x_2) = x_1^2 + x_2^2, \qquad H_f(\hat{x}_1, \hat{x}_2) = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$$

Hessian in 2d - Example 2



$$f(x_1, x_2) = -x_1^2 - x_2^2, \quad H_f(\hat{x}_1, \hat{x}_2) = \begin{pmatrix} -2 & 0 \\ 0 & -2 \end{pmatrix}$$

Hessian in 2d - Example 3



$$f(x_1, x_2) = x_1^2 - x_2^2, \quad H_f(\hat{x}_1, \hat{x}_2) = \begin{pmatrix} 2 & 0 \\ 0 & -2 \end{pmatrix}$$

Hessian in 2d - Examples 4 & 5

Other possibilities for definite matrices in $\mathbb{R}^{2\times 2}$:

Stationary Points

Points $\hat{\mathbf{x}}$ with $\nabla f(\hat{\mathbf{x}}) = (0, 0, \ldots, 0)^\top$ are called **stationary points**.

Depending on the properties of the Hessian we find:

- **positive definite:** local minimum
- **negative definite:** local maximum
- **indefinite:** saddle point
- **singular:** everything is possible (e.g. for positive/negative semi-definite Hessian)

Optimization in $\mathbb{R}^n$ - Example

$$f : \mathbb{R}^2 \to \mathbb{R}, \quad f(x, y) = \exp(x) \cdot (2x + y^2)$$

Introduction into Linear Regression

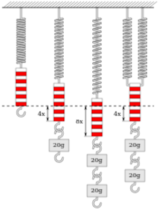
- Theory and experiment:
  How to confirm the congruence?

- Example:
  Elongation y [cm] of a spring subject to a force t [N]

  Hooke's law:

  $$y = y_0 + \frac{1}{D} t$$

  (D spring constant, describes stiffness of spring, y_0 pre-elongation of spring due to own weight)



Source: Wikipedia

- Are the free parameters D, y_0 constant over different experiments?

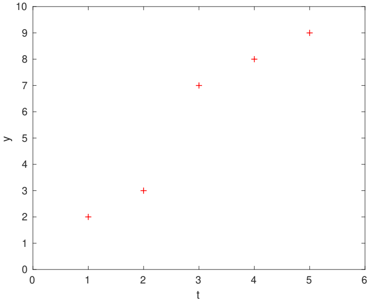
Linear Regression - Intro

$$\text{Theory: } y(t) = x_1 + x_2\, t$$

$$\text{Data: } (t_i, y_i)$$

$$\text{Error (residuum): } r_i = y_i - y(t_i)$$

i	t_i	y_i	$y(t_i)$	r_i	r_i^2
1	1	2			
2	2	3			
3	3	7			
4	4	8			
5	5	9			



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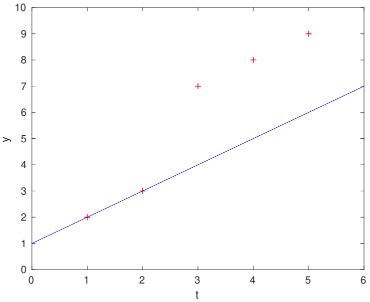
Linear Regression - 1st Try

Theory: $y(t) = 1 + t$

Data: (t_i, y_i)

Error (residuum): $r_i = y_i - y(t_i) = y_i - 1 - t_i$

i	t_i	y_i	$y(t_i)$	r_i	r_i^2
1	1	2	2	0	0
2	2	3	3	0	0
3	3	7	4	3	9
4	4	8	5	3	9
5	5	9	6	3	9
				$\Sigma_{i=1}^5 r_i^2$	$= 27$



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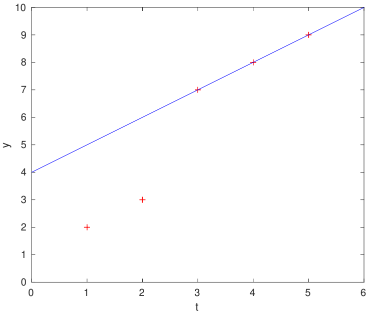
Linear Regression - 2nd Try

Theory: $y(t) = 4 + t$

Data: (t_i, y_i)

Error (residuum): $r_i = y_i - y(t_i) = y_i - 4 - t_i$

i	t_i	y_i	$y(t_i)$	r_i	r_i^2
1	1	2	5	−3	9
2	2	3	6	−3	9
3	3	7	7	0	0
4	4	8	8	0	0
5	5	9	9	0	0
				$\Sigma_{i=1}^{5} r_i^2$	$= 18$



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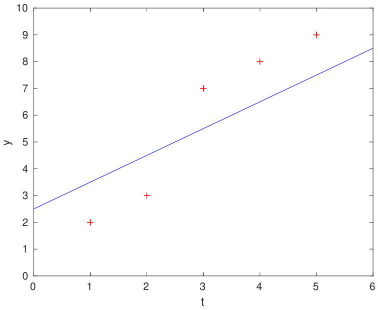
Linear Regression - 3rd Try

$$\text{Theory: } y(t) = 2.5 + t$$

$$\text{Data: } (t_i, y_i)$$

$$\text{Error (residuum): } r_i = y_i - y(t_i) = y_i - 2.5 - t_i$$

i	t_i	y_i	$y(t_i)$	r_i	r_i^2
1	1	2	3.5	-1.5	2.25
2	2	3	4.5	-1.5	2.25
3	3	7	5.5	1.5	2.25
4	4	8	6.5	1.5	2.25
5	5	9	7.5	1.5	2.25
				$\Sigma_{i=1}^{5} r_i^2 = 11.25$	



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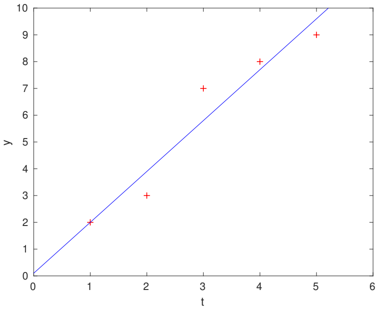
Linear Regression - Solved

$$\text{Theory: } y(t) = 0.1 + 1.9\,t$$

$$\text{Data: } (t_i, y_i)$$

$$\text{Error (residuum): } r_i = y_i - y(t_i) = y_i - 0.1 - 1.9\,t_i$$

i	t_i	y_i	$y(t_i)$	r_i	r_i^2
1	1	2	2	0	0
2	2	3	3.9	−0.9	0.81
3	3	7	5.8	1.2	1.44
4	4	8	7.7	0.3	0.09
5	5	9	9.6	−0.6	0.36
				$\Sigma_{i=1}^{5} r_i^2$	$= 2.7$



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Linear Regression: Normal Equations

In general (m arbitrary):

$$A^\top A = \begin{pmatrix} m & \sum_{i=1}^m t_i \\ \sum_{i=1}^m t_i & \sum_{i=1}^m t_i^2 \end{pmatrix}, \quad A^\top \mathbf{y} = \begin{pmatrix} \sum_{i=1}^m y_i \\ \sum_{i=1}^m t_i y_i \end{pmatrix}$$

$$x_1 = \frac{\sum_{i=1}^m t_i^2 \sum_{j=1}^m y_j - \sum_{i=1}^m t_i \sum_{j=1}^m t_j y_j}{m \sum_{i=1}^m t_i^2 - \left(\sum_{i=1}^m t_i\right)^2}$$

$$x_2 = \frac{m \sum_{i=1}^m t_i y_i - \sum_{i=1}^m t_i \sum_{j=1}^m y_j}{m \sum_{i=1}^m t_i^2 - \left(\sum_{i=1}^m t_i\right)^2}$$

Linear Regression: Motivation & Aims

We conclude:

- In general more data points y_i (here 5) as parameters x_i (here 2)
- Measurement of process/data collection afflicted with uncertainties (w/o systematical errors)
- Overdetermined LES $\rightsquigarrow$ in general no solution exists

Aims:

- Determine $\mathbf{x} = (x_1, \ldots, x_n)^\top$ "optimally" from data
- General method to do that

We call this **regression** (in particular in stochastics) or **curve fitting.**

Special case of a mathematical optimization method

Linear Regression: Stochastic Uncertainties

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Problem (Linear Regression)

Assume: linear relation (e.g. from physics)

$$y(t) = x_1 + x_2 t$$

Given: data points (t_i, y_i), $i = 1, \ldots, m$, afflicted with uncertainties (errors) ε_i. The uncertainties are random variables and 0 in average.

Searched for: $x_1, x_2 \in \mathbb{R}$, such that

$$\begin{pmatrix} 1 & t_1 \\ \vdots & \vdots \\ 1 & t_i \\ \vdots & \vdots \\ 1 & t_m \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} y_1 \\ \vdots \\ y_i \\ \vdots \\ y_m \end{pmatrix} + \begin{pmatrix} \varepsilon_1 \\ \vdots \\ \varepsilon_i \\ \vdots \\ \varepsilon_m \end{pmatrix}$$

We write

$$A\mathbf{x} = \mathbf{y} + \boldsymbol{\varepsilon}$$

with $A \in \mathbb{R}^{m \times 2}$, $\mathbf{x} \in \mathbb{R}^2$, $\mathbf{y}, \boldsymbol{\varepsilon} \in \mathbb{R}^m$.

Minimization Problem

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General situation: $A \in \mathbb{R}^{m\times n}$, $\mathbf{x} \in \mathbb{R}^n$, $\mathbf{y} \in \mathbb{R}^m$

Idea: determine $\mathbf{x} = (x_1, \ldots, x_n)^\top$, such that the error in the LES

$$\|A\mathbf{x} - \mathbf{y}\|_2 = \sqrt{\sum_{i=1}^{m}\left(\sum_{j=1}^{n} A_{ij}x_j - y_i\right)^2} \quad \text{bzw.} \quad \frac{1}{2}\|A\mathbf{x} - \mathbf{y}\|_2^2$$

is minimized.

The minimum is denoted by $\hat{\mathbf{x}}$.

This minimization problem is called a **linear regression problem** or **least-squares problem**.

Method of least squares, better **method of least residual sum of squares**
By C. F. Gauß and A.-M. Legendre (1805)

General problem

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Problem ($\star$) (Lin. regression as minimization problem)

Let be given a matrix $A \in \mathbb{R}^{m \times n}$ and a vector $\mathbf{y} \in \mathbb{R}^m$ with $m, n \in \mathbb{N}$.

We search for the solution $\hat{\mathbf{x}} \in \mathbb{R}^n$ of the minimization problem

$$\frac{1}{2}\|A\hat{\mathbf{x}} - \mathbf{y}\|_2^2 = \min_{x \in \mathbb{R}^n} \frac{1}{2}\|A\mathbf{x} - \mathbf{y}\|_2^2.$$

- If $m = n$ and A invertible, then $A\mathbf{x} = \mathbf{y}$ has a unique solution.
- The case $m > n$ is of uttermost importance in applications.
- In the case $m < n$ the LES $A\mathbf{x} = \mathbf{y}$ is underdetermined. It may be unsolvable, if $rank(A) \neq rank(A \mid \mathbf{y})$.

Moreover, other norms as $\|\cdot\|_2$ could be considered. Then the determination of solutions is harder in general, since differentiability might not be given.

Gaussian normal equations

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Theorem (Gaussian normal equations)

$\hat{x}$ solves Problem ($\star$) if and only iff the **normal equations**

$$A^\top A \hat{\mathbf{x}} = A^\top \mathbf{y}.$$

hold true.

$A^\top A \in \mathbb{R}^{n\times n}$ is symmetric and positive semi-definite.

Theorem (Uniqueness)

Let $m \geq n$. Suppose $A \in \mathbb{R}^{m\times n}$ has maximal rank,
d.h. $rank(A) = n$.
Exactly then the minimization problem ($\star$) or the normal equations, resp., are uniquely solvable.

Then $A^\top A \in \mathbb{R}^{n\times n}$ is invertible and positive definite.

(Non-)Linear Regression: TTF under Temperature Stress

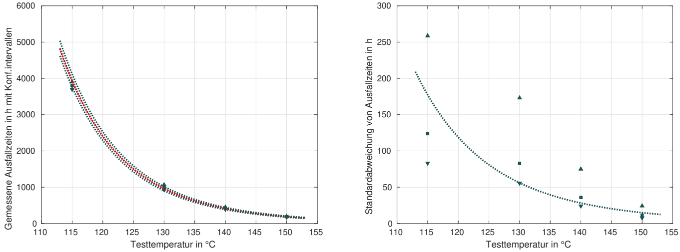

Figure: Curve fitting over different temperatures T compared with measured data points (squares) with confidence intervals for $q = 90\%$ (triangles). Left-hand side for $\mu_{krit}(T) \pm \sigma_{krit}(T)$, in red the fitted curve, right-hand side $\sigma_{krit}(T)$. [K., Dvorsky, Ließ, Avenhaus 2019]

Model based approach

$$f_{krit}(T) = t_{\ominus} + t_0 \exp\left(\left(\frac{T_a}{T - T_\infty}\right)^d\right)$$

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Lin. Regression: Transformation

Example (Measurement of TTF (Time-To-Failure) of Electrical Automotive Components)

T	[°C]	115	130	140	155
μ_{krit}	[h]	3791.62	987.74	439.66	189.94

Conjecture (model based): Arrhenius law

$$\mu_{krit}(T) = t_0 \exp\left(\frac{T_a}{T - T_\infty}\right)$$

(μ_{krit} TTF in h, t_0 reaction-kinetic period in h, T temperature in K, T_a activation temperature in K, $T_\infty = 173.15$ consolidation temperature in K)

We may transform this into an affine-linear relation

$$ln(\mu_{krit}(T)) = ln(t_0) + \frac{T_a}{T - T_\infty} \quad \Longleftrightarrow \quad y(t) = x_1 + x_2 t$$

By insertion of measured data we obtain a linear equation system (LES)

$$y_i = x_1 + x_2 t_i, \quad i = 1, \dots, 4.$$

Linear Regression: Example - Result

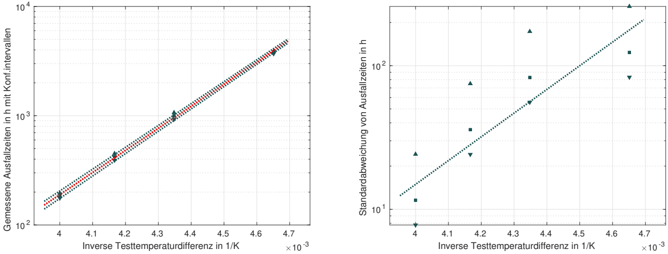

Figure: Curve fitting over different inverse temperature differences t, in semi-logarithmic representation and compared with measured data points (squares) together with confidence intervals for $q = 90\%$ (triangles). Left-hand side for $t_{krit}(1/t) \pm \sigma_{krit}(1/t)$, in red the fitted curve. Right-hand side $\sigma_{krit}(T)$. [K., Dvorsky, Ließ, Avenhaus 2019]

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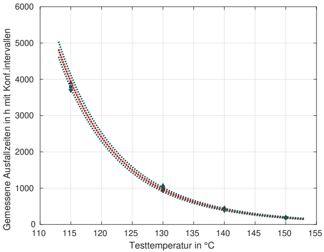
Linear Regression: Example - Re-transformed Result



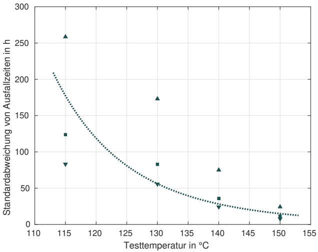


Figure: Curve fitting over different temperatures T, re-transformed in exponential representation and compared with measured data points (squares) together with confidence intervals for $q = 90\%$ (triangles). Left-hand side for $t_{krit}(T) \pm \sigma_{krit}(T)$, in red the fitted curve. Right-hand side $\sigma_{krit}(T)$. [K., Dvorsky, Ließ, Avenhaus 2019]

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Curves

A set $D \subseteq \mathbb{R}^n$ is called **(path-)connected**,
if for any $\mathbf{p}, \mathbf{q} \in D$ there exists
an interval $[a, b]$ and
a continuous function $r : [a, b] \to \mathbb{R}^n$,
such that:

- $r(t) \in D \quad$ for all $t \in [a, b]$
- $r(a) = \mathbf{p}$ and $r(b) = \mathbf{q}$

The set $r([a, b])$ (the range of r) is called a **curve.**

The mapping r itself is called **parametrization of the curve** or **path** from $\mathbf{p}$ to $\mathbf{q}$ in D.

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Curves and Connectedness

A curve is called **closed**, if $r(a) = r(b)$.

A set D is called **simply connected**, if any closed curve maybe continuously contracted (however this is defined rigorously) to a single point.

A **region** or domain[1] is an open and connected subset of $\mathbb{R}^n$.

[1] not to be confused with a domain of definition

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Examples for Connected Sets

Differentiation of Curves

We start with 2d:

Consider a parametrization $\mathbf{r}(t) = \begin{pmatrix} x(t) \\ y(t) \end{pmatrix}$

with x, y differentiable functions.

We call

$$\dot{\mathbf{r}}(t) = \lim_{h \to 0} \frac{1}{h} (\mathbf{r}(t+h) - \mathbf{r}(t)) = \begin{pmatrix} \dot{x}(t) \\ \dot{y}(t) \end{pmatrix}$$

a tangential vector of the curve.

It may interpreted as the limit vector of the secant vectors.

Analogously this may be generalized to 3d and higher dimensions.

Analysis 2
S.-J. Kimmerle
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Differentiation of Curves - Example

Motion of a mass point in 3d space

Position | Velocity | Acceleration

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   - Integration of Functions with Several Variables
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Curve Integrals, Areas of Sectors & Solids of Revolution

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Before turning to iterated integrals of functions of more than 1 variable,
we consider integrals of functions in 1 variable:

- Vector-valued functions:
  Curve integrals
- Real-valued functions of vectors, but with symmetry:
  Areas of sectors,
  Solids of revolution

Regular Parametrization of a Curve

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Let $D \subseteq \mathbb{R}^n$ open.

A mapping $\mathbf{r} : [a, b] \to D : t \mapsto \mathbf{r}(t) = (r_1(t), \ldots, r_n(t))^\top$ is called **regular parametrization** of a curve in D, if

- $\mathbf{r}$ is continuously differentiable and
- $\mathbf{r}'(t) \neq \mathbf{0} \in \mathbb{R}^n$ for all $t \in [a, b]$.

Different regular parametrizations exist.

The sense of circulation may be different.

Curve Integrals

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Let $D \subseteq \mathbb{R}^n$ open.

For any continuous function $\mathbf{f} : D \to \mathbb{R}^n$ and any regular parametrization $\mathbf{r} : [a, b] \to D$ of a curve $K := \mathbf{r}([a, b])$ we call

$$\int_K \mathbf{f}(\mathbf{x}) \bullet d\mathbf{x} := \int_a^b \mathbf{f}(\mathbf{r}(t)) \bullet \mathbf{r}'(t)\, dt$$

the **curve integral** of **f** along the curve K w.r.t. **r**.

The curve integral is independent from the parametrization, but its sign depends on the sense of circulation.

Arc Length - Parametrized Curve

Let K be a curve with a regular parametrization $(x(t), y(t))^\top$, $t \in [a, b]$,
i.e. with $x(t)$, $y(t)$ cont. diff.able on $[a, b]$ and

$$(\dot{x}(t))^2 + (\dot{y}(t))^2 \neq 0 \quad \text{for all } t \in [a, b].$$

Then the arc length is given by

$$L = \int_a^b \sqrt{\dot{x}(t))^2 + (\dot{y}(t))^2}\, dt.$$

In higher dimensions with $\mathbf{x}(t) \in \mathbb{R}^n$ there holds under analoguous assumptions:

Arc length in 2d - Cartesian Coordinates

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For the graph $y = f(\mathbf{x})$ of a cont. differentiable function $f : [a, b] \to \mathbb{R}$
the arc length is given by

$$L = \int_a^b \sqrt{1 + (y'(x))^2}\, dx.$$

Arc length in 2d - Polar Coordinates

For a curve with a regular parametrization $r(\phi)$, $\phi \in [\alpha, \beta]$, i.e. with $r(\phi)$ cont. differentiable on $[\alpha, \beta]$ and

$$r'(\phi) \neq 0 \quad \text{for all } \phi \in [\alpha, \beta].$$

$$L = \int_\alpha^\beta \sqrt{r(\phi)^2 + (\dot{r}(\phi))^2}\, d\phi.$$

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Consider $r : [\alpha, \beta] \to \mathbb{R}_0^+$ continuous, where $\alpha < \beta$. The sector enclosed by the 3 curves $r(\phi)$, $\phi = \alpha$, and $\phi = \beta$ has the area

$$A = \frac{1}{2} \int_\alpha^\beta (r(\phi))^2 \, d\phi.$$

Motivation:

$$\Delta A \approx \pi r^2 \cdot \frac{\Delta\phi}{2\pi}$$

$$A = \lim_{\Delta\phi \to 0} \sum \frac{1}{2} r^2 \Delta\phi$$

Areas of Sectors in Polar Coordinates - Example

Archimedean spiral (1 turn)

$$r(\phi) = a\phi, \quad a > 0, \quad \text{for } 0 \leq \phi \leq 2\pi$$

Areas of Sectors in Cartesian Coordinates

Leibniz sector formula

$$A = \frac{1}{2}\left|\int_{t_1}^{t_2} (x(t)y'(t) - y(t)x'(t))\ dt\right|$$

for a parametrized curve $K = \{(x(t), y(t)), t_1 \leq t \leq t_2\}$, where $x(t)$, $y(t)$ cont. differentiable

Solids of Revolution

Let $f : [a, b] \to \mathbb{R}$ continuous.

The solid of revolution generated by rotating the curve $y = f(x)$, $a \leq x \leq b$, around the x-axis has the volume

$$V = \pi \int_a^b (f(x))^2 \, dx$$

Motivation:

$$\Delta V = A(x) \cdot \Delta x \approx \pi (f(x))^2 \cdot \Delta x$$
$$V = \lim_{\Delta x \to 0} \sum \pi (f(x))^2 \cdot \Delta x$$

Remark: Rotations around other axes yield analogous formulas.

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Circular cone

$$f(x) = \frac{r}{h}x$$

Integration on $\mathbb{R}^n$

Up to now we have considered different cases of functions depending in principle on one variable, although the range might be higher dimensional, i.e. in $\mathbb{R}^n$.
We wish to enlarge this to several variables in $\mathbb{R}^m$.

We consider $f : B \subseteq \mathbb{R}^2 \to \mathbb{R}$.

$$S_n := \sum_{i=1}^{n} f(x_*^{[i]}, y_*^{[i]}) \cdot \Delta F_i \quad \text{with } (x_*^{[i]}, y_*^{[i]}) \in B$$

Small domains B_i with area $|B_i| = \Delta F_i$ with fineness δ

Double Integral

Idea: iterated Riemann integral

But why should we restrict us to an approximation by rectangles?

Like Riemann construction

$$\iint\limits_B f(x,y)\,dF = \lim_{\delta\to 0, n\to\infty} \sum_{i=1}^{n} f(x_*^{[i]}, y_*^{[i]}) \cdot \Delta F_i$$

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Important Double Integrals

Area integrals

$$A = \iint\limits_B 1 \, dA = \text{ area of } B$$

Volume integrals

$$V = \iiint\limits_C 1 \, dV = \text{ volume of } C$$

$$\stackrel{\text{special case}}{=} \iint\limits_B f(x,y) \, dA$$

$$= \text{volume of solid with base area } B$$

$$\text{and top area described by } f(B)$$

Note $A = |B|$, $V = |C|$

(Regular) Domains

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For a more formal approach, we need some preparation:

- Recall: A set $D \subseteq \mathbb{R}^n$ is called connected, iff for any 2 points $\mathbf{x}^{[0]}$ and $\mathbf{x}^{[1]}$ there exists a curve $k : [a, b] \to \mathbb{R}^n$ with $k(a) = \mathbf{x}^{[0]}$ and $k(b) = \mathbf{x}^{[1]}$.

  A **region** or domain[2] is an open and connected subset of $\mathbb{R}^n$.

- Normal areas (regular domains) $\rightsquigarrow$ see next slide

[2] not to be confused with a domain of definition

Normal areas

Normal areas are in 2D:

- Type I:
  $B_I = \{(x, y) \,|\, a \leq x \leq b$ and $g(x) \leq y \leq h(x)\}$
  with $a, b \in \mathbb{R}$, where $a < b$, and
  $g : [a, b] \to \mathbb{R}$, $h : [a, b] \to \mathbb{R}$ cont. differentiable.
- Type II:
  $B_{II} = \{(x, y) \,|\, c \leq y \leq d$ and $G(y) \leq y \leq H(y)\}$
  with $c, d \in \mathbb{R}$, where $c < d$, and
  $G : [c, d] \to \mathbb{R}$, $H : [c, d] \to \mathbb{R}$ cont. differentiable.

The roles of x and y are reversed.

This may be extended to higher dimensions.

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- We perform the integrations "from inside to outside". The integral and the differential work like a “bracket”.

- For practical computations it may be helpful to split the normal area B by cuts (that are parallel to the axes) into smaller (disjunct) normal areas, e.g. B_1 and B_2. The whole integral is then obtained by the additivity.

Fubini Theorem

The order of integration may not be exchanged in general, but:

Theorem (Fubini Theorem)

Let $R = \{(x,y) \,|\, a \leq x \leq b \text{ and } c \leq y \leq d\}$, $a,b,c,d \in \mathbb{R}$ a rectangle, and $f : \mathbb{R}^2 \to \mathbb{R}$ continuous.

Then there holds

$$\iint\limits_R f\,dA = \int_a^b \int_c^d f(x,y)\,dy\,dx = \int_c^d \int_a^b f(x,y)\,dx\,dy.$$

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Fubini Theorem - Example

Consider B bounded by the curves $y = x$, $y = \frac{1}{x}$, and $y = 2$.

$$A = \iint\limits_B dx\, dy = \iint\limits_B dy\, dx$$

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Multiple Integrals

Let $f : B \subseteq \mathbb{R}^n \to \mathbb{R}$,
B a normal area.

$$\begin{aligned}\int_B f(\mathbf{x})\, dF &:= \int \cdots \int_B f(\mathbf{x})\, d\mathbf{x} \\ &:= \int \cdots \int_B f(\mathbf{x})\, dx_1 \ldots dx_n \\ &= \lim_{\delta \to 0, n \to \infty} \sum_{i=1}^{n} f(\mathbf{x}^{[i]}) \cdot \Delta F_i\end{aligned}$$

Properties of Integrals I

The following properties transfer to multiple integrals.

Let $f, g : B \to \mathbb{R}$ integrable functions and $B \subseteq \mathbb{R}^n$ a normal area.

Linearity:
$\int_B f(\mathbf{x}) + g(\mathbf{x})\, d\mathbf{x} = \int_B f(\mathbf{x})\, d\mathbf{x} + \int_B g(\mathbf{x})\, d\mathbf{x}$

and (factor rule) $\int_B c\, f(\mathbf{x})\, d\mathbf{x} = c \int_B f(\mathbf{x})\, d\mathbf{x}$

Additivity for $B_1 \cup B_2 = B$ with $B_1 \cap B_2 = \emptyset$:

$$\int_{B_1} f(\mathbf{x})\, d\mathbf{x} + \int_{B_2} f(\mathbf{x})\, d\mathbf{x} = \int_B f(\mathbf{x})\, dx$$

Monotonicity: $f \leq g \implies \int_B f(\mathbf{x})\, d\mathbf{x} \leq \int_B g(\mathbf{x})\, d\mathbf{x}$

Properties of Integrals II

Inequalities:

"triangle inequality"

$$\left| \int_B f(\mathbf{x})\, d\mathbf{x} \right| \leq \int_B |f(\mathbf{x})|\, d\mathbf{x}$$

Cauchy-Schwarz

$$\left(\int_B f(\mathbf{x}) g(\mathbf{x})\, d\mathbf{x} \right)^2 \leq \left(\int_B f(\mathbf{x})^2\, d\mathbf{x} \right) \left(\int_B g(\mathbf{x})^2\, d\mathbf{x} \right)$$

Integration over a set N of measure "zero":

$$\int_N f(\mathbf{x})\, d\mathbf{x} = 0$$

We only give some examples in 2d:

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S.-J. Kimmerle
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Another Application: Barycenter

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The **center of mass s** of a mass distribution (mass density) $\rho : B \subseteq \mathbb{R}^n \to \mathbb{R}^+$ in space is the unique point where the weighted relative position of the distributed mass sums to zero:

$$\mathbf{s} := \frac{1}{M} \int_B \mathbf{x}\, \rho(\mathbf{x})\, d\mathbf{x}$$

where $M := \int_B \rho(\mathbf{x})\, d\mathbf{x}$.

Remarks:
A center of mass may be translated to any distribution ρ or a data set.
If $\rho = 1$, we obtain the so-called centroid (geometric center). The word **barycenter** comprises the terms "center of mass" and "centroid".

Example: Barycenter of

Area of a Surface in Space

If $f : B \subseteq \mathbb{R}^2 \to \mathbb{R}$ continuously partial differentiable, $B \subseteq \mathbb{R}^2$ regular,

then the surface (the graph of f) has the area

$$\int\int_B \sqrt{1 + \left(\frac{\partial f}{\partial x}(x,y)\right)^2 + \left(\frac{\partial f}{\partial y}(x,y)\right)^2}\, dx\, dy\,.$$

Remarks:

- For a $f : I \subseteq \mathbb{R} \to \mathbb{R}$ this reduces to the length of a curve.
- Surface integrals are a topic of their own.

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Transformation Formula: Coordinate Transformation

We consider a domain $S \subseteq \mathbb{R}^2$ generated by a **coordinate transformation**

$$x = x(u, v), y = y(u, v)$$

(being continuously differentiable, bijective, ... see literature) from a domain $B \subseteq \mathbb{R}^2$.

Let

$$g : \mathbb{R}^2 \to \mathbb{R}^2, \begin{pmatrix} u \\ v \end{pmatrix} \mapsto \begin{pmatrix} x(u,v) \\ y(u,v) \end{pmatrix}.$$

Analogously, we define coordinate transformations for 3d and higher dimensions.

Transformation Formula 2d

For such a coordinate transformation $g : \mathbb{R}^2 \to \mathbb{R}^2$,

we have for $f : S \subseteq \mathbb{R}^2 \to \mathbb{R}$ continuous

$$\iint_S f(x,y)\,dx\,dy$$

$$= \iint_B f(x(u,v), y(u,v)) \cdot \left|\det(J_g(u,v))\right| \,du\,dv\,.$$

Transformation from Polar Coordinates

For polar coordinates there holds

$$x = r\cos(\phi),$$
$$y = r\sin(\phi),$$

thus

$$g : \mathbb{R}^+ \times [0, 2\pi) \to \mathbb{R}^2, \begin{pmatrix} r \\ \phi \end{pmatrix} \mapsto \begin{pmatrix} x(r,\phi) \\ y(r,\phi) \end{pmatrix} = \begin{pmatrix} r\cos(\phi) \\ r\sin(\phi) \end{pmatrix}.$$

Hence the Jacobian determinant (functional determinant) is:

$$\det \begin{pmatrix} \cos(\phi) & -r\sin(\phi) \\ \sin(\phi) & r\cos(\phi) \end{pmatrix} = r\cos(\phi)^2 + r\sin(\phi)^2 = r$$

Since $r > 0$, we replace the "area element" $dx\,dy$ by $r\,dr\,d\phi$.

Example: Polar Coordinates

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Let $S = \{x^2 + y^2 \leq 1\}$.
We apply the transformation formula to compute

$$\iint_S \rho\, x^2\, dx\, dy$$

(the moment of inertia of the full circular disc w.r.t. the y-axis).

We assume $\rho = const$.

Transformation Formula 3d

For a suitable (see 2d case) coordinate transformation $g : \mathbb{R}^3 \to \mathbb{R}^3$,

we have for $f : S \subseteq \mathbb{R}^3 \to \mathbb{R}$ continuous

$$\iiint\limits_S f(x,y,z)\, dx\, dy\, dz$$

$$= \iiint\limits_B f(x(u,v,w), y(u,v,w)) \cdot \left|\det(J_g(u,v,w))\right|\, du\, dv\, dw\,.$$

Transformation from Cylinder Coordinates

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For cylinder coordinates there holds

$$\begin{aligned} x &= r\cos(\phi), \\ y &= r\sin(\phi), \\ z &= z \end{aligned}$$

thus

$$g : \mathbb{R}^+ \times (-\pi, \pi] \times \mathbb{R} \to \mathbb{R}^3, \begin{pmatrix} r \\ \phi \\ z \end{pmatrix} \mapsto \begin{pmatrix} x(r,\phi,z) \\ y(r,\phi,z) \\ z(r,\phi,z) \end{pmatrix} = \begin{pmatrix} r\cos(\phi) \\ r\sin(\phi) \\ z \end{pmatrix}.$$

Hence the Jacobian determinant (functional determinant) is:

$$\det \begin{pmatrix} \cos(\phi) & -r\sin(\phi) & 0 \\ \sin(\phi) & r\cos(\phi) & 0 \\ 0 & 0 & 1 \end{pmatrix} = \left(r\cos(\phi)^2 + r\sin(\phi)^2 \right) \cdot 1 = r$$

Since $r > 0$, we replace the "volume element" $dx\,dy\,dz$ by $r\,dr\,d\phi\,dz$.

Example: Cylinder Coordinates

We compute the volume of a cylinder with radius $R > 0$ and height $h > 0$:

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Transformation from Spherical Coordinates

For spherical coordinates there holds

$$\begin{aligned} x &= r\cos(\phi)\sin(\theta), \\ y &= r\sin(\phi)\sin(\theta), \\ z &= r\cos(\theta) \end{aligned}$$

thus

$$g : \mathbb{R}^+ \times (-\pi, \pi] \times [0, \pi] \to \mathbb{R}^3, \begin{pmatrix} r \\ \phi \\ \theta \end{pmatrix} \mapsto \begin{pmatrix} x(r,\phi,\theta) \\ y(r,\phi,\theta) \\ z(r,\phi,\theta) \end{pmatrix} = \begin{pmatrix} r\cos(\phi)\sin(\theta) \\ r\sin(\phi)\sin(\theta) \\ r\cos(\theta) \end{pmatrix}.$$

Hence the Jacobian determinant (functional determinant) is:

$$\det \begin{pmatrix} \cos(\phi)\sin(\theta) & -r\sin(\phi)\sin(\theta) & r\cos(\phi)\cos(\theta) \\ \sin(\phi)\sin(\theta) & r\cos(\phi)\sin(\theta) & r\sin(\phi)\cos(\theta) \\ \cos(\theta) & 0 & -r\sin(\theta) \end{pmatrix} = -r^2\sin(\theta)$$

Since $\sin(\theta) > 0$, we replace the “volume element” $dx\,dy\,dz$ by $r^2\,\sin(\theta)\,dr\,d\phi\,d\theta$.

Example: Spherical Coordinates

We compute the mass of a homogeneous sphere with radius $R > 0$.
Let $\rho(x, y, z) = \rho_0 = const$ be the constant mass density.

Bell Curve, Continued I

An improper integral important for stochastics is the integral over the Gauss bell curve:

$$f(x) = \frac{1}{\sqrt{2\pi} \cdot \sigma} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right), \quad \mu \in \mathbb{R}, \sigma > 0.$$

For a probability we have to check:

$$\int_{-\infty}^{\infty} f(x)\, dx = 1.$$

However, for $f(x)$ there exists no closed form for a primitive (cf. Analysis 1):

$$erf(x) = \frac{2}{\sqrt{\pi}} \int_{-\infty}^{x} \exp\left(-\frac{\tilde{x}^2}{2}\right) d\tilde{x}.$$

By now, we are able to check the normalization factor $\frac{1}{\sqrt{2\pi}}$ for the standard normal distribution ($\mu = 0$, $\sigma = 1$).

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Bell Curve, Continued II

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We consider the square of the sought-after integral and apply Fubini:

$$
\begin{aligned}
&\int_{\mathbb{R}} \exp\left(-\frac{1}{2}x_1^2\right) dx_1 \cdot \int_{\mathbb{R}} \exp\left(-\frac{1}{2}x_2^2\right) dx_2 \\
=&\int\int_{\mathbb{R}^2} \exp\left(-\frac{1}{2}(x_1^2+x_2^2)\right) dx_1\, dx_2 \\
=&\int_0^{2\pi}\int_0^{\infty} \exp\left(-\frac{1}{2}r^2\right) r\, dr\, d\phi \\
=&\int_0^{2\pi}\int_0^{\infty} -\exp\left(-\frac{1}{2}r^2\right)\frac{d}{dr}\left(-\frac{1}{2}r^2\right) dr\, d\phi \\
=&2\pi \cdot \lim_{b\to\infty}\left[-\exp\left(-\frac{1}{2}r^2\right)\right]_0^b \\
=&2\pi \cdot (0-(-1)) \\
=&2\pi
\end{aligned}
$$

Mean Value Theorem for Integration I

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Theorem (Mean Value Theorem for Definite Double Integrals)

Let $B \subseteq \mathbb{R}^2$ connected and closed, then there exists for any continuous function $f : B \to \mathbb{R}$ a point $(x^*, y^*) \in B$ such that

$$\iint_B f \, dA = f(x^*, y^*) A \quad \textit{with } A := \iint_B 1 \, dA$$

We call $\frac{1}{A} \iint f \, dA$ the **integral mean value.**

Mean Value Theorem for Integration II

Note that:

- The mean value theorem holds for higher dimensional domains $B \subseteq \mathbb{R}^n$ as well.
- But this theorem fails for vector-valued functions.
- We do not consider indefinite integrals here.

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Parameter Integrals

A **parameter integral** is an integral which integrand depends on parameters:

$$\int f(x_1, x_2, \ldots, x_n)\, dx_i, \quad i \in \{1, \ldots, n\}$$

Here x_i is considered as variable and all other x_j, $j \neq i$, are held fixed.
The x_j enter as parameters only.

In 2d we often write x for the variable and t for the parameter.

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A parameter integral is the inverse operation w.r.t. to partial differentiation:

For instance, let $f : [a, b] \times [c, d] \to \mathbb{R}$ continuous and $s \in [c, d]$

$$F(x, s) := \int_c^s f(x, t)\, dt,$$

then

$$\frac{\partial}{\partial s} F(x, s) = \frac{\partial}{\partial s} \int_c^s f(x, t)\, dt = f(x, s).$$

Note that improper parameter integrals are more subtle.

Parameter Integrals - Examples

- Gamma function:

$$\Gamma(x) = \int_0^\infty t^{x-1} \exp(-t)\,dt, \quad t > 0$$

- Bessel functions:

$$J_n(x) := \frac{1}{\pi} \int_0^\pi \cos(x \sin(t) - nt)\,dt, \quad n \in \mathbb{Z}$$

- Laplace transform of a given function f

$$F(s) = \int_0^\infty f(t) \exp(-st)\,dt$$

- Gravitational potential V generated by a solid $M \subset \mathbb{R}^3$ with variable density ρ in a point $x \in \mathbb{R}^3 \subset M$ (G the gravitational constant)

$$V(\mathbf{x}) = -G \iiint_M \frac{\rho(\mathbf{y})}{|\mathbf{x} - \mathbf{y}|}\,d\mathbf{y}$$

Parameter Integrals - Exchanging Integration & Differentiation

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Theorem (Leibniz Rule for Parameter Integrals)

Let $f : [a,b] \times [c,d] \to \mathbb{R}$ on $[a,b]$ continuously partial differentiable w.r.t. x,
then $F(x) := \int_c^d f(x,t)\,dt$ is differentiable (w.r.t. x) and

$$F'(x) = \frac{d}{dx} \int_c^d f(x,t)\,dt = \int_c^d \frac{\partial}{\partial x} f(x,t)\,dt.$$

We may exchange integration and differentiation in this situation.
In general the latter is not true.

The Fubini theorem may be demonstrated by considering in both orders one integral as a parameter integral.

Practical Computation of Integrals

- Using primitives
  See integral tables
- By transformation formula
- Numerical methods
  Relying on the Riemann approach, on interpolation, ...
- Special integrals
  Tabulated, e.g., the error function
- Using series
- ...

Various Concepts of Integration

- **Riemann integral**
  (mainly the approach of our lectures)
  $\rightsquigarrow$ advantage w.r.t. improper integrals
- Cauchy integral
- **Lebesgue integral**
  $\rightsquigarrow$ important for stochastics
- Stieltjes integral
- Bochner integral
- Itō integral (stochastic integral)
- ... any many more ...

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Vector Analysis

Let $D \subseteq \mathbb{R}^n$.
A function $\mathbf{F} : D \to \mathbb{R}^n$ with $n \geq 2$ is also called a **vector field**.

Example:
Let $f : D \to \mathbb{R}$, then ∇f is a vector field.

A vector field F is called **conservative** or **gradient field**, if there exists a function ϕ s.t.:

$$\mathbf{F} = \nabla\phi.$$

Then we call ϕ a (scalar) **potential (function)**.

Application of Potential Functions

Path independence:

Let D be a simply connected domain.

$$\int_{\mathbf{a}}^{\mathbf{b}} \mathbf{F} \cdot d\mathbf{s} = \phi(\mathbf{b}) - \phi(\mathbf{a})$$

for a sufficiently smooth curve from **a** to **b**.

Note that the integral does not depend on the curve, but only on the start and end points, **a** and **b**.

How can we decide whether a vector field is conservative?

Characterization of Potential Functions

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Consider a simply connected domain D.

The following statements are equivalent:

- $\int_{\mathbf{a}}^{\mathbf{b}} \mathbf{F} \cdot d\mathbf{s} = \phi(\mathbf{b}) - \phi(\mathbf{a})$ for a curve from **a** to **b**.
- The curve integral over **F** along any closed curve is zero.
- $\nabla \times \mathbf{F} = 0$

We suppose that the involved curves are sufficiently smooth.

Note that ϕ is unique up to an additive constant.

Examples: Potential

Fundamental Theorem (of Analysis)

The fundamental theorem of Analysis 1

$$F(x) := \int_a^x F'(\tilde{x})\, d\tilde{x}$$

or

$$\int_a^b F'(x)\, dx = F(b) - F(a)$$

cannot be easily generalized to several dimensions.

Integral Theorems

Some generalizations are:

- Gradient theorem ("1d")

$$\int_\gamma \nabla f(\mathbf{r}) \cdot d\mathbf{r} = f(\mathbf{r}(t_b)) - f(\mathbf{r}(t_a))$$

  (γ a curve from $\mathbf{a} = \mathbf{r}(t_a)$ to $\mathbf{b} = \mathbf{r}(t_b)$ in $\mathbb{R}^n$ with parametrization $\mathbf{r}$)
- Stokes theorem (2d)

$$\iint_M (\nabla \times \mathbf{F}) \cdot d\mathbf{A} = \int_{\partial M} \mathbf{F} \cdot d\boldsymbol{\gamma}$$

  (M a 2d submanifold of $\mathbb{R}^3$, bounded by a curve $\boldsymbol{\gamma}$ representing ∂M)
- Gauss divergence theorem in 3d

$$\iiint_K \nabla \cdot \mathbf{F}\, dV = \iint_{\partial K} \mathbf{F} \cdot d\mathbf{A}$$

  ($K \subseteq \mathbb{R}^3$ compact. May be generalized to $\mathbb{R}^n$.)

Important Differential Operators

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Summary - Outlook and Review

Recall: gradient

$$\mathit{grad}\, f(\mathbf{x}) = \nabla f(\mathbf{x}) = \left(\frac{\partial}{\partial_{x_1}} f(\mathbf{x}) \ldots, \frac{\partial}{\partial x_n} f(\mathbf{x}) \right)^\top$$

Divergence (sources or sinks)

$$\mathit{div}\, \mathbf{F}(\mathbf{x}) = \nabla \cdot \mathbf{F}(\mathbf{x}) = \sum_{i=1}^{n} \frac{\partial}{\partial x_i} F_i(\mathbf{x})$$

Curl or rot(ation), in $\mathbb{R}^3$ ($\mathbb{R}^2$ also possible):

$$\mathit{curl}\, \mathbf{F}(\mathbf{x}) = \nabla \times \mathbf{F}(\mathbf{x}) = \begin{pmatrix} \frac{\partial}{\partial x_2} F_3(\mathbf{x}) - \frac{\partial}{\partial x_3} F_2(\mathbf{x}) \\ \frac{\partial}{\partial x_3} F_1(\mathbf{x}) - \frac{\partial}{\partial x_1} F_3(\mathbf{x}) \\ \frac{\partial}{\partial x_1} F_2(\mathbf{x}) - \frac{\partial}{\partial x_2} F_1(\mathbf{x}) \end{pmatrix}$$

Laplace operator

$$\mathit{div}\, \mathit{grad}\, f(\mathbf{x}) = \nabla \cdot \nabla f(\mathbf{x}) = \Delta f(\mathbf{x}) = \sum_{i=1}^{n} \frac{\partial^2}{\partial x_i^2} f(\mathbf{x})$$

Integration by Parts

Integration by parts

$$\iiint\limits_V g\,\nabla\cdot\mathbf{f}\,dV = \iint\limits_{\partial V} g\mathbf{f}\cdot d\mathbf{A} - \iiint\limits_V \nabla g\cdot\mathbf{f}\,dV$$

(May be generalized to $\mathbb{R}^n$.)

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Summary - Outlook and Review

Fourier and Laplace transforms are useful tools for solving (partial) differential equations

Applications of the Fourier transform

- Information technology/electrical engineering: Low-pass filter
- Spectroscopy (NMR, FTIR, . . .)
- Acoustics
- Quantum mechanics
- ...
- Generalizes Fourier series from periodic to (some) non-periodic functions

Fourier Transform: Motivation I

Suppose

$$f(x) = \sum_{k=-\infty}^{\infty} c_k \exp(ik(\Delta\omega)x), \quad \Delta\omega = \frac{2\pi}{T}$$

with complex Fourier coefficients

$$\begin{aligned} c_k &= \frac{1}{T}\int_0^T f(x)\exp(-ik(\Delta\omega)x)\,dx \\ &= \frac{1}{T}\int_{-T/2}^{T/2} f(x)\overline{\exp(ik(\Delta\omega)x)}\,dx, \quad k \in \mathbb{Z} \end{aligned}$$

Introduce $\omega_k := k\Delta\omega$ and insert c_k into the series:

$$f(x) = \sum_{k=-\infty}^{\infty}\left(\frac{1}{T}\int_{-T/2}^{T/2} f(x)\overline{\exp(i\omega_k x)}\,dx\right)\exp(i\omega_k x) \quad = \ldots$$

Fourier Transform: Motivation II

$$
\begin{aligned}
f(x) &= \sum_{k=-\infty}^{\infty} \left(\frac{1}{T} \int_{-T/2}^{T/2} f(\xi) \overline{\exp(i\omega_k \xi)\, d\xi} \right) \exp(i\omega_k x) \\
&= \ldots \\
&= \frac{1}{2\pi} \sum_{k=-\infty}^{\infty} \left(\int_{-T/2}^{T/2} f(\xi) \overline{\exp(i\omega_k \xi)}\, d\xi \right) \exp(i\omega_k t) \Delta\omega
\end{aligned}
$$

The series may be interpreted as a limit of Riemann sums that approximate an integral on $[-\infty, \infty]$ with refinement $\Delta\omega$ and grid points ω_k, $k \in \mathbb{Z}$.

Fourier Transform - Definition

For $T \to \infty$ (and $\Delta\omega \to 0$) we may expect convergence to an improper integral:

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} F(\omega) \exp(i\omega x) \, d\omega$$

with

$$F(\omega) = \int_{-\infty}^{\infty} f(x) \overline{\exp(i\omega x)} \, dx$$

<u>Definition:</u>

$$F(\omega) := \mathcal{F}\{f(x)\} := \int_{-\infty}^{\infty} f(x) \exp(-i\omega x) \, dx$$

is called **Fourier transform** (or spectral function) of $f : \mathbb{R} \to \mathbb{C}$, if the integral exists for all $\omega \in \mathbb{R}$.

$$\mathcal{F}^{-1}\{F(\omega)\} := f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} F(\omega) \exp(i\omega x) \, d\omega$$

is called **inverse Fourier transform** of $F : \mathbb{R} \to \mathbb{C}$, if the integral exists for all $x \in \mathbb{R}$.

Fourier Transform - Properties

- Linearity
- Displacement
- Similarity
- Derivatives
- Modulation

Laplace Transform

Laplace transform

$$F(s) := \mathcal{L}\{f(t)\} := \int_0^\infty f(t)\exp(-st)\,dt,$$

is called **Laplace transform** of $f : \mathbb{R}^+ \to \mathbb{R}$,
if the integral exists for some $s \in \mathbb{R}$.

The inverse Laplace transform is hard to calculate.
Usually, reference tables are used.

The Laplace transform has similar properties as the Fourier transform,
in particular

$$\mathcal{L}\{y'(t)\} = s\mathcal{L}\{y(t)\} - y(0) = sY(s) - y(0)$$

transforming differential equations (incl. initial values) into algebraic equations

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Outlook and insight: What we did in Analysis 2

- **Differential calculus in higher dimensions (mainly 2d, 3d)**
- **Integral calculus in higher dimensions (mainly 2d, 3d)**
- Sequences of functions
- **Power series,**

  Taylor series/Taylor expansions

  Fourier series
- …

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What we did in Analysis 2 - More Details

- Sequences of functions, uniform convergence
- Power series,
  especially Taylor series, Fourier series,
  discrete Fourier transform
- Limits and continuity (for any d), curves (application: ECC)
- Differential calculus (for any d),
  especially optimization, linear regression
- Integrals along curves, on sectors; solids of revolution
- Integral calculus (for any d)
- Vector analysis (brief insight)
- Fourier transform (very brief insight)

What we have not discussed here

- Total differential, implicit functions, implicit differentiation
- Optimization with constraints, Lagrange multipliers
- Curvature
- **Differential equations**
- Integrals over curved surfaces, ...
- Laplace transform
- Fundamental theorem of Algebra
  to be proved by analytical methods ;)
- ...

... and all topics of this lecture may be discussed with all proofs and more details and extensions

References: recommended literature

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Formula collections are also available in English.

Further sources (for sake of completeness)

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Software packages

General mathematical software:

- SCILAB, free software, `scilab.org`)
- MATLAB, campus licence
- Wolfram Mathematica
- ...

Computer algebra, i.e. “symbolic calculators”:

- MAPLE
- MATLAB, symbolic toolbox, campus licence ???
- Wolfram Alpha
- ...

For optimization, finite element methods, machine learning, . . . specialized software packages exist.

Programming languages as Python, Java, C, . . . are always useful.